并行机器编程

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GPU、多核、集群

关于本书

为什么本书和其它的并行编程书籍不同呢？原因在于我们主要关注在实现层面：

- 这里几乎没有理论内容，诸如 O() 分析、最大理论加速、PRAM、有向无环图 (DAG) 等等。
- 书中使用的都是真实代码。
- 我们使用的都是主流的并行平台，包括 OpenMP、CUDA 和 MPI，而没有使用其它仍处于实验阶段的语言。
- 关于性能的主题——通信延迟、内存/网络连接、负载均衡等，在全书中交叉进行，并且都是在特定平台或应用的层面进行讨论的。
- 相当关注 debug 技术。

书中使用的主要编程语言 C/C++，但也使用了一些 R 代码。R 已经是最主流的用于数据分析的语言。作为一门脚本语言，R 可以用于快速原型构建。在本书中，我用 R 将可以一些例子表述得远远比用 C/C++ 要简洁，从而使得学生更容易的理解所使用的并行计算原则。出于同样的原因，学生们也可以更容易地编写并行代码，更加集中精力于这些原则之上。另外，R 也有相当丰富的并行库。

我们假设学生在编程方面是有相当经验的，并有包括线性代数在内的数学背景。附录里回顾了本书所需要的数学知识。另一个附录提供了不同系统问题的概述，包括进程调度和虚拟内存等。

需要特别说明的是，书中多数代码没有进行优化。我们主要关注的是技术和语言使用的清晰明了。然而，有很多影响速度的因素值得讨论，比如高速缓存一致性问题、网络延迟、GPU 内存结构等等。

这里展示了你可以如何使用书中的代码：本书使用 LATEX 排版，原始的 .tex 文件可以在 http://heather.cs.ucdavis.edu/~matloff/158/PLN 下载。请直接下载相关文件（文件名应该足够明），之后使用一个文本编辑器进行裁剪，从而得到感兴趣的代码。

为了向学生展示研究和教学的相互促进关系，我会时不时引用我的一些研究工作。

如同我的其它开源图书，本书是在**不停变动**中的。我会继续添加新的主题、新的示例等等，当然也会修补漏洞和改善说明。由于这个原因，所以保存本书最新版本的链接，http://heather.cs.ucdavis.edu/~matloff/158/PLN/ParProcBook.pdf，比保存一份拷贝更好。

同样出于这个原因，我非常希望得到反馈。这里我希望感谢 Stuart Ambler、Matt Butner、Stuart Hansen、Bill Hsu、Sameer Khan、Mikel McDaniel、Richard Minner、Lars Seeman、Marc Sosnick 和 Johan Wikström 的评论。特别感谢 Hsu 教授为我提供了高级的 GPU 设备。

各位可能对我另一本关于概览和统计的开源图书感兴趣，可以在 http://heather.cs.ucdavis.edu/probstatbook 下载。

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如果您使用了本书用于教学，我将很高兴您能通知我，这仅仅为了让我知道这些材料正在被使用当中，但这不是必须的。

作者简介

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Matloff 博士生于 Los Angeles，在 East Los Angeles 和 San Gabriel Valley 长大。他从 UCLA 得到了纯数学的博士学位，研究方向为概率论和统计他在计算机科学和统计学方面发表了大量论文，现在的研究方向是并行处理、统计学和回归方法。

Matloff 博士曾是 UNESCO 下的数据库安全国际委员会，IFIP Working Group 11.3 成员。他是戴维斯分校统计系的创始人之一，并参与了计算机系的建立。他在戴维斯分校被授予 Distinguished Teaching Award and Distinguished Public Service Award。

Matloff 博士是两本书的作者，并编写了大量广泛使用的网络教程，涉及 Linux 和 python 语言。他和 Peter Salzman 博士是《软件调试的艺术》[①]一书的作者。Matloff 博士关于 R 语言的《R 语言编程艺术》[②]一书已于 2011 年出版。他的新书，*Parallel Computation for Data Science* 会于 2014 年出版。他还写作了很多开源图书，包括 *From Algorithms to Z-Scores: Probabilistic and Statistical Modeling in Computer Science*（`http://heather.cs.ucdavis.edu/probstatbook`），和《并行机器编程》（`http://heather.cs.ucdavis.edu/~matloff/ParProcBook.pdf`）。

[①]The Art of Debugging with GDB, DDD, and Eclipse，中文版已由人民邮电出版社出版
[②]The Art of R Programming，中文版已由机械工业出版社出版

目录

第 1 章 并行处理入门

Parallel machines provide a wonderful opportunity for applications with large computational requirements. Effective use of these machines, though, requires a keen understanding of how they work. This chapter provides an overview of both the software and hardware.

1.1 Why Use Parallel Systems?

1.1.1 Execution Speed

There is an ever-increasing appetite among some types of computer users for faster and faster machines. This was epitomized in a statement by the late Steve Jobs, founder/CEO of Apple and Pixar. He noted that when he was at Apple in the 1980s, he was always worried that some other company would come out with a faster machine than his. But later at Pixar, whose graphics work requires extremely fast computers, he was always <u>hoping</u> someone would produce faster machines, so that he could use them!

A major source of speedup is the parallelizing of operations. Parallel operations can be either within-processor, such as with pipelining or having several ALUs within a processor, or between-processor, in which many processor work on different parts of a problem in parallel. Our focus here is on between-processor operations.

For example, the Registrar's Office at UC Davis uses shared-memory multiprocessors for processing its on-line registration work. Online registration involves an enormous amount of database computation. In order to handle this computation reasonably quickly, the program partitions the work to be done, assigning different portions of the database to different processors. The database field has contributed greatly to the commercial success of large shared-memory machines.

As the Pixar example shows, highly computation-intensive applications like computer graphics also have a need for these fast parallel computers. No one wants to wait hours just to generate a single

image, and the use of parallel processing machines can speed things up considerably. For example, consider **ray tracing** operations. Here our code follows the path of a ray of light in a scene, accounting for reflection and absorbtion of the light by various objects. Suppose the image is to consist of 1,000 rows of pixels, with 1,000 pixels per row. In order to attack this problem in a parallel processing manner with, say, 25 processors, we could divide the image into 25 squares of size 200x200, and have each processor do the computations for its square.

Note, though, that it may be much more challenging than this implies. First of all, the computation will need some communication between the processors, which hinders performance if it is not done carefully. Second, if one really wants good speedup, one may need to take into account the fact that some squares require more computation work than others. More on this below.

We are now in the era of Big Data, which requires Big Computation, thus again generating a major need for parallel processing.

1.1.2　Memory

Yes, execution speed is the reason that comes to most people's minds when the subject of parallel processing comes up. But in many applications, an equally important consideration is memory capacity. Parallel processing application often tend to use huge amounts of memory, and in many cases the amount of memory needed is more than can fit on one machine. If we have many machines working together, especially in the message-passing settings described below, we can accommodate the large memory needs.

1.1.3　Distributed Processing

In the above two subsections we've hit the two famous issues in computer science—time (speed) and space (memory capacity). But there is a third reason to do parallel processing, which actually has its own name, **distributed processing**. In a distributed database, for instance, parts of the database may be physically located in widely dispersed sites. If most transactions at a particular site arise locally, then we would make more efficient use of the network, and so on.

1.1.4　Our Focus Here

In this book, the primary emphasis is on processing speed.

1.2 Parallel Processing Hardware

This is a common scenario: Someone acquires a fancy new parallel machine, and excitedly writes a program to run on it—only to find that the parallel code is actually slower than the original serial version! This is due to lack of understanding of how the hardware works, at least at a high level.

This is not a hardware book, but since the goal of using parallel hardware is speed, the efficiency of our code is a major issue. That in turn means that we need a good understanding of the underlying hardware that we are programming. In this section, we give an overview of parallel hardware.

1.2.1 Shared-Memory Systems

Basic Architecture

Here many CPUs share the same physical memory. This kind of architecture is sometimes called MIMD, standing for Multiple Instruction (different CPUs are working independently, and thus typically are executing different instructions at any given instant), Multiple Data (different CPUs are generally accessing different memory locations at any given time).

Until recently, shared-memory systems cost hundreds of thousands of dollars and were affordable only by large companies, such as in the insurance and banking industries. The high-end machines are indeed still quite expensive, but now **multicore** machines, in which two or more CPUs share a common memory,[1] are commonplace in the home and even in cell phones!

Multiprocessor Topologies

A Symmetric Multiprocessor (SMP) system has the following structure:

The multicore setup is effectively the same as SMP, except that the processors are all on one chip, attached to the bus.

So-called NUMA architectures will be discussed in Chapter 3.

Memory Issues Etc.

Consider the SMP figure above.

- The Ps are processors, e.g. off-the-shelf chips such as Pentiums.

---

[1]The terminology gets confusing here. Although each core is a complete processor, people in the field tend to call the entire chip a "processor," referring to the cores, as, well, cores. In this book, the term *processor* will generally include cores, e.g. a dual-core chip will be considered to have two processors.

- The Ms are **memory modules**. These are physically separate objects, e.g. separate boards of memory chips. It is typical that there will be the same number of memory modules as processors. In the shared-memory case, the memory modules collectively form the entire shared address space, but with the addresses being assigned to the memory modules in one of two ways:

  - (a)

    High-order interleaving. Here consecutive addresses are in the <u>same</u> M (except at boundaries). For example, suppose for simplicity that our memory consists of addresses 0 through 1023, and that there are four Ms. Then M0 would contain addresses 0-255, M1 would have 256-511, M2 would have 512-767, and M3 would have 768-1023.

    We need 10 bits for addresses (since $1024 = 2^{10}$). The two most-significant bits would be used to select the module number (since $4 = 2^2$); hence the term *high-order* in the name of this design. The remaining eight bits are used to select the word within a module.

  - (b)

    Low-order interleaving. Here consecutive addresses are in consecutive memory modules (except when we get to the right end). In the example above, if we used low-order interleaving, then address 0 would be in M0, 1 would be in M1, 2 would be in M2, 3 would be in M3, 4 would be back in M0, 5 in M1, and so on.

    Here the two least-significant bits are used to determine the module number.

- To make sure only one processor uses the bus at a time, standard bus arbitration signals and/or arbitration devices are used.

- There may also be **coherent caches**, which we will discuss later.

All of the above issues can have major on the speed of our program, as will be seen later.

1.2.2 Message-Passing Systems

Basic Architecture

Here we have a number of independent CPUs, each with its own independent memory. The various processors communicate with each other via networks of some kind.

Example: Clusters

Here one has a set of commodity PCs and networks them for use as a parallel processing system. The PCs are of course individual machines, capable of the usual uniprocessor (or now multiprocessor)

applications, but by networking them together and using parallel-processing software environments, we can form very powerful parallel systems.

One factor which can be key to the success of a cluster is the use of a fast network, fast both in terms of hardware and network protocol. Ordinary Ethernet and TCP/IP are fine for the applications envisioned by the original designers of the Internet, e.g. e-mail and file transfer, but is slow in the cluster context. A good network for a cluster is, for instance, Infiniband.

Clusters have become so popular that there are now "recipes" on how to build them for the specific purpose of parallel processing. The term **Beowulf** come to mean a cluster of PCs, usually with a fast network connecting them, used for parallel processing. Software packages such as ROCKS (`http://www.rocksclusters.org/wordpress/`) have been developed to make it easy to set up and administer such systems.

1.2.3 SIMD

In contrast to MIMD systems, processors in SIMD—Single Instruction, Multiple Data—systems execute in lockstep. At any given time, all processors are executing the same machine instruction on different data.

Some famous SIMD systems in computer history include the ILLIAC and Thinking Machines Corporation's CM-1 and CM-2. Also, DSP ("digital signal processing") chips tend to have an SIMD architecture.

But today the most prominent example of SIMD is that of GPUs—graphics processing units. In addition to powering your PC's video cards, GPUs can now be used for general-purpose computation. The architecture is fundamentally shared-memory, but the individual processors do execute in lockstep, SIMD-fashion.

1.3 Programmer World Views

1.3.1 Example: Matrix-Vector Multiply

To explain the paradigms, we will use the term **nodes**, where roughly speaking one node corresponds to one processor, and use the following example:

Suppose we wish to multiply an nx1 vector X by an nxn matrix A, putting the product in an nx1 vector Y, and we have p processors to share the work.

In all the forms of parallelism, each node could be assigned some of the rows of A, and that node would multiply X by those rows, thus forming part of Y.

Note that in typical applications, the matrix A would be very large, say thousands of rows, possibly even millions. Otherwise the computation could be done quite satisfactorily in a **serial**, i.e. nonparallel manner, making parallel processing unnecessary..

1.3.2　Shared-Memory

Programmer View

In implementing the matrix-vector multiply example of Section 1.3.1 in the shared-memory paradigm, the arrays for A, X and Y would be held in common by all nodes. If for instance node 2 were to execute

```
1    Y[3] = 12;
```

and then node 15 were to subsequently execute

```
1    print("%d\n",Y[3]);
```

then the outputted value from the latter would be 12.

Computation of the matrix-vector product AX would then involve the nodes somehow deciding which nodes will handle which rows of A. Each node would then multiply its assigned rows of A times X, and place the result directly in the proper section of the shared Y.

Today, programming on shared-memory multiprocessors is typically done via **threading**. (Or, as we will see in other chapters, by higher-level code that runs threads underneath.) A **thread** is similar to a **process** in an operating system (OS), but with much less overhead. Threaded applications have become quite popular in even uniprocessor systems, and Unix,[2] Windows, Python, Java, Perl and now C++11 and R (via my Rdsm package) all support threaded programming.

In the typical implementation, a thread is a special case of an OS process. But the key difference is that the various threads of a program share memory. (One can arrange for processes to share memory too in some OSs, but they don't do so by default.)

On a uniprocessor system, the threads of a program take turns executing, so that there is only an illusion of parallelism. But on a multiprocessor system, one can genuinely have threads running in parallel.[3] Whenever a processor becomes available, the OS will assign some ready thread to it. So,

---

[2] Here and below, the term *Unix* includes Linux.

[3] There may be other processes running too. So the threads of our program must still take turns with other processes running on the machine.

among other things, this says that a thread might actually run on different processors during different turns.

Important note: Effective use of threads requires a basic understanding of how processes take turns executing. See Section **??** in the appendix of this book for this material.

One of the most popular threads systems is Pthreads, whose name is short for POSIX threads. POSIX is a Unix standard, and the Pthreads system was designed to standardize threads programming on Unix. It has since been ported to other platforms.

Example: Pthreads Prime Numbers Finder

Following is an example of Pthreads programming, in which we determine the number of prime numbers in a certain range. Read the comments at the top of the file for details; the threads operations will be explained presently.

```
1   // PrimesThreads.c
2
3   // threads-based program to find the number of primes between 2 and n;
4   // uses the Sieve of Eratosthenes, deleting all multiples of 2, all
5   // multiples of 3, all multiples of 5, etc.
6
7   // for illustration purposes only; NOT claimed to be efficient
8
9   // Unix compilation:  gcc -g -o primesthreads PrimesThreads.c -lpthread -lm
10
11  // usage:  primesthreads n num_threads
12
13  #include <stdio.h>
14  #include <math.h>
15  #include <pthread.h>  // required for threads usage
16
17  #define MAX_N 100000000
18  #define MAX_THREADS 25
19
20  // shared variables
21  int nthreads,  // number of threads (not counting main())
22      n,  // range to check for primeness
23      prime[MAX_N+1],  // in the end, prime[i] = 1 if i prime, else 0
24      nextbase;  // next sieve multiplier to be used
```

```
25  // lock for the shared variable nextbase
26  pthread_mutex_t nextbaselock = PTHREAD_MUTEX_INITIALIZER;
27  // ID structs for the threads
28  pthread_t id[MAX_THREADS];
29
30  // "crosses out" all odd multiples of k
31  void crossout(int k)
32  { int i;
33     for (i = 3; i*k <= n; i += 2)  {
34        prime[i*k] = 0;
35     }
36  }
37
38  // each thread runs this routine
39  void *worker(int tn)  // tn is the thread number (0,1,...)
40  { int lim,base,
41        work = 0;  // amount of work done by this thread
42     // no need to check multipliers bigger than sqrt(n)
43     lim = sqrt(n);
44     do  {
45        // get next sieve multiplier, avoiding duplication across threads
46        // lock the lock
47        pthread_mutex_lock(&nextbaselock);
48        base = nextbase;
49        nextbase += 2;
50        // unlock
51        pthread_mutex_unlock(&nextbaselock);
52        if (base <= lim)  {
53           // don't bother crossing out if base known composite
54           if (prime[base])  {
55              crossout(base);
56              work++;  // log work done by this thread
57           }
58        }
59        else return work;
60     } while (1);
61  }
62
63  main(int argc, char **argv)
```

```
64  {  int nprimes,  // number of primes found
65        i,work;
66     n = atoi(argv[1]);
67     nthreads = atoi(argv[2]);
68     // mark all even numbers nonprime, and the rest "prime until
69     // shown otherwise"
70     for (i = 3; i <= n; i++)  {
71        if (i%2 == 0) prime[i] = 0;
72        else prime[i] = 1;
73     }
74     nextbase = 3;
75     // get threads started
76     for (i = 0; i < nthreads; i++)  {
77        // this call says create a thread, record its ID in the array
78        // id, and get the thread started executing the function worker(),
79        // passing the argument i to that function
80        pthread_create(&id[i],NULL,worker,i);
81     }
82
83     // wait for all done
84     for (i = 0; i < nthreads; i++)  {
85        // this call says wait until thread number id[i] finishes
86        // execution, and to assign the return value of that thread to our
87        // local variable work here
88        pthread_join(id[i],&work);
89        printf("%d values of base done\n",work);
90     }
91
92     // report results
93     nprimes = 1;
94     for (i = 3; i <= n; i++)
95        if (prime[i])  {
96           nprimes++;
97        }
98     printf("the number of primes found was %d\n",nprimes);
99
100 }
```

To make our discussion concrete, suppose we are running this program with two threads. Suppose also the both threads are running simultaneously most of the time. This will occur if they aren't competing for turns with other threads, say if there are no other threads, or more generally if the number of other threads is less than or equal to the number of processors minus two. (Actually, the original thread is **main()**, but it lies dormant most of the time, as you'll see.)

Note the global variables:

```
int nthreads,  // number of threads (not counting main())
    n,  // range to check for primeness
    prime[MAX_N+1],  // in the end, prime[i] = 1 if i prime, else 0
    nextbase;  // next sieve multiplier to be used
pthread_mutex_t nextbaselock = PTHREAD_MUTEX_INITIALIZER;
pthread_t id[MAX_THREADS];
```

This will require some adjustment for those who've been taught that global variables are "evil."

In most threaded programs, all communication between threads is done via global variables.[④] So even if you consider globals to be evil, they are a necessary evil in threads programming.

Personally I have always thought the stern admonitions against global variables are overblown anyway; see `http://heather.cs.ucdavis.edu/~matloff/globals.html`. But as mentioned, those admonitions are routinely ignored in threaded programming. For a nice discussion on this, see the paper by a famous MIT computer scientist on an Intel Web page, at `http://software.intel.com/en-us/articles/global-variable-reconsidered/?wapkw=%28parallelism%29`.

As mentioned earlier, the globals are shared by all processors.[⑤] If one processor, for instance, assigns the value 0 to **prime[35]** in the function **crossout()**, then that variable will have the value 0 when accessed by any of the other processors as well. On the other hand, local variables have different values at each processor; for instance, the variable **i** in that function has a different value at each processor.

Note that in the statement

```
pthread_mutex_t nextbaselock = PTHREAD_MUTEX_INITIALIZER;
```

the right-hand side is not a constant. It is a macro call, and is thus something which is executed. In the code

---

[④]Technically one could use locals in **main()** (or whatever function it is where the threads are created) for this purpose, but this would be so unwieldy that it is seldom done.

[⑤]Technically, we should say "shared by all threads" here, as a given thread does not always execute on the same processor, but at any instant in time each executing thread is at some processor, so the statement is all right.

```
1  pthread_mutex_lock(&nextbaselock);
2  base = nextbase
3  nextbase += 2
4  pthread_mutex_unlock(&nextbaselock);
```

we see a **critical section** operation which is typical in shared-memory programming. In this context here, it means that we cannot allow more than one thread to execute the code

```
1  base = nextbase;
2  nextbase += 2;
```

at the same time. A common term used for this is that we wish the actions in the critical section to collectively be **atomic**, meaning not divisible among threads. The calls to **pthread_mutex_lock()** and **pthread_mutex_unlock()** ensure this. If thread A is currently executing inside the critical section and thread B tries to lock the lock by calling **pthread_mutex_lock()**, the call will block until thread B executes **pthread_mutex_unlock()**.

Here is why this is so important: Say currently **nextbase** has the value 11. What we want to happen is that the next thread to read **nextbase** will "cross out" all multiples of 11. But if we allow two threads to execute the critical section at the same time, the following may occur, in order:

- thread A reads **nextbase**, setting its value of **base** to 11

- thread B reads **nextbase**, setting its value of **base** to 11

- thread A adds 2 to **nextbase**, so that **nextbase** becomes 13

- thread B adds 2 to **nextbase**, so that **nextbase** becomes 15

Two problems would then occur:

- Both threads would do "crossing out" of multiples of 11, duplicating work and thus slowing down execution speed.

- We will never "cross out" multiples of 13.

Thus the lock is crucial to the correct (and speedy) execution of the program.

Note that these problems could occur either on a uniprocessor or multiprocessor system. In the uniprocessor case, thread A's turn might end right after it reads **nextbase**, followed by a turn by B which executes that same instruction. In the multiprocessor case, A and B could literally be running simultaneously, but still with the action by B coming an instant after A.

This problem frequently arises in parallel database systems. For instance, consider an airline reservation system. If a flight has only one seat left, we want to avoid giving it to two different

customers who might be talking to two agents at the same time. The lines of code in which the seat is finally assigned (the **commit** phase, in database terminology) is then a critical section.

A critical section is always a potential bottleneck in a parallel program, because its code is serial instead of parallel. In our program here, we may get better performance by having each thread work on, say, five values of **nextbase** at a time. Our line

```
nextbase += 2;
```

would become

```
nextbase += 10;
```

That would mean that any given thread would need to go through the critical section only one-fifth as often, thus greatly reducing overhead. On the other hand, near the end of the run, this may result in some threads being idle while other threads still have a lot of work to do.

Note this code.

```
for (i = 0; i < nthreads; i++)  {
    pthread_join(id[i],&work);
    printf("%d values of base done\n",work);
}
```

This is a special case of of **barrier**.

A barrier is a point in the code that all threads must reach before continuing. In this case, a barrier is needed in order to prevent premature execution of the later code

```
for (i = 3; i <= n; i++)
    if (prime[i])  {
        nprimes++;
    }
```

which would result in possibly wrong output if we start counting primes before some threads are done.

Actually, we could have used Pthreads' built-in barrier function. We need to declare a barrier variable, e.g.

```
pthread_barrier_t barr;
```

and then call it like this:

```
1  pthread_barrier_wait(&barr);
```

The **pthread_join()** function actually causes the given thread to exit, so that we then "join" the thread that created it, i.e. **main()**. Thus some may argue that this is not really a true barrier.

Barriers are very common in shared-memory programming, and will be discussed in more detail in Chapter 3.

Role of the OS

Let's again ponder the role of the OS here. What happens when a thread tries to lock a lock:

- The lock call will ultimately cause a system call, causing the OS to run.
- The OS keeps track of the locked/unlocked status of each lock, so it will check that status.
- Say the lock is unlocked (a 0). Then the OS sets it to locked (a 1), and the lock call returns. The thread enters the critical section.
- When the thread is done, the unlock call unlocks the lock, similar to the locking actions.
- If the lock is locked at the time a thread makes a lock call, the call will block. The OS will mark this thread as waiting for the lock. When whatever thread currently using the critical section unlocks the lock, the OS will relock it and unblock the lock call of the waiting thread. If several threads are waiting, of course only one will be unblock.

Note that **main()** is a thread too, the original thread that spawns the others. However, it is dormant most of the time, due to its calls to **pthread_join()**.

Finally, keep in mind that although the globals variables are shared, the locals are not. Recall that local variables are stored on a stack. Each thread (just like each process in general) has its own stack. When a thread begins a turn, the OS prepares for this by pointing the stack pointer register to this thread's stack.

Debugging Threads Programs

Most debugging tools include facilities for threads. Here's an overview of how it works in GDB.

First, as you run a program under GDB, the creation of new threads will be announced, e.g.

```
1  (gdb) r 100 2
2  Starting program: /debug/primes 100 2
3  [New Thread 16384 (LWP 28653)]
4  [New Thread 32769 (LWP 28676)]
```

```
5   [New Thread 16386 (LWP 28677)]
6   [New Thread 32771 (LWP 28678)]
```

You can do backtrace (**bt**) etc. as usual. Here are some threads-related commands:

- `info threads` (gives information on all current threads)
- `thread 3` (change to thread 3)
- `break 88 thread 3` (stop execution when thread 3 reaches source line 88)
- `break 88 thread 3 if x==y` (stop execution when thread 3 reaches source line 88 and the variables x and y are equal)

Of course, many GUI IDEs use GDB internally, and thus provide the above facilities with a GUI wrapper. Examples are DDD, Eclipse and NetBeans.

Higher-Level Threads

The OpenMP library gives the programmer a higher-level view of threading. The threads are there, but rather hidden by higher-level abstractions. We will study OpenMP in detail in Chapter 4, and use it frequently in the succeeding chapters, but below is an introductory example.

Example: Sampling Bucket Sort

This code implements the sampling bucket sort of Section 12.5.

```
1   // OpenMP introductory example: sampling bucket sort

2

3   // compile: gcc -fopenmp -o bsort bucketsort.c

4

5   // set the number of threads via the environment variable

6   // OMP_NUM_THREADS, e.g. in the C shell

7

8   // setenv OMP_NUM_THREADS 8

9

10  #include <omp.h> // required

11  #include <stdlib.h>

12

13  // needed for call to qsort()
```

```
14   int cmpints(int *u, int *v)
15   { if (*u < *v) return -1;
16      if (*u > *v) return 1;
17      return 0;
18   }
19
20   // adds xi to the part array, increments npart, the length of part
21   void grab(int xi, int *part, int *npart)
22   {
23      part[*npart] = xi;
24      *npart += 1;
25   }
26
27   // finds the min and max in y, length ny,
28   // placing them in miny and maxy
29   void findminmax(int *y, int ny, int *miny, int *maxy)
30   { int i,yi;
31      *miny = *maxy = y[0];
32      for (i = 1; i < ny; i++) {
33         yi = y[i];
34         if (yi < *miny) *miny = yi;
35         else if (yi > *maxy) *maxy = yi;
36      }
37   }
38
39   // sort the array x of length n
40   void bsort(int *x, int n)
41   { // these are local to this function, but shared among the threads
42      float *bdries; int *counts;
43      #pragma omp parallel
44      // entering this block activates the threads, each executing it
45      { // variables declared below are local to each thread
46         int me = omp_get_thread_num();
```

```
47    // have to do the next call within the block, while the threads
48    // are active
49    int nth = omp_get_num_threads();
50    int i,xi,minx,maxx,start;
51    int *mypart;
52    float increm;
53    int SAMPLESIZE;
54    // now determine the bucket boundaries; nth - 1 of them, by
55    // sampling the array to get an idea of its range
56    #pragma omp single // only 1 thread does this, implied barrier at end
57    {
58       if (n > 1000) SAMPLESIZE = 1000;
59       else SAMPLESIZE = n / 2;
60       findminmax(x,SAMPLESIZE,&minx,&maxx);
61       bdries = malloc((nth-1)*sizeof(float));
62       increm = (maxx - minx) / (float) nth;
63       for (i = 0; i < nth-1; i++)
64          bdries[i] = minx + (i+1) * increm;
65       // array to serve as the count of the numbers of elements of x
66       // in each bucket
67       counts = malloc(nth*sizeof(int));
68    }
69    // now have this thread grab its portion of the array; thread 0
70    // takes everything below bdries[0], thread 1 everything between
71    // bdries[0] and bdries[1], etc., with thread nth-1 taking
72    // everything over bdries[nth-1]
73    mypart = malloc(n*sizeof(int)); int nummypart = 0;
74    for (i = 0; i < n; i++) {
75       if (me == 0) {
76          if (x[i] <= bdries[0]) grab(x[i],mypart,&nummypart);
77       }
78       else if (me < nth-1) {
79          if (x[i] > bdries[me-1] && x[i] <= bdries[me])
```

```
80              grab(x[i],mypart,&nummypart);
81          } else
82             if (x[i] > bdries[me-1]) grab(x[i],mypart,&nummypart);
83        }
84        // now record how many this thread got
85        counts[me] = nummypart;
86        // sort my part
87        qsort(mypart,nummypart,sizeof(int),cmpints);
88        #pragma omp barrier // other threads need to know all of counts
89        // copy sorted chunk back to the original array; first find start point
90        start = 0;
91        for (i = 0; i < me; i++) start += counts[i];
92        for (i = 0; i < nummypart; i++) {
93           x[start+i] = mypart[i];
94        }
95     }
96     // implied barrier here; main thread won't resume until all threads
97     // are done
98  }
99
100 int main(int argc, char **argv)
101 {
102    // test case
103    int n = atoi(argv[1]), *x = malloc(n*sizeof(int));
104    int i;
105    for (i = 0; i < n; i++) x[i] = rand() % 50;
106    if (n < 100)
107       for (i = 0; i < n; i++) printf("%d\n",x[i]);
108    bsort(x,n);
109    if (n <= 100) {
110       printf("x after sorting:\n");
111       for (i = 0; i < n; i++) printf("%d\n",x[i]);
112    }
```

```
113  }
```

Details on OpenMP are presented in Chapter 4. Here is an overview of a few of the OpenMP constructs available:

- **#pragma omp for**

  In our example above, we wrote our own code to assign specific threads to do specific parts of the work. An alternative is to write an ordinary **for** loop that iterates over all the work to be done, and then ask OpenMP to assign specific iterations to specific threads. To do this, insert the above pragma just before the loop.

- **#pragma omp critical**

  The block that follows is implemented as a critical section. OpenMP sets up the locks etc. for you, alleviating you of work and alleviating your code of clutter.

Debugging OpenMP

Since there are threads underlying the OpenMP execution, you should be able to use your debugging tool's threads facilities. Note, though, that this may not work perfectly well.

Some versions of GCC/GDB, for instance, do not display some local variables. Let's consider two categories of such variables:

(a) Variables within a **parallel** block, such as **me** in **bsort()** in Section 1.3.2.

(b) Variables that are not in a **parallel** block, but which are still local to a function that contains such a block. An example is **counts** in **bsort()**.

You may find that when you try to use GDB's **print** command, GDB says there is no such variable.

The problem seems to arise from a combination of (i) optimzation, so that a variable is placed in a register and basically eliminated from the namespace, and (ii) some compilers implement OpenMP by actually making special versions of the function being debugged.

In GDB, one possible workaround is to use the **-gstabs+** option when compiling, instead of **-g**. But here is a more general workarounds. Let's consider variables of type (b) first.

The solution is to temporarily change these variables to globals, e.g.

```
1  int *counts;
2  void bsort(int *x, int n)
```

This would still be all right in terms of program correctness, because the variables in (b) are global to the threads anyway. (Of course, make sure not to have another global of the same name!) The switch

would only be temporary, during debugging, to be switched back later so that in the end **bsort()** is self-contained.

The same solution works for category (a) variables, with an added line:

```
int me;
#pragma omp threadprivate(me)
void bsort(int *x, int n)
```

What this does is make separate copies of **me** as global variables, one for each thread. As globals, GCC won't engage in any shenanigans with them. :-) One does have to keep in mind that they will retain there values upon exit from a parallel block etc., but the workaround does work.

1.3.3 Message Passing

Programmer View

Again consider the matrix-vector multiply example of Section 1.3.1. In contrast to the shared-memory case, in the message-passing paradigm all nodes would have <u>separate</u> copies of A, X and Y. Our example in Section 1.3.2 would now change. in order for node 2 to send this new value of Y[3] to node 15, it would have to execute some special function, which would be something like

```
send(15,12,"Y[3]");
```

and node 15 would have to execute some kind of **receive()** function.

To compute the matrix-vector product, then, would involve the following. One node, say node 0, would distribute the rows of A to the various other nodes. Each node would receive a different set of rows. The vector X would be sent to all nodes.[6] Each node would then multiply X by the node's assigned rows of A, and then send the result back to node 0. The latter would collect those results, and store them in Y.

Example: MPI Prime Numbers Finder

Here we use the MPI system, with our hardware being a cluster.

MPI is a popular public-domain set of interface functions, callable from C/C++, to do message passing. We are again counting primes, though in this case using a **pipelining** method. It is similar to hardware pipelines, but in this case it is done in software, and each "stage" in the pipe is a different computer.

---

[6]In a more refined version, X would be parceled out to the nodes, just as the rows of A are.

The program is self-documenting, via the comments.

```
/* MPI sample program; NOT INTENDED TO BE EFFICIENT as a prime
   finder, either in algorithm or implementation

   MPI (Message Passing Interface) is a popular package using
   the "message passing" paradigm for communicating between
   processors in parallel applications; as the name implies,
   processors communicate by passing messages using "send" and
   "receive" functions

   finds and reports the number of primes less than or equal to N

   uses a pipeline approach:  node 0 looks at all the odd numbers (i.e.
   has already done filtering out of multiples of 2) and filters out
   those that are multiples of 3, passing the rest to node 1; node 1
   filters out the multiples of 5, passing the rest to node 2; node 2
   then removes the multiples of 7, and so on; the last node must check
   whatever is left

   note that we should NOT have a node run through all numbers
   before passing them on to the next node, since we would then
   have no parallelism at all; on the other hand, passing on just
   one number at a time isn't efficient either, due to the high
   overhead of sending a message if it is a network (tens of
   microseconds until the first bit reaches the wire, due to
   software delay); thus efficiency would be greatly improved if
   each node saved up a chunk of numbers before passing them to
   the next node */

#include <mpi.h>  // mandatory

#define PIPE_MSG 0  // type of message containing a number to be checked
#define END_MSG 1  // type of message indicating no more data will be coming

int NNodes,  // number of nodes in computation
    N,  // find all primes from 2 to N
    Me;  // my node number
double T1,T2;  // start and finish times
```

```
39  void Init(int Argc,char **Argv)
40  {  int DebugWait;
41     N = atoi(Argv[1]);
42     // start debugging section
43     DebugWait = atoi(Argv[2]);
44     while (DebugWait) ;  // deliberate infinite loop; see below
45     /* the above loop is here to synchronize all nodes for debugging;
46        if DebugWait is specified as 1 on the mpirun command line, all
47        nodes wait here until the debugging programmer starts GDB at
48        all nodes (via attaching to OS process number), then sets
49        some breakpoints, then GDB sets DebugWait to 0 to proceed; */
50     // end debugging section
51     MPI_Init(&Argc,&Argv);  // mandatory to begin any MPI program
52     // puts the number of nodes in NNodes
53     MPI_Comm_size(MPI_COMM_WORLD,&NNodes);
54     // puts the node number of this node in Me
55     MPI_Comm_rank(MPI_COMM_WORLD,&Me);
56     // OK, get started; first record current time in T1
57     if (Me == NNodes-1) T1 = MPI_Wtime();
58  }
59
60  void Node0()
61  {  int I,ToCheck,Dummy,Error;
62     for (I = 1; I <= N/2; I++)  {
63        ToCheck = 2 * I + 1;  // latest number to check for div3
64        if (ToCheck > N) break;
65        if (ToCheck % 3 > 0)  // not divis by 3, so send it down the pipe
66           // send the string at ToCheck, consisting of 1 MPI integer, to
67           // node 1 among MPI_COMM_WORLD, with a message type PIPE_MSG
68           Error = MPI_Send(&ToCheck,1,MPI_INT,1,PIPE_MSG,MPI_COMM_WORLD);
69           // error not checked in this code
70     }
71     // sentinel
72     MPI_Send(&Dummy,1,MPI_INT,1,END_MSG,MPI_COMM_WORLD);
73  }
74
75  void NodeBetween()
76  {  int ToCheck,Dummy,Divisor;
77     MPI_Status Status;
```

```
78      // first received item gives us our prime divisor
79      // receive into Divisor 1 MPI integer from node Me-1, of any message
80      // type, and put information about the message in Status
81      MPI_Recv(&Divisor,1,MPI_INT,Me-1,MPI_ANY_TAG,MPI_COMM_WORLD,&Status);
82      while (1)  {
83         MPI_Recv(&ToCheck,1,MPI_INT,Me-1,MPI_ANY_TAG,MPI_COMM_WORLD,&Status);
84         // if the message type was END_MSG, end loop
85         if (Status.MPI_TAG == END_MSG) break;
86         if (ToCheck % Divisor > 0)
87            MPI_Send(&ToCheck,1,MPI_INT,Me+1,PIPE_MSG,MPI_COMM_WORLD);
88      }
89      MPI_Send(&Dummy,1,MPI_INT,Me+1,END_MSG,MPI_COMM_WORLD);
90   }
91
92   NodeEnd()
93   {  int ToCheck,PrimeCount,I,IsComposite,StartDivisor;
94      MPI_Status Status;
95      MPI_Recv(&StartDivisor,1,MPI_INT,Me-1,MPI_ANY_TAG,MPI_COMM_WORLD,&Status);
96      PrimeCount = Me + 2;  /* must account for the previous primes, which
97                               won't be detected below */
98      while (1)  {
99         MPI_Recv(&ToCheck,1,MPI_INT,Me-1,MPI_ANY_TAG,MPI_COMM_WORLD,&Status);
100        if (Status.MPI_TAG == END_MSG) break;
101        IsComposite = 0;
102        for (I = StartDivisor; I*I <= ToCheck; I += 2)
103           if (ToCheck % I == 0)  {
104              IsComposite = 1;
105              break;
106           }
107        if (!IsComposite) PrimeCount++;
108     }
109     /* check the time again, and subtract to find run time */
110     T2 = MPI_Wtime();
111     printf("elapsed time = %f\n",(float)(T2-T1));
112     /* print results */
113     printf("number of primes = %d\n",PrimeCount);
114  }
115
116  int main(int argc,char **argv)
```

```
117  {  Init(argc,argv);
118     // all nodes run this same program, but different nodes take
119     // different actions
120     if (Me == 0) Node0();
121     else if (Me == NNodes-1) NodeEnd();
122         else NodeBetween();
123     // mandatory for all MPI programs
124     MPI_Finalize();
125  }
126
127  /* explanation of "number of items" and "status" arguments at the end
128     of MPI_Recv():
129
130     when receiving a message you must anticipate the longest possible
131     message, but the actual received message may be much shorter than
132     this; you can call the MPI_Get_count() function on the status
133     argument to find out how many items were actually received
134
135     the status argument will be a pointer to a struct, containing the
136     node number, message type and error status of the received
137     message
138
139     say our last parameter is Status; then Status.MPI_SOURCE
140     will contain the number of the sending node, and
141     Status.MPI_TAG will contain the message type; these are
142     important if used MPI_ANY_SOURCE or MPI_ANY_TAG in our
143     node or tag fields but still have to know who sent the
144     message or what kind it is */
```

The set of machines can be heterogeneous, but MPI "translates" for you automatically. If say one node has a big-endian CPU and another has a little-endian CPU, MPI will do the proper conversion.

1.3.4   Scatter/Gather

Technically, the **scatter/gather** programmer world view is a special case of message passing. However, it has become so pervasive as to merit its own section here.

In this paradigm, one node, say node 0, serves as a **manager**, while the others serve as **workers**. The parcels out work to the workers, who process their respective chunks of the data and return the results to the manager. The latter receives the results and combines them into the final product.

The matrix-vector multiply example in Section 1.3.3 is an example of scatter/gather.

As noted, scatter/gather is very popular. Here are some examples of packages that use it:

- MPI includes scatter and gather functions (Section 7.4).
- Hadoop/MapReduce Computing (Chapter **??**) is basically a scatter/gather operation.
- The **snow** package (Section 1.3.4) for the R language is also a scatter/gather operation.

R snow Package

Base R does not include parallel processing facilities, but includes the **parallel** library for this purpose, and a number of other parallel libraries are available as well. The **parallel** package arose from the merger (and slight modifcation) of two former user-contributed libraries, **snow** and **multicore**. The former (and essentially the latter) uses the scatter/gather paradigm, and so will be introduced in this section; see Section 1.3.4 for further details. for convenience, I'll refer to the portion of **parallel** that came from **snow** simply as **snow**.

Let's use matrix-vector multiply as an example to learn from:

```
1  > library(parallel)
2  > c2 <- makePSOCKcluster(rep("localhost",2))
3  > c2
4  socket cluster with 2 nodes on host  ''localhost
5  > mmul
6  function(cls,u,v) {
7      rowgrps <- splitIndices(nrow(u),length(cls))
8      grpmul <- function(grp) u[grp,] %*% v
9      mout <- clusterApply(cls,rowgrps,grpmul)
10     Reduce(c,mout)
11 }
12 > a <- matrix(sample(1:50,16,replace=T),ncol=2)
13 > a
14      [,1] [,2]
15 [1,] 34 41
16 [2,] 10 28
17 [3,] 44 23
18 [4,] 7 29
```

```
19  [5,] 6 24
20  [6,] 28 29
21  [7,] 21 1
22  [8,] 38 30
23  > b <- c(5,-2)
24  > b
25  [1] 5 -2
26  > a %*% b # serial multiply
27       [,1]
28  [1,] 88
29  [2,] -6
30  [3,] 174
31  [4,] -23
32  [5,] -18
33  [6,] 82
34  [7,] 103
35  [8,] 130
36  > clusterExport(c2,c("a","b")) # send a,b to workers
37  > clusterEvalQ(c2,a) # check that they have it
38  [[1]]
39       [,1] [,2]
40  [1,] 34 41
41  [2,] 10 28
42  [3,] 44 23
43  [4,] 7 29
44  [5,] 6 24
45  [6,] 28 29
46  [7,] 21 1
47  [8,] 38 30
48
49  [[2]]
50       [,1] [,2]
51  [1,] 34 41
```

```
52  [2,] 10 28
53  [3,] 44 23
54  [4,] 7 29
55  [5,] 6 24
56  [6,] 28 29
57  [7,] 21 1
58  [8,] 38 30
59  > mmul(c2,a,b) # test our parallel code
60  [1] 88 -6 174 -23 -18 82 103 130
```

What just happened?

First we set up a **snow** cluster. The term should not be confused with hardware systems we referred to as "clusters" earlier. We are simply setting up a group of R processes that will communicate with each other via TCP/IP sockets.

In this case, my cluster consists of two R processes running on the machine from which I invoked **makePSOCKcluster()**. (In TCP/IP terminology, **localhost** refers to the local machine.) If I were to run the Unix **ps** command, with appropriate options, say **ax**, I'd see three R processes. I saved the cluster in **c2**.

On the other hand, my **snow** cluster could indeed be set up on a real cluster, e.g.

```
1  c3 <- makePSOCKcluster(c("pc28","pc29","pc29"))
```

where **pc28** etc. are machine names.

In preparing to test my parallel code, I needed to ship my matrices **a** and **b** to the workers:

```
1  > clusterExport(c2,c("a","b")) # send a,b to workers
```

Note that this function assumes that **a** and **b** are global variables at the invoking node, i.e. the manager, and it will place copies of them in the global workspace of the worker nodes.

Note that the copies are independent of the originals; if a worker changes, say, **b[3]**, that change won't be made at the manager or at the other worker. This is a message-passing system, indeed.

So, how does the **mmul** code work? Here's a handy copy:

```
1  mmul <- function(cls,u,v) {
2    rowgrps <- splitIndices(nrow(u),length(cls))
3    grpmul <- function(grp) u[grp,] %*% v
4    mout <- clusterApply(cls,rowgrps,grpmul)
```

```
5    Reduce(c,mout)
6  }
```

As discussed in Section 1.3.1, our strategy will be to partition the rows of the matrix, and then have different workers handle different groups of rows. Our call to **splitIndices()** sets this up for us.

That function does what its name implies, e.g.

```
1  > splitIndices(12,5)
2  [[1]]
3  [1] 1 2 3
4
5  [[2]]
6  [1] 4 5
7
8  [[3]]
9  [1] 6 7
10
11 [[4]]
12 [1] 8 9
13
14 [[5]]
15 [1] 10 11 12
```

Here we asked the function to partition the numbers 1,...,12 into 5 groups, as equal-sized as possible, which you can see is what it did. Note that the type of the return value is an R list.

So, after executing that function in our **mmul()** code, **rowgrps** will be an R list consisting of a partitioning of the row numbers of **u**, exactly what we need.

The call to **clusterApply()** is then where the actual work is assigned to the workers. The code

```
1  mout <- clusterApply(cls,rowgrps,grpmul)
```

instructs **snow** to have the first worker process the rows in **rowgrps[[1]]**, the second worker to work on **rowgrps[[2]]**, and so on. The **clusterApply()** function expects its second argument to be an R list, which is the case here.

Each worker will then multiply **v** by its row group, and return the product to the manager.

However, the product will again be a list, one component for each worker, so we need **Reduce()** to string everything back together.

Note that R does allow functions defined within functions, which the locals and arguments of the outer function becoming global to the inner function.

Note that **a** here could have been huge, in which case the export action could slow down our program. If **a** were not needed at the workers other than for this one-time matrix multiply, we may wish to change to code so that we send each worker only the rows of **a** that we need:

```
mmul1 <- function(cls,u,v) {
  rowgrps <- splitIndices(nrow(u),length(cls))
  uchunks <- Map(function(grp) u[grp,],rowgrps)
  mulchunk <- function(uc) uc %*% v
  mout <- clusterApply(cls,uchunks,mulchunk)
  Reduce(c,mout)
}
```

Let's test it:

```
> a <- matrix(sample(1:50,16,replace=T),ncol=2)
> b <- c(5,-2)
> clusterExport(c2,"b") # don't send a
 a
     [,1] [,2]
[1,] 10 26
[2,] 1 34
[3,] 49 30
[4,] 39 41
[5,] 12 14
[6,] 2 30
[7,] 33 23
[8,] 44 5
> a %*% b
     [,1]
[1,] -2
[2,] -63
```

```
18  [3,] 185
19  [4,] 113
20  [5,] 32
21  [6,] -50
22  [7,] 119
23  [8,] 210
24  > mmul1(c2,a,b)
25  [1] -2 -63 185 113 32 -50 119 210
```

Note that we did not need to use **clusterExport()** to send the chunks of **a** to the workers, as the call to **clusterApply()** does this, since it sends the arguments,

第 2 章 Recurring Performance Issues

2.1 "Embarrassingly Parallel"" Applications

第 3 章 Shared Memory Parallelism

Shared-memory programming is considered by many in the parallel processing community as being the clearest of the various parallel paradigms available.

Note: To get the most of this section—which is used frequently in the rest of this book—you may wish to read the material on array storage in the appendix of this book, Section **??**.

3.1 What Is Shared?

The term **shared memory** means that the processors all share a common address space. Say this is occurring at the hardware level, and we are using Intel Pentium CPUs. Suppose processor P3 issues the instruction

```
1   movl 200, %ebx
```

which reads memory location 200 and places the result in the EAX register in the CPU. If processor P4 does the same, they both will be referring to the same physical memory cell. (Note, however, that each CPU has a separate register set, so each will have its own independent EAX.) In non-shared-memory machines, each processor has its own private memory, and each one will then have its own location 200, completely independent of the locations 200 at the other processors' memories.

Say a program contains a global variable **X** and a local variable **Y** on share-memory hardware (and we use shared-memory software). If for example the compiler assigns location 200 to the variable **X**, i.e. `&X = 200`, then the point is that all of the processors will have that variable in common, because any processor which issues a memory operation on location 200 will access the same physical memory cell.

On the other hand, each processor will have its own separate run-time stack. All of the stacks are in shared memory, but they will be accessed separately, since each CPU has a different value in its SP (Stack Pointer) register. Thus each processor will have its own independent copy of the local variable **Y**.

To make the meaning of "shared memory" more concrete, suppose we have a bus-based system, with all the processors and memory attached to the bus. Let us compare the above variables **X** and **Y** here. Suppose again that the compiler assigns **X** to memory location 200. Then in the machine language code for the program, every reference to **X** will be there as 200. Every time an instruction that writes to **X** is executed by a CPU, that CPU will put 200 into its Memory Address Register (MAR), from which the 200 flows out on the address lines in the bus, and goes to memory. This will happen in the same way no matter which CPU it is. Thus the same physical memory location will end up being accessed, no matter which CPU generated the reference.

By contrast, say the compiler assigns a local variable **Y** to something like ESP+8, the third item on the stack (on a 32-bit machine), 8 bytes past the word pointed to by the stack pointer, ESP. The OS will assign a different ESP value to each thread, so the stacks of the various threads will be separate. Each CPU has its own ESP register, containing the location of the stack for whatever thread that CPU is currently running. So, the value of **Y** will be different for each thread.

3.2   Memory Modules

Parallel execution of a program requires, to a large extent, parallel accessing of memory. To some degree this is handled by having a cache at each CPU, but it is also facilitated by dividing the memory into separate **modules** or **banks**. This way several memory accesses can be done simultaneously.

In this section, assume for simplicity that our machine has 32-bit words. This is still true for many GPUs, in spite of the widespread use of 64-bit general-purpose machines today, and in any case, the numbers here can easily be converted to the 64-bit case.

Note that this means that consecutive words differ in address by 4. Let's thus define the word-address of a word to be its ordinary address divided by 4. Note that this is also its address with the lowest two bits deleted.

3.2.1   Interleaving

There is a question of how to divide up the memory into banks. There are two main ways to do this:

(a) **High-order interleaving:** Here consecutive words are in the <u>same</u> bank (except at boundaries). For example, suppose for simplicity that our memory consists of word-addresses 0 through 1023, and that there are four banks, M0 through M3. Then M0 would contain word-addresses 0-255, M1 would have 256-511, M2 would have 512-767, and M3 would have 768-1023.

(b) **Low-order interleaving:** Here consecutive addresses are in consecutive banks (except when we get to the right end). In the example above, if we used low-order interleaving, then word-address 0 would be in M0, 1 would be in M1, 2 would be in M2, 3 would be in M3, 4 would be back in M0, 5 in M1, and so on.

Say we have eight banks. Then under high-order interleaving, the first three bits of a word-address would be taken to be the bank number, with the remaining bits being address within bank. Under low-order interleaving, the three least significant bits would be used to determine bank number.

Low-order interleaving has often been used for **vector processors**. On such a machine, we might have both a regular add instruction, ADD, and a vector version, VADD. The latter would add two vectors together, so it would need to read two vectors from memory. If low-order interleaving is used, the elements of these vectors are spread across the various banks, so fast access is possible.

A more modern use of low-order interleaving, but with the same motivation as with the vector processors, is in GPUs (Chapter 5).

High-order interleaving might work well in matrix applications, for instance, where we can partition the matrix into blocks, and have different processors work on different blocks. In image processing applications, we can have different processors work on different parts of the image. Such partitioning almost never works perfectly—e.g. computation for one part of an image may need information from another part—but if we are careful we can get good results.

3.2.2   Bank Conflicts and Solutions

Consider an array **x** of 16 million elements, whose sum we wish to compute, say using 16 threads. Suppose we have four memory banks, with low-order interleaving.

A naive implementation of the summing code might be

```
1   parallel for thr = 0 to 15
2       localsum = 0
3       for j = 0 to 999999
4           localsum += x[thr*1000000+j]
5       grandsum += localsumsum
```

In other words, thread 0 would sum the first million elements, thread 1 would sum the second million, and so on. After summing its portion of the array, a thread would then add its sum to a grand total. (The threads *could* of course add to **grandsum** directly in each iteration of the loop, but this would cause too much traffic to memory, thus causing slowdowns.)

Suppose for simplicity that there is one address per word (it is usually one address per byte).

Suppose also for simplicity that the threads run in lockstep, so that they all attempt to access memory at once. On a multicore/multiprocessor machine, this may not occur, but it in fact typically *will* occur in a GPU setting.

A problem then arises. To make matters simple, suppose that **x** starts at an address that is a multiple of 4, thus in bank 0. (The reader should think about how to adjust this to the other three cases.) On the very first memory access, thread 0 accesses **x[0]** in bank 0, thread 1 accesses **x[1000000]**, also in bank 0, and so on—and *these will all be in memory bank 0*! Thus there will be major conflicts, hence major slowdown.

A better approach might be to have any given thread work on every sixteenth element of **x**, instead of on contiguous elements. Thread 0 would work on **x[1000000]**, **x[1000016]**, **x[10000032**,...; thread 1 would handle **x[1000001]**, **x[1000017]**, **x[10000033**,...; and so on:

```
1  parallel for thr = 0 to 15
2     localsum = 0
3     for j = 0 to 999999
4        localsum += x[16*j+thr]
5     grandsum += localsumsum
```

Here, consecutive threads work on consecutive elements in **x**.[1] That puts them in separate banks, thus no conflicts, hence speedy performance.

In general, avoiding bank conflicts is an art, but there are a couple of approaches we can try.

- We can rewrite our algorithm, e.g. use the second version of the above code instead of the first.

- We can add **padding** to the array. For instance in the first version of our code above, we could lengthen the array from 16 million to 16000016, placing padding in words 1000000, 2000001 and so on. We'd tweak our array indices in our code accordingly, and eliminate bank conflicts that way.

In the first approach above, the concept of **stride** often arises. It is defined to be the distance betwwen array elements in consecutive accesses by a thread. In our original code to compute **grandsum**, the stride was 1, since each array element accessed by a thread is 1 past the last access by that thread. In our second version, the stride was 16.

Strides of greater than 1 often arise in code that deals with multidimensional arrays. Say for example we have two-dimensional array with 16 columns. In C/C++, which uses row-major order, access of an entire column will have a stride of 16. Access down the main diagonal will have a stride of 17.

---

[1] Here thread 0 is considered "consecutive" to thread 15, in a wraparound manner.

Suppose we have b banks, again with low-order interleaving. You should experiment a bit to see that an array access with a stride of s will access s different banks if and only if s and b are relatively prime, i.e. the greatest common divisor of s and b is 1. This can be proven with group theory.

Another strategy, useful for collections of complex objects, is to set up **structs of arrays** rather than **arrays of structs**. Say for instance we are working with data on workers, storing for each worker his name, salary and number of years with the firm. We might naturally write code like this:

```
struct {
   char name[25];
   float salary;
   float yrs;
} x[100];
```

That gives a 100 structs for 100 workers. Again, this is very natural, but it may make for poor memory access patterns. Salary values for the various workers will no longer be contiguous, for instance, even though the **struct**s are contiguous. This could cause excessive cache misses.

One solution would be to add padding to each **struct**, so that the salary values are a word apart in memory. But another approach would be to replace the above arrays of **struct**s by a **struct** of arrays:

```
struct {
   char *name[]100;
   float salary[100];
   float yrs[100];
}
```

3.2.3 Example: Code to Implement Padding

As discussed above, array padding is used to try to get better parallel access to memory banks. The code below is aimed to provide utilities to assist in this. Details are explained in the comments.

```

// routines to initialize, read and write
// padded versions of a matrix of floats;
// the matrix is nominally mxn, but its
// rows will be padded on the right ends,
```

```
6   // so as to enable a stride of s down each
7   // column; it is assumed that s >= n
8
9   // allocate space for the padded matrix,
10  // initially empty
11  float *padmalloc(int m, int n, int s) {
12    return(malloc(m*s*sizeof(float)));
13  }
14
15  // store the value tostore in the matrix q,
16  // at row i, column j; m, n and
17  // s are as in padmalloc() above
18  void setter(float *q, int m, int n, int s,
19      int i, int j, float tostore) {
20    *(q + i*s+j) = tostore;
21  }
22
23  // fetch the value in the matrix q,
24  // at row i, column j; m, n and s are
25  // as in padmalloc() above
26  float getter(float *q, int m, int n, int s,
27      int i, int j) {
28    return *(q + i*s+j);
29  }
```

3.3　Interconnection Topologies

3.3.1　SMP Systems

A Symmetric Multiprocessor (SMP) system has the following structure:

bus
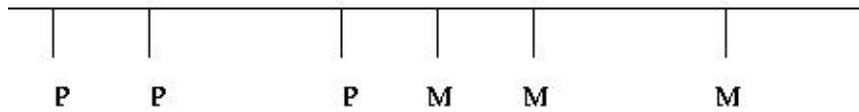
Here and below:

- The Ps are processors, e.g. off-the-shelf chips such as Pentiums.
- The Ms are **memory modules**. These are physically separate objects, e.g. separate boards of memory chips. It is typical that there will be the same number of Ms as Ps.
- To make sure only one P uses the bus at a time, standard bus arbitration signals and/or arbitration devices are used.
- There may also be **coherent caches**, which we will discuss later.

3.3.2 NUMA Systems

In a **Nonuniform Memory Access** (NUMA) architecture, each CPU has a memory module physically next to it, and these processor/memory (P/M) pairs are connected by some kind of network.

Here is a simple version:

bus
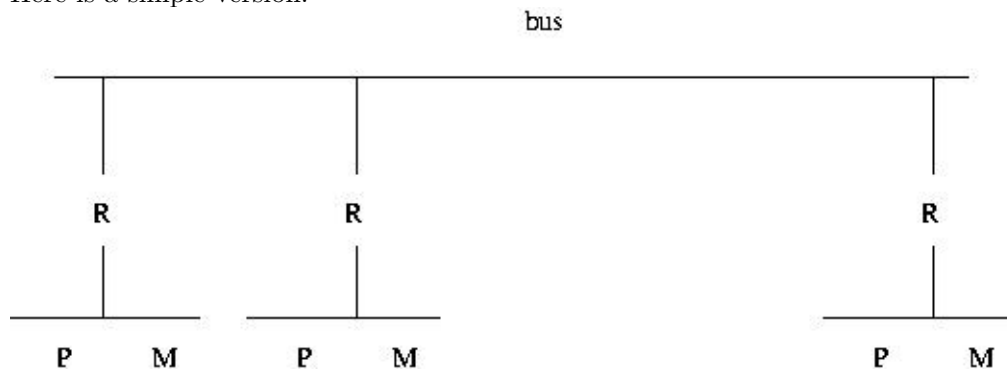
Each P/M/R set here is called a **processing element** (PE). Note that each PE has its own local bus, and is also connected to the global bus via R, the router.

Suppose for example that P3 needs to access location 200, and suppose that high-order interleaving is used. If location 200 is in M3, then P3's request is satisfied by the local bus.[2] On the other hand, suppose location 200 is in M8. Then the R3 will notice this, and put the request on the global bus, where it will be seen by R8, which will then copy the request to the local bus at PE8, where the request will be satisfied. (E.g. if it was a read request, then the response will go back from M8 to R8 to the global bus to R3 to P3.)

---

[2] This sounds similar to the concept of a cache. However, it is very different. A cache contains a local copy of some data stored elsewhere. Here it is the data itself, not a copy, which is being stored locally.

It should be obvious now where NUMA gets its name. P8 will have much faster access to M8 than P3 will to M8, if none of the buses is currently in use—and if say the global bus is currently in use, P3 will have to wait a long time to get what it wants from M8.

Today almost all high-end MIMD systems are NUMAs. One of the attractive features of NUMA is that by good programming we can exploit the nonuniformity. In matrix problems, for example, we can write our program so that, for example, P8 usually works on those rows of the matrix which are stored in M8, P3 usually works on those rows of the matrix which are stored in M3, etc. In order to do this, we need to make use of the C language's & address operator, and have some knowledge of the memory hardware structure, i.e. the interleaving.

3.3.3　NUMA Interconnect Topologies

The problem with a bus connection, of course, is that there is only one pathway for communication, and thus only one processor can access memory at the same time. If one has more than, say, two dozen processors are on the bus, the bus becomes saturated, even if traffic-reducing methods such as adding caches are used. Thus multipathway topologies are used for all but the smallest systems. In this section we look at two alternatives to a bus topology.

Crossbar Interconnects

Consider a shared-memory system with n processors and n memory modules. Then a crossbar connection would provide n^2 pathways. E.g. for n = 8:
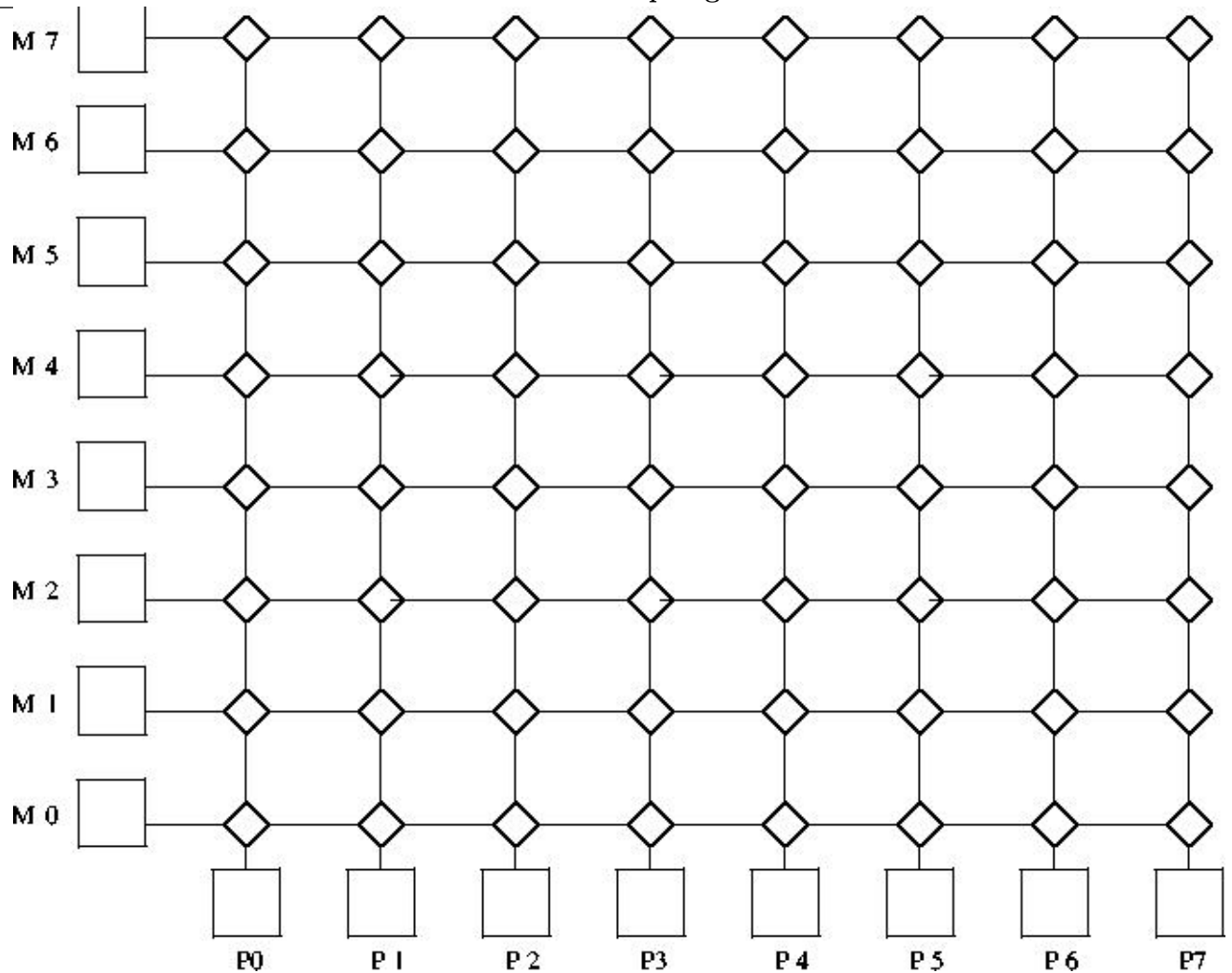
Generally serial communication is used from node to node, with a packet containing information on both source and destination address. E.g. if P2 wants to read from M5, the source and destination will be 3-bit strings in the packet, coded as 010 and 101, respectively. The packet will also contain bits which specify which word within the module we wish to access, and bits which specify whether we wish to do a read or a write. In the latter case, additional bits are used to specify the value to be written.

Each diamond-shaped node has two inputs (bottom and right) and two outputs (left and top), with buffers at the two inputs. If a buffer fills, there are two design options: (a) Have the node from which the input comes block at that output. (b) Have the node from which the input comes discard the packet, and retry later, possibly outputting some other packet for now. If the packets at the heads of the two buffers both need to go out the same output, the one (say) from the bottom input will be given priority.

There could also be a return network of the same type, with this one being memory $\rightarrow$ processor, to return the result of the read requests.[3]

Another version of this is also possible. It is not shown here, but the difference would be that at the bottom edge we would have the PEi and at the left edge the memory modules Mi would be replaced by lines which wrap back around to PEi, similar to the Omega network shown below.

Crossbar switches are too expensive for large-scale systems, but are useful in some small systems. The 16-CPU Sun Microsystems Enterprise 10000 system includes a 16x16 crossbar.

Omega (or Delta) Interconnects

These are multistage networks similar to crossbars, but with fewer paths. Here is an example of a NUMA 8x8 system:
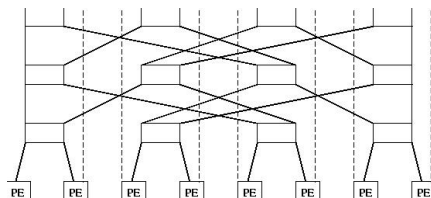
Recall that each PE is a processor/memory pair. PE3, for instance, consists of P3 and M3.

Note the fact that at the third stage of the network (top of picture), the outputs are routed back to the PEs, each of which consists of a processor and a memory module.[4]

At each network node (the nodes are the three rows of rectangles), the output routing is done by destination bit. Let's number the stages here 0, 1 and 2, starting from the bottom stage, number the nodes within a stage 0, 1, 2 and 3 from left to right, number the PEs from 0 to 7, left to right, and number the bit positions in a destination address 0, 1 and 2, starting from the most significant bit. Then at stage i, bit i of the destination address is used to determine routing, with a 0 meaning routing out the left output, and 1 meaning the right one.

Say P2 wishes to read from M5. It sends a read-request packet, including $5 = 101$ as its destination address, to the switch in stage 0, node 1. Since the first bit of 101 is 1, that means that this switch will route the packet out its right-hand output, sending it to the switch in stage 1, node 3. The latter switch will look at the next bit in 101, a 0, and thus route the packet out its left output, to the switch in stage 2, node 2. Finally, that switch will look at the last bit, a 1, and output out its right-hand

---

[3]For safety's sake, i.e. fault tolerance, even writes are typically acknowledged in multiprocessor systems.

[4]The picture may be cut off somewhat at the top and left edges. The upper-right output of the rectangle in the top row, leftmost position should connect to the dashed line which leads down to the second PE from the left. Similarly, the upper-left output of that same rectangle is a dashed lined, possibly invisible in your picture, leading down to the leftmost PE.

output, sending it to PE5, as desired. M5 will process the read request, and send a packet back to PE2, along the same

Again, if two packets at a node want to go out the same output, one must get priority (let's say it is the one from the left input).

Here is how the more general case of N = 2^n PEs works. Again number the rows of switches, and switches within a row, as above. So, S_{ij} will denote the switch in the i-th row from the bottom and j-th column from the left (starting our numbering with 0 in both cases). Row i will have a total of N input ports I_{ik} and N output ports O_{ik}, where k = 0 corresponds to the leftmost of the N in each case. Then if row i is not the last row ($i < n - 1$), O_{ik} will be connected to I_{jm}, where j = i+1 and

$$m = (2k + \lfloor (2k)/N \rfloor) \ mod \ N \tag{3.1}$$

If row i is the last row, then O_{ik} will be connected to, PE k.

3.3.4   Comparative Analysis

In the world of parallel architectures, a key criterion for a proposed feature is **scalability**, meaning how well the feature performs as we go to larger and larger systems. Let n be the system size, either the number of processors and memory modules, or the number of PEs. Then we are interested in how fast the latency, bandwidth and cost grow with n:

criterion	bus	Omega	crossbar
latency	O(1)	O($\log_2$ n)	O(n)
bandwidth	O(1)	O(n)	O(n)
cost	O(1)	O(n $\log_2$ n)	O(n^2)

Let us see where these expressions come from, beginning with a bus: No matter how large n is, the time to get from, say, a processor to a memory module will be the same, thus O(1). Similarly, no matter how large n is, only one communication can occur at a time, thus again O(1).[5]

Again, we are interested only in "O( )" measures, because we are only interested in growth rates as the system size n grows. For instance, if the system size doubles, the cost of a crossbar will quadruple; the $O(n^2)$ cost measure tells us this, with any multiplicative constant being irrelevant.

For Omega networks, it is clear that $log_2 n$ network rows are needed, hence the latency value given. Also, each row will have n/2 switches, so the number of network nodes will be O(n $log_2 n$). This figure

---

[5] Note that the '1' in "O(1)" does not refer to the fact that only one communication can occur at a time. If we had, for example, a two-bus system, the bandwidth would still be O(1), since multiplicative constants do not matter. What O(1) means, again, is that as n grows, the bandwidth stays at a multiple of 1, i.e. stays constant.

then gives the cost (in terms of switches, the main expense here). It also gives the bandwidth, since the maximum number of simultaneous transmissions will occur when all switches are sending at once.

Similar considerations hold for the crossbar case.

The crossbar's big advantage is that it is guaranteed that n packets can be sent simultaneously, providing they are to distinct destinations.

That is <u>not</u> true for Omega-networks. If for example, PE0 wants to send to PE3, and at the same time PE4 wishes to sent to PE2, the two packets will clash at the leftmost node of stage 1, where the packet from PE0 will get priority.

On the other hand, a crossbar is very expensive, and thus is dismissed out of hand in most modern systems. Note, though, that an equally troublesom aspect of crossbars is their high latency value; this is a big drawback when the system is not heavily loaded.

The bottom line is that Omega-networks amount to a compromise between buses and crossbars, and for this reason have become popular.

3.3.5   Why Have Memory in Modules?

In the shared-memory case, the Ms collectively form the entire shared address space, but with the addresses being assigned to the Ms in one of two ways:

- (a)

  High-order interleaving. Here consecutive addresses are in the <u>same</u> M (except at boundaries). For example, suppose for simplicity that our memory consists of addresses 0 through 1023, and that there are four Ms. Then M0 would contain addresses 0-255, M1 would have 256-511, M2 would have 512-767, and M3 would have 768-1023.

- (b)

  Low-order interleaving. Here consecutive addresses are in consecutive M's (except when we get to the right end). In the example above, if we used low-order interleaving, then address 0 would be in M0, 1 would be in M1, 2 would be in M2, 3 would be in M3, 4 would be back in M0, 5 in M1, and so on.

The idea is to have several modules busy at once, say in conjunction with a **split-transaction bus**. Here, after a processor makes a memory request, it relinquishes the bus, allowing others to use it while the memory does the requested work. Without splitting the memory into modules, this wouldn't achieve parallelism. The bus does need extra lines to identify which processor made the request.

3.4 Synchronization Hardware

Avoidance of race conditions, e.g. implementation of locks, plays such a crucial role in shared-memory parallel processing that hardware assistance is a virtual necessity. Recall, for instance, that critical sections can effectively serialize a parallel program. Thus efficient implementation is crucial.

3.4.1 Test-and-Set Instructions

Consider a bus-based system. In addition to whatever memory read and memory write instructions the processor included, there would also be a TAS instruction.[⑥] This instruction would control a TAS pin on the processor chip, and the pin in turn would be connected to a TAS line on the bus.

Applied to a location L in memory and a register R, say, TAS does the following:

```
1    copy L to R
2    if R is 0 then write 1 to L
```

And most importantly, these operations are done in an **atomic** manner; no bus transactions by other processors may occur between the two steps.

The TAS operation is applied to variables used as locks. Let's say that 1 means locked and 0 unlocked. Then the guarding of a critical section C by a lock variable L, using a register R, would be done by having the following code in the program being run:

```
1    TRY:  TAS R,L
2          JNZ TRY
3      C:  ...   ; start of critical section
4          ...
5          ...   ; end of critical section
6          MOV 0,L  ; unlock
```

where of course JNZ is a jump-if-nonzero instruction, and we are assuming that the copying from the Memory Data Register to R results in the processor N and Z flags (condition codes) being affected.

LOCK Prefix on Intel Processors

On Pentium machines, the LOCK prefix can be used to get atomicity for certain instructions: ADD, ADC, AND, BTC, BTR, BTS, CMPXCHG, DEC, INC, NEG, NOT, OR, SBB, SUB, XOR, XADD. The bus will be locked for the duration of the execution of the instruction, thus setting up atomic operations. There is a special LOCK line in the control bus for this purpose. (Locking thus only

---

[⑥]This discussion is for a mythical machine, but any real system works in this manner.

applies to these instructions in forms in which there is an operand in memory.) By the way, XCHG asserts this LOCK# bus signal even if the LOCK prefix is not specified.

For example, consider our count-the-2s example on page **??**. If we store **mycount** in a register, say EDX, then

```
1  lock add %edx, overallcount
```

would replace the code we had earlier,

```
1  pthread_mutex_lock(&nextbaselock);
2  overallcount += mylocalcount;
3  pthread_mutex_unlock(&nextbaselock);
```

without locks!

Here is how we could implement a lock if needed. The lock would be in a variable named, say, **lockvar**.

```
1    movl $lockvar, %ebx
2    movl $1, %ecx
3  top:
4    movl $0, %eax
5    lock cmpxchg (%ebx), %ecx
6    jz top # else leave the loop and enter the critical section
```

The operation CMPXCHG has EAX as an unnamed operand. The instruction basically does (here **source** is ECX and **destination** is **lockvar**)

```
1  if c(EAX) != c(destination) # sorry, lock is already locked
2    c(EAX) <- c(destination)
3    ZF <- 0 # the Zero Flag in the EFLAGS register
4  else
5    c(destination) <- c(source) # lock the lock
6    ZF <- 1
```

The LOCK prefix locks the bus for the entire duration of the instruction. Note that the ADD instruction here involves two memory transactions—one to read the old value of **overallcount**, and the second the write the new, incremented value back to **overallcount**. So, we are locking for a rather

long time, potentially compromising performance when other threads want to access memory, but the benefits can be huge.

Locks with More Complex Interconnects

In crossbar or Ω-network systems, some 2-bit field in the packet must be devoted to transaction type, say 00 for Read, 01 for Write and 10 for TAS. In a sytem with 16 CPUs and 16 memory modules, say, the packet might consist of 4 bits for the CPU number, 4 bits for the memory module number, 2 bits for the transaction type, and 32 bits for the data (for a write, this is the data to be written, while for a read, it would be the requested value, on the trip back from the memory to the CPU).

But note that the atomicity here is best done at the memory, i.e. some hardware should be added at the memory so that TAS can be done; otherwise, an entire processor-to-memory path (e.g. the bus in a bus-based system) would have to be locked up for a fairly long time, obstructing even the packets which go to other memory modules.

3.4.2 May Not Need the Latest

Note carefully that in many settings it may not be crucial to get the most up-to-date value of a variable. For example, a program may have a data structure showing work to be done. Some processors occasionally add work to the queue, and others take work from the queue. Suppose the queue is currently empty, and a processor adds a task to the queue, just as another processor is checking the queue for work. As will be seen later, it is possible that even though the first processor has written to the queue, the new value won't be visible to other processors for some time. But the point is that if the second processor does not see work in the queue (even though the first processor has put it there), the program will still work correctly, albeit with some performance loss.

3.4.3 Fetch-and-Add Instructions

Another form of interprocessor synchronization is a **fetch-and-add** (FA) instruction. The idea of FA is as follows. For the sake of simplicity, consider code like

```
1  LOCK(K);
2  Y = X++;
3  UNLOCK(K);
```

Suppose our architecture's instruction set included an F&A instruction. It would add 1 to the specified location in memory, and return the old value (to **Y**) that had been in that location before being incremented. And all this would be an atomic operation.

We would then replace the code above by a library call, say,

```
1  FETCH_AND_ADD(X,1);
```

The C code above would compile to, say,

```
1  F&A X,R,1
```

where **R** is the register into which the old (pre-incrementing) value of **X** would be returned.

There would be hardware adders placed at each memory module. That means that the whole operation could be done in one round trip to memory. Without F&A, we would need two round trips to memory just for the

```
1  X++;
```

(we would load **X** into a register in the CPU, increment the register, and then write it back to **X** in memory), and then the LOCK() and UNLOCK() would need trips to memory too. This could be a huge time savings, especially for long-latency interconnects.

3.5   Cache Issues

If you need a review of cache memories or don't have background in that area at all, read Section **??** in the appendix of this book before continuing.

3.5.1   Cache Coherency

Consider, for example, a bus-based system. Relying purely on TAS for interprocessor synchronization would be unthinkable: As each processor contending for a lock variable spins in the loop shown above, it is adding tremendously to bus traffic.

An answer is to have caches at each processor.[7] These will store copies of the values of lock variables. (Of course, non-lock variables are stored too. However, the discussion here will focus on effects on lock variables.) The point is this: Why keep looking at a lock variable L again and again, using up the bus bandwidth? L may not change value for a while, so why not keep a copy in the cache, avoiding use of the bus?

The answer of course is that eventually L <u>will</u> change value, and this causes some delicate problems. Say for example that processor P5 wishes to enter a critical section guarded by L, and that processor

---

[7]The reader may wish to review the basics of caches. See for example `http://heather.cs.ucdavis.edu/~matloff/50/PLN/CompOrganization.pdf`.

P2 is already in there. During the time P2 is in the critical section, P5 will spin around, always getting the same value for L (1) from C5, P5's cache. When P2 leaves the critical section, P2 will set L to 0—and now C5's copy of L will be incorrect. This is the **cache coherency problem**, inconsistency between caches.

A number of solutions have been devised for this problem. For bus-based systems, **snoopy** protocols of various kinds are used, with the word "snoopy" referring to the fact that all the caches monitor ("snoop on") the bus, watching for transactions made by <u>other</u> caches.

The most common protocols are the **invalidate** and **update** types. This relation between these two is somewhat analogous to the relation between **write-back** and **write-through** protocols for caches in uniprocessor systems:

- Under an invalidate protocol, when a processor writes to a variable in a cache, it first (i.e. before actually doing the write) tells each other cache to mark as invalid its cache line (if any) which contains a copy of the variable.[8] Those caches will be updated only later, the next time their processors need to access this cache line.

- For an update protocol, the processor which writes to the variable tells all other caches to immediately update their cache lines containing copies of that variable with the new value.

Let's look at an outline of how one implementation (many variations exist) of an invalidate protocol would operate:

In the scenario outlined above, when P2 leaves the critical section, it will write the new value 0 to L. Under the invalidate protocol, P2 will post an invalidation message on the bus. All the other caches will notice, as they have been monitoring the bus. They then mark their cached copies of the line containing L as invalid.

Now, the next time P5 executes the TAS instruction—which will be very soon, since it is in the loop shown above—P5 will find that the copy of L in C5 is invalid. It will respond to this cache miss by going to the bus, and requesting P2 to supply the "real" (and valid) copy of the line containing L.

But there's more. Suppose that all this time P6 had also been executing the loop shown above, along with P5. Then P5 and P6 may have to contend with each other. Say P6 manages to grab possession of the bus first.[9] P6 then executes the TAS again, which finds L = 0 and changes L back to 1. P6 then relinquishes the bus, and enters the critical section. Note that in changing L to 1, P6 also sends an invalidate signal to all the other caches. So, when P5 tries its execution of the TAS again, it

---

[8]We will follow commonly-used terminology here, distinguishing between a *cache line* and a *memory block*. Memory is divided in blocks, some of which have copies in the cache. The cells in the cache are called *cache lines*. So, at any given time, a given cache line is either empty or contains a copy (valid or not) of some memory block.

[9]Again, remember that ordinary bus arbitration methods would be used.

will have to ask P6 to send a valid copy of the block. P6 does so, but L will be 1, so P5 must resume executing the loop. P5 will then continue to use its valid local copy of L each time it does the TAS, until P6 leaves the critical section, writes 0 to L, and causes another cache miss at P5, etc.

At first the update approach seems obviously superior, and actually, if our shared, cacheable[10] variables were only lock variables, this might be true.

But consider a shared, cacheable vector. Suppose the vector fits into one block, and that we write to each vector element sequentially. Under an update policy, we would have to send a new message on the bus/network for each component, while under an invalidate policy, only one message (for the first component) would be needed. If during this time the other processors do not need to access this vector, all those update messages, and the bus/network bandwidth they use, would be wasted.

Or suppose for example we have code like

```
1    Sum += X[I];
```

in the middle of a **for** loop. Under an update protocol, we would have to write the value of Sum back many times, even though the other processors may only be interested in the final value when the loop ends. (This would be true, for instance, if the code above were part of a critical section.)

Thus the invalidate protocol works well for some kinds of code, while update works better for others. The CPU designers must try to anticipate which protocol will work well across a broad mix of applications.[11]

Now, how is cache coherency handled in non-bus shared-memory systems, say crossbars? Here the problem is more complex. Think back to the bus case for a minute: The very feature which was the biggest negative feature of bus systems—the fact that there was only one path between components made bandwidth very limited—is a very <u>positive</u> feature in terms of cache coherency, because it makes <u>broadcast</u> very easy: Since everyone is attached to that single pathway, sending a message to all of them costs no more than sending it to just one—we get the others for free. That's no longer the case for multipath systems. In such systems, extra copies of the message must be created for each path, adding to overall traffic.

A solution is to send messages only to "interested parties." In **directory-based** protocols, a list is kept of all caches which currently have valid copies of all blocks. In one common implementation, for example, while P2 is in the critical section above, it would be the **owner** of the block containing L. (Whoever is the latest node to write to L would be considered its current owner.) It would maintain a directory of all caches having valid copies of that block, say C5 and C6 in our story here. As soon as

---

[10] Many modern processors, including Pentium and MIPS, allow the programmer to mark some blocks as being noncacheable.

[11] Some protocols change between the two modes dynamically.

P2 wrote to L, it would then send either invalidate or update packets (depending on which type was being used) to C5 and C6 (and <u>not</u> to other caches which didn't have valid copies).

There would also be a directory at the memory, listing the current owners of all blocks. Say for example P0 now wishes to "join the club," i.e. tries to access L, but does not have a copy of that block in its cache C0. C0 will thus not be listed in the directory for this block. So, now when it tries to access L and it will get a cache miss. P0 must now consult the **home** of L, say P14. The home might be determined by L's location in main memory according to high-order interleaving; it is the place where the main-memory version of L resides. A table at P14 will inform P0 that P2 is the current owner of that block. P0 will then send a message to P2 to add C0 to the list of caches having valid copies of that block. Similarly, a cache might "resign" from the club, due to that cache line being replaced, e.g. in a LRU setting, when some other cache miss occurs.

3.5.2   Example: the MESI Cache Coherency Protocol

Many types of cache coherency protocols have been proposed and used, some of them quite complex. A relatively simple one for snoopy bus systems which is widely used is MESI, which for example is the protocol used in the Pentium series.

MESI is an invalidate protocol for bus-based systems. Its name stands for the four states a given cache line can be in for a given CPU:

- Modified
- Exclusive
- Shared
- Invalid

Note that *each memory block* has such a state at *each cache*. For instance, block 88 may be in state S at P5's and P12's caches but in state I at P1's cache.

Here is a summary of the meanings of the states:

state	meaning
M	written to more than once; no other copy valid
E	valid; no other cache copy valid; memory copy valid
S	valid; at least one other cache copy valid
I	invalid (block either not in the cache or present but incorrect)

Following is a summary of MESI state changes.[12] When reading it, keep in mind again that there is a separate state for each cache/memory block combination.

In addition to the terms **read hit**, **read miss**, **write hit**, **write miss**, which you are already familiar with, there are also **read snoop** and **write snoop**. These refer to the case in which our CPU observes on the bus a block request by another CPU that has attempted a read or write action but encountered a miss in its own cache; if our cache has a valid copy of that block, we must provide it to the requesting CPU (and in some cases to memory).

So, here are various events and their corresponding state changes:

If our CPU does a read:

present state	event	new state
M	read hit	M
E	read hit	E
S	read hit	S
I	read miss; no valid cache copy at any other CPU	E
I	read miss; at least one valid cache copy in some other CPU	S

If our CPU does a memory write:

present state	event	new state
M	write hit; do not put invalidate signal on bus; do not update memory	M
E	same as M above	M
S	write hit; put invalidate signal on bus; update memory	E
I	write miss; update memory but do nothing else	I

If our CPU does a read or write snoop:

present state	event	newstat
M	read snoop; write line back to memory, picked up by other CPU	S
M	write snoop; write line back to memory, signal other CPU now OK to do its write	I
E	read snoop; put shared signal on bus; no memory action	S
E	write snoop; no memory action	I
S	read snoop	S
S	write snoop	I
I	any snoop	I

Note that a write miss does NOT result in the associated block being brought in from memory.

---

[12]See *Pentium Processor System Architecture*, by D. Anderson and T. Shanley, Addison-Wesley, 1995. We have simplified the presentation here, by eliminating certain programmable options.

Example: Suppose a given memory block has state M at processor A but has state I at processor B, and B attempts to write to the block. B will see that its copy of the block is invalid, so it notifies the other CPUs via the bus that it intends to do this write. CPU A sees this announcement, tells B to wait, writes its own copy of the block back to memory, and then tells B to go ahead with its write. The latter action means that A's copy of the block is not correct anymore, so the block now has state I at A. B's action does not cause loading of that block from memory to its cache, so the block still has state I at B.

3.5.3   The Problem of "False Sharing"

Consider the C declaration

```
int W,Z;
```

Since **W** and **Z** are declared adjacently, most compilers will assign them contiguous memory addresses. Thus, unless one of them is at a memory block boundary, when they are cached they will be stored in the same cache line. Suppose the program writes to **Z**, and our system uses an invalidate protocol. Then **W** will be considered invalid at the other processors, even though its values at those processors' caches are correct. This is the **false sharing** problem, alluding to the fact that the two variables are sharing a cache line even though they are not related.

This can have very adverse impacts on performance. If for instance our variable **W** is now written to, then **Z** will suffer unfairly, as its copy in the cache will be considered invalid even though it is perfectly valid. This can lead to a "ping-pong" effect, in which alternate writing to two variables leads to a cyclic pattern of coherency transactions.

One possible solution is to add padding, e.g. declaring **W** and **Z** like this:

```
int W,U[1000],Z;
```

to separate **W** and **Z** so that they won't be in the same cache block. Of course, we must take block size into account, and check whether the compiler really has placed the two variables are in widely separated locations. To do this, we could for instance run the code

```
printf("%x %x\n",&W,&Z);
```

3.6   Memory-Access Consistency Policies

Though the word *consistency* in the title of this section may seem to simply be a synonym for *coherency* from the last section, and though there actually is some relation, the issues here are quite

different. In this case, it is a timing issue: After one processor changes the value of a shared variable, when will that value be visible to the other processors?

There are various reasons why this is an issue. For example, many processors, especially in multiprocessor systems, have **write buffers**, which save up writes for some time before actually sending them to memory. (For the time being, let's suppose there are no caches.) The goal is to reduce memory access costs. Sending data to memory in groups is generally faster than sending one at a time, as the overhead of, for instance, acquiring the bus is amortized over many accesses. Reads following a write may proceed, without waiting for the write to get to memory, except for reads to the same address. So in a multiprocessor system in which the processors use write buffers, there will often be some delay before a write actually shows up in memory.

A related issue is that operations may occur, or appear to occur, out of order. As noted above, a read which follows a write in the program may execute before the write is sent to memory. Also, in a multiprocessor system with multiple paths between processors and memory modules, two writes might take different paths, one longer than the other, and arrive "out of order." In order to simplify the presentation here, we will focus on the case in which the problem is due to write buffers, though.

The designer of a multiprocessor system must adopt some **consistency model** regarding situations like this. The above discussion shows that the programmer must be made aware of the model, or risk getting incorrect results. Note also that different consistency models will give different levels of performance. The "weaker" consistency models make for faster machines but require the programmer to do more work.

The strongest consistency model is Sequential Consistency. It essentially requires that memory operations done by one processor are observed by the other processors to occur in the same order as executed on the first processor. Enforcement of this requirement makes a system slow, and it has been replaced on most systems by weaker models.

One such model is **release consistency**. Here the processors' instruction sets include instructions ACQUIRE and RELEASE. Execution of an ACQUIRE instruction at one processor involves telling all other processors to flush their write buffers. However, the ACQUIRE won't execute until pending RELEASEs are done. Execution of a RELEASE basically means that you are saying, "I'm done writing for the moment, and wish to allow other processors to see what I've written." An ACQUIRE waits for all pending RELEASEs to complete before it executes.[13]

A related model is **scope consistency**. Say a variable, say **Sum**, is written to within a critical section guarded by LOCK and UNLOCK instructions. Then under scope consistency any changes

---

[13]There are many variants of all of this, especially in the software distibuted shared memory realm, to be discussed later.

made by one processor to **Sum** within this critical section would then be visible to another processor when the latter next enters this critical section. The point is that memory update is postponed until it is actually needed. Also, a barrier operation (again, executed at the hardware level) forces all pending memory writes to complete.

All modern processors include instructions which implement consistency operations. For example, Sun Microsystems' SPARC has a MEMBAR instruction. If used with a STORE operand, then all pending writes at this processor will be sent to memory. If used with the LOAD operand, all writes will be made visible to this processor.

Now, how does cache coherency fit into all this? There are many different setups, but for example let's consider a design in which there is a write buffer between each processor and its cache. As the processor does more and more writes, the processor saves them up in the write buffer. Eventually, some programmer-induced event, e.g. a MEMBAR instruction,[14] will cause the buffer to be flushed. Then the writes will be sent to "memory"—actually meaning that they go to the cache, and then possibly to memory.

The point is that (in this type of setup) before that flush of the write buffer occurs, the cache coherency system is quite unaware of these writes. Thus the cache coherency operations, e.g. the various actions in the MESI protocol, won't occur until the flush happens.

To make this notion concrete, again consider the example with **Sum** above, and assume release or scope consistency. The CPU currently executing that code (say CPU 5) writes to **Sum**, which is a memory operation—it affects the cache and thus eventually the main memory—but that operation will be invisible to the cache coherency protocol for now, as it will only be reflected in this processor's write buffer. But when the unlock is finally done (or a barrier is reached), the write buffer is flushed and the writes are sent to this CPU's cache. That then triggers the cache coherency operation (depending on the state). The point is that the cache coherency operation would occur only now, not before.

What about reads? Suppose another processor, say CPU 8, does a read of **Sum**, and that page is marked invalid at that processor. A cache coherency operation will then occur. Again, it will depend on the type of coherency policy and the current state, but in typical systems this would result in **Sum**'s cache block being shipped to CPU 8 from whichever processor the cache coherency system thinks has a valid copy of the block. That processor may or may not be CPU 5, but even if it is, that block won't show the recent change made by CPU 5 to **Sum**.

The analysis above assumed that there is a write buffer between each processor and its cache. There would be a similar analysis if there were a write buffer between each cache and memory.

---

[14]We call this "programmer-induced," since the programmer will include some special operation in her C/C++ code which will be translated to MEMBAR.

Note once again the performance issues. Instructions such as ACQUIRE or MEMBAR will use a substantial amount of interprocessor communication bandwidth. A consistency model must be chosen carefully by the system designer, and the programmer must keep the communication costs in mind in developing the software.

The recent Pentium models use Sequential Consistency, with any write done by a processor being immediately sent to its cache as well.

3.7 Fetch-and-Add Combining within Interconnects

In addition to read and write operations being specifiable in a network packet, an F&A operation could be specified as well (a 2-bit field in the packet would code which operation was desired). Again, there would be adders included at the memory modules, i.e. the addition would be done at the memory end, not at the processors. When the F&A packet arrived at a memory module, our variable **X** would have 1 added to it, while the old value would be sent back in the return packet (and put into R).

Another possibility for speedup occurs if our system uses a multistage interconnection network such as a crossbar. In that situation, we can design some intelligence into the network nodes to do **packet combining**: Say more than one CPU is executing an F&A operation at about the same time for the same variable **X**. Then more than one of the corresponding packets may arrive at the same network node at about the same time. If each one requested an incrementing of **X** by 1, the node can replace the two packets by one, with an increment of 2. Of course, this is a delicate operation, and we must make sure that different CPUs get different return values, etc.

3.8 Multicore Chips

A recent trend has been to put several CPUs on one chip, termed a **multicore** chip. As of March 2008, dual-core chips are common in personal computers, and quad-core machines are within reach of the budgets of many people. Just as the invention of the integrated circuit revolutionized the computer industry by making computers affordable for the average person, multicore chips will undoubtedly revolutionize the world of parallel programming.

A typical dual-core setup might have the two CPUs sharing a common L2 cache, with each CPU having its own L1 cache. The chip may interface to the bus or interconnect network of via an L3 cache.

Multicore is extremely important these days. However, they are just SMPs, for the most part, and thus should not be treated differently.

3.9   Optimal Number of Threads

A common question involves the best number of threads to run in a shared-memory setting. Clearly there is no general magic answer, but here are some considerations:[15]

- If your application does a lot of I/O, CPUs or cores may stay idle while waiting for I/O events. It thus makes sense to have many threads, so that computation threads can run when the I/O threads are tied up.

- In a purely computational application, one generally should not have more threads than cores. However, a program with a lot of virtual memory page faults may benefit from setting up extra threads, as page replacement involves (disk) I/O.

- Applications in which there is heavy interthread communication, say due to having a lot of lock variable, access, may benefit from setting up fewer threads than the number of cores.

- Many Intel processors include hardware for *hypertheading.* These are not full threads in the sense of having separate cores, but rather involve a limited amount of resource duplication within a core. The performance gain from this is typically quite modest. In any case, be aware of it; some software systems count these as threads, and assume for instance that there are 8 cores when the machine is actually just quad core.

- With GPUs (Chapter 5), most memory accesses have long latency and thus are I/O-like. Typically one needs very large numbers of threads for good performance.

3.10   Processor Affinity

With a timesharing OS, a given thread may run on different cores during different timeslices. If so, the cache for a given core may need a lot of refreshing, each time a new thread runs on that core. To avoid this slowdown, one might designate a preferred core for each thread, in the hope of reusing cache contents. Setting this up is dependent on the chip and the OS. OpenMP 3.1 has some facility for this.

---

[15]As with many aspects of parallel programming, a good basic knowledge of operating systems is key. See the reference on page 7.

3.11　Illusion of Shared-Memory through Software

Software Distributed Shared Memory

There are also various shared-memory software packages that run on message-passing hardware such as NOWs, called **software distributed shared memory** (SDSM) systems. Since the platforms do not have any physically shared memory, the shared-memory view which the programmer has is just an illusion. But that illusion is very useful, since the shared-memory paradigm is believed to be the easier one to program in. Thus SDSM allows us to have "the best of both worlds"—the convenience of the shared-memory world view with the inexpensive cost of some of the message-passing hardware systems, particularly networks of workstations (NOWs).

SDSM itself is divided into two main approaches, the **page-based** and **object-based** varieties. The page-based approach is generally considered clearer and easier to program in, and provides the programmer the "look and feel" of shared-memory programming better than does the object-based type.[16] We will discuss only the page-based approach here. The most popular SDSM system today is the page-based Treadmarks (Rice University). Another excellent page-based system is JIAJIA (Academy of Sciences, China).

To illustrate how page-based SDSMs work, consider the line of JIAJIA code

```
1  Prime = (int *) jia_alloc(N*sizeof(int));
```

The function **jia_alloc()** is part of the JIAJIA library, **libjia.a**, which is linked to one's application program during compilation.

At first this looks a little like a call to the standard **malloc()** function, setting up an array **Prime** of size **N**. In fact, it does indeed allocate some memory. Note that each node in our JIAJIA group is executing this statement, so each node allocates some memory at that node. Behind the scenes, not visible to the programmer, each node will then have its own copy of **Prime**.

However, JIAJIA sets things up so that when one node later accesses this memory, for instance in the statement

```
1  Prime[I] = 1;
```

this action will eventually trigger a network transaction (not visible to the programmer) to the other JIAJIA nodes.[17] This transaction will then update the copies of **Prime** at the other nodes.[18]

---

[16] The term *object-based* is not related to the term *object-oriented programming*.

[17] There are a number of important issues involved with this word *eventually*, as we will see later.

[18] The update may not occur immediately. More on this later.

How is all of this accomplished? It turns out that it relies on a clever usage of the nodes' virtual memory (VM) systems. To understand this, you need a basic knowledge of how VM systems work. If you lack this, or need review, read Section **??** in the appendix of this book before continuing.

Here is how VM is exploited to develop SDSMs on Unix systems. The SDSM will call a system function such as **mprotect()**. This allows the SDSM to deliberately mark a page as nonresident (even if the page *is* resident). Basically, anytime the SDSM knows that a node's local copy of a variable is invalid, it will mark the page containing that variable as nonresident. Then, the next time the program at this node tries to access that variable, a page fault will occur.

As mentioned in the review above, normally a page fault causes a jump to the OS. However, technically any page fault in Unix is handled as a signal, specifically SIGSEGV. Recall that Unix allows the programmer to write his/her own signal handler for any signal type. In this case, that means that the programmer—meaning the people who developed JIAJIA or any other page-based SDSM—writes his/her own page fault handler, which will do the necessary network transactions to obtain the latest valid value for **X**.

Note that although SDSMs are able to create an illusion of almost all aspects of shared memory, it really is not possible to create the illusion of shared pointer variables. For example on shared memory hardware we might have a variable like **P**:

```
1  int Y,*P;
2  ...
3  ...
4  P = &Y;
5  ...
```

There is no simple way to have a variable like **P** in an SDSM. This is because a pointer is an address, and each node in an SDSM has its own memory separate address space. The problem is that even though the underlying SDSM system will keep the various copies of **Y** at the different nodes consistent with each other, **Y** will be at a potentially different address on each node.

All SDSM systems must deal with a software analog of the cache coherency problem. Whenever one node modifies the value of a shared variable, that node must notify the other nodes that a change has been made. The designer of the system must choose between update or invalidate protocols, just as in the hardware case.[19] Recall that in non-bus-based shared-memory multiprocessors, one needs to maintain a directory which indicates at which processor a valid copy of a shared variable exists. Again, SDSMs must take an approach similar to this.

---

[19]Note, though, that we are not actually dealing with a cache here. Each node in the SDSM system will have a cache, of course, but a node's cache simply stores parts of that node's set of pages. The coherency across nodes is across pages, not caches. We must insure that a change made to a given page is eventually propropagated to pages on other nodes which correspond to this one.

Similarly, each SDSM system must decide between sequential consistency, release consistency etc. More on this later.

Note that in the NOW context the internode communication at the SDSM level is typically done by TCP/IP network actions. Treadmarks uses UDP, which is faster than TCP. but still part of the slow TCP/IP protocol suite. TCP/IP was simply not designed for this kind of work. Accordingly, there have been many efforts to use more efficient network hardware and software. The most popular of these is the Virtual Interface Architecture (VIA).

Not only are coherency actions more expensive in the NOW SDSM case than in the shared-memory hardware case due to network slowness, there is also expense due to granularity. In the hardware case we are dealing with cache blocks, with a typical size being 512 bytes. In the SDSM case, we are dealing with pages, with a typical size being 4096 bytes. The overhead for a cache coherency transaction can thus be large.

Case Study: JIAJIA

Programmer Interface

We will not go into detail on JIAJIA programming here. There is a short tutorial on JIAJIA at `http://heather.cs.ucdavis.edu/~matloff/jiajia.html`, but here is an overview:

- One writes in C/C++ (or FORTRAN), making calls to the JIAJIA library, which is linked in upon compilation.

- The library calls include standard shared-memory operations for lock, unlock, barrier, processor number, etc., plus some calls aimed at improving performance.

Following is a JIAJIA example program, performing Odd/Even Transposition Sort. This is a variant on Bubble Sort, sometimes useful in parallel processing contexts.[20] The algorithm consists of n phases, in which each processor alternates between trading with its left and right neighbors.

```
1   // JIAJIA example program:  Odd-Even Tranposition Sort
2
3   // array is of size n, and we use n processors; this would be more
4   // efficient in a "chunked" versions, of course (and more suited for a
5   // message-passing context anyway)
6
7   #include <stdio.h>
8   #include <stdlib.h>
9   #include <jia.h>  // required include; also must link via -ljia
10
```

---

[20]Though, as mentioned in the comments, it is aimed more at message-passing contexts.

```
11   // pointer to shared variable
12   float *x;  // array to be sorted
13
14   int n,  // range to check for primeness
15       debug;  // 1 for debugging, 0 else
16
17
18   // does sort of m-element array y
19   void oddeven(float *y, int m)
20   {  int i,left=jiapid-1,right=jiapid+1;
21      float newval;
22      for (i=0; i < m; i++)  {
23         if ((i+jiapid)%2 == 0)  {
24            if (right < m)
25               if (y[jiapid] > y[right]) newval = y[right];
26         }
27         else  {
28            if (left >= 0)
29               if (y[jiapid] < y[left]) newval = y[left];
30         }
31         jia_barrier();
32         if ((i+jiapid)%2 == 0 && right < m || (i+jiapid)%2 == 1 && left >= 0)
33               y[jiapid] = newval;
34         jia_barrier();
35      }
36   }
37
38   main(int argc, char **argv)
39   {  int i,mywait=0;
40      jia_init(argc,argv);  // required init call
41      // get command-line arguments (shifted for nodes > 0)
42      if (jiapid == 0)  {
43         n = atoi(argv[1]);
44         debug = atoi(argv[2]);
45      }
46      else  {
47         n = atoi(argv[2]);
48         debug = atoi(argv[3]);
49      }
50      jia_barrier();
51      // create a shared array x of length n
52      x = (float *) jia_alloc(n*sizeof(float));
53      // barrier recommended after allocation
54      jia_barrier();
55      // node 0 gets simple test array from command-line
56      if (jiapid == 0)  {
57         for (i = 0; i < n; i++)
```

```
58          x[i] = atoi(argv[i+3]);
59        }
60     jia_barrier();
61     if (debug && jiapid == 0)
62         while (mywait == 0)  { ; }
63     jia_barrier();
64     oddeven(x,n);
65     if (jiapid == 0)  {
66        printf("\nfinal array\n");
67        for (i = 0; i < n; i++)
68           printf("%f\n",x[i]);
69     }
70     jia_exit();
71  }
```

System Workings

JIAJIA's main characteristics as an SDSM are:

- page-based

- scope consistency

- home-based

- multiple writers

Let's take a look at these.

As mentioned earlier, one first calls **jia_alloc()** to set up one's shared variables. Note that this will occur at each node, so there are multiple copies of each variable; the JIAJIA system ensures that these copies are consistent with each other, though of course subject to the laxity afforded by scope consistency.

Recall that under scope consistency, a change made to a shared variable at one processor is guaranteed to be made visible to another processor if the first processor made the change between lock/unlock operations and the second processor accesses that variable between lock/unlock operations on that same lock.[21]

Each page—and thus each shared variable—has a **home** processor. If another processor writes to a page, then later when it reaches the unlock operation it must send all changes it made to the page back to the home node. In other words, the second processor calls **jia_unlock()**, which sends the

---

[21]Writes will also be propagated at barrier operations, but two successive arrivals by a processor to a barrier can be considered to be a lock/unlock pair, by considering a departure from a barrier to be a "lock," and considering reaching a barrier to be an "unlock." So, we'll usually not mention barriers separately from locks in the remainder of this subsection.

changes to its sister invocation of **jia_unlock()** at the home processor.[22] Say later a third processor calls **jia_lock()** on that same lock, and then attempts to read a variable in that page. A page fault will occur at that processor, resulting in the JIAJIA system running, which will then obtain that page from the first processor.

Note that all this means the JIAJIA system at each processor must maintain a page table, listing where each home page resides.[23] At each processor, each page has one of three states: Invalid, Read-Only, Read-Write. State changes, though, are reported when lock/unlock operations occur. For example, if CPU 5 writes to a given page which had been in Read-Write state at CPU 8, the latter will not hear about CPU 5's action until some CPU does a lock. This CPU need not be CPI 8. When one CPU does a lock, it must coordinate with all other nodes, at which time state-change messages will be piggybacked onto lock-coordination messages.

Note also that JIAJIA allows the programmer to specify which node should serve as the home of a variable, via one of several forms of the **jia_alloc()** call. The programmer can then tailor his/her code accordingly. For example, in a matrix problem, the programmer may arrange for certain rows to be stored at a given node, and then write the code so that most writes to those rows are done by that processor.

The general principle here is that writes performed at one node can be made visible at other nodes on a "need to know" basis. If for instance in the above example with CPUs 5 and 8, CPU 2 does not access this page, it would be wasteful to send the writes to CPU 2, or for that matter to even inform CPU 2 that the page had been written to. This is basically the idea of all non-Sequential consistency protocols, even though they differ in approach and in performance for a given application.

JIAJIA allows multiple writers of a page. Suppose CPU 4 and CPU 15 are simultaneously writing to a particular page, and the programmer has relied on a subsequent barrier to make those writes visible to other processors.[24] When the barrier is reached, each will be informed of the writes of the other.[25] Allowing multiple writers helps to reduce the performance penalty due to false sharing.

---

[22]The set of changes is called a **diff**, remiscent of the Unix file-compare command. A copy, called a **twin**, had been made of the original page, which now will be used to produce the diff. This has substantial overhead. The Treadmarks people found that it took 167 microseconds to make a twin, and as much as 686 microseconds to make a diff.

[23]In JIAJIA, that location is normally fixed, but JIAJIA does include advanced programmer options which allow the location to migrate.

[24]The only other option would be to use lock/unlock, but then their writing would not be simultaneous.

[25]If they are writing to the same variable, not just the same page, the programmer would use locks instead of a barrier, and the situation would not arise.

3.12 Barrier Implementation

Recall that a **barrier** is program code[20] which has a processor do a wait-loop action until all processors have reached that point in the program.[27]

A function **Barrier()** is often supplied as a library function; here we will see how to implement such a library function in a correct and efficient manner. Note that since a barrier is a serialization point for the program, efficiency is crucial to performance.

Implementing a barrier in a fully correct manner is actually a bit tricky. We'll see here what can go wrong, and how to make sure it doesn't.

In this section, we will approach things from a shared-memory point of view. But the methods apply in the obvious way to message-passing systems as well, as will be discused later.

3.12.1 A Use-Once Version

```
1  struct BarrStruct {
2     int NNodes, // number of threads participating in the barrier
3         Count, // number of threads that have hit the barrier so far
4         EvenOdd,  // "parity"
5         pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
6  } ;
7
8  Barrier(struct BarrStruct *PB)
9  {  pthread_mutex_lock(&PB->Lock);
10    PB->Count++;
11    pthread_mutex_unlock(&PB->Lock);
12    while (PB->Count < PB->NNodes) ;
13 }
```

This is very simple, actually overly so. This implementation will work once, so if a program using it doesn't make two calls to **Barrier()** it would be fine. But not otherwise. If, say, there is a call to **Barrier()** in a loop, we'd be in trouble.

What is the problem? Clearly, something must be done to reset **Count** to 0 at the end of the call, but doing this safely is not so easy, as seen in the next section.

---

[20]Some hardware barriers have been proposed.

[27]I use the word *processor* here, but it could be just a thread on the one hand, or on the other hand a processing element in a message-passing context.

3.12.2 An Attempt to Write a Reusable Version

Consider the following attempt at fixing the code for **Barrier()**:

```
1  Barrier(struct BarrStruct *PB)
2  {  int OldCount;
3     pthread_mutex_lock(&PB->Lock);
4     OldCount = PB->Count++;
5     pthread_mutex_unlock(&PB->Lock);
6     if (OldCount == PB->NNodes-1)  PB->Count = 0;
7     else while (PB->Count < PB->NNodes) ;
8  }
```

Unfortunately, this doesn't work either. To see why, consider a loop with a barrier call at the end:

```
1  struct BarrStruct B;  // global variable
2  ........
3  while (.......) {
4     .........
5     Barrier(&B);
6     .........
7  }
```

At the end of the first iteration of the loop, all the processors will wait at the barrier until everyone catches up. After this happens, one processor, say 12, will reset **B.Count** to 0, as desired. But if we are unlucky, some other processor, say processor 3, will then race ahead, perform the second iteration of the loop in an extremely short period of time, and then reach the barrier and increment the **Count** variable before processor 12 resets it to 0. This would result in disaster, since processor 3's increment would be canceled, leaving us one short when we try to finish the barrier the second time.

Another disaster scenario which might occur is that one processor might reset **B.Count** to 0 before another processor had a chance to notice that **B.Count** had reached **B.NNodes**.

3.12.3 A Correct Version

One way to avoid this would be to have *two* **Count** variables, and have the processors alternate using one then the other. In the scenario described above, processor 3 would increment the *other* **Count**

variable, and thus would not conflict with processor 12's resetting. Here is a safe barrier function based on this idea:

```
struct BarrStruct {
    int NNodes, // number of threads participating in the barrier
        Count[2], // number of threads that have hit the barrier so far
        pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
} ;

Barrier(struct BarrStruct *PB)
{  int Par,OldCount;
   Par = PB->EvenOdd;
   pthread_mutex_lock(&PB->Lock);
   OldCount = PB->Count[Par]++;
   if (OldCount == PB->NNodes-1)  {
      PB->Count[Par] = 0;
      PB->EvenOdd = 1 - Par;
      pthread_mutex_unlock(&PB->Lock);
   }
   else {
      pthread_mutex_unlock(&PB->Lock);
      while (PB->Count[Par] > 0) ;
   }
}
```

3.12.4   Refinements

Use of Wait Operations

The code

```
else while (PB->Count[Par] > 0) ;
```

is harming performance, since it has the processor spining around doing no useful work. In the Pthreads context, we can use a condition variable:

```
struct BarrStruct {
   int NNodes, // number of threads participating in the barrier
       Count[2], // number of threads that have hit the barrier so far
       pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
       pthread_cond_t CV = PTHREAD_COND_INITIALIZER;
} ;


Barrier(struct BarrStruct *PB)
{  int Par,I;
   Par = PB->EvenOdd;
   pthread_mutex_lock(&PB->Lock);
   PB->Count[Par]++;
   if (PB->Count < PB->NNodes)
      pthread_cond_wait(&PB->CV,&PB->Lock);
   else  {
      PB->Count[Par] = 0;
      PB->EvenOdd = 1 - Par;
      for (I = 0; I < PB->NNodes-1; I++)
         pthread_cond_signal(&PB->CV);
   }
   pthread_mutex_unlock(&PB->Lock);
}
```

Here, if a thread finds that not everyone has reached the barrier yet, it still waits for the rest, but does so passively, via the wait for the condition variable **CV**. This way the thread is not wasting valuable time on that processor, which can run other useful work.

Note that the call to **pthread_cond_wait()** requires use of the lock. Your code must lock the lock before making the call. The call itself immediately unlocks that lock after it registers the wait with the threads manager. But the call blocks until awakened when another thread calls **pthread_cond_signal()** or **pthread_cond_broadcast()**.

It is required that your code lock the lock before calling **pthread_cond_signal()**, and that it unlock the lock after the call.

By using **pthread_cond_wait()** and placing the unlock operation later in the code, as seen above, we actually could get by with just a single **Count** variable, as before.

Even better, the **for** loop could be replaced by a single call

```
pthread_cond_broadcast(&PB->CV);
```

This still wakes up the waiting threads one by one, but in a much more efficient way, and it makes for clearer code.

Parallelizing the Barrier Operation

Tree Barriers   It is clear from the code above that barriers can be costly to performance, since they rely so heavily on critical sections, i.e. serial parts of a program. Thus in many settings it is worthwhile to parallelize not only the general computation, but also the barrier operations themselves.

Consider for instance a barrier in which 16 threads are participating. We could speed things up by breaking this barrier down into two sub-barriers, with eight threads each. We would then set up three barrier operations: one of the first group of eight threads, another for the other group of eight threads, and a third consisting of a "competition" between the two groups. The variable **NNodes** above would have the value 8 for the first two barriers, and would be equal to 2 for the third barrier.

Here thread 0 could be the representative for the first group, with thread 4 representing the second group. After both groups's barriers were hit by all of their members, threads 0 and 4 would participated in the third barrier.

Note that then the notification phase would the be done in reverse: When the third barrier was complete, threads 0 and 4 would notify the members of their groups.

This would parallelize things somewhat, as critical-section operations could be executing simultaneously for the first two barriers. There would still be quite a bit of serial action, though, so we may wish to do further splitting, by partitioning each group of four threads into two subroups of two threads each.

In general, for n threads (with n, say, equal to a power of 2) we would have a tree structure, with $log_2 n$ levels in the tree. The ith level (starting with the root as level 0) with consist of 2^i parallel barriers, each one representing $n/2^i$ threads.

Butterfly Barriers   Another method basically consists of each node "shaking hands" with every other node. In the shared-memory case, handshaking could be done by having a global array **Reached-Barrier**. When thread 3 and thread 7 shake hands, for instance, would reach the barrier, thread 3 would set **ReachedBarrier[3]** to 1, and would then wait for **ReachedBarrier[7]** to become 1. The wait, as before, could either be a **while** loop or a call to **pthread_cond_wait()**. Thread 7 would do the opposite.

If we have n nodes, again with n being a power of 2, then the barrier process would consist of $log_2 n$ phases, which we'll call phase 0, phase 1, etc. Then the process works as follows.

For any node i, let i(k) be the number obtained by inverting bit k in the binary representation of i, with bit 0 being the least significant bit. Then in the kth phase, node i would shake hands with node i(k).

For example, say n = 8. In phase 0, node $5 = 101_2$, say, would shake hands with node $4 = 100_2$. Actually, a butterfly exchange amounts to a number of simultaneously tree operations.

第 4 章   Introduction to OpenMP

OpenMP has become the *de facto* standard for shared-memory programming.

4.1   Overview

OpenMP has become the environment of choice for many, if not most, practitioners of shared-memory parallel programming. It consists of a set of directives which are added to one's C/C++/FORTRAN code that manipulate threads, without the programmer him/herself having to deal with the threads directly. This way we get "the best of both worlds"—the true parallelism of (nonpreemptive) threads and the pleasure of avoiding the annoyances of threads programming.

Most OpenMP constructs are expressed via **pragmas**, i.e. directives. The syntax is

```
1  #pragma omp ......
```

The number sign must be the first nonblank character in the line.

4.2   Example: Dijkstra Shortest-Path Algorithm

The following example, implementing Dijkstra's shortest-path graph algorithm, will be used throughout this tutorial, with various OpenMP constructs being illustrated later by modifying this code:

```
1  // Dijkstra.c
2
3  // OpenMP example program:  Dijkstra shortest-path finder in a
4  // bidirectional graph; finds the shortest path from vertex 0 to all
5  // others
6
7  // usage:  dijkstra nv print
8
9  // where nv is the size of the graph, and print is 1 if graph and min
```

```
10    // distances are to be printed out, 0 otherwise
11
12    #include <omp.h>
13
14    // global variables, shared by all threads by default; could placed them
15    // above the "parallel" pragma in dowork()
16
17    int nv,  // number of vertices
18        *notdone, // vertices not checked yet
19        nth,  // number of threads
20        chunk,  // number of vertices handled by each thread
21        md,  // current min over all threads
22        mv,  // vertex which achieves that min
23        largeint = -1;  // max possible unsigned int
24
25    unsigned *ohd,  // 1-hop distances between vertices; "ohd[i][j]" is
26            // ohd[i*nv+j]
27            *mind;  // min distances found so far
28
29    void init(int ac, char **av)
30    {  int i,j,tmp;
31       nv = atoi(av[1]);
32       ohd = malloc(nv*nv*sizeof(int));
33       mind = malloc(nv*sizeof(int));
34       notdone = malloc(nv*sizeof(int));
35       // random graph
36       for (i = 0; i < nv; i++)
37          for (j = i; j < nv; j++)  {
38             if (j == i) ohd[i*nv+i] = 0;
39             else  {
40                ohd[nv*i+j] = rand() % 20;
41                ohd[nv*j+i] = ohd[nv*i+j];
42             }
43          }
44       for (i = 1; i < nv; i++)  {
45          notdone[i] = 1;
46          mind[i] = ohd[i];
47       }
48    }
49
50    // finds closest to 0 among notdone, among s through e
51    void findmymin(int s, int e, unsigned *d, int *v)
52    {  int i;
53       *d = largeint;
54       for (i = s; i <= e; i++)
55          if (notdone[i] && mind[i] < *d)  {
56             *d = mind[i];
```

```
57          *v = i;
58      }
59 }
60
61 // for each i in [s,e], ask whether a shorter path to i exists, through
62 // mv
63 void updatemind(int s, int e)
64 { int i;
65    for (i = s; i <= e; i++)
66        if (mind[mv] + ohd[mv*nv+i] < mind[i])
67            mind[i] = mind[mv] + ohd[mv*nv+i];
68 }
69
70 void dowork()
71 {
72    #pragma omp parallel
73    { int startv,endv,  // start, end vertices for my thread
74          step,  // whole procedure goes nv steps
75          mymv,  // vertex which attains the min value in my chunk
76          me = omp_get_thread_num();
77          unsigned mymd;  // min value found by this thread
78      #pragma omp single
79      { nth = omp_get_num_threads();  // must call inside parallel block
80          if (nv % nth != 0) {
81              printf("nv must be divisible by nth\n");
82              exit(1);
83          }
84          chunk = nv/nth;
85          printf("there are %d threads\n",nth);
86      }
87      startv = me * chunk;
88      endv = startv + chunk - 1;
89      for (step = 0; step < nv; step++)  {
90          // find closest vertex to 0 among notdone; each thread finds
91          // closest in its group, then we find overall closest
92          #pragma omp single
93          { md = largeint; mv = 0;  }
94          findmymin(startv,endv,&mymd,&mymv);
95          // update overall min if mine is smaller
96          #pragma omp critical
97          { if (mymd < md)
98                { md = mymd; mv = mymv;  }
99          }
100         #pragma omp barrier
101         // mark new vertex as done
102         #pragma omp single
103         { notdone[mv] = 0;  }
```

```
104          // now update my section of mind
105          updatemind(startv,endv);
106          #pragma omp barrier
107       }
108    }
109  }
110
111  int main(int argc, char **argv)
112  {  int i,j,print;
113     double startime,endtime;
114     init(argc,argv);
115     startime = omp_get_wtime();
116     // parallel
117     dowork();
118     // back to single thread
119     endtime = omp_get_wtime();
120     printf("elapsed time:  %f\n",endtime-startime);
121     print = atoi(argv[2]);
122     if (print)  {
123        printf("graph weights:\n");
124        for (i = 0; i < nv; i++)  {
125           for (j = 0; j < nv; j++)
126              printf("%u  ",ohd[nv*i+j]);
127           printf("\n");
128        }
129        printf("minimum distances:\n");
130        for (i = 1; i < nv; i++)
131           printf("%u\n",mind[i]);
132     }
133  }
```

The constructs will be presented in the following sections, but first the algorithm will be explained.

4.2.1   The Algorithm

The code implements the Dijkstra algorithm for finding the shortest paths from vertex 0 to the other vertices in an N-vertex undirected graph. Pseudocode for the algorithm is shown below, with the array G assumed to contain the one-hop distances between vertices.

```
1  Done = {0}  # vertices checked so far
2  NewDone = None  # currently checked vertex
3  NonDone = {1,2,...,N-1}  # vertices not checked yet
4  for J = 0 to N-1 Dist[J] = G(0,J)  # initialize shortest-path lengths
5
6  for Step = 1 to N-1
```

```
7      find J such that Dist[J] is min among all J in NonDone
8      transfer J from NonDone to Done
9      NewDone = J
10     for K = 1 to N-1
11        if K is in NonDone
12           # check if there is a shorter path from 0 to K through NewDone
13           # than our best so far
14           Dist[K] = min(Dist[K],Dist[NewDone]+G[NewDone,K])
```

At each iteration, the algorithm finds the closest vertex J to 0 among all those not yet processed, and then updates the list of minimum distances to each vertex from 0 by considering paths that go through J. Two obvious potential candidate part of the algorithm for parallelization are the "find J" and "for K" lines, and the above OpenMP code takes this approach.

4.2.2　The OpenMP `parallel` Pragma

As can be seen in the comments in the lines

```
1      // parallel
2      dowork();
3      // back to single thread
```

the function **main()** is run by a **master thread**, which will then branch off into many threads running **dowork()** in parallel. The latter feat is accomplished by the directive in the lines

```
1   void dowork()
2   {
3      #pragma omp parallel
4      { int startv,endv,  // start, end vertices for this thread
5            step,  // whole procedure goes nv steps
6            mymv,  // vertex which attains that value
7            me = omp_get_thread_num();
```

That directive sets up a team of threads (which includes the master), all of which execute the block following the directive in parallel.[①] Note that, unlike the **for** directive which will be discussed below, the **parallel** directive leaves it up to the programmer as to how to partition the work. In our case here, we do that by setting the range of vertices which this thread will process:

```
1         startv = me * chunk;
2         endv = startv + chunk - 1;
```

[①]There is an issue here of thread startup time. The OMPi compiler sets up threads at the outset, so that that startup time is incurred only once. When a **parallel** construct is encountered, they are awakened. At the end of the construct, they are suspended again, until the next **parallel** construct is reached.

Again, keep in mind that *all* of the threads execute this code, but we've set things up with the variable **me** so that different threads will work on different vertices. This is due to the OpenMP call

```
1         me = omp_get_thread_num();
```

which sets **me** to the thread number for this thread.

4.2.3 Scope Issues

Note carefully that in

```
1    #pragma omp parallel
2    {  int startv,endv,  // start, end vertices for this thread
3           step,  // whole procedure goes nv steps
4           mymv,  // vertex which attains that value
5           me = omp_get_thread_num();
```

the pragma comes *before* the declaration of the local variables. That means that all of them are "local" to each thread, i.e. not shared by them. But if a work sharing directive comes within a function but *after* declaration of local variables, those variables are actually "global" to the code in the directive, i.e. they *are* shared in common among the threads.

This is the default, but you can change these properties, e.g. using the **private** keyword and its cousins. For instance,

```
1    #pragma omp parallel private(x,y)
```

would make **x** and **y** nonshared even if they were declared above the directive line. You may wish to modify that a bit, so that **x** and **y** have initial values that were shared before the directive; use **firstprivate** for this.

It is crucial to keep in mind that variables which are global to the program (in the C/C++ sense) are automatically global to all threads. This is the primary means by which the threads communicate with each other.

4.2.4 The OpenMP `single` Pragma

In some cases we want just one thread to execute some code, even though that code is part of a **parallel** or other **work sharing** block.[2] We use the **single** directive to do this, e.g.:

---

[2]This is an OpenMP term. The **for** directive is another example of it. More on this below.

```
1    #pragma omp single
2    { nth = omp_get_num_threads();
3       if (nv % nth != 0) {
4          printf("nv must be divisible by nth\n");
5          exit(1);
6       }
7       chunk = nv/nth;
8       printf("there are %d threads\n",nth);  }
```

Since the variables **nth** and **chunk** are global and thus shared, we need not have all threads set them, hence our use of **single**.

4.2.5 The OpenMP `barrier` Pragma

As see in the example above, the **barrier** implements a standard barrier, applying to all threads.

4.2.6 Implicit Barriers

Note that there is an implicit barrier at the end of each **single** block, which is also the case for **parallel**, **for**, and **sections** blocks. This can be overridden via the **nowait** clause, e.g.

```
1  #pragma omp for nowait
```

Needless to say, the latter should be used with care, and in most cases will not be usable. On the other hand, putting in a barrier where it is not needed would severely reduce performance.

4.2.7 The OpenMP `critical` Pragma

The last construct used in this example is **critical**, for critical sections.

```
1        #pragma omp critical
2        { if (mymd < md)
3            { md = mymd; mv = mymv;  }
4        }
```

It means what it says, allowing entry of only one thread at a time while others wait. Here we are updating global variables **md** and **mv**, which has to be done atomically, and **critical** takes care of that for us. This is much more convenient than setting up lock variables, etc., which we would do if we were programming threads code directly.

4.3 The OpenMP `for` Pragma

This one breaks up a C/C++ **for** loop, assigning various iterations to various threads. (The threads, of course, must have already been set up via the **omp parallel** pragma.) This way the iterations are done in parallel. Of course, that means that they need to be independent iterations, i.e. one iteration cannot depend on the result of another.

4.3.1 Example: Dijkstra with Parallel for Loops

Here's how we could use this construct in the Dijkstra program :

```
1   // Dijkstra.c
2
3   // OpenMP example program (OMPi version):  Dijkstra shortest-path finder
4   // in a bidirectional graph; finds the shortest path from vertex 0 to
5   // all others
6
7   // usage:  dijkstra nv print
8
9   // where nv is the size of the graph, and print is 1 if graph and min
10  // distances are to be printed out, 0 otherwise
11
12  #include <omp.h>
13
14  // global variables, shared by all threads by default
15
16  int nv,  // number of vertices
17      *notdone, // vertices not checked yet
18      nth,  // number of threads
19      chunk,  // number of vertices handled by each thread
20      md,  // current min over all threads
21      mv,  // vertex which achieves that min
22      largeint = -1;  // max possible unsigned int
23
24  unsigned *ohd,  // 1-hop distances between vertices; "ohd[i][j]" is
25                  // ohd[i*nv+j]
26          *mind;  // min distances found so far
27
28  void init(int ac, char **av)
29  {  int i,j,tmp;
30     nv = atoi(av[1]);
31     ohd = malloc(nv*nv*sizeof(int));
32     mind = malloc(nv*sizeof(int));
33     notdone = malloc(nv*sizeof(int));
34     // random graph
```

```
35       for (i = 0; i < nv; i++)
36          for (j = i; j < nv; j++)  {
37             if (j == i) ohd[i*nv+i] = 0;
38             else  {
39                ohd[nv*i+j] = rand() % 20;
40                ohd[nv*j+i] = ohd[nv*i+j];
41             }
42          }
43       for (i = 1; i < nv; i++)  {
44          notdone[i] = 1;
45          mind[i] = ohd[i];
46       }
47    }
48
49    void dowork()
50    {
51       #pragma omp parallel
52       { int step,  // whole procedure goes nv steps
53             mymv,  // vertex which attains that value
54             me = omp_get_thread_num(),
55             i;
56          unsigned mymd;  // min value found by this thread
57          #pragma omp single
58          { nth = omp_get_num_threads();
59             printf("there are %d threads\n",nth);  }
60          for (step = 0; step < nv; step++)  {
61             // find closest vertex to 0 among notdone; each thread finds
62             // closest in its group, then we find overall closest
63             #pragma omp single
64             { md = largeint; mv = 0;  }
65             mymd = largeint;
66             #pragma omp for nowait
67             for (i = 1; i < nv; i++)  {
68                if (notdone[i] && mind[i] < mymd)  {
69                   mymd = ohd[i];
70                   mymv = i;
71                }
72             }
73             // update overall min if mine is smaller
74             #pragma omp critical
75             { if (mymd < md)
76                  { md = mymd; mv = mymv;  }
77             }
78             // mark new vertex as done
79             #pragma omp single
80             { notdone[mv] = 0;  }
81             // now update ohd
```

```
82              #pragma omp for
83              for (i = 1; i < nv; i++)
84                  if (mind[mv] + ohd[mv*nv+i] < mind[i])
85                      mind[i] = mind[mv] + ohd[mv*nv+i];
86          }
87       }
88  }
89
90  int main(int argc, char **argv)
91  {  int i,j,print;
92     init(argc,argv);
93     // parallel
94     dowork();
95     // back to single thread
96     print = atoi(argv[2]);
97     if (print)  {
98        printf("graph weights:\n");
99        for (i = 0; i < nv; i++)  {
100           for (j = 0; j < nv; j++)
101               printf("%u  ",ohd[nv*i+j]);
102           printf("\n");
103        }
104        printf("minimum distances:\n");
105        for (i = 1; i < nv; i++)
106           printf("%u\n",mind[i]);
107     }
108  }
109
```

The work which used to be done in the function **findmymin()** is now done here:

```
1              #pragma omp for
2              for (i = 1; i < nv; i++)  {
3                 if (notdone[i] && mind[i] < mymd)  {
4                    mymd = ohd[i];
5                    mymv = i;
6                 }
7              }
```

Each thread executes one or more of the iterations, i.e. takes responsibility for one or more values of i. This occurs in parallel, so as mentioned earlier, the programmer must make sure that the iterations are independent; there is no predicting which threads will do which values of **i**, in which order. By the way, for obvious reasons OpenMP treats the loop index, **i** here, as private even if by context it would be shared.

4.3.2 Nested Loops

If we use the **for** pragma to nested loops, by default the pragma applies only to the outer loop. We can of course insert another **for** pragma inside, to parallelize the inner loop.

Or, starting with OpenMP version 3.0, one can use the **collapse** clause, e.g.

```
1  #pragma omp parallel for collapse(2)
```

to specify two levels of nesting in the assignment of threads to tasks.

4.3.3 Controlling the Partitioning of Work to Threads: the schedule Clause

In this default version of the **for** construct, iterations are executed by threads *in unpredictable order*; the OpenMP standard does not specify which threads will execute which iterations in which order. But this can be controlled by the programmer, using the **schedule** clause. OpenMP provides three choices for this:

- **static:** The iterations are grouped into chunks, and assigned to threads in round-robin fashion. Default chunk size is approximately the number of iterations divided by the number of threads.

- **dynamic:** Again the iterations are grouped into chunks, but here the assignment of chunks to threads is done dynamically. When a thread finishes working on a chunk, it asks the OpenMP runtime system to assign it the next chunk in the queue. Default chunk size is 1.

- **guided:** Similar to dynamic, but with the chunk size decreasing as execution proceeds.

For instance, our original version of our program in Section 4.2 broke the work into chunks, with chunk size being the number vertices divided by the number of threads.

For the Dijkstra algorithm, for instance, we could get the same operation with less code by asking OpenMP to do the chunking for us, say with a chunk size of 8:

```
1   ...
2           #pragma omp for schedule(static)
3           for (i = 1; i < nv; i++)  {
4             if (notdone[i] && mind[i] < mymd)  {
5                mymd = ohd[i];
6                mymv = i;
7             }
8           }
9   ...
10          #pragma omp for schedule(static)
11          for (i = 1; i < nv; i++)
12            if (mind[mv] + ohd[mv*nv+i] < mind[i])
```

```
13            mind[i] = mind[mv] + ohd[mv*nv+i];
14    ...
```

Note again that this would have the same effect as our original code, which each thread handling one chunk of contiguous iterations within a loop. So it's just a programming convenience for us in this case. (If the number of threads doesn't evenly divide the number of iterations, OpenMP will fix that up for us too.)

The more general form is

```
1   #pragma omp for schedule(static,chunk)
```

Here **static** is still a keyword but **chunk** is an actual argument. However, setting the chunk size in the **schedule()** clause is a *compile-time* operation. If you wish to have the chunk size set at run time, call **omp_set_schedule()** in conjunction with the **runtime** clause. Example:

```
1   int main(int argc, char **argv)
2   {
3      ...
4      n = atoi(argv[1]);
5      int chunk = atoi(argv[2]);
6      omp_set_schedule(omp_sched_static, chunk);
7      #pragma omp parallel
8      {
9         ...
10        #pragma omp for schedule(runtime)
11        for (i = 1; i < n; i++) {
12           ...
13        }
14        ...
15     }
16  }
```

Or set the **OMP_SCHEDULE** environment variable.

The syntax is the same for **dynamic** and **guided**.

As discussed in Section **??**, on the one hand, large chunks are good, due to there being less overhead—every time a thread finishes a chunk, it must go through the critical section, which serializes our parallel program and thus slows things down. On the other hand, if chunk sizes are large, then

toward the end of the work, some threads may be working on their last chunks while others have finished and are now idle, thus foregoing potential speed enhancement. So it would be nice to have large chunks at the beginning of the run, to reduce the overhead, but smaller chunks at the end. This can be done using the **guided** clause.

For the Dijkstra algorithm, for instance, we could have this:

```
...
        #pragma omp for schedule(guided)
        for (i = 1; i < nv; i++)  {
          if (notdone[i] && mind[i] < mymd)  {
             mymd = ohd[i];
             mymv = i;
          }
        }
...
        #pragma omp for schedule(guided)
        for (i = 1; i < nv; i++)
          if (mind[mv] + ohd[mv*nv+i] < mind[i])
             mind[i] = mind[mv] + ohd[mv*nv+i];
...
```

There are other variations of this available in OpenMP. However, in Section **??**, I showed that these would seldom be necessary or desirable; having each thread handle a single chunk would be best.

See Section **??** for a timing example.

```
setenv OMP_SCHEDULE "static,20"
```

4.3.4 Example: In-Place Matrix Transpose

This method works in-place, a virtue if we are short on memory. Its cache performance is probably poor, though. It may be better to look at horizontal slabs above the diagonal, say, and trade them with vertical ones below the diagonal.

```
#include <omp.h>

// translate from 2-D to 1-D indices
int onedim(int n,int i,int j) { return n * i + j; }

void transp(int *m, int n)
{
```

```
8      #pragma omp parallel
9      { int i,j,tmp;
10        // walk through all the above-diagonal elements, swapping them
11        // with their below-diagonal counterparts
12        #pragma omp for
13        for (i = 0; i < n; i++) {
14           for (j = i+1; j < n; j++) {
15              tmp = m[onedim(n,i,j)];
16              m[onedim(n,i,j)] = m[onedim(n,j,i)];
17              m[onedim(n,j,i)] = tmp;
18           }
19        }
20     }
21  }
```

4.3.5 The OpenMP `reduction` Clause

The name of this OpenMP clause alludes to the term **reduction** in functional programming. Many parallel programming languages include such operations, to enable the programmer to more conveniently (and often more efficiently) have threads/processors cooperate in computing sums, products, etc. OpenMP does this via the **reduction** clause.

For example, consider

```
1  int z;
2  ...
3  #pragma omp for reduction(+:z)
4  for (i = 0; i < n; i++)  z += x[i];
```

The pragma says that the threads will share the work as in our previous discussion of the **for** pragma. In addition, though, there will be independent copies of **z** maintained for each thread, each initialized to 0 before the loop begins. When the loop is entirely done, the values of **z** from the various threads will be summed, of course in an atomic manner.

Note that the **+** operator not only indicates that the values of **z** are to be summed, but also that their initial values are to be 0. If the operator were *****, say, then the product of the values would be computed, and their initial values would be 1.

One can specify several reduction variables to the right of the colon, separated by commas.

Our use of the **reduction** clause here makes our programming much easier. Indeed, if we had old serial code that we wanted to parallelize, we would have to make no change to it! OpenMP is taking care of both the work splitting across values of **i**, and the atomic operations. Moreover—note this carefully—it is efficient, because by maintaining separate copies of **z** until the loop is done, we are reducing the number of serializing atomic actions, and are avoiding time-costly cache coherency transactions and the like.

Without this construct, we would have to do

```
1   int z,myz=0;
2   ...
3   #pragma omp for private(myz)
4   for (i = 0; i < n; i++)  myz += x[i];
5   #pragma omp critical
6   { z += myz; }
```

Here are the eligible operators and the corresponding initial values:

In C/C++, you can use **reduction** with +, -, *, &, |, && and || (and the exclusive-or operator).

operator	initial value
+	0
-	0
*	1
&	bit string of 1s
|	bit string of 0s
^	0
&&	1
||	0

The lack of other operations typically found in other parallel programming languages, such as min and max, is due to the lack of these operators in C/C++. The FORTRAN version of OpenMP does have min and max.[3]

Note that the reduction variables must be shared by the threads, and apparently the only acceptable way to do so in this case is to declare them as global variables.

A reduction variable must be scalar, in C/C++. It can be an array in FORTRAN.

---

[3]Note, though, that plain min and max would not help in our Dijkstra example above, as we not only need to find the minimum value, but also need the vertex which attains that value.

4.4   Example: Mandelbrot Set

Here's the code for the timings in Section **??**:

```
1   // compile with -D, e.g.
2   //
3   // gcc -fopenmp -o manddyn Gove.c -DDYNAMIC
4   //
5   // to get the version that uses dynamic scheduling
6
7   #include <omp.h>
8   #include <complex.h>
9
10  #include <time.h>
11  float timediff(struct timespec t1, struct timespec t2)
12  { if (t1.tv_nsec > t2.tv_nsec) {
13        t2.tv_sec -= 1;
14        t2.tv_nsec += 1000000000;
15     }
16     return t2.tv_sec-t1.tv_sec + 0.000000001 * (t2.tv_nsec-t1.tv_nsec);
17  }
18
19  #ifdef RC
20  // finds chunk among 0,...,n-1 to assign to thread number me among nth
21  // threads
22  void findmyrange(int n,int nth,int me,int *myrange)
23  { int chunksize = n / nth;
24     myrange[0] = me * chunksize;
25     if (me < nth-1) myrange[1] = (me+1) * chunksize - 1;
26     else myrange[1] = n - 1;
27  }
28
29  #include <stdlib.h>
30  #include <stdio.h>
```

```
31  // from http://www.cis.temple.edu/~ingargio/cis71/code/randompermute.c
32  // It returns a random permutation of 0..n-1
33  int * rpermute(int n) {
34    int *a = (int *)(int *) malloc(n*sizeof(int));
35    // int *a = malloc(n*sizeof(int));
36    int k;
37    for (k = 0; k < n; k++)
38      a[k] = k;
39    for (k = n-1; k > 0; k--) {
40      int j = rand() % (k+1);
41      int temp = a[j];
42      a[j] = a[k];
43      a[k] = temp;
44    }
45    return a;
46  }
47  #endif
48
49  #define MAXITERS 1000
50
51  // globals
52  int count = 0;
53  int nptsside;
54  float side2;
55  float side4;
56
57  int inset(double complex c) {
58    int iters;
59    float rl,im;
60    double complex z = c;
61    for (iters = 0; iters < MAXITERS; iters++) {
62      z = z*z + c;
63      rl = creal(z);
```

```
64       im = cimag(z);
65       if (rl*rl + im*im > 4) return 0;
66    }
67    return 1;
68 }
69
70 int *scram;
71
72 void dowork()
73 {
74    #ifdef RC
75    #pragma omp parallel reduction(+:count)
76    #else
77    #pragma omp parallel
78    #endif
79    {
80       int x,y; float xv,yv;
81       double complex z;
82       #ifdef STATIC
83       #pragma omp for reduction(+:count) schedule(static)
84       #elif defined DYNAMIC
85       #pragma omp for reduction(+:count) schedule(dynamic)
86       #elif defined GUIDED
87       #pragma omp for reduction(+:count) schedule(guided)
88       #endif
89       #ifdef RC
90       int myrange[2];
91       int me = omp_get_thread_num();
92       int nth = omp_get_num_threads();
93       int i;
94       findmyrange(nptsside,nth,me,myrange);
95       for (i = myrange[0]; i <= myrange[1]; i++) {
96          x = scram[i];
```

```
97       #else
98       for (x=0; x<nptsside; x++) {
99       #endif
100        for ( y=0; y<nptsside; y++) {
101           xv = (x - side2) / side4;
102           yv = (y - side2) / side4;
103           z = xv + yv*I;
104           if (inset(z)) {
105              count++;
106           }
107        }
108      }
109    }
110  }
111
112  int main(int argc, char **argv)
113  {
114     nptsside = atoi(argv[1]);
115     side2 = nptsside / 2.0;
116     side4 = nptsside / 4.0;
117
118     struct timespec bgn,nd;
119     clock_gettime(CLOCK_REALTIME, &bgn);
120
121     #ifdef RC
122     scram = rpermute(nptsside);
123     #endif
124
125     dowork();
126
127     // implied barrier
128     printf("%d\n",count);
129     clock_gettime(CLOCK_REALTIME, &nd);
```

```
130      printf("%f\n",timediff(bgn,nd));
131  }
```

The code is similar to that of a number of books and Web sites, such as the Gove book cited in Section **??**. Here RC is the random chunk method discussed in Section **??**.

4.5   The Task Directive

This is new to OpenMP 3.0. The basic idea is to set up a task queue: When a thread encounters a **task** directive, it arranges for some thread to execute the associated block—at some time. The first thread can continue. Note that the task might not execute right away; it may have to wait for some thread to become free after finishing another task. Also, there may be more tasks than threads, also causing some threads to wait.

Note that we could arrange for all this ourselves, without **task**. We'd set up our own work queue, as a shared variable, and write our code so that whenever a thread finished a unit of work, it would delete the head of the queue. Whenever a thread generated a unit of work, it would add it to the que. Of course, the deletion and addition would have to be done atomically. All this would amount to a lot of coding on our part, so **task** really simplifies the programming.

4.5.1   Example: Quicksort

```
1   // OpenMP example program:  quicksort; not necessarily efficient
2
3   void swap(int *yi, int *yj)
4   {  int tmp = *yi;
5      *yi = *yj;
6      *yj = tmp;
7   }
8
9   int *separate(int *x, int low, int high)
10  {  int i,pivot,last;
11     pivot = x[low];  // would be better to take, e.g., median of 1st 3 elts
12     swap(x+low,x+high);
13     last = low;
14     for (i = low; i < high; i++) {
15        if (x[i] <= pivot) {
16           swap(x+last,x+i);
17           last += 1;
18        }
19     }
```

```
20      swap(x+last,x+high);
21      return last;
22  }
23
24  // quicksort of the array z, elements zstart through zend; set the
25  // latter to 0 and m-1 in first call, where m is the length of z;
26  // firstcall is 1 or 0, according to whether this is the first of the
27  // recursive calls
28  void qs(int *z, int zstart, int zend, int firstcall)
29  {
30      #pragma omp parallel
31      { int part;
32        if (firstcall == 1) {
33          #pragma omp single nowait
34          qs(z,0,zend,0);
35        } else {
36          if (zstart < zend) {
37            part = separate(z,zstart,zend);
38            #pragma omp task
39            qs(z,zstart,part-1,0);
40            #pragma omp task
41            qs(z,part+1,zend,0);
42          }
43
44        }
45      }
46  }
47
48  // test code
49  main(int argc, char**argv)
50  { int i,n,*w;
51      n = atoi(argv[1]);
52      w = malloc(n*sizeof(int));
53      for (i = 0; i < n; i++) w[i] = rand();
54      qs(w,0,n-1,1);
55      if (n < 25)
56        for (i = 0; i < n; i++) printf("%d\n",w[i]);
57  }
```

The code

```
1  if (firstcall == 1) {
2     #pragma omp single nowait
3     qs(z,0,zend,0);
```

gets things going. We want only one thread to execute the root of the recursion tree, hence the need for the **single** clause. After that, the code

```
1  part = separate(z,zstart,zend);
2  #pragma omp task
3  qs(z,zstart,part-1,0);
```

sets up a call to a subtree, with the **task** directive stating, "OMP system, please make sure that this subtree is handled by some thread."

There are various refinements, such as the barrier-like **taskwait** clause.

4.6   Other OpenMP Synchronization Issues

Earlier we saw the **critical** and **barrier** constructs. There is more to discuss, which we do here.

4.6.1   The OpenMP `atomic` Clause

The **critical** construct not only serializes your program, but also it adds a lot of overhead. If your critical section involves just a one-statement update to a shared variable, e.g.

```
1  x += y;
```

etc., then the OpenMP compiler can take advantage of an atomic hardware instruction, e.g. the LOCK prefix on Intel, to set up an extremely efficient critical section, e.g.

```
1  #pragma omp atomic
2  x += y;
```

Since it is a single statement rather than a block, there are no braces.

The eligible operators are:

```
1  ++, --, +=, *=, <<=, &=, |=
```

4.6.2   Memory Consistency and the `flush` Pragma

Consider a shared-memory multiprocessor system with coherent caches, and a shared, i.e. global, variable **x**. If one thread writes to **x**, you might think that the cache coherency system will ensure that the new value is visible to other threads. But as discussed in Section 3.6, it is is not quite so simple as this.

For example, the compiler may store **x** in a register, and update **x** itself at certain points. In between such updates, since the memory location for **x** is not written to, the cache will be unaware of the new value, which thus will not be visible to other threads. If the processors have write buffers etc., the same problem occurs.

In other words, we must account for the fact that our program could be run on different kinds of hardware with different memory consistency models. Thus OpenMP must have its own memory consistency model, which is then translated by the compiler to mesh with the hardware.

OpenMP takes a **relaxed consistency** approach, meaning that it forces updates to memory ("flushes") at all synchronization points, i.e. at:

- **barrier**
- entry/exit to/from **critical**
- entry/exit to/from **ordered**
- entry/exit to/from **parallel**
- exit from **parallel for**
- exit from **parallel sections**
- exit from **single**

In between synchronization points, one can force an update to **x** via the **flush** pragma:

```
1  #pragma omp flush (x)
```

The flush operation is obviously architecture-dependent. OpenMP compilers will typically have the proper machine instructions available for some common architectures. For the rest, it can force a flush at the hardware level by doing lock/unlock operations, though this may be costly in terms of time.

4.7   Combining Work-Sharing Constructs

In our examples of the **for** pragma above, that pragma would come within a block headed by a **parallel** pragma. The latter specifies that a team of theads is to be created, with each one executing the given block, while the former specifies that the various iterations of the loop are to be distributed among the threads. As a shortcut, we can combine the two pragmas:

```
1  #pragma omp parallel for
```

This also works with the **sections** pragma.

4.8   The Rest of OpenMP

There is much, much more to OpenMP than what we have seen here. To see the details, there are many Web pages you can check, and there is also the excellent book, *Using OpenMP: Portable*

Shared Memory Parallel Programming, by Barbara Chapman, Gabriele Jost and Ruud Van Der Pas, MIT Press, 2008. The book by Gove cited in Section **??** also includes coverage of OpenMP.

4.9 Compiling, Running and Debugging OpenMP Code

4.9.1 Compiling

There are a number of open source compilers available for OpenMP, including:

- Omni: This is available at (`http://phase.hpcc.jp/Omni/`). To compile an OpenMP program in **x.c** and create an executable file **x**, run

```
1  omcc -g -o x x.c
```

   Note: Apparently declarations of local variables cannot be made in the midst of code; they must precede all code within a block.

- Ompi: You can download this at `http://www.cs.uoi.gr/~ompi/index.html`. Compile **x.c** by

```
1  ompicc -g -o x x.c
```

- GCC, version 4.2 or later:[④] Compile **x.c** via

```
1  gcc -fopenmp -g -o x x.c
```

   You can also use **-lgomp** instead of **-fopenmp**.

4.9.2 Running

Just run the executable as usual.

The number of threads will be the number of processors, by default. To change that value, set the OMP_NUM_THREADS environment variable. For example, to get four threads in the C shell, type

```
1  setenv OMP_NUM_THREADS 4
```

4.9.3 Debugging

Since OpenMP is essentially just an interface to threads, your debugging tool's threads facilities should serve you well. See Section 1.3.2 for the GDB case.

A possible problem, though, is that OpenMP's use of pragmas makes it difficult for the compilers to maintain your original source code line numbers, and your function and variable names. But with

---

[④]You may find certain subversions of GCC 4.1 can be used too.

a little care, a symbolic debugger such as GDB can still be used. Here are some tips for the compilers mentioned above, using GDB as our example debugging tool:

- GCC: GCC maintains line numbers and names well. In earlier versions, it had a problem in that it did not not retain names of local variables within blocks controlled by **omp parallel** at all. That problem was fixed in version 4.4 of the GCC suite, but seems to have slipped back in with some later versions! This may be due to compiler optimizations that place variables in registers.

- Omni: The function **main()** in your executable is actually in the OpenMP library, and your function **main()** is renamed **__ompc_main()**. So, when you enter GDB, first set a breakpoint at your own code:

```
(gdb) b _ompc_main
```

  Then run your program to this breakpoint, and set whatever other breakpoints you want.
  You should find that your other variable and function names are unchanged.

- Ompi: Older versions also changed your function names, but the current version (1.2.0) doesn't. Works fine in GDB.

4.10   Performance

As is usually the case with parallel programming, merely parallelizing a program won't necessarily make it faster, even on shared-memory hardware. Operations such as critical sections, barriers and so on serialize an otherwise-parallel program, sapping much of its speed. In addition, there are issues of cache coherency transactions, false sharing etc.

4.10.1   The Effect of Problem Size

To illustrate this, I ran our original Dijkstra example (Section 4.2 on various graph sizes, on a quad core machine. Here are the timings:

nv	nth	time
1000	1	0.005472
1000	2	0.011143
1000	4	0.029574

The more parallelism we had, the *slower* the program ran! The synchronization overhead was just too much to be compensated by the parallel computation.

However, parallelization did bring benefits on larger problems:

nv	nth	time
25000	1	2.861814
25000	2	1.710665
25000	4	1.453052

4.10.2   Some Fine Tuning

How could we make our Dijkstra code faster? One idea would be to eliminate the critical section. Recall that in each iteration, the threads compute their local minimum distance values **md** and **mv**, and then update the global values **md** and **mv**. Since the update must be atomic, this causes some serialization of the program. Instead, we could have the threads store their values **mymd** and **mymv** in a global array **mymins**, with each thread using a separate pair of locations within that array, and then at the end of the iteration we could have just one task scan through **mymins** and update **md** and **mv**.

Here is the resulting code:

```
1   // Dijkstra.c
2
3   // OpenMP example program:  Dijkstra shortest-path finder in a
4   // bidirectional graph; finds the shortest path from vertex 0 to all
5   // others
6
7   // **** in this version, instead of having a critical section in which
8   // each thread updates md and mv, the threads record their mymd and mymv
9   // values in a global array mymins, which one thread then later uses to
10  // update md and mv
11
12  // usage:  dijkstra nv print
13
14  // where nv is the size of the graph, and print is 1 if graph and min
15  // distances are to be printed out, 0 otherwise
16
17  #include <omp.h>
18
19  // global variables, shared by all threads by default
20
21  int nv,  // number of vertices
22      *notdone, // vertices not checked yet
23      nth,  // number of threads
24      chunk,  // number of vertices handled by each thread
25      md,  // current min over all threads
26      mv,  // vertex which achieves that min
27      largeint = -1;  // max possible unsigned int
28
```

```
29    int *mymins;  // (mymd,mymv) for each thread; see dowork()

30

31    unsigned *ohd,  // 1-hop distances between vertices; "ohd[i][j]" is
32              // ohd[i*nv+j]
33              *mind;  // min distances found so far

34

35    void init(int ac, char **av)
36    {  int i,j,tmp;
37       nv = atoi(av[1]);
38       ohd = malloc(nv*nv*sizeof(int));
39       mind = malloc(nv*sizeof(int));
40       notdone = malloc(nv*sizeof(int));
41       // random graph
42       for (i = 0; i < nv; i++)
43          for (j = i; j < nv; j++)  {
44             if (j == i) ohd[i*nv+i] = 0;
45             else  {
46                ohd[nv*i+j] = rand() % 20;
47                ohd[nv*j+i] = ohd[nv*i+j];
48             }
49          }
50       for (i = 1; i < nv; i++)  {
51          notdone[i] = 1;
52          mind[i] = ohd[i];
53       }
54    }

55

56    // finds closest to 0 among notdone, among s through e
57    void findmymin(int s, int e, unsigned *d, int *v)
58    {  int i;
59       *d = largeint;
60       for (i = s; i <= e; i++)
61          if (notdone[i] && mind[i] < *d)  {
62             *d = ohd[i];
63             *v = i;
64          }
65    }

66

67    // for each i in [s,e], ask whether a shorter path to i exists, through
68    // mv
69    void updatemind(int s, int e)
70    {  int i;
71       for (i = s; i <= e; i++)
72          if (mind[mv] + ohd[mv*nv+i] < mind[i])
73             mind[i] = mind[mv] + ohd[mv*nv+i];
74    }

75
```

```
76    void dowork()
77    {
78       #pragma omp parallel
79       { int startv,endv,  // start, end vertices for my thread
80             step,  // whole procedure goes nv steps
81             me,
82             mymv;  // vertex which attains the min value in my chunk
83             unsigned mymd;  // min value found by this thread
84          int i;
85          me = omp_get_thread_num();
86          #pragma omp single
87          { nth = omp_get_num_threads();
88             if (nv % nth != 0) {
89                printf("nv must be divisible by nth\n");
90                exit(1);
91             }
92             chunk = nv/nth;
93             mymins = malloc(2*nth*sizeof(int));
94          }
95          startv = me * chunk;
96          endv = startv + chunk - 1;
97          for (step = 0; step < nv; step++)  {
98             // find closest vertex to 0 among notdone; each thread finds
99             // closest in its group, then we find overall closest
100            findmymin(startv,endv,&mymd,&mymv);
101            mymins[2*me] = mymd;
102            mymins[2*me+1] = mymv;
103            #pragma omp barrier
104            // mark new vertex as done
105            #pragma omp single
106            { md = largeint; mv = 0;
107               for (i = 1; i < nth; i++)
108                  if (mymins[2*i] < md) {
109                     md = mymins[2*i];
110                     mv = mymins[2*i+1];
111                  }
112               notdone[mv] = 0;
113            }
114            // now update my section of mind
115            updatemind(startv,endv);
116            #pragma omp barrier
117         }
118      }
119   }
120
121   int main(int argc, char **argv)
122   { int i,j,print;
```

```
123      double startime,endtime;
124      init(argc,argv);
125      startime = omp_get_wtime();
126      // parallel
127      dowork();
128      // back to single thread
129      endtime = omp_get_wtime();
130      printf("elapsed time:  %f\n",endtime-startime);
131      print = atoi(argv[2]);
132      if (print)  {
133         printf("graph weights:\n");
134         for (i = 0; i < nv; i++)  {
135            for (j = 0; j < nv; j++)
136               printf("%u  ",ohd[nv*i+j]);
137            printf("\n");
138         }
139         printf("minimum distances:\n");
140         for (i = 1; i < nv; i++)
141            printf("%u\n",mind[i]);
142      }
143   }
```

Let's take a look at the latter part of the code for one iteration;

```
1          findmymin(startv,endv,&mymd,&mymv);
2          mymins[2*me] = mymd;
3          mymins[2*me+1] = mymv;
4          #pragma omp barrier
5          // mark new vertex as done
6          #pragma omp single
7          {  notdone[mv] = 0;
8             for (i = 1; i < nth; i++)
9                if (mymins[2*i] < md) {
10                  md = mymins[2*i];
11                  mv = mymins[2*i+1];
12               }
13          }
14          // now update my section of mind
15          updatemind(startv,endv);
16          #pragma omp barrier
```

The call to **findmymin()** is as before; this thread finds the closest vertex to 0 among this thread's range of vertices. But instead of comparing the result to **md** and possibly updating it and **mv**, the thread simply stores its **mymd** and **mymv** in the global array **mymins**. After all threads have done this and then waited at the barrier, we have just one thread update **md** and **mv**.

Let's see how well this tack worked:

nv	nth	time
25000	1	2.546335
25000	2	1.449387
25000	4	1.411387

This brought us about a 15% speedup in the two-thread case, though less for four threads.

What else could we do? Here are a few ideas:

- False sharing could be a problem here. To address it, we could make **mymins** much longer, changing the places at which the threads write their data, leaving most of the array as padding.

- We could try the modification of our program in Section 4.3.1, in which we use the OpenMP **for** pragma, as well as the refinements stated there, such as **schedule**.

- We could try combining all of the ideas here.

4.10.3   OpenMP Internals

We may be able to write faster code if we know a bit about how OpenMP works inside.

You can get some idea of this from your compiler. For example, if you use the **-t** option with the Omni compiler, or **-k** with Ompi, you can inspect the result of the preprocessing of the OpenMP pragmas.

Here for instance is the code produced by Omni from the call to **findmymin()** in our Dijkstra program:

```
# 93 "Dijkstra.c"
findmymin(startv,endv,&(mymd),&(mymv));{
_ompc_enter_critical(&__ompc_lock_critical);
# 96 "Dijkstra.c"
if((mymd)<(((unsigned )(md)))){

# 97 "Dijkstra.c"
(md)=(((int )(mymd)));
# 97 "Dijkstra.c"
(mv)=(mymv);
}_ompc_exit_critical(&__ompc_lock_critical);
```

Fortunately Omni saves the line numbers from our original source file, but the pragmas have been replaced by calls to OpenMP library functions.

With Ompi, while preprocessing of your file **x.c**, the compiler produces an intermediate file **x_ompi.c**, and the latter is what is actually compiled. Your function **main** is renamed to **_ompi_originalMain()** Your other functions and variables are renamed. For example in our Dijkstra code, the function

dowork() is renamed to **dowork_parallel_0**. And by the way, all indenting is lost! So it's a bit hard to read, but can be very instructive.

The document, *The GNU OpenMP Implementation*, `http://pl.postech.ac.kr/~gla/cs700-07f/ ref/openMp/libgomp.pdf`, includes good outline of how the pragmas are translated.

4.11   Example: Root Finding

The application is described in the comments, but here are a couple of things to look for in particular:

- The variables **curra** and **currb** are shared by all the threads, but due to the nature of the application, no critical sections are needed.

- On the other hand, the barrier is essential. The reader should ponder what calamities would occur without it.

Note the disclaimer in the comments, to the effect that parallelizing this application will be fruitful only if the functioin f() is very time-consuming to evaluate. It might be the output of some complex simulation, for instance, with the argument to f() being some simulation parameter.

```
1  #include<omp.h>
2  #include<math.h>
3
4  // OpenMP example: root finding
5
6  // the function f() is known to be negative
7  // at a, positive at b, and thus has at
8  // least one root in (a,b); if there are
9  // multiple roots, only one is found;
10 // the procedure runs for niters iterations
11
12 // strategy: in each iteration, the current
13 // interval is split into nth equal parts,
14 // and each thread checks its subinterval
15 // for a sign change of f(); if one is
16 // found, this subinterval becomes the
```

```
17   // new current interval; the current guess
18   // for the root is the left endpoint of the
19   // current interval
20
21   // of course, this approach is useful in
22   // parallel only if f() is very expensive
23   // to evaluate
24
25   // for simplicity, assumes that no endpoint
26   // of a subinterval will ever exactly
27   // coincide with a root
28
29   float root(float(*f)(float),
30      float inita, float initb, int niters) {
31      float curra = inita;
32      float currb = initb;
33      #pragma omp parallel
34      {
35         int nth = omp_get_num_threads();
36         int me = omp_get_thread_num();
37         int iter;
38         for (iter = 0; iter < niters; iter++) {
39            #pragma omp barrier
40            float subintwidth =
41               (currb - curra) / nth;
42            float myleft =
43               curra + me * subintwidth;
44            float myright = myleft + subintwidth;
45            if ((*f)(myleft) < 0 &&
46               (*f)(myright) > 0) {
47               curra = myleft;
48               currb = myright;
49            }
```

```
50          }
51       }
52       return curra;
53  }
54
55  float testf(float x) {
56       return pow(x-2.1,3);
57  }
58
59  int main(int argc, char **argv)
60  { printf("%f\n",root(testf,-4.1,4.1,1000)); }
```

4.12   Example: Mutual Outlinks

Consider the example of Section **??**. We have a network graph of some kind, such as Web links. For any two vertices, say any two Web sites, we might be interested in mutual outlinks, i.e. outbound links that are common to two Web sites.

The OpenMP code below finds the mean number of mutual outlinks, among all pairs of sites in a set of Web sites. Note that it uses the method for load balancing presented in Section **??**.

```
1   #include <omp.h>
2   #include <stdio.h>
3
4   // OpenMP example:  finds mean number of mutual outlinks, among all
5   // pairs of Web sites in our set
6
7   int n,  // number of sites (will assume n is even)
8       nth,  // number of threads (will assume n/2 divisible by nth)
9       *m, // link matrix
10      tot = 0; // grand total of matches
11
12  // processes row pairs (i,i+1), (i,i+2), ...
13  int procpairs(int i)
14  { int j,k,sum=0;
15      for (j = i+1; j < n; j++) {
16         for (k = 0; k < n; k++)
17            sum += m[n*i+k] * m[n*j+k];
18      }
19      return sum;
```

```
20   }
21
22   float dowork()
23   {
24      #pragma omp parallel
25      {  int pn1,pn2,i,mysum=0;
26         int me = omp_get_thread_num();
27         nth = omp_get_num_threads();
28         // in checking all (i,j) pairs, partition the work according to i;
29         // to get good load balance, this thread me will handle all i that equal
30         // me mod nth
31         for (i = me; i < n; i += nth) {
32            mysum += procpairs(i);
33         }
34         #pragma omp atomic
35         tot += mysum;
36         #pragma omp barrier
37      }
38      int divisor = n * (n-1) / 2;
39      return ((float) tot)/divisor;
40   }
41
42   int main(int argc, char **argv)
43   {  int n2 = n/2,i,j;
44      n = atoi(argv[1]);  // number of matrix rows/cols
45      int msize = n * n * sizeof(int);
46      m = (int *) malloc(msize);
47      // as a test, fill matrix with random 1s and 0s
48      for (i = 0; i < n; i++) {
49         m[n*i+i] = 0;
50         for (j = 0; j < n; j++) {
51            if (j != i) m[i*n+j] = rand() % 2;
52         }
53      }
54      if (n < 10) {
55         for (i = 0; i < n; i++) {
56            for (j = 0; j < n; j++) printf("%d  ",m[n*i+j]);
57            printf("\n");
58         }
59      }
60      tot = 0;
61      float meanml = dowork();
62      printf("mean = %f\n",meanml);
63   }
```

4.13　Example: Transforming an Adjacency Matrix

Say we have a graph with adjacency matrix

$$
\begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}
\tag{4.1}
$$

with row and column numbering starting at 0, not 1. We'd like to transform this to a two-column matrix that displays the links, in this case

$$
\begin{pmatrix}
0 & 1 \\
1 & 0 \\
1 & 3 \\
2 & 1 \\
2 & 3 \\
3 & 0 \\
3 & 1 \\
3 & 2
\end{pmatrix}
\tag{4.2}
$$

For instance, there is a 1 on the far right, second row of the above matrix, meaning that in the graph there is an edge from vertex 1 to vertex 3. This results in the row (1,3) in the transformed matrix seen above.

Suppose further that we require this listing to be in lexicographical order, sorted on source vertex and then on destination vertex. Here is code to do this computation in OpenMP:

```
1   // takes a graph adjacency matrix for a directed graph, and converts it
2   // to a 2-column matrix of pairs (i,j), meaning an edge from vertex i to
3   // vertex j; the output matrix must be in lexicographical order
4
5   // not claimed efficient, either in speed or in memory usage
6
7   #include <omp.h>
8
9   // needs -lrt link flag for C++
10  #include <time.h>
```

```
11  float timediff(struct timespec t1, struct timespec t2)
12  { if (t1.tv_nsec > t2.tv_nsec) {
13        t2.tv_sec -= 1;
14        t2.tv_nsec += 1000000000;
15     }
16     return t2.tv_sec-t1.tv_sec + 0.000000001 * (t2.tv_nsec-t1.tv_nsec);
17  }
18
19  // transgraph() does this work
20  // arguments:
21  // adjm: the adjacency matrix (NOT assumed symmetric), 1 for edge, 0
22  // otherwise; note: matrix is overwritten by the function
23  // n: number of rows and columns of adjm
24  // nout: output, number of rows in returned matrix
25  // return value: pointer to the converted matrix
26  int *transgraph(int *adjm, int n, int *nout)
27  {
28     int *outm, // to become the output matrix
29        *num1s, // i-th element will be the number of 1s in row i of adjm
30        *cumul1s; // cumulative sums in num1s
31     #pragma omp parallel
32     { int i,j,m;
33        int me = omp_get_thread_num(),
34           nth = omp_get_num_threads();
35        int myrows[2];
36        int tot1s;
37        int outrow,num1si;
38        #pragma omp single
39        {
40           num1s = malloc(n*sizeof(int));
41           cumul1s = malloc((n+1)*sizeof(int));
42        }
43        // determine the rows in adjm to be handled by this thread
```

```
44        findmyrange(n,nth,me,myrows);
45        // start the action
46        for (i = myrows[0]; i <= myrows[1]; i++) {
47           tot1s = 0;
48           for (j = 0; j < n; j++)
49              if (adjm[n*i+j] == 1) {
50                 adjm[n*i+(tot1s++)] = j;
51              }
52           num1s[i] = tot1s;
53        }
54        #pragma omp barrier
55        #pragma omp single
56        {
57           cumul1s[0] = 0;
58           // now calculate where the output of each row in adjm
59           // should start in outm
60           for (m = 1; m <= n; m++) {
61              cumul1s[m] = cumul1s[m-1] + num1s[m-1];
62           }
63           *nout = cumul1s[n];
64           outm = malloc(2*(*nout) * sizeof(int));
65        }
66        // now fill in this thread's portion
67        for (i = myrows[0]; i <= myrows[1]; i++) {
68           outrow = cumul1s[i];
69           num1si = num1s[i];
70           for (j = 0; j < num1si; j++) {
71              outm[2*(outrow+j)] = i;
72              outm[2*(outrow+j)+1] = adjm[n*i+j];
73           }
74        }
75        #pragma omp barrier
76     }
```

```
77      return outm;
78   }
79
80   int main(int argc, char **argv)
81   { int i,j;
82      int *adjm;
83      int n = atoi(argv[1]);
84      int nout;
85      int *outm;
86      adjm = malloc(n*n*sizeof(int));
87      for (i = 0; i < n; i++)
88         for (j = 0; j < n; j++)
89            if (i == j) adjm[n*i+j] = 0;
90            else adjm[n*i+j] = rand() % 2;
91
92      struct timespec bgn,nd;
93      clock_gettime(CLOCK_REALTIME, &bgn);
94
95      outm = transgraph(adjm,n,&nout);
96      printf("number of output rows: %d\n",nout);
97
98      clock_gettime(CLOCK_REALTIME, &nd);
99      printf("%f\n",timediff(bgn,nd));
100
101     if (n <= 10)
102        for (i = 0; i < nout; i++)
103           printf("%d %d\n",outm[2*i],outm[2*i+1]);
104  }
105
106  // finds chunk among 0,...,n-1 to assign to thread number me among nth
107  // threads
108  void findmyrange(int n,int nth,int me,int *myrange)
109  { int chunksize = n / nth;
```

```
110     myrange[0] = me * chunksize;
111     if (me < nth-1) myrange[1] = (me+1) * chunksize - 1;
112     else myrange[1] = n - 1;
113   }
```

4.14   Locks with OpenMP

Though one of OpenMP's best virtues is that you can avoid working with those pesky lock variables needed for straight threads programming, there are still some instances in which lock variables may be useful. OpenMP does provide for locks:

- declare your locks to be of type `omp_lock_t`
- call `omp_set_lock()` to lock the lock
- call `omp_unset_lock()` to unlock the lock

4.15   Other Examples of OpenMP Code in This Book

There are additional OpenMP examples in later sections of this book, such as:[5]

- sampling bucket sort, Section 1.3.2
- parallel prefix sum/run-length decoding, Section 10.3.
- matrix multiplication, Section 11.3.2.
- Jacobi algorithm for solving systems of linear equations, with a good example of the OpenMP **reduction** clause, Section 11.5.4
- another implementation of Quicksort, Section 12.1.2

---

[5]If you are reading this presentation on OpenMP separately from the book, the book is at `http://heather.cs.ucdavis.edu/~matloff/158/PLN/ParProcBook.pdf`

第 5 章　Introduction to GPU Programming with CUDA

Even if you don't play video games, you can be grateful to the game players, as their numbers have given rise to a class of highly powerful parallel processing devices—**graphics processing units** (GPUs). Yes, you program right on the video card in your computer, even though your program may have nothing to do with graphics or games.

5.1　Overview

The video game market is so lucrative that the industry has developed ever-faster GPUs, in order to handle ever-faster and ever-more visually detailed video games. These actually are parallel processing hardware devices, so around 2003 some people began to wonder if one might use them for parallel processing of nongraphics applications.

Originally this was cumbersome. One needed to figure out clever ways of mapping one's application to some kind of graphics problem, i.e. ways to disguising one's problem so that it appeared to be doing graphics computations. Though some high-level interfaces were developed to automate this transformation, effective coding required some understanding of graphics principles.

But current-generation GPUs separate out the graphics operations, and now consist of multiprocessor elements that run under the familiar shared-memory threads model. Thus they are easily programmable. Granted, effective coding still requires an intimate knowledge of the hardwre, but at least it's (more or less) familiar hardware, not requiring knowledge of graphics.

Moreover, unlike a multicore machine, with the ability to run just a few threads at one time, e.g. four threads on a quad core machine, GPUs can run *hundreds or thousands* of threads at once. There are various restrictions that come with this, but you can see that there is fantastic potential for speed here.

NVIDIA has developed the CUDA language as a vehicle for programming on their GPUs. It's basically just a slight extension of C, and has become very popular. More recently, the OpenCL language has been developed by Apple, AMD and others (including NVIDIA). It too is a slight extension of C, and it aims to provide a uniform interface that works with multicore machines in addition to GPUs. OpenCL is not yet in as broad use as CUDA, so our discussion here focuses on CUDA and NVIDIA GPUs.

Also, the discussion will focus on NVIDIA's Tesla line. This then led to the second generation, Fermi, and then Kepler. Unless otherwise stated, all statements here refer to Tesla.

Some terminology:

- A CUDA program consists of code to be run on the **host**, i.e. the CPU, and code to run on the **device**, i.e. the GPU.
- A function that is called by the host to execute on the device is called a **kernel**.
- Threads in an application are grouped into **blocks**. The entirety of blocks is called the **grid** of that application.

5.2   Example: Calculate Row Sums

Here's a sample program. And I've kept the sample simple: It just finds the sums of all the rows of a matrix.

```
1  #include <stdio.h>
2  #include <stdlib.h>
3  #include <cuda.h>
4
5  // CUDA example: finds row sums of an integer matrix m
6
7  // find1elt() finds the rowsum of one row of the nxn matrix m, storing the
8  // result in the corresponding position in the rowsum array rs; matrix
9  // stored as 1-dimensional, row-major order
10
11  __global__ void find1elt(int *m, int *rs, int n)
12  {
13     int rownum = blockIdx.x; // this thread will handle row # rownum
```

```
14      int sum = 0;
15      for (int k = 0; k < n; k++)
16         sum += m[rownum*n+k];
17      rs[rownum] = sum;
18   }
19
20   int main(int argc, char **argv)
21   {
22      int n = atoi(argv[1]); // number of matrix rows/cols
23      int *hm, // host matrix
24          *dm, // device matrix
25          *hrs, // host rowsums
26          *drs; // device rowsums
27      int msize = n * n * sizeof(int); // size of matrix in bytes
28      // allocate space for host matrix
29      hm = (int *) malloc(msize);
30      // as a test, fill matrix with consecutive integers
31      int t = 0,i,j;
32      for (i = 0; i < n; i++) {
33         for (j = 0; j < n; j++) {
34            hm[i*n+j] = t++;
35         }
36      }
37      // allocate space for device matrix
38      cudaMalloc((void **)&dm,msize);
39      // copy host matrix to device matrix
40      cudaMemcpy(dm,hm,msize,cudaMemcpyHostToDevice);
41      // allocate host, device rowsum arrays
42      int rssize = n * sizeof(int);
43      hrs = (int *) malloc(rssize);
44      cudaMalloc((void **)&drs,rssize);
45      // set up parameters for threads structure
46      dim3 dimGrid(n,1); // n blocks
```

```
47      dim3 dimBlock(1,1,1); // 1 thread per block
48      // invoke the kernel
49      find1elt<<<dimGrid,dimBlock>>>(dm,drs,n);
50      // wait for kernel to finish
51      cudaThreadSynchronize();
52      // copy row vector from device to host
53      cudaMemcpy(hrs,drs,rssize,cudaMemcpyDeviceToHost);
54      // check results
55      if (n < 10) for(int i=0; i<n; i++) printf("%d\n",hrs[i]);
56      // clean up
57      free(hm);
58      cudaFree(dm);
59      free(hrs);
60      cudaFree(drs);
61   }
```

This is mostly C, with a bit of CUDA added here and there. Here's how the program works:

- Our **main()** runs on the host.

- Kernel functions are identified by **___global___ void**. They are called by the host and run on the device, thus serving as entries to the device.

   We have only one kernel invocation here, but could have many, say with the output of one serving as input to the next.

- Other functions that will run on the device, called by functions running on the device, must be identified by **___device___**, e.g.

```
1   __device__ int sumvector(float *x, int n)
```

   Note that unlike kernel functions, device functions can have return values, e.g. **int** above.

- When a kernel is called, each thread runs it. Each thread receives the same arguments.

- Each block and thread has an ID, stored in programmer-accessible structs **blockIdx** and **threadIdx**. We'll discuss the details later, but for now, we'll just note that here the statement

```
1   int rownum = blockIdx.x;
```

   picks up the block number, which our code in this example uses to determine which row to sum.

- One calls **cudaMalloc()** on the host to dynamically allocate space on the device's memory.[①] Execution of the statement

```
1  cudaMalloc((void **)&drs,rssize);
```

  allocates space *on the device*, pointed to by **drs**, a variable in the *host's* address space.

  The space allocated by a **cudaMalloc()** call on the device is global to all kernels, and resides in the global memory of the device (details on memory types later).

  One can also allocate device memory statically. For example, the statement

```
1  __device int z[100];
```

  appearing outside any function definition would allocate space on device global memory, with scope global to all kernels. However, it is not accessible to the host.

- Data is transferred to and from the host and device memories via **cudaMemcpy()**. The fourth argument specifies the direction, e.g. cudaMemcpyHostToDevice, cudaMemcpyDeviceToHost or cudaMemcpyDeviceToDevice.

- Kernels return **void** values, so values are returned via a kernel's arguments.

- Device functions (which we don't have here) can return values. They are called only by kernel functions or other device functions.

- Note carefully that a call to the kernel doesn't block; it returns immediately. For that reason, the code above has a host barrier call, to avoid copying the results back to the host from the device before they're ready:

```
1  cudaThreadSynchronize();
```

  On the other hand, if our code were to have another kernel call, say on the next line after

```
1  find1elt<<<dimGrid,dimBlock>>>(dm,drs,n);
```

  and if some of the second call's input arguments were the outputs of the first call, there would be an implied barrier betwwen the two calls; the second would not start execution before the first finished.

  Calls like **cudaMemcpy()** do block until the operation completes.

  There is also a thread barrier available for the threads themselves, at the block level. The call is

```
1  __syncthreads();
```

  This can only be invoked by threads within a block, not across blocks. In other words, this is barrier synchronization within blocks.

[①]This function cannot be called from the device itself. However, **malloc()** is available from the device, and device memory allocated by it can be copied to the host. See the NVIDIA programming guide for details.

- I've written the program so that each thread will handle one row of the matrix. I've chosen to store the matrix in one-dimensional form in row-major order, and the matrix is of size n x n, so the loop

```
1   for (int k = 0; k < n; k++)
2       sum += m[rownum*n+k];
```

will indeed traverse the n elements of row number **rownum**, and compute their sum. That sum is then placed in the proper element of the output array:

```
1   rs[rownum] = sum;
```

- After the kernel returns, the host must copy the result back from the device memory to the host memory, in order to access the results of the call.

5.3   Understanding the Hardware Structure

Scorecards, get your scorecards here! You can't tell the players without a scorecard—classic cry of vendors at baseball games

Know thy enemy—Sun Tzu, *The Art of War*

The enormous computational potential of GPUs cannot be unlocked without an intimate understanding of the hardware. This of course is a fundamental truism in the parallel processing world, but it is acutely important for GPU programming. This section presents an overview of the hardware.

5.3.1   Processing Units

A GPU consists of a large set of **streaming multiprocessors** (SMs). Since each SM is essentially a multicore machine in its own right, you might say the GPU is a multi-multiprocessor machine.

Each SM consists of a number of **streaming processors** (SPs), individual cores. The cores run threads, as with ordinary cores, but threads in an SM run in lockstep, to be explained below.

It is important to understand the motivation for this SM/SP hierarchy: Two threads located in different SMs cannot synchronize with each other in the barrier sense. Though this sounds like a negative at first, it is actually a great advantage, as the independence of threads in separate SMs means that the hardware can run faster. So, if the CUDA application programmer can write his/her algorithm so as to have certain independent chunks, and those chunks can be assigned to different SMs (we'll see how, shortly), then that's a "win."

Note that at present, word size is 32 bits. Thus for instance floating-point operations in hardware were originally in single precision only, though newer devices are capable of double precision.

5.3.2   Thread Operation

GPU operation is highly threaded, and again, understanding of the details of thread operation is key to good performance.

SIMT Architecture

When you write a CUDA application program, you partition the threads into groups called **blocks**. The hardware will assign an entire block to a single SM, though several blocks can run in the same SM. The hardware will then divide a block into **warps**, 32 threads to a warp. Knowing that the hardware works this way, the programmer controls the block size and the number of blocks, and in general writes the code to take advantage of how the hardware works.

The central point is that *all the threads in a warp run the code in lockstep.* During the machine instruction fetch cycle, the same instruction will be fetched for all of the threads in the warp. Then in the execution cycle, each thread will either execute that particular instruction or execute nothing. The execute-nothing case occurs in the case of branches; see below. This is the classical **single instruction, multiple data** (SIMD) pattern used in some early special-purpose computers such as the ILLIAC; here it is called **single instruction, multiple thread** (SIMT).

The syntactic details of grid and block configuration will be presented in Section 5.3.4.

The Problem of Thread Divergence

The SIMT nature of thread execution has major implications for performance. Consider what happens with if/then/else code. If some threads in a warp take the "then" branch and others go in the "else" direction, they cannot operate in lockstep. That means that some threads must wait while others execute. This renders the code at that point serial rather than parallel, a situation called **thread divergence**. As one CUDA Web tutorial points out, this can be a "performance killer." (On the other hand, threads in the same block but in different warps can diverge with no problem.)

"OS in Hardware"

Each SM runs the threads on a timesharing basis, just like an operating system (OS). This time-sharing is implemented in the hardware, though, not in software as in the OS case.

The "hardware OS" runs largely in analogy with an ordinary OS:

- A process in an ordinary OS is given a fixed-length timeslice, so that processes take turns running. In a GPU's hardware OS, warps take turns running, with fixed-length timeslices.

- With an ordinary OS, if a process reaches an input/output operation, the OS suspends the process while I/O is pending, even if its turn is not up. The OS then runs some other process instead, so as to avoid wasting CPU cycles during the long period of time needed for the I/O.

  With an SM, though, the analogous situation occurs when there is a long memory operation, to global memory; if a a warp of threads needs to access global memory (including local memory; see below), the SM will schedule some other warp while the memory access is pending.

The hardware support for threads is extremely good; a context switch takes very little time, quite a contrast to the OS case. Moreover, as noted above, the long latency of global memory may be solvable by having a lot of threads that the hardware can timeshare to hide that latency; while one warp is fetching data from memory, another warp can be executing, thus not losing time due to the long fetch delay. For these reasons, CUDA programmers typically employ a large number of threads, each of which does only a small amount of work—again, quite a contrast to something like OpenMP.

5.3.3 Memory Structure

The GPU memory hierarchy plays a key role in performance. Let's discuss the most important two types of memory first—shared and global.

Shared and Global Memory

Here is a summary:

type	shared	global
scope	glbl. to block	glbl. to app.
size	small	large
location	on-chip	off-chip
speed	blinding	molasses
lifetime	kernel	application
host access?	no	yes
cached?	no	no

In prose form:

- Shared memory: All the threads in an SM share this memory, and use it to communicate among themselves, just as is the case with threads in CPUs. Access is very fast, as this memory is on-chip. It is declared inside the kernel, or in the kernel call (details below).

  On the other hand, shared memory is small, currently 16K bytes per SM, and the data stored

in it are valid only for the life of the currently-executing kernel. Also, shared memory cannot be accessed by the host.

- Global memory: This is shared by all the threads in an entire application, and is persistent across kernel calls, throughout the life of the application, i.e. until the program running on the host exits. It is usually much larger than shared memory. It is accessible from the host. Pointers to global memory can (but do not have to) be declared outside the kernel.

  On the other hand, global memory is off-chip and very slow, taking hundreds of clock cycles per access instead of just a few. As noted earlier, this can be ameliorated by exploiting latency hiding; we will elaborate on this in Section 5.3.3.

The reader should pause here and reread the above comparison between shared and global memories. *The key implication is that shared memory is used essentially as a programmer-managed cache.* Data will start out in global memory, but if a variable is to be accessed multiple times by the GPU code, it's probably better for the programmer to write code that copies it to shared memory, and then access the copy instead of the original. If the variable is changed and is to be eventually transmitted back to the host, the programmer must include code to copy it back to global memory.

Accesses to global and shared memory are done via half-warps, i.e. an attempt is made to do all memory accesses in a half-warp simultaneously. In that sense, only threads in a half-warp run simultaneously, but the full warp is *scheduled* to run contemporaneously by the hardware OS, first one half-warp and then the other.

The host can access global memory via **cudaMemcpy()**, as seen earlier. It cannot access shared memory. Here is a typical pattern:

```
__global__ void abckernel(int *abcglobalmem)
{
   __shared__ int abcsharedmem[100];
   // ... code to copy some of abcglobalmem to some of abcsharedmem
   // ... code for computation
   // ... code to copy some of abcsharedmem to some of abcglobalmem
}
```

Typically you would write the code so that each thread deals with its own portion of the shared data, e.g. its own portion of **abcsharedmem** and **abcglobalmem** above. However, all the threads in that block can read/write any element in **abcsharedmem**.

Shared memory consistency (recall Section 3.6) is sequential within a thread, but **relaxed** among threads in a block: A write by one thread is not guaranteed to be visible to the others in a block until **___syncthreads()** is called. On the other hand, writes by a thread *will* be visible to that same thread

in subsequent reads without calling **___syncthreads()**. Among the implications of this is that if each thread writes only to portions of shared memory that are not read by other threads in the block, then **___syncthreads()** need not be called.

In the code fragment above, we allocated the shared memory through a C-style declaration:

```
__shared__ int abcsharedmem[100];
```

It is also possible to allocate shared memory in the kernel call, along with the block and thread configuration. Here is an example:

```
#include <stdio.h>
#include <stdlib.h>
#include <cuda.h>

// CUDA example: illustrates kernel-allocated shared memory; does
// nothing useful, just copying an array from host to device global,
// then to device shared, doubling it there, then copying back to device
// global then host

__global__ void doubleit(int *dv, int n)
{ extern __shared__ int sv[];
   int me = threadIdx.x;
   // threads share in copying dv to sv, with each thread copying one
   // element
   sv[me] = 2 * dv[me];
   dv[me] = sv[me];
}

int main(int argc, char **argv)
{
   int n = atoi(argv[1]); // number of matrix rows/cols
   int *hv, // host array
       *dv; // device array
   int vsize = n * sizeof(int); // size of array in bytes
   // allocate space for host array
```

```
26      hv = (int *) malloc(vsize);
27      // fill test array with consecutive integers
28      int t = 0,i;
29      for (i = 0; i < n; i++)
30        hv[i] = t++;
31      // allocate space for device array
32      cudaMalloc((void **)&dv,vsize);
33      // copy host array to device array
34      cudaMemcpy(dv,hv,vsize,cudaMemcpyHostToDevice);
35      // set up parameters for threads structure
36      dim3 dimGrid(1,1);
37      dim3 dimBlock(n,1,1); // all n threads in the same block
38      // invoke the kernel; third argument is amount of shared memory
39      doubleit<<<dimGrid,dimBlock,vsize>>>(dv,n);
40      // wait for kernel to finish
41      cudaThreadSynchronize();
42      // copy row array from device to host
43      cudaMemcpy(hv,dv,vsize,cudaMemcpyDeviceToHost);
44      // check results
45      if (n < 10) for(int i=0; i<n; i++) printf("%d\n",hv[i]);
46      // clean up
47      free(hv);
48      cudaFree(dv);
49    }
```

Here the variable **sv** is kernel allocated. It's declared in the statement

```
1  extern __shared__ int sv[];
```

but actually allocated during the kernel invocation

```
1  doubleit<<<dimGrid,dimBlock,vsize>>>(dv,n);
```

in that third argument within the chevrons, **vsize**.

Note that one can only directly declare one region of space in this manner. This has two implications:

- Suppose we have two **___device___** functions, each declared an **extern ___shared___** array like this. Those two arrays will occupy the same place in memory!

- Suppose within one **___device___** function, we wish to have two **extern ___shared___** arrays. We cannot do that literally, but we can share the space via subarrays, e.g.:

```
1  int *x = &sv[120];
```

would set up **x** as a subarray of **sv** above, starting at element 120.

One can also set up shared arrays of fixed length in the same code. Declare them before the variable-length one.

In our example above, the array **sv** is syntactically local to the function **doubleit()**, but is shared by all invocations of that function in the block, thus acting "global" to them in a sense. But the point is that it is not accessible from within *other* functions running in that block. In order to achieve the latter situation, a shared array can be declared outside any function.

Global-Memory Performance Issues

As noted, the latency (Section **??**) for global memory is quite high, on the order of hundreds of clock cycles. However, the hardware attempts to ameliorate this problem in a couple of ways.

First, as mentioned earlier, if a warp has requested a global memory access that will take a long time, the hardware will schedule another warp to run while the first is waiting for the memory access to complete. This is an example of a common parallel processing technique called **latency hiding**.

Second, the bandwidth (Section **??**) to global memory can be high, due to hardware actions called **coalescing**. This simply means that if the hardware sees that the threads in this half-warp (or at least the ones currently accessing global memory) are accessing consecutive words, the hardware can execute the memory requests in groups of up to 32 words at a time. This works because the memory is low-order interleaved (Section 3.2.1), and is true for both reads and writes.

The newer GPUs go even further, coalescing much more general access patterns, not just to consecutive words.

The programmer may be able to take advantage of coalescing, by a judicious choice of algorithms and/or by inserting padding into arrays (Section 3.2.2).

Shared-Memory Performance Issues

Shared memory is divided into banks, in a low-order interleaved manner (recall Section 3.2): Words with consecutive addresses are stored in consecutive banks, mod the number of banks, i.e. wrapping

back to 0 when hitting the last bank. If for instance there are 8 banks, addresses 0, 8, 16,... will be in bank 0, addresses 1, 9, 17,... will be in bank 1 and so on. (Actually, older devices have 16 banks, while newer ones have 32.) The fact that all memory accesses in a half-warp are attempted simultaneously implies that the best access to shared memory arises when the accesses are to different banks, just as for the case of global memory.

An exception occurs in **broadcast**. If all threads in the block wish to read from the same word in the same bank, the word will be sent to all the requestors simultaneously without conflict. However, if only some theads try to read the same word, there may or may not be a conflict, as the hardware chooses a bank for broadcast in some unspecified way.

As in the discussion of global memory above, we should write our code to take advantage of these structures.

The biggest performance issue with shared memory is its size, as little as 16K per SM in many GPU cards. And remember, this is divvied up among the blocks on a given SM. If we have 4 blocks running on an SM, each one can only use 16K/4 = 4K bytes of shared memory.

Host/Device Memory Transfer Performance Issues

Copying data between host and device can be a major bottleneck. One way to ameliorate this is to use **cudaMallocHost()** instead of **malloc()** when allocating memory on the host. This sets up page-locked memory, meaning that it cannot be swapped out by the OS' virtual memory system. This allows the use of DMA hardware to do the memory copy, said to make **cudaMemcpy()** twice as fast.

Other Types of Memory

There are also other types of memory. Again, let's start with a summary:

type	registers	local	constant	texture
scope	single thread	single thread	glbl. to app.	glbl. to app.
location	device	device	host+device cache	host+device cache
speed	fast	molasses	fast if cache hit	fast if cache hit
lifetime	kernel	kernel	application	application
host access?	no	no	yes	yes
device access?	read/write	read/write	read	read

- **Registers:**

  Each SM has a set of registers, much more numerous than in a CPU. Access to them is very fast, said to be slightly faster than to shared memory.

The compiler normally stores the local variables for a device function in registers, but there are exceptions. An array won't be placed in registers if the array is too large, or if the array has variable index values, such as

```
1  int z[20],i;
2  ...
3  y = z[i];
```

Since registers are not indexable by the hardware, the compiler cannot allocate **z** to registers in this case. If on the other hand, the only code accessing **z** has constant indices, e.g. **z[8]**, the compiler may put **z** in registers.

- **Local memory:**

  This is physically part of global memory, but is an area within that memory that is allocated by the compiler for a given thread. As such, it is slow, and accessible only by that thread. The compiler allocates this memory for local variables in a device function if the compiler cannot store them in registers. This is called **register spill**.

- **Constant memory:**

  As the name implies, it's read-only from the device (read/write by the host), for storing values that will not be changed by device code. It is off-chip, thus potentially slow, but has a cache on the chip. At present, the size is 64K.

  One designates this memory with **___constant___**, as a global variable in the source file. One sets its contents from the host via **cudaMemcpyToSymbol()**, whose (simple form for the) call is

```
1  cudaMemcpyToSymbol(var_name,pointer_to_source,number_bytes_copy,cudaMemcpyHostToDevice)
```

  For example:

```
1  __constant__ int x;  // not contained in any function
2
3  // host code
4  int y = 3;
5  cudaMemcpyToSymbol("x",&y,sizeof(int));
6  ...
7
8  // device code
9  int z;
10 z = x;
```

  Note again that the name Constant refers to the fact that device code cannot change it. But host code certainly can change it between kernel calls. This might be useful in iterative algorithms like this:

```
1   / host code
2   for 1 to number of iterations
3       set Constant array x
4       call kernel (do scatter op)
5       cudaThreadSynchronize()
6       do gather op, using kernel results to form new x
7
8   // device code
9   use x together with thread-specific data
10  return results to host
```

- **Texture:**

  This is similar to constant memory, in the sense that it is read-only and cached. The difference is that the caching is two-dimensional. The elements **a[i][j]** and **a[i+1][j]** are far from each other in the global memory, but since they are "close" in a two-dimensional sense, they may reside in the same cache line.

5.3.4   Threads Hierarchy

Following the hardware, threads in CUDA software follow a hierarchy:

- The entirety of threads for an application is called a **grid**.

- A grid consists of one or more **blocks** of threads.

- Each block has its own ID within the grid, consisting of an "x coordinate" and a "y coordinate."

- Likewise each thread has x, y and z coordinates within whichever block it belongs to.

- Just as an ordinary CPU thread needs to be able to sense its ID, e.g. by calling **omp_get_thread_num()** in OpenMP, CUDA threads need to do the same. A CUDA thread can access its block ID via the built-in variables **blockIdx.x** and **blockIdx.y**, and can access its thread ID within its block via **threadIdx.x**, **threadIdx.y** and **threadIdx.z**.

- The programmer specifies the grid size (the numbers of rows and columns of blocks within a grid) and the block size (numbers of rows, columns and layers of threads within a block). In the first example above, this was done by the code

```
1   dim3 dimGrid(n,1);
2   dim3 dimBlock(1,1,1);
3   find1elt<<<dimGrid,dimBlock>>>(dm,drs,n);
```

  Here the grid is specified to consist of n ($n \times 1$) blocks, and each block consists of just one ($1 \times 1 \times 1$) thread.

  That last line is of course the call to the kernel. As you can see, CUDA extends C syntax to allow

specifying the grid and block sizes. CUDA will store this information in structs of type **dim3**, in this case our variables **gridDim** and **blockDim**, accessible to the programmer, again with member variables for the various dimensions, e.g. **blockDim.x** for the size of the X dimension for the number of threads per block.

- All threads in a block run in the same SM, though more than one block might be on the same SM.

- The "coordinates" of a block within the grid, and of a thread within a block, are merely abstractions. If for instance one is programming computation of heat flow across a two-dimensional slab, the programmer may find it clearer to use two-dimensional IDs for the threads. *But this does not correspond to any physical arrangement in the hardware.*

As noted, the motivation for the two-dimensional block arrangment is to make coding conceptually simpler for the programmer if he/she is working an application that is two-dimensional in nature.

For example, in a matrix application one's parallel algorithm might be based on partitioning the matrix into rectangular submatrices (**tiles**), as we'll do in Section 11.2. In a small example there, the matrix

$$A = \begin{pmatrix} 1 & 5 & 12 \\ 0 & 3 & 6 \\ 4 & 8 & 2 \end{pmatrix} \tag{5.1}$$

is partitioned as

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}, \tag{5.2}$$

where

$$A_{00} = \begin{pmatrix} 1 & 5 \\ 0 & 3 \end{pmatrix}, \tag{5.3}$$

$$A_{01} = \begin{pmatrix} 12 \\ 6 \end{pmatrix}, \tag{5.4}$$

$$A_{10} = \begin{pmatrix} 4 & 8 \end{pmatrix} \tag{5.5}$$

and

$$A_{11} = \left(\ 2\ \right). \tag{5.6}$$

We might then have one block of threads handle A_{00}, another block handle A_{01} and so on. CUDA's two-dimensional ID system for blocks makes life easier for programmers in such situations.

5.3.5 What's NOT There

We're not in Kansas anymore, Toto—character Dorothy Gale in *The Wizard of Oz*

It looks like C, it feels like C, and for the most part, it *is* C. But in many ways, it's quite different from what you're used to:

- You don't have access to the C library, e.g. **printf()** (the library consists of host machine language, after all). There are special versions of math functions, however, e.g. **___sin()**.
- No recursion.
- No stack. Functions are essentially inlined, rather than their calls being handled by pushes onto a stack.
- No pointers to functions.

5.4 Synchronization, Within and Between Blocks

As mentioned earlier, a barrier for the threads in the same block is available by calling **___syncthreads()**. Note carefully that if one thread writes a variable to shared memory and another then reads that variable, one must call this function (from both threads) in order to get the latest value. Keep in mind that within a block, different warps will run at different times, making synchronization vital.

Remember too that threads across blocks cannot sync with each other in this manner. There are, though, several **atomic** operations—read/modify/write actions that a thread can execute without **pre-emption**, i.e. without interruption—available on both global and shared memory. For example, **atomicAdd()** performs a fetch-and-add operation, as described in Section 3.4.3 of this book. The call is

```
1   atomicAdd(address of integer variable,inc);
```

where **address of integer variable** is the address of the (device) variable to add to, and **inc** is the amount to be added. The return value of the function is the value originally at that address before the operation.

There are also **atomicExch()** (exchange the two operands), **atomicCAS()** (if the first operand equals the second, replace the first by the third), **atomicMin()**, **atomicMax()**, **atomicAnd()**, **atomicOr()**, and so on.

Use **-arch=sm_11** when compiling, e.g.

```
1  nvcc -g -G yoursrc.cu -arch=sm_11
```

Though a barrier could in principle be constructed from the atomic operations, its overhead would be quite high. In earlier models that was near a microsecond, and though that problem has been ameliorated in more recent models, implementing a barrier in this manner . would not be not much faster than attaining interblock synchronization by returning to the host and calling **cudaThreadSynchronize()** there. Recall that the latter *is* a possible way to implement a barrier, since global memory stays intact in between kernel calls, but again, it would be slow.

So, what if synchronization is really needed? This is the case, for instance, for iterative algorithms, where all threads must wait at the end of each iteration.

If you have a small problem, maybe you can get satisfactory performance by using just one block. You'll have to use a larger granularity, i.e. more work assigned to each thread. But using just one block means you're using only one SM, thus only a fraction of the potential power of the machine.

If you use multiple blocks, though, your only feasible option for synchronization is to rely on returns to the host, where synchronization occurs via **cudaThreadSynchronize()**. You would then have the situation outlined in the discussion of Constant memory in Section 5.3.3.

5.5 More on the Blocks/Threads Tradeoff

Resource size considerations must be kept in mind when you design your code and your grid configuration. In particular, note the following:

- Each block in your code is assigned to some SM. It will be tied to that SM during the entire execution of your kernel, though of course it will not constantly be running during that time.
- If there are more blocks than can be accommodated by all the SMs, then some blocks will need to wait for assignment; when a block finishes, that block's resources, e.g. shared memory, can now be assigned to a waiting block.
- The programmer has no control over which block is assigned to which SM.
- Within a block, threads execute by the warp, 32 threads. At any give time, the SM is running one warp, chosen by the GPU OS.

- The GPU has a limit on the number of threads that can run on a single block, typically 512, and on the total number of threads running on an SM, 786.

- If a block contains fewer than 32 threads, only part of the processing power of the SM it's running on will be used. So block size should normally be at least 32. Moreover, for the same reason, block size should ideally be a multiple of 32.

- If your code makes used of shared memory, or does within-block synchronization, the larger the block size, the better.

- We want to use the full power of the GPU, with its many SMs, thus implying a need to use at least as many blocks as there are SMs (which may require smaller blocks).

- Moreover, due to the need for latency hiding in memory access, we want to have lots of warps, so that some will run while others are doing memory access.

- Two threads doing unrelated work, or the same work but with many if/elses, would cause a lot of thread divergence if they were in the same block.

- A commonly-cited rule of thumb is to have between 128 and 256 threads per block.

Though there is a limit on the number of blocks, this limit will be much larger than the number of SMs. So, you may have multiple blocks running on the same SM. Since execution is scheduled by the warp anyway, there appears to be no particular drawback to having more than one block on the same SM.

5.6   Hardware Requirements, Installation, Compilation, Debugging

You do need a suitable NVIDIA video card. There is a list at `http://www.nvidia.com/object/cuda_gpus.html`; see also the Wikipedia entry, `http://en.wikipedia.org/wiki/CUDA#Supported_GPUs`. If you have a Linux system, run **lspci** to determine what kind you have.[2]

Download the CUDA toolkit from NVIDIA. Just plug "CUDA download" into a Web search engine to find the site. Install as directed.

You'll need to set your search and library paths to include the CUDA **bin** and **lib** directories.

To compile **x.cu** (and yes, use the **.cu** suffix), type

```
1   $ nvcc -g -G x.cu
```

---

[2]It might be in **/sbin**.

The **-g -G** options are for setting up debugging, the first for host code, the second for device code. You may also need to specify

```
-I/your_CUDA_include_path
```

to pick up the file **cuda.h**. Run the code as you normally would.

You may need to take special action to set your library path properly. For example, on Linux machines, set the environment variable **LD_LIBRARY_PATH** to include the CUDA library.

To determine the limits, e.g. maximum number of threads, for your device, use code like this:

```
cudaDeviceProp Props;
cudaGetDeviceProperties(&Props,0);
```

The 0 is for device 0, assuming you only have one device. The return value of **cudaGetDeviceProperties()** is a complex C struct whose components are listed at `http://developer.download. nvidia.com/compute/cuda/2_3/toolkit/docs/online/group__CUDART__DEVICE_g5aa4f47938af8276f08074d0 html`.

Here's a simple program to check some of the properties of device 0:

```
#include<cuda.h>
#include <stdio.h>

int main()
{
   cudaDeviceProp Props;
   cudaGetDeviceProperties( &Props,0);

   printf("shared mem: %d\n", Props.sharedMemPerBlock);
   printf("max threads/block: %d\n",Props.maxThreadsPerBlock);
   printf("max blocks: %d\n",Props.maxGridSize[0]);
   printf("total Const mem: %d\n",Props.totalConstMem);
}
```

Under older versions of CUDA, such as 2.3, one can debug using GDB as usual. You must compile your program in emulation mode, using the **-deviceemu** command-line option. This is no longer available as of version 3.2. CUDA also includes a special version of GDB, CUDA-GDB (invoked as **cuda-gdb**) for real-time debugging. However, on Unix-family platforms it runs only if X11 is not

running. Short of dedicating a machine for debugging, you may find it useful to install a version 2.3 in addition to the most recent one to use for debugging.

5.7 Example: Improving the Row Sums Program

The issues involving coalescing in Section 5.3.3 would suggest that our rowsum code might run faster with column sums, to take advantage of the memory banking. (So the user would either need to take the transpose first, or have his code set up so that the matrix is in transpose form to begin with.) As two threads in the same half-warp march down adjoining columns in lockstep, they will always be accessing adjoining words in memory.

So, I modified the program accordingly (not shown), and compiled the two versions, as **rs** and **cs**, the row- and column-sum versions of the code, respectively.

This did produce a small improvement (confirmed in subsequent runs, needed in any timing experiment):

```
1  pc5:~/CUDA% time rs 20000
2  2.585u 1.753s 0:04.54 95.3%    0+0k 7104+0io 54pf+0w
3  pc5:~/CUDA% time cs 20000
4  2.518u 1.814s 0:04.40 98.1%    0+0k 536+0io 5pf+0w
```

But let's compare it to a version running only on the CPU,

```
1  #include <stdio.h>
2  #include <stdlib.h>
3
4  // non-CUDA example: finds col sums of an integer matrix m
5
6  // find1elt() finds the colsum of one col of the nxn matrix m, storing the
7  // result in the corresponding position in the colsum array cs; matrix
8  // stored as 1-dimensional, row-major order
9
10 void find1elt(int *m, int *cs, int n)
11 {
12    int sum=0;
13    int topofcol;
14    int col,k;
```

```
15    for (col = 0; col < n; col++) {
16      topofcol = col;
17      sum = 0;
18      for (k = 0; k < n; k++)
19        sum += m[topofcol+k*n];
20      cs[col] = sum;
21    }
22  }
23
24  int main(int argc, char **argv)
25  {
26    int n = atoi(argv[1]); // number of matrix cols/cols
27    int *hm, // host matrix
28        *hcs; // host colsums
29    int msize = n * n * sizeof(int); // size of matrix in bytes
30    // allocate space for host matrix
31    hm = (int *) malloc(msize);
32    // as a test, fill matrix with consecutive integers
33    int t = 0,i,j;
34    for (i = 0; i < n; i++) {
35      for (j = 0; j < n; j++) {
36        hm[i*n+j] = t++;
37      }
38    }
39    int cssize = n * sizeof(int);
40    hcs = (int *) malloc(cssize);
41    find1elt(hm,hcs,n);
42    if (n < 10) for(i=0; i<n; i++) printf("%d\n",hcs[i]);
43    // clean up
44    free(hm);
45    free(hcs);
46  }
```

How fast does this non-CUDA version run?

```
1  pc5:~/CUDA% time csc 20000
2  61.110u 1.719s 1:02.86 99.9%    0+0k 0+0io 0pf+0w
```

Very impressive! No wonder people talk of CUDA in terms like "a supercomputer on our desktop." And remember, this includes the time to copy the matrix from the host to the device (and to copy the output array back). And we didn't even try to optimize thread configuration, memory coalescing and bank usage, making good use of memory hierarchy, etc.[3]

On the other hand, remember that this is an "embarrassingly parallel" application, and in many applications we may have to settle for a much more modest increase, and work harder to get it.

5.8 Example: Finding the Mean Number of Mutual Outlinks

As in Sections **??** and 4.12, consider a network graph of some kind, such as Web links. For any two vertices, say any two Web sites, we might be interested in mutual outlinks, i.e. outbound links that are common to two Web sites. The CUDA code below finds the mean number of mutual outlinks, among all pairs of sites in a set of Web sites.

```
1   #include <cuda.h>
2   #include <stdio.h>
3
4   // CUDA example: finds mean number of mutual outlinks, among all pairs
5   // of Web sites in our set; in checking all (i,j) pairs, thread k will
6   // handle all i such that i mod totth = k, where totth is the number of
7   // threads
8
9   // procpairs() processes all pairs for a given thread
10  __global__ void procpairs(int *m, int *tot, int n)
11  { int totth = gridDim.x * blockDim.x, // total number of threads
12        me = blockIdx.x * blockDim.x + threadIdx.x; // my thread number
13     int i,j,k,sum = 0;
14     for (i = me; i < n; i += totth) { // do various rows i
15        for (j = i+1; j < n; j++) { // do all rows j > i
16           for (k = 0; k < n; k++)
```

---

[3]Neither has the CPU-only version of the program been optimized. As pointed out by Bill Hsu, the row-major version of that program should run faster than the column-major one, due to cache consideration.

```
17         sum += m[n*i+k] * m[n*j+k];
18       }
19     }
20     atomicAdd(tot,sum);
21 }
22
23 int main(int argc, char **argv)
24 { int n = atoi(argv[1]), // number of vertices
25       nblk = atoi(argv[2]); // number of blocks
26    int *hm, // host matrix
27       *dm, // device matrix
28       htot, // host grand total
29       *dtot; // device grand total
30    int msize = n * n * sizeof(int); // size of matrix in bytes
31    // allocate space for host matrix
32    hm = (int *) malloc(msize);
33    // as a test, fill matrix with random 1s and 0s
34    int i,j;
35    for (i = 0; i < n; i++) {
36      hm[n*i+i] = 0;
37      for (j = 0; j < n; j++) {
38         if (j != i) hm[i*n+j] = rand() % 2;
39      }
40    }
41    // allocate space for device matrix
42    cudaMalloc((void **)&dm,msize);
43    // copy host matrix to device matrix
44    cudaMemcpy(dm,hm,msize,cudaMemcpyHostToDevice);
45    htot = 0;
46    // set up device total and initialize it
47    cudaMalloc((void **)&dtot,sizeof(int));
48    cudaMemcpy(dtot,&htot,sizeof(int),cudaMemcpyHostToDevice);
49    // set up parameters for threads structure
```

```
50     dim3 dimGrid(nblk,1);
51     dim3 dimBlock(192,1,1);
52     // invoke the kernel
53     procpairs<<<dimGrid,dimBlock>>>(dm,dtot,n);
54     // wait for kernel to finish
55     cudaThreadSynchronize();
56     // copy total from device to host
57     cudaMemcpy(&htot,dtot,sizeof(int),cudaMemcpyDeviceToHost);
58     // check results
59     if (n <= 15) {
60        for (i = 0; i < n; i++) {
61           for (j = 0; j < n; j++)
62              printf("%d ",hm[n*i+j]);
63           printf("\n");
64        }
65     }
66     printf("mean = %f\n",htot/float((n*(n-1))/2));
67     // clean up
68     free(hm);
69     cudaFree(dm);
70     cudaFree(dtot);
71  }
```

Again we've used the method in Section **??** to partition the various pairs (i,j) to the different threads. Note the use of **atomicAdd()**.

The above code is hardly optimal. The reader is encouraged to find improvements.

5.9   Example: Finding Prime Numbers

The code below finds all the prime numbers from 2 to **n**.

```
1  #include <stdio.h>
2  #include <stdlib.h>
3  #include <cuda.h>
4
```

```
5  // CUDA example: illustration of shared memory allocation at run time;
6  // finds primes using classical Sieve of Erathosthenes: make list of
7  // numbers 2 to n, then cross out all multiples of 2 (but not 2 itself),
8  // then all multiples of 3, etc.; whatever is left over is prime; in our
9  // array, 1 will mean "not crossed out" and 0 will mean "crossed out"
10
11 // IMPORTANT NOTE: uses shared memory, in a single block, without
12 // rotating parts of array in and out of shared memory; thus limited to
13 // n <= 4000 if have 16K shared memory
14
15 // initialize sprimes, 1s for the odds, 0s for the evens; see sieve()
16 // for the nature of the arguments
17 __device__ void initsp(int *sprimes, int n, int nth, int me)
18 {
19    int chunk,startsetsp,endsetsp,val,i;
20    sprimes[2] = 1;
21    // determine sprimes chunk for this thread to init
22    chunk = (n-1) / nth;
23    startsetsp = 2 + me*chunk;
24    if (me < nth-1) endsetsp = startsetsp + chunk - 1;
25    else endsetsp = n;
26    // now do the init
27    val = startsetsp % 2;
28    for (i = startsetsp; i <= endsetsp; i++) {
29       sprimes[i] = val;
30       val = 1 - val;
31    }
32    // make sure sprimes up to date for all
33    __syncthreads();
34 }
35
36 // copy sprimes back to device global memory; see sieve() for the nature
37 // of the arguments
```

```
38  __device__ void cpytoglb(int *dprimes, int *sprimes, int n, int nth, int me)
39  {
40     int startcpy,endcpy,chunk,i;
41     chunk = (n-1) / nth;
42     startcpy = 2 + me*chunk;
43     if (me < nth-1) endcpy = startcpy + chunk - 1;
44     else endcpy = n;
45     for (i = startcpy; i <= endcpy; i++) dprimes[i] = sprimes[i];
46     __syncthreads();
47  }
48
49  // finds primes from 2 to n, storing the information in dprimes, with
50  // dprimes[i] being 1 if i is prime, 0 if composite; nth is the number
51  // of threads (threadDim somehow not recognized)
52  __global__ void sieve(int *dprimes, int n, int nth)
53  {
54     extern __shared__ int sprimes[];
55     int me = threadIdx.x;
56     int nth1 = nth - 1;
57     // initialize sprimes array, 1s for odds, 0 for evens
58     initsp(sprimes,n,nth,me);
59     // "cross out" multiples of various numbers m, with each thread doing
60     // a chunk of m's; always check first to determine whether m has
61     // already been found to be composite; finish when m*m > n
62     int maxmult,m,startmult,endmult,chunk,i;
63     for (m = 3; m*m <= n; m++) {
64        if (sprimes[m] != 0) {
65           // find largest multiple of m that is <= n
66           maxmult = n / m;
67           // now partition 2,3,...,maxmult among the threads
68           chunk = (maxmult - 1) / nth;
69           startmult = 2 + me*chunk;
70           if (me < nth1) endmult = startmult + chunk - 1;
```

```
71        else endmult = maxmult;
72      }
73      // OK, cross out my chunk
74      for (i = startmult; i <= endmult; i++) sprimes[i*m] = 0;
75    }
76    __syncthreads();
77    // copy back to device global memory for return to host
78    cpytoglb(dprimes,sprimes,n,nth,me);
79 }
80
81 int main(int argc, char **argv)
82 {
83    int n = atoi(argv[1]), // will find primes among 1,...,n
84        nth = atoi(argv[2]); // number of threads
85    int *hprimes, // host primes list
86        *dprimes; // device primes list
87    int psize = (n+1) * sizeof(int); // size of primes lists in bytes
88    // allocate space for host list
89    hprimes = (int *) malloc(psize);
90    // allocate space for device list
91    cudaMalloc((void **)&dprimes,psize);
92    dim3 dimGrid(1,1);
93    dim3 dimBlock(nth,1,1);
94    // invoke the kernel, including a request to allocate shared memory
95    sieve<<<dimGrid,dimBlock,psize>>>(dprimes,n,nth);
96    // check whether we asked for too much shared memory
97    cudaError_t err = cudaGetLastError();
98    if(err != cudaSuccess) printf("%s\n",cudaGetErrorString(err));
99    // wait for kernel to finish
100   cudaThreadSynchronize();
101   // copy list from device to host
102   cudaMemcpy(hprimes,dprimes,psize,cudaMemcpyDeviceToHost);
103   // check results
```

```
104      if (n <= 1000) for(int i=2; i<=n; i++)
105         if (hprimes[i] == 1) printf("%d\n",i);
106      // clean up
107      free(hprimes);
108      cudaFree(dprimes);
109   }
```

This code has been designed with some thought as to memory speed and thread divergence. Ideally, we would like to use device shared memory if possible, and to exploit the lockstep, SIMD nature of the hardware.

The code uses the classical Sieve of Erathosthenes, "crossing out" multiples of 2, 3, 5, 7 and so on to get rid of all the composite numbers. However, the code here differs from that in Section 1.3.2, even though both programs use the Sieve of Erathosthenes.

Say we have just two threads, A and B. In the earlier version, thread A might cross out all multiples of 19 while B handles multiples of 23. In this new version, thread A deals with only some multiples of 19 and B handles the others for 19. Then they both handle their own portions of multiples of 23, and so on. The thinking here is that the second version will be more amenable to lockstep execution, thus causing less thread divergence.

Thus in this new version, each thread handles a chunk of multiples of the given prime. Note the contrast of this with many CUDA examples, in which each thread does only a small amount of work, such as computing a single element in the product of two matrices.

In order to enhance memory performance, this code uses device shared memory. All the "crossing out" is done in the shared memory array **sprimes**, and then when we are all done, that is copied to the device global memory array **dprimes**, which is in turn copies to host memory. By the way, note that the amount of shared memory here is determined dynamically.

However, device shared memory consists only of 16K bytes, which would limit us here to values of **n** up to about 4000. Moreover, by using just one block, we are only using a small part of the CPU. Extending the program to work for larger values of **n** would require some careful planning if we still wish to use shared memory.

5.10   Example: Finding Cumulative Sums

Here we wish to compute cumulative sums. For instance, if the original array is (3,1,2,0,3,0,1,2), then it is changed to (3,4,6,6,9,9,10,12).

(Note: This is a special case of the *prefix scan* problem, covered in Chapter **??**.)

The general plan is for each thread to operate on one chunk of the array. A thread will find cumulative sums for its chunk, and then adjust them based on the high values of the chunks that precede it. In the above example, for instance, say we have 4 threads. The threads will first produce (3,4), (2,2), (3,3) and (1,3). Since thread 0 found a cumulative sum of 4 in the end, we must add 4 to each element of (2,2), yielding (6,6). Thread 1 had found a cumulative sum of 2 in the end, which together with the 4 found by thread 0 makes 6. Thus thread 2 must add 6 to each of its elements, i.e. add 6 to (3,3), yielding (9,9). The case of thread 3 is similar.

Below is code for the special case of a single block:

```
// for this simple illustration, it is assumed that the code runs in
// just one block, and that the number of threads evenly divides n

// improvements that could be made:
// 1. change to multiple blocks, to try to use all SMs
// 2. possibly use shared memory
// 3. have each thread work on staggered elements of dx, rather than
// on contiguous ones, to get more efficient bank access

#include <cuda.h>
#include <stdio.h>

__global__ void cumulker(int *dx, int n)
{
   int me = threadIdx.x;
   int csize = n / blockDim.x;
   int start = me * csize;
   int i,j,base;
   for (i = 1; i < csize; i++) {
      j = start + i;
      dx[j] = dx[j-1] + dx[j];
   }
   __syncthreads();
   if (me > 0) {
```

```
25      base = 0;
26      for (j = 0; j < me; j++)
27        base += dx[(j+1)*csize-1];
28    }
29    __syncthreads();
30    if (me > 0) {
31      for (i = start; i < start + csize; i++)
32        dx[i] += base;
33    }
34  }
```

5.11   When Is it Advantageous to Use Shared Memory

Shared memory only helps if we are doing multiple accesses to the data. If for instance our code does a single read and a single write to an element of an array, then transferring it back and forth between global and shared memory isn't worthwhile.

Would the cumulative-sums program in Section 5.10 benefit from the use of shared memory? (Put aside the fact that the code runs in just one block, making use of just a sliver of the machine.) The answer appears to be that a modest imrprovement might be obtained. Each thread (except the first) reads many elements of **dx** twice, some of them three times. There are also writes.

The case of the prime-finder program in Section 5.9 is less clear, and probably quite dependent on whether we are using the more advanced GPUs, which feature at least some L1 cache space.

5.12   Example: Transforming an Adjacency Matrix

Here is a CUDA version of the code in Section 4.13.

```
1  // CUDA example
2
3  // takes a graph adjacency matrix for a directed graph, and converts it
4  // to a 2-column matrix of pairs (i,j), meaning an edge from vertex i to
5  // vertex j; the output matrix must be in lexicographical order
6
7  // not claimed efficient, either in speed or in memory usage
```

```
 8
 9  #include <cuda.h>
10  #include <stdio.h>
11
12  // needs -lrt link flag for C++
13  #include <time.h>
14  float timediff(struct timespec t1, struct timespec t2)
15  { if (t1.tv_nsec > t2.tv_nsec) {
16          t2.tv_sec -= 1;
17          t2.tv_nsec += 1000000000;
18      }
19      return t2.tv_sec-t1.tv_sec + 0.000000001 * (t2.tv_nsec-t1.tv_nsec);
20  }
21
22
23  // kernel transgraph() does this work
24  // arguments:
25  // adjm: the adjacency matrix (NOT assumed symmetric), 1 for edge, 0
26  // otherwise; note: matrix is overwritten by the function
27  // n: number of rows and columns of adjm
28  // adjmout: output matrix
29  // nout: number of rows in adjmout
30
31  __global__ void tgkernel1(int *dadjm, int n, int *dcounts)
32  { int tot1s,j;
33      int me = blockDim.x * blockIdx.x + threadIdx.x;
34      tot1s = 0;
35      for (j = 0; j < n; j++) {
36          if (dadjm[n*me+j] == 1) {
37              dadjm[n*me+tot1s++] = j;
38          }
39      dcounts[me] = tot1s;
40      }
```

```
41  }
42
43  __global__ void tgkernel2(int *dadjm, int n,
44     int *dcounts, int *dstarts, int *doutm)
45  { int outrow,num1si,j;
46     // int me = threadIdx.x;
47     int me = blockDim.x * blockIdx.x + threadIdx.x;
48     // fill in this thread's portion of doutm
49     outrow = dstarts[me];
50     num1si = dcounts[me];
51     if (num1si > 0) {
52       for (j = 0; j < num1si; j++) {
53         doutm[2*outrow+2*j] = me;
54         doutm[2*outrow+2*j+1] = dadjm[n*me+j];
55       }
56     }
57  }
58
59  // replaces counts by cumulative counts
60  void cumulcounts(int *c, int *s, int n)
61  { int i;
62     s[0] = 0;
63     for (i = 1; i < n; i++) {
64       s[i] = s[i-1] + c[i-1];
65     }
66  }
67
68  int *transgraph(int *hadjm, int n, int *nout, int gsize, int bsize)
69  { int *dadjm; // device adjacency matrix
70     int *houtm; // host output matrix
71     int *doutm; // device output matrix
72     int *hcounts; // host counts vector
73     int *dcounts; // device counts vector
```

```
74    int *hstarts; // host starts vector
75    int *dstarts; // device starts vector
76    hcounts = (int *) malloc(n*sizeof(int));
77    hstarts = (int *) malloc(n*sizeof(int));
78    cudaMalloc((void **)&dadjm,n*n*sizeof(int));
79    cudaMalloc((void **)&dcounts,n*sizeof(int));
80    cudaMalloc((void **)&dstarts,n*sizeof(int));
81    houtm = (int *) malloc(n*n*sizeof(int));
82    cudaMalloc((void **)&doutm,n*n*sizeof(int));
83    cudaMemcpy(dadjm,hadjm,n*n*sizeof(int),cudaMemcpyHostToDevice);
84    dim3 dimGrid(gsize,1);
85    dim3 dimBlock(bsize,1,1);
86    // calculate counts and starts first
87    tgkernel1<<<dimGrid,dimBlock>>>(dadjm,n,dcounts);
88    // cudaMemcpy(hadjm,dadjm,n*n*sizeof(int),cudaMemcpyDeviceToHost);
89    cudaMemcpy(hcounts,dcounts,n*sizeof(int),cudaMemcpyDeviceToHost);
90    cumulcounts(hcounts,hstarts,n);
91    *nout = hstarts[n-1] + hcounts[n-1];
92    cudaMemcpy(dstarts,hstarts,n*sizeof(int),cudaMemcpyHostToDevice);
93    tgkernel2<<<dimGrid,dimBlock>>>(dadjm,n,dcounts,dstarts,doutm);
94    cudaMemcpy(houtm,doutm,2*(*nout)*sizeof(int),cudaMemcpyDeviceToHost);
95    free(hcounts);
96    free(hstarts);
97    cudaFree(dadjm);
98    cudaFree(dcounts);
99    cudaFree(dstarts);
100   return houtm;
101 }
102
103 int main(int argc, char **argv)
104 { int i,j;
105   int *adjm; // host adjacency matrix
106   int *outm; // host output matrix
```

```
107    int n = atoi(argv[1]);
108    int gsize = atoi(argv[2]);
109    int bsize = atoi(argv[3]);
110    int nout;
111    adjm = (int *) malloc(n*n*sizeof(int));
112    for (i = 0; i < n; i++)
113      for (j = 0; j < n; j++)
114        if (i == j) adjm[n*i+j] = 0;
115        else adjm[n*i+j] = rand() % 2;
116    if (n < 10) {
117      printf("adjacency matrix: \n");
118      for (i = 0; i < n; i++) {
119        for (j = 0; j < n; j++) printf("%d ",adjm[n*i+j]);
120        printf("\n");
121      }
122    }
123
124    struct timespec bgn,nd;
125    clock_gettime(CLOCK_REALTIME, &bgn);
126
127    outm = transgraph(adjm,n,&nout,gsize,bsize);
128    printf("num rows in out matrix = %d\n",nout);
129    if (nout < 50) {
130      printf("out matrix: \n");
131      for (i = 0; i < nout; i++)
132        printf("%d %d\n",outm[2*i],outm[2*i+1]);
133    }
134
135    clock_gettime(CLOCK_REALTIME, &nd);
136    printf("%f\n",timediff(bgn,nd));
137 }
```

5.13   Error Checking

Every CUDA call (except for kernel invocations) returns an error code of type **cudaError_t**. One can view the nature of the error by calling **cudaGetErrorString()** and printing its output.

For kernel invocations, one can call **cudaGetLastError()**, which does what its name implies. A call would typically have the form

```
1  cudaError_t err = cudaGetLastError();
2  if(err != cudaSuccess) printf("%s\n",cudaGetErrorString(err));
```

You may also wish to **cutilSafeCall()**, which is used by wrapping your regular CUDA call. It automatically prints out error messages as above.

Each CUBLAS call returns a potential error code, of type **cublasStatus**, not checked here.

5.14   Loop Unrolling

Loop unrolling is an old technique used on uniprocessor machines to achieve speedup due to branch elimination and the like. Branches make it difficult to do instruction or data prefetching, so eliminating them may speed things up.

The CUDA compiler provides the programmer with the **unroll** pragma to request loop unrolling. Here an n-iteration **for** loop is changed to k copies of the body of the loop, each working on about n/k iterations. If n and k are known constant, GPU registers can be used to implement the unrolled loop.

For example, the loop

```
1  for (i = 0; i < 2; i++ {
2      sum += x[i];
3      sum2 += x[i]*x[i];
4  }
```

could be unrolled to

```
1  sum += x[1];
2  sum2 += x[1]*x[1];
3  sum += x[2];
4  sum2 += x[2]*x[2];
```

Here n = k = 2. If **x** is local to this function, then unrolling will allow the compiler to store it in a register, which could be a great performance enhancer.

The compiler will try to do loop unrolling even if the programmer doesn't request it, but the programmer can try to control things by using the pragma:

```
1  #pragma unroll k
```

suggest to the compiler a k-fold unrolling. Setting k = 1 will instruct the compiler *not* to unroll.

5.15   Short Vectors

In CUDA, there are types such as **int4**, **char2** and so on, up to four elements each. So, an **uint4** type is a set of four unsigned **int**s. These are called **short vectors**.

The key point is that a short vector can be treated as a single word in terms of memory access and GPU instructions. It may be possible to reduce time by a factor of 4 by dividing arrays into chunks of four contiguous words and making short vectors from them.

5.16   The New Generation

The latest GPU architecture from NVIDIA is called Kepler. Many of the advances are of the "bigger and faster than before" type. These are important, but be sure to note the significant architectural changes, including:

- Host memory, device global memory and device shared memory share a unifed address space.
- On-chip memory can be apportioned to both shared memory and cache memory. Since shared memory is in essence a programmer-managed cache, this gives the programmer access to a real cache, a great convenience to the programmer though with a possible sacrifice in speed. Note by the way that this cache is aimed at spatial locality, not temporal locality.

5.17   CUDA from a Higher Level

CUDA programming can involve a lot of work, and one is never sure that one's code is fully efficient. Fortunately, a number of libraries of tight code have been developed for operations that arise often in parallel programming.

You are of course using CUDA code at the bottom, but without explicit kernel calls. And again, remember, the contents of device global memory are persistent across kernel calls in the same application. Therefore you can mix explicit CUDA code and calls to these libraries. Your program might have multiple kernel invocations, some CUDA and others to the libraries, with each using data in device global memory that was written by earlier kernels. In some cases, you may need to do a conversion to get the proper type.

These packages can be deceptively simple. **Remember, each call to a function in these packages involves a CUDA kernel call—with the associated overhead.**

Programming in these libraries is typically much more convenient than in direct CUDA. Note, though, that even though these libraries have been highly optimized for what they are intended to do, they will not generally give you the fastest possible code for any given CUDA application.

We'll discuss a few such libraries in this section.

5.17.1 CUBLAS

CUDA includes some parallel linear algebra routines callable from straight C code. In other words, you can get the benefit of GPU in linear algebra contexts without directly programming in CUDA.

Example: Row Sums Once Again

Below is an example **RowSumsCB.c**, the matrix row sums example again, this time using CUBLAS. We can find the vector of row sums of the matrix A by post-multiplying A by a column vector of all 1s.

I compiled the code by typing

```
gcc -g -I/usr/local/cuda/include -L/usr/local/cuda/lib RowSumsCB.c -lcublas -lcudart
```

You should modify for your own CUDA locations accordingly. Users who merely wish to use CUBLAS will find the above more convenient, but if you are mixing CUDA and CUBLAS, you would use **nvcc**:

```
nvcc -g -G RowSumsCB.c -lcublas
```

Here is the code:

```
#include <stdio.h>
#include <cublas.h> // required include

int main(int argc, char **argv)
{
   int n = atoi(argv[1]); // number of matrix rows/cols
   float *hm, // host matrix
         *hrs, // host rowsums vector
         *ones, // 1s vector for multiply
```

```
10        *dm, // device matrix
11        *drs; // device rowsums vector
12    // allocate space on host
13    hm = (float *) malloc(n*n*sizeof(float));
14    hrs = (float *) malloc(n*sizeof(float));
15    ones = (float *) malloc(n*sizeof(float));
16    // as a test, fill hm with consecutive integers, but in column-major
17    // order for CUBLAS; also put 1s in ones
18    int i,j;
19    float t = 0.0;
20    for (i = 0; i < n; i++) {
21        ones[i] = 1.0;
22        for (j = 0; j < n; j++)
23            hm[j*n+i] = t++;
24    }
25    cublasInit(); // required init
26    // set up space on the device
27    cublasAlloc(n*n,sizeof(float),(void**)&dm);
28    cublasAlloc(n,sizeof(float),(void**)&drs);
29    // copy data from host to device
30    cublasSetMatrix(n,n,sizeof(float),hm,n,dm,n);
31    cublasSetVector(n,sizeof(float),ones,1,drs,1);
32    // matrix times vector ("mv")
33    cublasSgemv('n',n,n,1.0,dm,n,drs,1,0.0,drs,1);
34    // copy result back to host
35    cublasGetVector(n,sizeof(float),drs,1,hrs,1);
36    // check results
37    if (n < 20) for (i = 0; i < n; i++) printf("%f\n",hrs[i]);
38    // clean up on device (should call free() on host too)
39    cublasFree(dm);
40    cublasFree(drs);
41    cublasShutdown();
42 }
```

As noted in the comments, CUBLAS assumes FORTRAN-style, i.e. column-major order, for matrices.

Now that you know the basic format of CUDA calls, the CUBLAS versions will look similar. In the call

```
1  cublasAlloc(n*n,sizeof(float),(void**)&dm);
```

for instance, we are allocating space on the device for an n x n matrix of **float**s.

The call

```
1  cublasSetMatrix(n,n,sizeof(float),hm,n,dm,n);
```

is slightly more complicated. Here we are saying that we are copying **hm**, an n x n matrix of **float**s on the host, to **dm** on the host. The **n** arguments in the last and third-to-last positions again say that the two matrices each have **n** dimensioned rows. This seems redundant, but this is needed in cases of matrix tiling, where the number of rows of a tile would be less than the number of rows of the matrix as a whole.

The 1s in the call

```
1  cublasSetVector(n,sizeof(float),ones,1,drs,1);
```

are needed for similar reasons. We are saying that in our source vector **ones**, for example, the elements of interest are spaced 1 elements apart, i.e. they are contiguous. But if we wanted our vector to be some row in a matrix with, say, 500 rows, the elements of any particular row of interest would be spaced 500 elements apart, again keeping in mind that column-major order is assumed.

The actual matrix multiplication is done here:

```
1  cublasSgemv('n',n,n,1.0,dm,n,drs,1,0.0,drs,1);
```

The "mv" in "cublasSgemv" stands for "matrix times vector." Here the call says: no ('n'), we do not want the matrix to be transposed; the matrix has **n** rows and **n** columns; we wish the matrix to be multiplied by 1.0 (if 0, the multiplication is not actually performed, which we could have here); the matrix is at **dm**; the number of dimensioned rows of the matrix is **n**; the vector is at **drs**; the elements of the vector are spaced 1 word apart; we wish the vector to not be multiplied by a scalar (see note above); the resulting vector will be stored at **drs**, 1 word apart.

Further information is available in the CUBLAS manual.

5.17.2　Thrust

The Thrust library is usable not only with CUDA but also to general OpenMP code! So I've put my coverage of Thrust in a separate chapter, Chapter 6.

5.17.3   CUDPP

CUDPP is similar to Thrust (though CUDPP was developed earlier) in terms of operations offered. It is perhaps less flexible than Thrust, but is easier to learn and is said to be faster.

(No examples yet, as the author did not have access to a CUDPP system yet.)

5.17.4   CUFFT

CUFFT does for the Fast Fourier Transform what CUBLAS does for linear algebra, i.e. it provides CUDA-optimized FFT routines.

5.18   Other CUDA Examples in This Book

There are additional CUDA examples in later sections of this book. These include:[4]

- Prof. Richard Edgar's matrix-multiply code, optimized for use of shared memory, Section 11.3.2.
- Odd/even transposition sort, Section 12.3.3, showing a typical CUDA pattern for iterative algorithms.
- Gaussian elimination for linear systems, Section 11.5.1.

---

[4]If you are reading this presentation on CUDA separately from the book, the book is at `http://heather.cs.ucdavis.edu/~matloff/158/PLN/ParProcBook.pdf`

第 6 章   Introduction to Thrust Programming

In the spirit of CUBLAS (Section 5.17.1) and other packages, the CUDA people have brought in another package to ease CUDA programming, Thrust. It uses the C++ STL library as a model, and Thrust is indeed a C++ template library. It includes various data manipulation routines, such as for sorting and prefix scan operations.

6.1   Compiling Thrust Code

Thrust allows the programmer a choice of *back ends*, i.e. platforms on which the executable code will run. In addition to the CUDA back end, for running on the GPU, one can also choose OpenMP as the back end. The latter choice allows the high-level expressive power of Thrust to be used on multicore machines. A third choice is Intel's TBB language.

6.1.1   Compiling to CUDA

If your CUDA version is at least 4.0, then Thrust is included, which will be assumed here. In that case, you compile Thrust code with **nvcc**, no special link commands needed.

6.1.2   Compiling to OpenMP

You can use Thrust to generate OpenMP code. The Thrust "include" files work without having a GPU. Here for instance is how you would compile the first example program below:[1]

```
1   g++ -g -O2 -o unqcount unqcount.cpp -fopenmp -lgomp \
```

---

[1]Note that we used a **.cpp** suffix for the source file name, instead of **.cu**. Or, we can use the **-x cu** if compiling with **nvcc**.

```
2      -DTHRUST_DEVICE_BACKEND=THRUST_DEVICE_BACKEND_OMP \
3      -I/usr/home/matloff/Tmp/tmp1
```

I had no CUDA-capable GPU on this machine, but put the Thrust include directory tree in **/usr/home/matloff/Tmp/tmp1**, and then compiled as with any other include file.

The result is real OpenMP code.[2] Everywhere you set up a Thrust vector, you'll be using OpenMP, i.e. the threads set up by Thrust will be OpenMP threads on the CPU rather than CUDA threads on the GPU.[3] You set the number of threads as you do with any OpenMP program, e.g. with the environment variable OMP_NUM_THREADS.

6.2 Example: Counting the Number of Unique Values in an Array

As our first example, suppose we wish to determine the number of distinct values in an integer array. The following code may not be too efficient, but as an introduction to Thrust fundamental building blocks, we'll take the following approach:

(a) sort the array

(b) compare the array to a shifted version of itself, so that changes from one distinct element to another can be detected, producing an array of 1s (change) and 0s (no change)

(c) count the number of 1s

Here's the code:

```
1   // various Thrust includes
2   #include <thrust/host_vector.h>
3   #include <thrust/device_vector.h>
4   #include <thrust/generate.h>
5   #include <thrust/sort.h>
6   #include <thrust/copy.h>
7   #include <thrust/count.h>
8   #include <cstdlib>
9
10  int rand16() // generate random integers mod 16
```

---

[2]If you search through the Thrust source code, you'll fine **omp** pragmas.

[3]Threads will not be set up if you use host arraysvectors.

```
11    { return rand() % 16; }

12

13    // C++ functor, to be called from thrust::transform(); compares
14    // corresponding elements of the arrays x and y, yielding 0 when they
15    // match, 1 when they don't
16    struct finddiff
17    {
18       __device__ int operator()(const int& x, const int&y)
19       { return x == y?0:1; }
20    };

21

22    int main(void)
23    {
24       // generate test data, 1000 random numbers, on the host, int type
25       thrust::host_vector<int> hv(1000);
26       thrust::generate(hv.begin(), hv.end(), rand16);

27

28       // copy data to the device, creating a vector there
29       thrust::device_vector<int> dv = hv;

30

31       // sort data on the device
32       thrust::sort(dv.begin(), dv.end());

33

34       // create device vector to hold differences, with length 1 less than
35       // dv's length
36       thrust::device_vector<int> diffs(dv.size()-1);

37

38       // find the diffs; note that the syntax is finddiff(), not finddiff
39       thrust::transform(dv.begin(),dv.end()-1,
40          dv.begin()+1,diffs.begin(),finddiff());

41

42       // count the 1s, by removing 0s and checking new length
43       // (or could use thrust::count())
```

```
44      int ndiffs = thrust::reduce(diffs.begin(), diffs.end(), (int) 0,
45        thrust::plus<int>());
46      printf("# distinct: %d\n",ndiffs+1);
47
48      // we've achieved our goal, but let's do a little more
49      // transfer data back to host
50      thrust::copy(dv.begin(), dv.end(), hv.begin());
51
52      printf("the sorted array:\n");
53      for (int i = 0; i < 1000; i++) printf("%d\n",hv[i]);
54
55      return 0;
56  }
```

After generating some random data on a host array **hv**, we copy it to the device, creating a vector **dv** there. This code is certainly much simpler to write than slogging through calls to **cudaMalloc()** and **cudaMemcpy()**!

The heart of the code is the call to **thrust::transform()**, which is used to implement step (b) in our outline above. It performs a "map" operation as in functional programming, taking one or two arrays (the latter is the case here) as input, and outputting an array of the same size.

This example, as is typical in Thrust code, defines a **functor**. Well, what is a functor? This is a C++ mechanism to produce a callable function, largely similar in goal to using a pointer to a function. In the context above, we are turning a C++ struct into a callable function, and we can do so with classes too. Since structs and classes can have member variables, we can store needed data in them, and that is what distinguishes functors from function pointers.

The transform function does elementwise operation—it calls the functor on each corresponding pair of elements from the two input arguments (0th element with 0th element, 1st with 1st, etc.), placing the results in the output array. So we must thus design our functor to do the map operation. In this case, we want to compare successive elements of our array (after sorting it), so we must find a way to do this through some element-by-element operation. The solution is to do elementwise comparison of the array and its shifted version. The call is

```
1   thrust::transform(dv.begin(),dv.end()-1,
2        dv.begin()+1,diffs.begin(),finddiff());
```

Note the parentheses in "finddiff()." This is basically a constructor, creating an instance of a **finddiff** object and returning a pointer to it. By contrast, in the code

```
thrust::generate(hv.begin(), hv.end(), rand16);
```

rand16() is an ordinary function, not a functor, so we just write its name here, thus passing a pointer to the function.

In the code

```
__device__ int operator()(const int& x, const int&y)
{ return x == y?0:1; }
```

the C++ keyword **operator** says we are defining a function, which in this case has two **int** inputs and an **int** output. We stated earlier that functors are callable structs, and this is what gets called.

Thrust vectors have built-in member functions **begin()** and **end()**, that specify the start and the place 1 element past the end of the array. Note that we didn't actually create our shifted array in

```
thrust::transform(dv.begin(),dv.end()-1,
    dv.begin()+1,diffs.begin(),finddiff());
```

Instead, we specified "the array beginning 1 element past the start of **dv**."

The "places" returned by calling **begin()** and **end()** above are formally called **iterators**, and work in a manner similar to pointers. Note again that **end()** returns a pointer to the location just *after* the last element of the array. The pointers are of type **thrust::device_vector<int>::iterator** here, with similar expressions for cases other than **int** type.

The transform function, in this case the comparison operation, will be done in parallel, on the GPU or other backend, as was the sorting. All that's left is to count the 1s. We want to do that in parallel too, and Thrust provides another functional programming operation, reduction (as in OpenMP). We specify Thrust's built-in addition function (we could have defined our own if it were a more complex situation) as the operation, and 0 as the initial value:

```
int ndiffs = thrust::reduce(diffs.begin(), diffs.end(), (int) 0, thrust::plus<int
    >());
```

We also could have used Thrust's **thrust::count()** function for further convenience.

Below is a shorter version of our unique-values-counter program, using **thrust::unique()**. Note that that function only removes *consecutive* duplicates, so the preliminary sort is still needed.

```
1  // various Thrust includes
2  #include <thrust/host_vector.h>
3  #include <thrust/device_vector.h>
4  #include <thrust/generate.h>
5  #include <thrust/sort.h>
6  #include <thrust/copy.h>
7  #include <thrust/unique.h>
8  #include <cstdlib>
9
10 int rand16()
11 { return rand() % 16; }
12
13 int main(void)
14 {
15    thrust::host_vector<int> hv(1000);
16    thrust::generate(hv.begin(), hv.end(), rand16);
17    thrust::device_vector<int> dv = hv;
18    thrust::sort(dv.begin(), dv.end());
19    thrust::device_vector<int>::iterator newend =
20       thrust::unique(dv.begin(),dv.end());
21    printf("# distinct: %d\n",newend - dv.begin());
22    return 0;
23 }
```

Note the line

```
1  thrust::device_vector<int>::iterator newend =
2     thrust::unique(dv.begin(),dv.end());
```

The **unique()** function returns an iterator pointing to (one element past) the end of the result of applying the unique-ifying operation. We can then "subtract" iterator values to get our desired count:

```
1  printf("# distinct: %d\n",newend - dv.begin());
```

6.3　Example: A Plain-C Wrapper for Thrust sort()

We may wish to wrap utility Thrust code in a function callable from a purely C/C++ program. The code below does that for the Thrust sort function.

```
1  // definitely needed
2  extern "C" void tsort(int *x, int *nx);
3
4  #include <thrust/device_vector.h>
5  #include <thrust/sort.h>
6
7  // nx set up as pointer so can call from R
8  void tsort(int *x, int *nx)
9  { int n = *nx;
10    // set up device vector and copy x to it
11    thrust::device_vector<int> dx(x,x+n);
12    // sort, then copy back to x
13    thrust::sort(dx.begin(), dx.end());
14    thrust::copy(dx.begin(), dx.end(),x);
15  }
```

To compile in the CUDA case, run **nvcc -c** and then run **gcc** (or whatever) as usual, making sure to link with the CUDA library. For instance,

```
1  nvcc -c SortForC.cu
2  gcc Main.c S*o -L/usr/local/cuda/lib -lcudart
```

Here's an example:

```
1  // TestSort.cpp: interface to Thrust sort from non-CUDA callers
2
3  #include <stdio.h>
4
5  extern "C" void tsort(int *x, int *nx);
6
7  // test
```

```
8   int main()
9   { int x[5] = {12,13,5,8,88};
10    int n=5,*nx; nx = &n;
11    int i;
12    tsort(x,nx);
13    for (i = 0; i < 5; i++) printf("%d\n",x[i]);
14  }
```

Compile and run for the OpenMP case:

```
1   g++ -g -mcmodel=medium -fopenmp -lgomp \
2     -DTHRUST_DEVICE_BACKEND=THRUST_DEVICE_BACKEND_OMP \
3     -I/home/matloff/Thrust SortForC.cpp -o sort.o -c
4   g++ -g -mcmodel=medium TestSort.cpp sort.o -fopenmp -lgomp
5   % a.out
6   5
7   8
8   12
9   13
10  88
```

And for the CUDA case:

```
1   nvcc SortForC.cu -c -o sfc.o
2   gcc -g TestSort.c sfc.o -L/usr/local/cuda/lib -lcudart
3   % a.out
4   5
5   8
6   12
7   13
8   88
```

6.4　Example: Calculating Percentiles in an Array

One of the most useful types of Thrust operations is that provided by conditional functions. For instance, **copy_if()** acts as a filter, copying from an array only those elements that satisfy a predicate. In the example below, for instance, we can copy every third element of an array, or every eighth etc.

```
1  // illustration of copy_if()
2
3  // find every k-th element in given array, going from smallest to
4  // largest; k obtained from command line and fed into ismultk() functor
5
6  // these are the the ik/n * 100 percentiles, i = 1, 2, ...
7
8  #include <stdio.h>
9
10 #include <thrust/device_vector.h>
11 #include <thrust/sort.h>
12 #include <thrust/sequence.h>
13 #include <thrust/remove.h> // for copy_if() but not copy_if.h
14
15 // functor
16 struct ismultk {
17    const int increm; // k in above comments
18    // get k from call
19    ismultk(int _increm): increm(_increm) {}
20    __device__
21    bool operator()(const int i)
22    { return i != 0 && (i % increm) == 0;
23    }
24 };
25
26 // test
27 int main(int argc, char **argv)
28 { int x[15] = {6,12,5,13,3,5,4,5,8,88,1,11,9,22,168};
```

```
29    int n=15;
30    thrust::device_vector<int> dx(x,x+n);
31    thrust::sort(dx.begin(),dx.end());
32    thrust::device_vector<int> seq(n);
33    thrust::sequence(seq.begin(),seq.end(),0);
34    thrust::device_vector<int> out(n);
35    int incr = atoi(argv[1]); // k
36    // for each i in seq, call ismultk() on this i, and if get a true
37    // result, put dx[i] into out
38    thrust::device_vector<int>::iterator newend =
39       thrust::copy_if(dx.begin(),dx.end(),seq.begin(),out.begin(),
40          ismultk(incr));
41    thrust::copy(out.begin(), newend,
42       std::ostream_iterator<int>(std::cout, " "));
43    std::cout << "\n";
44 }
```

The **sequence()** function simply generates an array consisting of 0,1,2,...,n-1.

Our functor here is a little more advanced than the one we saw earlier. It now has an argument, which is **incr** in the case of our call,

```
1 thrust::copy_if(dx.begin(),dx.end(),seq,out,ismultk(incr));
```

That is then used to set a member variable in the struct:

```
1 const int increm; // k in above comments
2 ismultk(int _increm): increm(_increm) {}
```

This is in a sense the *second*, though nonexplicit, argument to our calls to **ismultk()**. For example, in our call,

```
1 thrust::copy_if(hx.begin(),hx.end(),seq,out,ismultk(incr));
```

the function designated by **operator** within the **ismultk** struct will be called individually on each element in **hx**, each one playing role of **i** in

```
1 bool operator()(const int i)
2 { return i != 0 && (i % increm) == 0;
```

```
3 }
```

Since this code references **increm**, the value **incr** in our call above is used as well. The variable **increm** acts as a "global" variable to all the actions of the operator.

6.5 Mixing Thrust and CUDA Code

In order to mix Thrust and CUDA code, Thrust has the function **thrust::raw_pointer_cast()** to convert from a Thrust device pointer type to a CUDA device pointer type, and has **thrust::device_ptr** to convert in the other direction.

In our example in Section 6.6, we convert from Thrust to an ordinary address on the device:

```
1 int *wd;
2 ...
3 wd = thrust::raw_pointer_cast(&w[0]);
4 ...
5 { if (i != 0 && (i % increm) == 0) wd[i] = 2 * wd[i];
```

In the other direction, say we start with a CUDA pointer, and want to use it in Thrust. We might have something like

```
1 int *dz;
2 ...
3 cudaMalloc(&dz,100*sizeof(int));
4 ...
5 thrust::device_ptr<int> tz(dz);
6 ...
7 int k = thrust::reduce(tz,tz+100, (int) 0, thrust::plus<int>());
```

6.6 Example: Doubling Every kth Element of an Array

Let's adapt the code from the last section in order to illustrate another technique.

Suppose instead of copying every kth element of an array (after this first one), we wish to merely double each such element. There are various ways we could do this, but here we'll use an approach that shows another way we can use functors.

```
1   // double every k-th element in given array; k obtained from command
2   // line
3
4   #include <stdio.h>
5
6   #include <thrust/device_vector.h>
7   #include <thrust/sequence.h>
8   #include <thrust/remove.h> // for copy_if()
9
10  // functor
11  struct ismultk
12  {
13     const int increm; // k in above comments
14     const thrust::device_vector<int>::iterator w; // "pointer" to our array
15     int *wd;
16     // get "pointer," k
17     ismultk(thrust::device_vector<int>::iterator _w, int _increm):
18        w(_w), increm(_increm) {
19           wd = thrust::raw_pointer_cast(&w[0]);
20        }
21     __device__
22     bool operator()(const int i) // bool is phony, but void doesn't work
23     { if (i != 0 && (i % increm) == 0) wd[i] = 2 * wd[i];
24     }
25  };
26
27  // test
28  int main(int argc, char **argv)
29  { // test case:
30     int x[15] = {6,12,5,13,3,5,4,5,8,88,1,11,9,22,168};
31     int n=15;
32     thrust::device_vector<int> dx(x,x+n);
33     thrust::device_vector<int> seq(n);
```

```
34     thrust::sequence(seq.begin(),seq.end(),0);
35     thrust::device_vector<int> out(n);
36     int incr = atoi(argv[1]); // k
37     // for each i in seq, call ismultk() on this i, and if get a true
38     // result, put 0 in dx[i]
39     thrust::copy_if(dx.begin(),dx.end(),seq.begin(),out.begin(),
40        ismultk(dx.begin(),incr));
41     // did it work?
42     thrust::copy(dx.begin(), dx.end(),
43        std::ostream_iterator<int>(std::cout, " "));
44     std::cout << "\n";
45  }
```

Our functor here is quite different from before.

First, one of the functor's arguments is an iterator, rather than a simple type like **int**. This is really just like passing an array pointer to an ordinary C function.

Second, we've converted that iterator to a simple device array

```
1  const thrust::device_vector<int>::iterator w; // "pointer" to our array
2  int *wd;
3  ...
4     wd = thrust::raw_pointer_cast(&w[0]);
```

Our call to **copy_if()** doesn't actually do any copying. We are exploiting the "if" in "copy if," not the "copy."

6.7 Scatter and Gather Operations

These basically act as permuters; see the comments in the following small examples.
scatter:

```
1  // illustration of thrust::scatter(); permutes an array according to a
2  // map array
3
4  #include <stdio.h>
5  #include <thrust/device_vector.h>
```

```
6   #include <thrust/scatter.h>

7

8   int main()
9   { int x[5] = {12,13,5,8,88};
10      int n=5;
11      thrust::device_vector<int> dx(x,x+n);
12      // allocate map vector
13      thrust::device_vector<int> dm(n);
14      // allocate vector for output of gather
15      thrust::device_vector<int> hdst(n);
16      // example map
17      int m[5] = {3,2,4,1,0};
18      thrust::copy(m,m+n,dm.begin());
19      thrust::scatter(dx.begin(),dx.end(),dm.begin(),ddst.begin());
20      // the original x[0] should now be at position 3, the original x[1]
21      // now at position 2, etc., i.e. 88,8,13,12;,5 check it:
22      thrust::copy(ddst.begin(), ddst.end(),
23         std::ostream_iterator<int>(std::cout, " "));
24      std::cout << "\n";
25   }
```

gather():

```
1   // illustrations of thrust::gather(); permutes an array according to a
2   // map array

3

4   #include <stdio.h>
5   #include <thrust/device_vector.h>
6   #include <thrust/gather.h>

7

8   int main()
9   { int x[5] = {12,13,5,8,88};
10      int n=5;
11      thrust::device_vector<int> dx(x,x+n);
12      // allocate map vector
```

```
13     thrust::device_vector<int> dm(n);
14     // allocate vector for output of gather
15     thrust::device_vector<int> ddst(n);
16     // example map
17     int m[5] = {3,2,4,1,0};
18     thrust::copy(m,m+n,dm.begin());
19     thrust::gather(dm.begin(),dm.end(),dx.begin(),ddst.begin());
20     // the original x[3] should now be at position 0, the original x[2]
21     // now at position 1, etc., i.e. 8,5,88,13,12; check it:
22     thrust::copy(ddst.begin(), ddst.end(),
23        std::ostream_iterator<int>(std::cout, " "));
24     std::cout << "\n";
25   }
```

6.7.1   Example: Matrix Transpose

Here's an example of **scatter()**, applying it to transpose a matrix:

```
1  // matrix transpose, using scatter()
2
3  // similar to (though less efficient than) code included in the examples
4  // in the Thrust package
5
6  // matrices assumed stored in one dimension, row-major order
7
8  #include <stdio.h>
9  #include <thrust/device_vector.h>
10 #include <thrust/scatter.h>
11 #include <thrust/sequence.h>
12
13 struct transidx {
14    const int nr; // number of rows in input
15    const int nc; // number of columns in input
16    // set nr, nc
```

```
17    __host__ __device__
18    transidx(int _nr, int _nc): nr(_nr), nc(_nc) {};
19    // element i in input should map to which element in output?
20    __host__ __device__
21    int operator()(const int i)
22    { int r = i / nc; int c = i % nc; // row r, col c in input
23      // that will be row c and col r in output, which has nr cols
24      return c * nr + r;
25    }
26 };
27
28 int main()
29 { int mat[6] = { // test data
30      5, 12, 13,
31      3, 4, 5};
32    int nrow=2,ncol=3,n=nrow*ncol;
33    thrust::device_vector<int> dmat(mat,mat+n);
34    // allocate map vector
35    thrust::device_vector<int> dmap(n);
36    // allocate vector for output of gather
37    thrust::device_vector<int> ddst(n);
38    // construct map; element r of input matrix goes to s of output
39    thrust::device_vector<int> seq(n);
40    thrust::sequence (seq.begin(),seq.end());
41    thrust::transform(seq.begin(),seq.end(),dmap.begin(),transidx(nrow,ncol));
42    thrust::scatter(dmat.begin(),dmat.end(),dmap.begin(),ddst.begin());
43    // ddst should now hold the transposed matrix, 5,3,12,4,13,5; check it:
44    thrust::copy(ddst.begin(), ddst.end(), std::ostream_iterator<int>(std::cout, "
          "));
45    std::cout << "\n";
46 }
```

The idea is to determine, for each index in the original matrix, the index for that element in the transposed matrix. Not much new here in terms of Thrust, just more complexity.

It should be mentioned that the performance of this algorithm with a GPU backend would likely be better if matrix tiling were used (Section 11.2).

6.8   Advanced ("Fancy") Iterators

Since each Thrust call invokes considerable overhead, Thrust offers some special iterators to reduce memory access time and memory space requirements. Here are a few:

- **Counting iterators:** These play the same role as `thrust::sequence()`, but without actually setting up an array, thus avoiding the memory issues.

- **Transform iterators:** If your code first calls **thrust:transform()** and then makes another Thrust call on the result, you can combine them, which the Thrust people call **fusion**.

- **Zip iterators:** These essentially "zip" together two arrays (picture two halves of a zipper lining up parallel to each other as you zip up a coat). This is often useful when one needs to retain information on the position of an element within its array.

- **Discard iterators:** Sometimes we call **transform()** but don't need its output. Discard iterators then act in a manner similar to **/dev/null**.

6.8.1   Example: Matrix Transpose Again

Let's re-do the example of Section 6.7.1, this time using fusion.

```
1  // matrices assumed stored in one dimension, row-major order
2
3  #include <stdio.h>
4  #include <thrust/device_vector.h>
5  #include <thrust/scatter.h>
6  #include <thrust/sequence.h>
7  #include <thrust/iterator/transform_iterator.h>
8
9  struct transidx : public thrust::unary_function<int,int>
10 {
11    const int nr; // number of rows in input
12    const int nc; // number of columns in input
13    // set nr, nc
```

```
14     __host__ __device__
15     transidx(int _nr, int _nc): nr(_nr), nc(_nc) {};
16     // element i in input should map to which element in output?
17     __host__ __device__
18     int operator()(int i)
19     { int r = i / nc; int c = i % nc; // row r, col c in input
20       // that will be row c and col r in output, which has nr cols
21       return c * nr + r;
22     }
23  };
24
25  int main()
26  { int mat[6] = {
27       5, 12, 13,
28       3, 4, 5};
29     int nrow=2,ncol=3,n=nrow*ncol;
30     thrust::device_vector<int> dmat(mat,mat+n);
31     // allocate map vector
32     thrust::device_vector<int> dmap(n);
33     // allocate vector for output of gather
34     thrust::device_vector<int> ddst(n);
35     // construct map; element r of input matrix goes to s of output
36     thrust::device_vector<int> seq(n);
37     thrust::sequence (seq.begin(),seq.end());
38     thrust::scatter(
39        dmat.begin(),dmat.end(),
40        thrust::make_transform_iterator(seq.begin(),transidx(nrow,ncol)),
41        ddst.begin());
42     thrust::copy(ddst.begin(), ddst.end(),
43        std::ostream_iterator<int>(std::cout, " "));
44     std::cout << "\n";
45  }
```

The key new code here is:

```
1   thrust::scatter(
2     dmat.begin(),dmat.end(),
3     thrust::make_transform_iterator(seq.begin(),transidx(nrow,ncol)),
4     ddst.begin());
```

Fusion requires a special type of iterator, whose type is horrendous to write. So, Thrust provides the **make_transform_iterator()** function, which we call to produce the special iterator needed, and then put the result directly into the second phase of our fusion, in this case into **scatter()**.

Essentially our use of **make_transform_iterator()** is telling Thrust, "Don't apply **transidx()** to **seq** yet. Instead, perform that operation as you go along, and feed each result of **transidx()** directly into **scatter()**." That word *direct* is the salient one here; it means we save n memory reads and n memory writes.[④] Moreover, we save the overhead of the kernel call, if our backend is CUDA.

Note that we also had to be a little bit more elaborate with data typing issues, writing the first line of our struct declaration as

```
1   struct transidx : public thrust::unary_function<int,int>
```

It won't work without this!

It would be nice to be able to use a counting iterator in the above code, but apparently the compiler encounters problems with determining where the end of the counting sequence is. There is similar code in the examples directory that comes with Thrust, and that one uses **gather()** instead of **scatter()**. Since the former specifies a beginning and an end for the map array, counting interators work fine.

6.9　A Timing Comparison

Let's look at matrix transpose one more time. First, we'll use the method, shown in earlier sections, of passing a device vector iterator to a functor. For variety, let's use Thrust's **for_each()** function. The following will be known as Code 1:

```
1   // matrix transpose, for_each version
2
3   #include <stdio.h>
4   #include <thrust/device_vector.h>
5
```

[④]We are still writing to temporary storage, but that will probably be in registers (since we don't create the entire map at once), thus fast to access.

```
6   // functor; holds iterators for the input and output matrices, and each
7   // invocation of the function copies from one element from the former to
8   // the latter
9   struct copyelt2xp
10  {
11     int nrow;
12     int ncol;
13     const thrust::device_vector<int>::iterator m; // input matrix
14     const thrust::device_vector<int>::iterator mxp; // output matrix
15     int *m1,*mxp1;
16     copyelt2xp(thrust::device_vector<int>::iterator _m,
17            thrust::device_vector<int>::iterator _mxp,
18            int _nr, int _nc):
19       m(_m), mxp(_mxp), nrow(_nr), ncol(_nc) {
20          m1 = thrust::raw_pointer_cast(&m[0]);
21          mxp1 = thrust::raw_pointer_cast(&mxp[0]);
22       }
23     __device__
24     void operator()(const int i)
25     // copies the i-th element of the input matrix to the output matrix
26     { // elt i in input is row r, col c there
27        int r = i / ncol; int c = i % ncol;
28        // that elt will be row c and col r in output, which has nrow
29        // cols, so copy as follows
30        mxp1[c*nrow+r] = m1[r*ncol+c];
31     }
32  };
33
34  // transpose nr x nc inmat to outmat
35  void transp(int *inmat, int *outmat, int nr, int nc)
36  {
37     thrust::device_vector<int> dmat(inmat,inmat+nr*nc);
38     // make space for the transpose
```

```
39     thrust::device_vector<int> dxp(nr*nc);
40     thrust::counting_iterator<int> seqb(0);
41     thrust::counting_iterator<int> seqe = seqb + nr*nc;
42     // for each i in seq, copy the matrix elt to its spot in the
43     // transpose
44     thrust::for_each(seqb,seqe,
45        copyelt2xp(dmat.begin(),dxp.begin(),nr,nc));
46     thrust::copy(dxp.begin(),dxp.end(),outmat);
47  }
48
49  int rand16() // generate random integers mod 16
50  { return rand() % 16; }
51
52  // test code: cmd line args are matrix size, then row, col of elt to be
53  // checked
54
55  int main(int argc, char **argv)
56  { int nr = atoi(argv[1]); int nc = nr;
57     int *mat = (int *) malloc(nr*nc*sizeof(int));
58     int *matxp = (int *) malloc(nr*nc*sizeof(int));
59     thrust::generate(mat,mat+nr*nc,rand16);
60     int checkrow = atoi(argv[2]);
61     int checkcol = atoi(argv[3]);
62     printf("%d\n",mat[checkrow*nc+checkcol]);
63     transp(mat,matxp,nr,nc);
64     printf("%d\n",matxp[checkcol*nc+checkrow]);
65  }
```

The **for_each()** function does what the name implies: It calls a function/functor for each element in a sequence, doing so in a parallel manner. Note that this also obviates our earlier need to use a discard iterator.

For comparison, we'll use the matrix transpose code that is included in Thrust's **examples/** file, to be referred to as Code 2:

```
1  // matrix transpose, from the Thrust package examples
```

```
 2
 3   #include <thrust/host_vector.h>
 4   #include <thrust/device_vector.h>
 5   #include <thrust/functional.h>
 6   #include <thrust/gather.h>
 7   #include <thrust/scan.h>
 8   #include <thrust/iterator/counting_iterator.h>
 9   #include <thrust/iterator/transform_iterator.h>
10   #include <iostream>
11   #include <iomanip>
12   #include <stdio.h>
13
14   // convert a linear index to a linear index in the transpose
15   struct transpose_index : public thrust::unary_function<size_t,size_t>
16   {
17     size_t m, n;
18
19     __host__ __device__
20     transpose_index(size_t _m, size_t _n) : m(_m), n(_n) {}
21
22     __host__ __device__
23     size_t operator()(size_t linear_index)
24     {
25         size_t i = linear_index / n;
26         size_t j = linear_index % n;
27
28         return m * j + i;
29     }
30   };
31
32   // convert a linear index to a row index
33   struct row_index : public thrust::unary_function<size_t,size_t>
34   {
```

```
35    size_t n;

36

37    __host__ __device__
38    row_index(size_t _n) : n(_n) {}

39

40    __host__ __device__
41    size_t operator()(size_t i)
42    {
43        return i / n;
44    }
45  };

46

47  // transpose an M-by-N array
48  template <typename T>
49  void transpose(size_t m, size_t n, thrust::device_vector<T>& src, thrust::
        device_vector<T>& dst)
50  {
51    thrust::counting_iterator<size_t> indices(0);

52

53    thrust::gather
54      (thrust::make_transform_iterator(indices, transpose_index(n, m)),
55       thrust::make_transform_iterator(indices, transpose_index(n, m)) + dst.size()
            ,
56      src.begin(),
57      dst.begin());
58  }

59

60  void transp(int *inmat, int *outmat, int nr, int nc)
61  {
62    thrust::device_vector<int> dmat(inmat,inmat+nr*nc);
63    // make space for the transpose
64    thrust::device_vector<int> dxp(nr*nc);
65    transpose(nr,nc,dmat,dxp);
```

```
66     thrust::copy(dxp.begin(),dxp.end(),outmat);
67  }
68
69  int rand16() // generate random integers mod 16
70  { return rand() % 16; }
71
72  // test code: cmd line args are matrix size, then row, col of elt to be
73  // checked
74  int main(int argc, char **argv)
75  { int nr = atoi(argv[1]); int nc = nr;
76     int *mat = (int *) malloc(nr*nc*sizeof(int));
77     int *matxp = (int *) malloc(nr*nc*sizeof(int));
78     thrust::generate(mat,mat+nr*nc,rand16);
79     int checkrow = atoi(argv[2]);
80     int checkcol = atoi(argv[3]);
81     printf("%d\n",mat[checkrow*nc+checkcol]);
82     transp(mat,matxp,nr,nc);
83     printf("%d\n",matxp[checkcol*nc+checkrow]);
84  }
```

This approach is more efficient than ours in Section 6.7.1, making use of **gather()** instead of **scatter()**. It also takes advantage of fusion etc.

Code 1 is a lot easier to program than Code 2, but is it efficient? It turns out, though, that—good news!–the simpler code, i.e. Code 1, is actually a little faster than Code 2 in the case of a CUDA backend, and a lot faster in the OpenMP case.

Here we ran on CUDA backends, on a 10000x10000 matrix:

device	Code 1	Code 2
GeForce 9800 GTX	3.67	3.75
Tesla C2050	3.43	3.50

What about OpenMP? Here are some timing runs on a multicore machine (many more cores than the 16 we tried), using an input matrix of size 6000x6000:

# threads	Code 1	Code 2
2	9.57	23.01
4	5.17	10.62
8	3.01	7.42
16	1.99	3.35

6.10   Example: Transforming an Adjacency Matrix

Here is a Thrust approach to the example of Sections 4.13 and 5.12. To review, here is the problem: Say we have a graph with adjacency matrix

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \tag{6.1}$$

with row and column numbering starting at 0, not 1. We'd like to transform this to a two-column matrix that displays the links, in this case

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 3 \\ 2 & 1 \\ 2 & 3 \\ 3 & 0 \\ 3 & 1 \\ 3 & 2 \end{pmatrix} \tag{6.2}$$

For instance, there is a 1 on the far right, second row of the above matrix, meaning that in the graph there is an edge from vertex 1 to vertex 3. This results in the row (1,3) in the transformed matrix seen above.

Here's Thrust code to do this:

```
1  // transgraph problem, using Thrust
2
3  #include <stdio.h>
4
```

```
5   #include <thrust/device_vector.h>

6   #include <thrust/transform.h>

7   #include <thrust/remove.h>

8   #include <thrust/iterator/discard_iterator.h>

9

10  // forms one row of the output matrix

11  struct makerow {

12      const thrust::device_vector<int>::iterator outmat;

13      int *om;

14      const int nc; // number of columns

15      makerow(thrust::device_vector<int>::iterator _outmat,int _nc) :

16          outmat(_outmat), nc(_nc) { om = thrust::raw_pointer_cast(&outmat[0]); }

17      __device__

18      // the j-th 1 is in position i of the orig matrix

19      bool operator()(const int i, const int j)

20      { om[2*j] = i / nc;

21          om[2*j+1] = i % nc;

22      }

23  };

24

25  int main(int argc, char **argv)

26  { int x[12] = {

27          0,1,1,0,

28          1,0,0,1,

29          1,1,0,0};

30      int nr=3,nc=4,nrc = nr*nc,i;

31      thrust::device_vector<int> dx(x,x+nrc);

32      thrust::device_vector<int> ones(x,x+nrc);

33      thrust::counting_iterator<int> seqb(0);

34      thrust::counting_iterator<int> seqe = seqb + nrc;

35      // get 1-D indices of the 1s

36      thrust::device_vector<int>::iterator newend =

37          thrust::copy_if(seqb,seqe,dx.begin(),ones.begin(),
```

```
38        thrust::identity<int>());
39     int n1s = newend - ones.begin();
40     thrust::device_vector<int> newmat(2*n1s);
41     thrust::device_vector<int> out(n1s);
42     thrust::counting_iterator<int> seq2b(0);
43     thrust::transform(ones.begin(),newend,seq2b,
44        thrust::make_discard_iterator(), makerow(newmat.begin(),nc));
45     thrust::copy(newmat.begin(), newmat.end(),
46        std::ostream_iterator<int>(std::cout, " "));
47     std::cout << "\n";
48  }
```

One new feature here is the use of counting iterators. First, we create two of them in the code

```
1  thrust::counting_iterator<int> seqb(0);
2  thrust::counting_iterator<int> seqe = seqb + nrc;
```

Here **seqb** (virtually) points to the 0 in 0,1,2,... Actually no array is set up, but references to **seqb** will act as if there is an array there. The counting iterator **seqb** starts at **nrc**, but its role here is simply to demarcate the end of the (virtual) array.

Now, how does the code work? The call to **copy_if()** has the goal of indentifying where in **dx** the 1s are located. This is accomplished by calling Thrust's **identity()** function, which just does f(x) = x, which is enough, as it will return either 1 or 0, the latter interpreted as True. In other words, the values between **seqb** and **seqe** will be copied whenever the corresponding values in **dx** are 1s. The copied values are then placed into our array **ones**, which will now tell us where in **dx** the 1s are. Each such value, recall, will correspond to one row of our output matrix. The construction of the latter action is done by calling **transform()**:

```
1  thrust::transform(ones.begin(),newend,seq2b,
2    thrust::make_discard_iterator(), makerow(newmat.begin(),nc));
```

The construction of the output matrix, **newmat**, is actually done as a side effect of calling **makerow()**. For this reason, we've set our third parameter to **thrust::make_discard_iterator()**. Since we never use the output from **transform()** itself, and it thus would be wasteful—of both memory space and memory bandwidth—to store that output in a real array. Hence we use a discard array instead.

Our algorithm consists of two stages—first finding the locations of the 1s, and then calculating the output matrix. Could we combine the two stages? Possibly, but there are difficulties to deal with.

The biggest problem is that we don't know the size of the output matrix in advance; counting the 1s separately gives us that information. Without that, we'd either have to make the output matrix too large initially and then shrink it, or continually expand it as we go through the computation. The latter would probably result in a major slowdown, as memory allocation takes time.

6.11   Prefix Scan

Thrust includes functions for prefix scan (see Chapter 10):

```
1  // illustration of parallel prefix sum
2
3  #include <stdio.h>
4
5  #include <thrust/device_vector.h>
6  #include <thrust/scan.h>
7
8  int main(int argc, char **argv)
9  { int x[7] = {6,12,5,13,3,5,4};
10    int n=7,i;
11    thrust::device_vector<int> hx(x,x+n);
12    // in-place scan; default operation is +
13    thrust::inclusive_scan(hx.begin(),hx.end(),hx.begin());
14    thrust::copy(hx.begin(), hx.end(),
15      std::ostream_iterator<int>(std::cout, " "));
16    std::cout << "\n";
17  }
```

6.12   More on Use of Thrust for a CUDA Backend

6.12.1   Synchronicity

Thrust calls are in fact CUDA kernel calls, and thus entail some latency. Other than the **transform()**-family functions, the calls are all synchronous.

6.13   Error Messages

A message like

```
1  terminate called after throwing an instance of 'std::bad_alloc'
2   what(): std::bad_alloc
```

may mean that Thrust wasn't able to allocate your large array on the GPU.

Also, beware of the following. Consider the code

```
1  thrust::device_vector<int> seq(n);
2  thrust::copy_if(hx.begin(),hx.end(),seq,out,ismultk(hx.begin(),incr));
```

We forgot the **.begin()** for **seq**! If **seq** had been a non-Thrust array, declared as

```
1  int seq[n];
```

it would have been fine, but not for a Thrust array.

Unfortunately, the compiler gives us a very long megillah as an error message, a highly uninformative one. Keep this in mind if you get a 30-line compiler error.

The same thing happens if we forget to state the proper "include" files.

6.14   Other Examples of Thrust Code in This Book

- An application of Thrust's prefix-scan functionality is presented in Section 10.5

第 7 章　Message Passing Systems

Message passing systems are probably the most common platforms for parallel processing today.

7.1　Overview

Traditionally, shared-memory hardware has been extremely expensive, with a typical system costing hundreds of thousands of dollars. Accordingly, the main users were for very large corporations or government agencies, with the machines being used for heavy-duty server applications, such as for large databases and World Wide Web sites. The conventional wisdom is that these applications require the efficiency that good shared-memory hardware can provide.

But the huge expense of shared-memory machines led to a quest for high-performance message-passing alternatives, first in hypercubes and then in networks of workstations (NOWs).

The situation changed radically around 2005, when "shared-memory hardware for the masses" became available in dual-core commodity PCs. Chips of higher core multiplicity are commercially available, with a decline of price being inevitable. Ordinary users will soon be able to afford shared-memory machines featuring dozens of processors.

Yet the message-passing paradigm continues to thrive. Many people believe it is more amenable to writing really fast code, and the the advent of **cloud computing** has given message-passing a big boost. In addition, many of the world's very fastest systems (see `www.top500.org` for the latest list) are in fact of the message-passing type.

In this chapter, we take a closer look at this approach to parallel processing.

7.2　A Historical Example: Hypercubes

A popular class of parallel machines in the 1980s and early 90s was that of **hypercubes**. Intel sold them, for example, as did a subsidiary of Oracle, nCube. A hypercube would consist of some number

of ordinary Intel processors, with each processor having some memory and serial I/O hardware for connection to its "neighbor" processors.

Hypercubes proved to be too expensive for the type of performance they could achieve, and the market was small anyway. Thus they are not common today, but they are still important, both for historical reasons (in the computer field, old techniques are often recycled decades later), and because the algorithms developed for them have become quite popular for use on general machines. In this section we will discuss architecture, algorithms and software for such machines.

7.2.1 Definitions

A **hypercube** of dimension d consists of $D = 2^d$ **processing elements** (PEs), i.e. processor-memory pairs, with fast serial I/O connections between neighboring PEs. We refer to such a cube as a **d-cube**.

The PEs in a d-cube will have numbers 0 through D-1. Let $(c_{d-1}, ..., c_0)$ be the base-2 representation of a PE's number. The PE has fast point-to-point links to d other PEs, which we will call its **neighbors**. Its i*th* neighbor has number $(c_{d-1}, ..., 1 - c_{i-1}, ..., c_0)$.[1]

For example, consider a hypercube having D = 16, i.e. d = 4. The PE numbered 1011, for instance, would have four neighbors, 0011, 1111, 1001 and 1010.
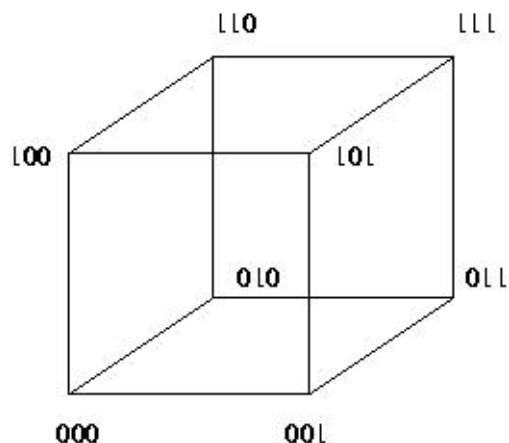
It is sometimes helpful to build up a cube from the lower-dimensional cases. To build a (d+1)-dimensional cube from two d-dimensional cubes, just follow this recipe:

(a) Take a d-dimensional cube and duplicate it. Call these two cubes subcube 0 and subcube 1.

---

[1] Note that we number the digits from right to left, with the rightmost digit being digit 0.

(b) For each pair of same-numbered PEs in the two subcubes, add a binary digit 0 to the front of the number for the PE in subcube 0, and add a 1 in the case of subcube 1. Add a link between them.

The following figure shows how a 4-cube can be constructed in this way from two 3-cubes:
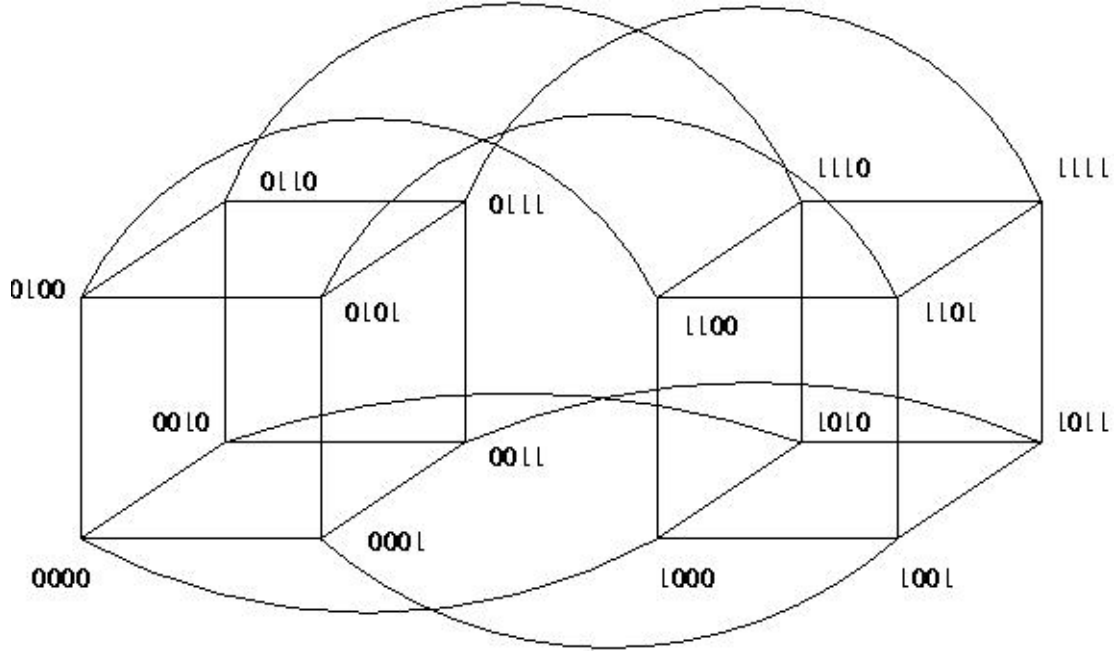
Given a PE of number $(c_{d-1}, ..., c_0)$ in a d-cube, we will discuss the i-cube to which this PE belongs, meaning all PEs whose first d-i digits match this PE's.[2] Of all these PEs, the one whose last i digits are all 0s is called the **root** of this i-cube.

For the 4-cube and PE 1011 mentioned above, for instance, the 2-cube to which that PE belongs consists of 1000, 1001, 1010 and 1011—i.e. all PEs whose first two digits are 10—and the root is 1000.

Given a PE, we can split the i-cube to which it belongs into two (i-1)-subcubes, one consisting of those PEs whose digit i-1 is 0 (to be called subcube 0), and the other consisting of those PEs whose digit i-1 is 1 (to be called subcube 1). Each given PE in subcube 0 has as its **partner** the PE in subcube 1 whose digits match those of the given PE, except for digit i-1.

To illustrate this, again consider the 4-cube and the PE 1011. As an example, let us look at how the 3-cube it belongs to will split into two 2-cubes. The 3-cube to which 1011 belongs consists of 1000, 1001, 1010, 1011, 1100, 1101, 1110 and 1111. This 3-cube can be split into two 2-cubes, one being 1000, 1001, 1010 and 1011, and the other being 1100, 1101, 1110 and 1111. Then PE 1000 is partners with PE 1100, PE 1001 is partners with PE 1101, and so on.

---

[2]Note that this is indeed an i-dimensional cube, because the last i digits are free to vary.

Each link between two PEs is a dedicated connection, much preferable to the shared link we have when we run, say, MPI, on a collection of workstations on an Ethernet. On the other hand, if one PE needs to communicate with a <u>non</u>-neighbor PE, multiple links (as many as d of them) will need to be traversed. Thus the nature of the communications costs here is much different than for a network of workstations, and this must be borne in mind when developing programs.

7.3   Networks of Workstations (NOWs)

The idea here is simple: Take a bunch of commodity PCs and network them for use as parallel processing systems. They are of course individual machines, capable of the usual uniprocessor, nonparallel applications, but by networking them together and using message-passing software environments such as MPI, we can form very powerful parallel systems.

The networking does result in a significant loss of performance, but the price/performance ratio in NOW can be much superior in many applications to that of shared-memory or hypercube hardware of comparable number of CPUs.

7.3.1   The Network Is Literally the Weakest Link

Still, one factor which can be key to the success of a NOW is to use a fast network, both in terms of hardware and network protocol. Ordinary Ethernet and TCP/IP are fine for the applications envisioned by the original designers of the Internet, e.g. e-mail and file transfer, but they are slow in the NOW context.

A popular network for a NOW today is Infiniband (IB) (`www.infinibandta.org`). It features low latency, about 1.0-3.0 microseconds, high bandwidth, about 1.0-2.0 gigaBytes per second), and uses a low amount of the CPU's cycles, around 5-10%.

The basic building block of IB is a switch, with many inputs and outputs, similar in concept to Ω-net. You can build arbitrarily large and complex topologies from these switches.

A central point is that IB, as with other high-performance networks designed for NOWs, uses RDMA (Remote Direct Memory Access) read/write, which eliminates the extra copying of data between the application program's address space to that of the operating system.

IB has high performance and scalable[3] implementations of distributed locks, semaphores, collective communication operations. An atomic operation takes about 3-5 microseconds.

---

[3]The term *scalable* arises frequently in conversations on parallel processing. It means that this particular method of dealing with some aspect of parallel processing continues to work well as the system size increases. We say that the method *scales*.

IB implements true **multicast**, i.e. the simultaneous sending of messages to many nodes. Note carefully that even though MPI has its **MPI_Bcast()** function, it will send things out one at a time unless your network hardware is capable of multicast, and the MPI implementation you use is configured specifically for that hardware.

For information on network protocols, e.g. for example `www.rdmaconsortium.org`. A research paper evaluating a tuned implementation of MPI on IB is available at `nowlab.cse.ohio-state.edu/publications/journal-papers/2004/liuj-ijpp04.pdf`.

7.3.2 Other Issues

Increasingly today, the workstations themselves are multiprocessor machines, so a NOW really is a hybrid arrangement. They can be programmed either purely in a message-passing manner—e.g. running eight MPI processes on four dual-core machines—or in a mixed way, with a shared-memory approach being used within a workstation but message-passing used between them.

NOWs have become so popular that there are now "recipes" on how to build them for the specific purpose of parallel processing. The term **Beowulf** come to mean a NOW, usually with a fast network connecting them, used for parallel processing. The term *NOW* itself is no longer in use, replaced by *cluster*. Software packages such as ROCKS (`http://www.rocksclusters.org/wordpress/`) have been developed to make it easy to set up and administer such systems.

7.4 Scatter/Gather Operations

Writing message-passing code is a lot of work, as the programmer must explicitly arrange for transfer of data. Contrast that, for instance, to shared-memory machines, in which cache coherency transactions will cause data transfers, but which are not arranged by the programmer and not even seen by him/her.

In order to make coding on message-passing machines easier, higher-level systems have been devised. These basically operate in the **scatter/gather** paradigm, in which a "manager" node sends out chunks of work to the other nodes, serving as "workers," and then collects and assembles the results sent back the workers.

MPI includes scatter/gather operations in its wide offering of functions, and they are used in many MPI applications. R's **snow** package, which will be discussed in Section 9.5, is based entirely on scatter/gather, as is MapReduce, to be discussed below.

第 8 章 Introduction to MPI

MPI is the *de facto* standard for message-passing software.

8.1 Overview

8.1.1 History

Though (small) shared-memory machines have come down radically in price, to the point at which a dual-core PC is now commonplace in the home, historically shared-memory machines were available only to the "very rich"—large banks, national research labs and so on. This led to interest in message-passing machines.

The first "affordable" message-machine type was the Hypercube, developed by a physics professor at Cal Tech. It consisted of a number of **processing elements** (PEs) connected by fast serial I/O cards. This was in the range of university departmental research labs. It was later commercialized by Intel and NCube.

Later, the notion of **networks of workstations** (NOWs) became popular. Here the PEs were entirely independent PCs, connected via a standard network. This was refined a bit, by the use of more suitable network hardware and protocols, with the new term being **clusters**.

All of this necessitated the development of standardized software tools based on a message-passing paradigm. The first popular such tool was Parallel Virtual Machine (PVM). It still has its adherents today, but has largely been supplanted by the Message Passing Interface (MPI).

MPI itself later became MPI 2. Our document here is intended mainly for the original.

8.1.2   Structure and Execution

MPI is merely a set of Application Programmer Interfaces (APIs), called from user programs written in C, C++ and other languages. It has many implementations, with some being open source and generic, while others are proprietary and fine-tuned for specific commercial hardware.

Suppose we have written an MPI program **x**, and will run it on four machines in a cluster. Each machine will be running its own copy of **x**. Official MPI terminology refers to this as four **processes**. Now that multicore machines are commonplace, one might indeed run two or more cooperating MPI processes—where now we use the term *processes* in the real OS sense—on the same multicore machine. In this document, we will tend to refer to the various MPI processes as **nodes**, with an eye to the cluster setting.

Though the nodes are all running the same program, they will likely be working on different parts of the program's data. This is called the Single Program Multiple Data (SPMD) model. This is the typical approach, but there could be different programs running on different nodes. Most of the APIs involve a node sending information to, or receiving information from, other nodes.

8.1.3   Implementations

Two of the most popular implementations of MPI are MPICH and LAM. MPICH offers more tailoring to various networks and other platforms, while LAM runs on networks. Introductions to MPICH and LAM can be found, for example, at `http://heather.cs.ucdavis.edu/~matloff/MPI/NotesMPICH.NM.html` and `http://heather.cs.ucdavis.edu/~matloff/MPI/NotesLAM.NM.html`, respectively.

LAM is no longer being developed, and has been replaced by Open MPI (not to be confused with OpenMP). Personally, I still prefer the simplicity of LAM. It is still being maintained.

Note carefully: If your machine has more than one MPI implementation, make absolutely sure one is not interfering with the other. Make sure all execution and library paths all include one and only one implementation at a time.

8.1.4   Performance Issues

Mere usage of a parallel language on a parallel platform does not guarantee a performance improvement over a serial version of your program. The central issue here is the overhead involved in internode communication.

Infiniband, one of the fastest cluster networks commercially available, has a **latency** of about

1.0-3.0 microseconds, meaning that it takes the first bit of a packet that long to get from one node on an Infiniband switch to another. Comparing that to the nanosecond time scale of CPU speeds, one can see that the communications overhead can destroy a program's performance. And Ethernet is quite a bit slower than Infiniband.

Latency is quite different from **bandwidth**, which is the number of bits sent per second. Say the latency is 1.0 microsecond and the bandwidth is 1 gigabit, i.e. 1000000000 bits per second or 1000 bits per microsecond. Say the message is 2000 bits long. Then the first bit of the message arrives after 1 microsecond, and the last bit arrives after an additional 2 microseconds. In other words, the message is does not arrive fully at the destination until 3 microseconds after it is sent.

In the same setting, say bandwidth is 10 gigabits. Now the message would need 1.2 seconds to arrive fully, in spite of a 10-fold increase in bandwidth. So latency is a major problem even if the bandwidth is high.

For this reason, the MPI applications that run well on networks tend to be of the "embarrassingly parallel" type, with very little communication between the processes.

Of course, if your platform is a shared-memory multiprocessor (especially a multicore one, where communication between cores is particularly fast) and you are running all your MPI processes on that machine, the problem is less severe. In fact, some implementations of MPI communicate directly through shared memory in that case, rather than using the TCP/IP or other network protocol.

8.2   Review of Earlier Example

Though the presentation in this chapter is self-contained, you may wish to look first at the somewhat simpler example in Section 1.3.3, a pipelined prime number finder.

8.3   Example: Dijkstra Algorithm

8.3.1   The Algorithm

The code implements the Dijkstra algorithm for finding the shortest paths in an undirected graph. Pseudocode for the algorithm is

```
1  Done = {0}
2  NonDone = {1,2,...,N-1}
3  for J = 1 to N-1 Dist[J] = infinity`
4  Dist[0] = 0
5  for Step = 1 to N-1
```

```
6        find J such that Dist[J] is min among all J in NonDone
7        transfer J from NonDone to Done
8        NewDone = J
9        for K = 1 to N-1
10          if K is in NonDone
11             Dist[K] = min(Dist[K],Dist[NewDone]+G[NewDone,K])
```

At each iteration, the algorithm finds the closest vertex J to 0 among all those not yet processed, and then updates the list of minimum distances to each vertex from 0 by considering paths that go through J. Two obvious potential candidate part of the algorithm for parallelization are the "find J" and "for K" lines, and the above OpenMP code takes this approach.

8.3.2 The MPI Code

```
1   // Dijkstra.c
2
3   // MPI example program:  Dijkstra shortest-path finder in a
4   // bidirectional graph; finds the shortest path from vertex 0 to all
5   // others
6
7   // command line arguments:  nv print dbg
8
9   // where:  nv is the size of the graph; print is 1 if graph and min
10  // distances are to be printed out, 0 otherwise; and dbg is 1 or 0, 1
11  // for debug
12
13  // node 0 will both participate in the computation and serve as a
14  // "manager"
15
16  #include <stdio.h>
17  #include <mpi.h>
18
19  #define MYMIN_MSG 0
20  #define OVRLMIN_MSG 1
21  #define COLLECT_MSG 2
22
23  // global variables (but of course not shared across nodes)
24
25  int nv,  // number of vertices
26      *notdone, // vertices not checked yet
27      nnodes,  // number of MPI nodes in the computation
28      chunk,  // number of vertices handled by each node
29      startv,endv,  // start, end vertices for this node
30      me,  // my node number
31      dbg;
```

```
32   unsigned largeint,  // max possible unsigned int
33           mymin[2],   // mymin[0] is min for my chunk,
34                       // mymin[1] is vertex which achieves that min
35           othermin[2],  // othermin[0] is min over the other chunks
36                         // (used by node 0 only)
37                         // othermin[1] is vertex which achieves that min
38           overallmin[2],  // overallmin[0] is current min over all nodes,
39                           // overallmin[1] is vertex which achieves that min
40           *ohd,  // 1-hop distances between vertices; "ohd[i][j]" is
41               // ohd[i*nv+j]
42           *mind;  // min distances found so far
43
44   double T1,T2;  // start and finish times
45
46   void init(int ac, char **av)
47   {  int i,j,tmp; unsigned u;
48      nv = atoi(av[1]);
49      dbg = atoi(av[3]);
50      MPI_Init(&ac,&av);
51      MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
52      MPI_Comm_rank(MPI_COMM_WORLD,&me);
53      chunk = nv/nnodes;
54      startv = me * chunk;
55      endv = startv + chunk - 1;
56      u = -1;
57      largeint = u >> 1;
58      ohd = malloc(nv*nv*sizeof(int));
59      mind = malloc(nv*sizeof(int));
60      notdone = malloc(nv*sizeof(int));
61      // random graph
62      // note that this will be generated at all nodes; could generate just
63      // at node 0 and then send to others, but faster this way
64      srand(9999);
65      for (i = 0; i < nv; i++)
66         for (j = i; j < nv; j++)  {
67            if (j == i) ohd[i*nv+i] = 0;
68            else  {
69               ohd[nv*i+j] = rand() % 20;
70               ohd[nv*j+i] = ohd[nv*i+j];
71            }
72         }
73      for (i = 0; i < nv; i++)  {
74         notdone[i] = 1;
75         mind[i] = largeint;
76      }
77      mind[0] = 0;
78      while (dbg) ;  // stalling so can attach debugger
```

```
79   }
80
81   // finds closest to 0 among notdone, among startv through endv
82   void findmymin()
83   {  int i;
84      mymin[0] = largeint;
85      for (i = startv; i <= endv; i++)
86         if (notdone[i] && mind[i] < mymin[0])  {
87            mymin[0] = mind[i];
88            mymin[1] = i;
89         }
90   }
91
92   void findoverallmin()
93   {  int i;
94      MPI_Status status;  // describes result of MPI_Recv() call
95      // nodes other than 0 report their mins to node 0, which receives
96      // them and updates its value for the global min
97      if (me > 0)
98         MPI_Send(mymin,2,MPI_INT,0,MYMIN_MSG,MPI_COMM_WORLD);
99      else  {
100        // check my own first
101        overallmin[0] = mymin[0];
102        overallmin[1] = mymin[1];
103        // check the others
104        for (i = 1; i < nnodes; i++)  {
105           MPI_Recv(othermin,2,MPI_INT,i,MYMIN_MSG,MPI_COMM_WORLD,&status);
106           if (othermin[0] < overallmin[0])  {
107              overallmin[0] = othermin[0];
108              overallmin[1] = othermin[1];
109           }
110        }
111     }
112  }
113
114  void updatemymind()  // update my mind segment
115  {  // for each i in [startv,endv], ask whether a shorter path to i
116     // exists, through mv
117     int i, mv = overallmin[1];
118     unsigned md = overallmin[0];
119     for (i = startv; i <= endv; i++)
120        if (md + ohd[mv*nv+i] < mind[i])
121           mind[i] = md + ohd[mv*nv+i];
122  }
123
124  void disseminateoverallmin()
125  {  int i;
```

```
126     MPI_Status status;
127     if (me == 0)
128        for (i = 1; i < nnodes; i++)
129           MPI_Send(overallmin,2,MPI_INT,i,OVRLMIN_MSG,MPI_COMM_WORLD);
130     else
131        MPI_Recv(overallmin,2,MPI_INT,0,OVRLMIN_MSG,MPI_COMM_WORLD,&status);
132  }
133
134  void updateallmind()  // collects all the mind segments at node 0
135  { int i;
136     MPI_Status status;
137     if (me > 0)
138        MPI_Send(mind+startv,chunk,MPI_INT,0,COLLECT_MSG,MPI_COMM_WORLD);
139     else
140        for (i = 1; i < nnodes; i++)
141           MPI_Recv(mind+i*chunk,chunk,MPI_INT,i,COLLECT_MSG,MPI_COMM_WORLD,
142              &status);
143  }
144
145  void printmind()  // partly for debugging (call from GDB)
146  { int i;
147     printf("minimum distances:\n");
148     for (i = 1; i < nv; i++)
149        printf("%u\n",mind[i]);
150  }
151
152  void dowork()
153  { int step,  // index for loop of nv steps
154          i;
155     if (me == 0) T1 = MPI_Wtime();
156     for (step = 0; step < nv; step++)  {
157        findmymin();
158        findoverallmin();
159        disseminateoverallmin();
160        // mark new vertex as done
161        notdone[overallmin[1]] = 0;
162        updatemymind(startv,endv);
163     }
164     updateallmind();
165     T2 = MPI_Wtime();
166  }
167
168  int main(int ac, char **av)
169  { int i,j,print;
170     init(ac,av);
171     dowork();
172     print = atoi(av[2]);
```

```
173      if (print && me == 0)  {
174         printf("graph weights:\n");
175         for (i = 0; i < nv; i++)  {
176            for (j = 0; j < nv; j++)
177               printf("%u  ",ohd[nv*i+j]);
178            printf("\n");
179         }
180         printmind();
181      }
182      if (me == 0) printf("time at node 0: %f\n",(float)(T2-T1));
183      MPI_Finalize();
184   }
185
```

The various MPI functions will be explained in the next section.

8.3.3   Introduction to MPI APIs

MPI_Init() and MPI_Finalize()

These are required for starting and ending execution of an MPI program. Their actions may be implementation-dependent. For instance, if our platform is an Ethernet-based cluster , **MPI_Init()** will probably set up the TCP/IP sockets via which the various nodes communicate with each other. On an Infiniband-based cluster, connections in the special Infiniband network protocol will be established. On a shared-memory multiprocessor, an implementation of MPI that is tailored to that platform would take very different actions.

MPI_Comm_size() and MPI_Comm_rank()

In our function **init()** above, note the calls

```
1   MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
2   MPI_Comm_rank(MPI_COMM_WORLD,&me);
```

The first call determines how many nodes are participating in our computation, placing the result in our variable **nnodes**. Here **MPI_COMM_WORLD** is our node group, termed a **communicator** in MPI parlance. MPI allows the programmer to subdivide the nodes into groups, to facilitate performance and clarity of code. Note that for some operations, such as barriers, the only way to apply the operation to a proper subset of all nodes is to form a group. The totality of all groups is denoted by **MPI_COMM_WORLD**. In our program here, we are not subdividing into groups.

The second call determines this node's ID number, called its **rank**, within its group. As mentioned earlier, even though the nodes are all running the same program, they are typically working on different parts of the program's data. So, the program needs to be able to sense which node it is running on, so as to access the appropriate data. Here we record that information in our variable **me**.

MPI_Send()

To see how MPI's basic send function works, consider our line above,

```
1  MPI_Send(mymin,2,MPI_INT,0,MYMIN_MSG,MPI_COMM_WORLD);
```

Let's look at the arguments:

mymin: We are sending a set of bytes. This argument states the address at which these bytes begin.

2, MPI_INT: This says that our set of bytes to be sent consists of 2 objects of type **MPI_INT**. That means 8 bytes on 32-bit machines, so why not just collapse these two arguments to one, namely the number 8? Why did the designers of MPI bother to define data types? The answer is that we want to be able to run MPI on a heterogeneous set of machines, with MPI serving as the "broker" between them in case different architectures among those machines handle data differently.

First of all, there is the issue of **endianness**. Intel machines, for instance, are **little-endian**, which means that the least significant byte of a memory word has the smallest address among bytes of the word. Sun SPARC chips, on the other hand, are **big-endian**, with the opposite storage scheme. If our set of nodes included machines of both types, straight transmission of sequences of 8 bytes might mean that some of the machines literally receive the data backwards! Secondly, these days 64-bit machines are becoming more and more common. Again, if our set of nodes were to include both 32-bit and 64-bit words, some major problems would occur if no conversion were done.

0: We are sending to node 0.

MYMIN_MSG: This is the message type, programmer-defined in our line

```
1  #define MYMIN_MSG 0
```

Receive calls, described in the next section, can ask to receive only messages of a certain type.

OMM_WORLD: This is the node group to which the message is to be sent. Above, where we said we are sending to node 0, we technically should say we are sending to node 0 within the group **MPI_COMM_WORLD**.

MPI_Recv()

Let's now look at the arguments for a basic receive:

```
1  MPI_Recv(othermin,2,MPI_INT,i,MYMIN_MSG,MPI_COMM_WORLD,&status);
```

othermin: The received message is to be placed at our location **othermin**.

2,MPI_INT: Two objects of **MPI_INT** type are to be received.

i: Receive only messages from node **i**. If we did not care what node we received a message from, we could specify the value **MPI_ANY_SOURCE**.

MYMIN_MSG: Receive only messages of type **MYMIN_MSG**. If we did not care what type of message we received, we would specify the value **MPI_ANY_TAG**.

OMM_WORLD: Group name.

status: Recall our line

```
1  MPI_Status status;  // describes result of MPI_Recv() call
```

The type is an MPI **struct** containing information about the received message. Its primary fields of interest are **MPI_SOURCE**, which contains the identity of the sending node, and **MPI_TAG**, which contains the message type. These would be useful if the receive had been done with **MPI_ANY_SOURCE** or **MPI_ANY_TAG**; the status argument would then tell us which node sent the message and what type the message was.

8.4 Example: Removing 0s from an Array

```
1   #include <mpi.h>
2   #include <stdlib.h>
3
4   #define MAX_N 100000
5   #define MAX_NPROCS 100
6   #define DATA_MSG 0
7   #define NEWDATA_MSG 1
8
9   int nnodes, // number of MPI processes
10      n, // size of original array
11      me, // my MPI ID
12      has0s[MAX_N], // original data
13      no0s[MAX_N], // 0-free data
14      nno0s; // number of non-0 elements
```

```
15
16  int debug;
17
18  init(int argc, char **argv)
19  {
20     int i;
21     MPI_Init(&argc,&argv);
22     MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
23     MPI_Comm_rank(MPI_COMM_WORLD,&me);
24     n = atoi(argv[1]);
25     if (me == 0) {
26        for (i = 0; i < n; i++)
27           has0s[i] = rand() % 4;
28     } else {
29        debug = atoi(argv[2]);
30        while (debug) ;
31     }
32  }
33
34  void managernode()
35  {
36     MPI_Status status;
37     int i;
38     int lenchunk;
39     lenchunk = n / (nnodes-1); // assumed divides evenly
40     for (i = 1; i < nnodes; i++) {
41        MPI_Send(has0s+(i-1)*lenchunk,lenchunk,
42           MPI_INT,i,DATA_MSG,MPI_COMM_WORLD);
43     }
44     int k = 0;
45     for (i = 1; i < nnodes; i++) {
46        MPI_Recv(no0s+k,MAX_N,
47           MPI_INT,i,NEWDATA_MSG,MPI_COMM_WORLD,&status);
```

```
48        MPI_Get_count(&status,MPI_INT,&lenchunk);
49        k += lenchunk;
50     }
51     nno0s = k;
52  }
53
54  void remov0s(int *oldx, int n, int *newx, int *nnewx)
55  { int i,count = 0;
56     for (i = 0; i < n; i++)
57        if (oldx[i] != 0) newx[count++] = oldx[i];
58     *nnewx = count;
59  }
60
61  void workernode()
62  {
63     int lenchunk;
64     MPI_Status status;
65     MPI_Recv(has0s,MAX_N,
66        MPI_INT,0,DATA_MSG,MPI_COMM_WORLD,&status);
67     MPI_Get_count(&status,MPI_INT,&lenchunk);
68     remov0s(has0s,lenchunk,no0s,&nno0s);
69     MPI_Send(no0s,nno0s,
70        MPI_INT,0,NEWDATA_MSG,MPI_COMM_WORLD);
71  }
72
73  int main(int argc,char **argv)
74  {
75     int i;
76     init(argc,argv);
77     if (me == 0 && n < 25) {
78        for (i = 0; i < n; i++) printf("%d ",has0s[i]);
79        printf("\n");
80     }
```

```
81    if (me == 0) managernode();
82    else workernode();
83    if (me == 0 && n < 25) {
84       for (i = 0; i < n; i++) printf("%d ",noOs[i]);
85       printf("\n");
86    }
87    MPI_Finalize();
88 }
```

8.5　Debugging MPI Code

If you are using GDB—either directly, or via an IDE such as Eclipse or Netbeans—the trick with MPI is to **attach** GDB to your running MPI processes.

Set up code like that we've seen in our examples here:

```
1 while (dbg) ;
```

This deliberately sets up an infinite loop of **dbg** is nonzero, for reasons to be discussed below.

For instance, suppose I'm running an MPI program **a.out**, on machines A, B and C. I would start the processes as usual, and have three terminal windows open. I'd log in to machine A, find the process number for **a.out**, using for example a command like **ps ax** on Unix-family systems, then attach GDB to that process. Say the process number is 88888. I'd attach by running the command

```
1 % gdb a.out 88888
```

That would start GDB, in the midst of my already-running process, thus stuck in the infinite loop seen above. I hit ctrl-c to interrupt it, which gives me the GDB prompt, (gdb). I then type

```
1 (gdb) set var dbg = 0
```

which means when I next hit the **c** command in GDB, the program will proceed, not stuck in the loop anymore. But first I set my breakpoints.

8.6　Collective Communications

MPI features a number of **collective communication** capabilities, a number of which are used in the following refinement of our Dijkstra program:

8.6.1   Example: Refined Dijkstra Code

```
1   // Dijkstra.coll1.c
2
3   // MPI example program:  Dijkstra shortest-path finder in a
4   // bidirectional graph; finds the shortest path from vertex 0 to all
5   // others; this version uses collective communication
6
7   // command line arguments:  nv print dbg
8
9   // where:  nv is the size of the graph; print is 1 if graph and min
10  // distances are to be printed out, 0 otherwise; and dbg is 1 or 0, 1
11  // for debug
12
13  // node 0 will both participate in the computation and serve as a
14  // "manager"
15
16  #include <stdio.h>
17  #include <mpi.h>
18
19  // global variables (but of course not shared across nodes)
20
21  int nv,  // number of vertices
22      *notdone, // vertices not checked yet
23      nnodes,  // number of MPI nodes in the computation
24      chunk,  // number of vertices handled by each node
25      startv,endv,  // start, end vertices for this node
26      me,  // my node number
27      dbg;
28  unsigned largeint,  // max possible unsigned int
29          mymin[2],  // mymin[0] is min for my chunk,
30                     // mymin[1] is vertex which achieves that min
31          overallmin[2],  // overallmin[0] is current min over all nodes,
32                     // overallmin[1] is vertex which achieves that min
33          *ohd,  // 1-hop distances between vertices; "ohd[i][j]" is
34              // ohd[i*nv+j]
35          *mind;  // min distances found so far
36
37  double T1,T2;  // start and finish times
38
39  void init(int ac, char **av)
40  {  int i,j,tmp; unsigned u;
41     nv = atoi(av[1]);
42     dbg = atoi(av[3]);
43     MPI_Init(&ac,&av);
44     MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
45     MPI_Comm_rank(MPI_COMM_WORLD,&me);
```

```
46       chunk = nv/nnodes;
47       startv = me * chunk;
48       endv = startv + chunk - 1;
49       u = -1;
50       largeint = u >> 1;
51       ohd = malloc(nv*nv*sizeof(int));
52       mind = malloc(nv*sizeof(int));
53       notdone = malloc(nv*sizeof(int));
54       // random graph
55       // note that this will be generated at all nodes; could generate just
56       // at node 0 and then send to others, but faster this way
57       srand(9999);
58       for (i = 0; i < nv; i++)
59          for (j = i; j < nv; j++)  {
60             if (j == i) ohd[i*nv+i] = 0;
61             else  {
62                ohd[nv*i+j] = rand() % 20;
63                ohd[nv*j+i] = ohd[nv*i+j];
64             }
65          }
66       for (i = 0; i < nv; i++)  {
67          notdone[i] = 1;
68          mind[i] = largeint;
69       }
70       mind[0] = 0;
71       while (dbg) ;  // stalling so can attach debugger
72    }
73
74    // finds closest to 0 among notdone, among startv through endv
75    void findmymin()
76    {  int i;
77       mymin[0] = largeint;
78       for (i = startv; i <= endv; i++)
79          if (notdone[i] && mind[i] < mymin[0])  {
80             mymin[0] = mind[i];
81             mymin[1] = i;
82          }
83    }
84
85    void updatemymind()  // update my mind segment
86    {  // for each i in [startv,endv], ask whether a shorter path to i
87       // exists, through mv
88       int i, mv = overallmin[1];
89       unsigned md = overallmin[0];
90       for (i = startv; i <= endv; i++)
91          if (md + ohd[mv*nv+i] < mind[i])
92             mind[i] = md + ohd[mv*nv+i];
```

```
 93  }
 94
 95  void printmind()  // partly for debugging (call from GDB)
 96  { int i;
 97     printf("minimum distances:\n");
 98     for (i = 1; i < nv; i++)
 99        printf("%u\n",mind[i]);
100  }
101
102  void dowork()
103  { int step,  // index for loop of nv steps
104          i;
105     if (me == 0) T1 = MPI_Wtime();
106     for (step = 0; step < nv; step++)  {
107        findmymin();
108        MPI_Reduce(mymin,overallmin,1,MPI_2INT,MPI_MINLOC,0,MPI_COMM_WORLD);
109        MPI_Bcast(overallmin,1,MPI_2INT,0,MPI_COMM_WORLD);
110        // mark new vertex as done
111        notdone[overallmin[1]] = 0;
112        updatemymind(startv,endv);
113     }
114     // now need to collect all the mind values from other nodes to node 0
115     MPI_Gather(mind+startv,chunk,MPI_INT,mind,chunk,MPI_INT,0,MPI_COMM_WORLD);
116     T2 = MPI_Wtime();
117  }
118
119  int main(int ac, char **av)
120  { int i,j,print;
121     init(ac,av);
122     dowork();
123     print = atoi(av[2]);
124     if (print && me == 0)  {
125        printf("graph weights:\n");
126        for (i = 0; i < nv; i++)  {
127           for (j = 0; j < nv; j++)
128              printf("%u  ",ohd[nv*i+j]);
129           printf("\n");
130        }
131        printmind();
132     }
133     if (me == 0) printf("time at node 0: %f\n",(float)(T2-T1));
134     MPI_Finalize();
135  }
```

The new calls will be explained in the next section.

8.6.2 MPI_Bcast()

In our original Dijkstra example, we had a loop

```
1  for (i = 1; i < nnodes; i++)
2      MPI_Send(overallmin,2,MPI_INT,i,OVRLMIN_MSG,MPI_COMM_WORLD);
```

in which node 0 sends to all other nodes. We can replace this by

```
1  MPI_Bcast(overallmin,2,MPI_INT,0,MPI_COMM_WORLD);
```

In English, this call would say,

> At this point all nodes participate in a broadcast operation, in which node 0 sends 2 objects of type **MPI_INT** to each node (including itself). The source of the data will be located at address **overallmin** at node 0, and the other nodes will receive the data at a location of that name.

Note my word "participate" above. The name of the function is "broadcast," which makes it sound like only node 0 executes this line of code, which is not the case; all the nodes in the group (in this case that means all nodes in our entire computation) execute this line. The only difference is the action; most nodes participate by receiving, while node 0 participates by sending.

Actually, this call to **MPI_Bcast()** is doing more than replacing the loop, since the latter had been part of an if-then-else that checked whether the given process had rank 0 or not.

Why might this be preferable to using an explicit loop? First, it would obviously be much clearer. That makes the program easier to write, easier to debug, and easier for others (and ourselves, later) to read.

But even more importantly, using the broadcast may improve performance. We may, for instance, be using an implementation of MPI which is tailored to the platform on which we are running MPI. If for instance we are running on a network designed for parallel computing, such as Myrinet or Infiniband, an optimized broadcast may achieve a much higher performance level than would simply a loop with individual send calls. On a shared-memory multiprocessor system, special machine instructions specific to that platform's architecture can be exploited, as for instance IBM has done for its shared-memory machines. Even on an ordinary Ethernet, one could exploit Ethernet's own broadcast mechanism, as had been done for PVM, a system like MPI (G. Davies and N. Matloff, Network-Specific Performance Enhancements for PVM, *Proceedings of the Fourth IEEE International Symposium on High-Performance Distributed Computing*, 1995, 205-210; N. Matloff, Analysis of a Programmed Backoff Method for Parallel Processing on Ethernets, in *Network-Based Parallel Computing*).

8.6.3   MPI_Reduce()/MPI_Allreduce()

Look at our call

```
1  MPI_Reduce(mymin,overallmin,1,MPI_2INT,MPI_MINLOC,0,MPI_COMM_WORLD);
```

above. In English, this would say,

At this point all nodes in this group participate in a "reduce" operation. The type of reduce operation is **MPI_MINLOC**, which means that the minimum value among the nodes will be computed, and the index attaining that minimum will be recorded as well. Each node contributes a value to be checked, and an associated index, from a location **mymin** in their programs; the type of the pair is **MPI_2INT**. The overall min value/index will be computed by combining all of these values at node 0, where they will be placed at a location **overallmin**.

MPI also includes a function **MPI_Allreduce()**, which does the same operation, except that instead of just depositing the result at one node, it does so at all nodes. So for instance our code above,

```
1  MPI_Reduce(mymin,overallmin,1,MPI_2INT,MPI_MINLOC,0,MPI_COMM_WORLD);
2  MPI_Bcast(overallmin,1,MPI_2INT,0,MPI_COMM_WORLD);
```

could be replaced by

```
1  MPI_Allreduce(mymin,overallmin,1,MPI_2INT,MPI_MINLOC,MPI_COMM_WORLD);
```

Again, these can be optimized for particular platforms.

Here is a table of MPI reduce operations:

MPI_MAX	max
MPI_MIN	min
MPI_SUM	sum
MPI_PROD	product
MPI_LAND	wordwise boolean and
MPI_LOR	wordwise boolean or
MPI_LXOR	wordwise exclusive or
MPI_BAND	bitwise boolean and
MPI_BOR	bitwise boolean or
MPI_BXOR	bitwise exclusive or
MPI_MAXLOC	max value and location
MPI_MINLOC	min value and location

8.6.4 MPI_Gather()/MPI_Allgather()

A classical approach to parallel computation is to first break the data for the application into chunks, then have each node work on its chunk, and then gather all the processed chunks together at some node. The MPI function **MPI_Gather()** does this.

In our program above, look at the line

```
1  MPI_Gather(mind+startv,chunk,MPI_INT,mind,chunk,MPI_INT,0,MPI_COMM_WORLD);
```

In English, this says,

At this point all nodes participate in a gather operation, in which each node (including Node 0) contributes **chunk** number of MPI integers, from a location **mind+startv** in that node's program. Node 0 then receives **chunk** items sent from each node, stringing everything together in node order and depositing it all at **mind** in the program running at Node 0.

(Yes, the fifth argument is redundant with the second; same for the thrid and sixth.)

There is also **MPI_Allgather()**, which places the result at all nodes, not just one. Its call form is the same as **MPI_Gather()**, but with one fewer argument (since the identity of "the" gathering node is no longer meaningful):

```
1  int MPI_Allgather(srcbuf, srccount, srctype, destbuf, destcount, desttype,
     communicator)
```

8.6.5 The MPI_Scatter()

This is the opposite of **MPI_Gather()**, i.e. it breaks long data into chunks which it parcels out to individual nodes. For example, in the code in the next section, the call

```
1  MPI_Scatter(oh, lenchunk, MPI_INT, ohchunk, lenchunk, MPI_INT, 0,
2    MPI_COMM_WORLD);
```

means

Node 0 will break up the array **oh** of type MPI_INT into chunks of length **lenchunk**, sending the ith chunk to Node i, where **lenchunk** items will be deposited at **ohchunk**.

8.6.6   Example: Count the Number of Edges in a Directed Graph

Below is MPI code to count the number of edges in a directed graph. ("Directed" means that a link from i to j does not necessarily imply one from j to i.)

In the context here, **me** is the node's rank; **nv** is the number of vertices; **oh** is the one-hop distance matrix; and **nnodes** is the number of MPI processes. At the beginning only the process of rank 0 has a copy of **oh**, but it sends that matrix out in chunks to the other nodes, each of which stores its chunk in an array **ohchunk**.

```
1  lenchunk = nv / nnodes;
2  MPI_Scatter(oh, lenchunk, MPI_INT, ohchunk, lenchunk, MPI_INT, 0,
3    MPI_COMM_WORLD);
4  mycount = 0;
5  for (i = 0; i < nv*nv/nnodes)
6    if (ohchunk[i] != 0) mycount++;
7  MPI_Reduce(&mycount,&numedge,1,MPI_INT,MPI_SUM,0,MPI_COMM_WORLD);
8  if (me == 0) printf("there are %d edges\n",numedge);
```

8.6.7   Example: Cumulative Sums

Here we find cumulative sums. For instance, if the original array is (3,1,2,0,3,0,1,2), then it is changed to (3,4,6,6,9,9,10,12). (This topic is pursued in depth in Chapter 10.)

```
1  // finds cumulative sums in the array x
2
3  #include <mpi.h>
4  #include <stdlib.h>
5
6  #define MAX_N 10000000
7  #define MAX_NODES 10
8
9  int nnodes, // number of MPI processes
10     n, // size of x
11     me, // MPI rank of this node
12     // full data for node 0, part for the rest
```

```
13     x[MAX_N],
14     csums[MAX_N], // cumulative sums for this node
15     maxvals[MAX_NODES]; // the max values at the various nodes
16
17  int debug;
18
19  init(int argc, char **argv)
20  {
21     int i;
22     MPI_Init(&argc,&argv);
23     MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
24     MPI_Comm_rank(MPI_COMM_WORLD,&me);
25     n = atoi(argv[1]);
26     // test data
27     if (me == 0) {
28        for (i = 0; i < n; i++)
29           x[i] = rand() % 32;
30     }
31     debug = atoi(argv[2]);
32     while (debug) ;
33  }
34
35  void cumulsums()
36  {
37     MPI_Status status;
38     int i,lenchunk,sum,node;
39     lenchunk = n / nnodes; // assumed to divide evenly
40     // note that node 0 will participate in the computation too
41     MPI_Scatter(x,lenchunk,MPI_INT,x,lenchunk,MPI_INT,
42        0,MPI_COMM_WORLD);
43     sum = 0;
44     for (i = 0; i < lenchunk; i++) {
45        csums[i] = sum + x[i];
```

```
46        sum += x[i];
47     }
48     MPI_Gather(&csums[lenchunk-1],1,MPI_INT,
49        maxvals,1,MPI_INT,0,MPI_COMM_WORLD);
50     MPI_Bcast(maxvals,nnodes,MPI_INT,0,MPI_COMM_WORLD);
51     if (me > 0) {
52        sum = 0;
53        for (node = 0; node < me; node++) {
54           sum += maxvals[node];
55        }
56        for (i = 0; i < lenchunk; i++)
57           csums[i] += sum;
58     }
59     MPI_Gather(csums,lenchunk,MPI_INT,csums,lenchunk,MPI_INT,
60        0,MPI_COMM_WORLD);
61  }
62
63  int main(int argc,char **argv)
64  {
65     int i;
66     init(argc,argv);
67     if (me == 0 && n < 25) {
68        for (i = 0; i < n; i++) printf("%d ",x[i]);
69        printf("\n");
70     }
71     cumulsums();
72     if (me == 0 && n < 25) {
73        for (i = 0; i < n; i++) printf("%d ",csums[i]);
74        printf("\n");
75     }
76     MPI_Finalize();
77  }
```

8.6.8 Example: an MPI Solution to the Mutual Outlinks Problem

Consider the example of Section **??**. We have a network graph of some kind, such as Web links. For any two vertices, say any two Web sites, we might be interested in mutual outlinks, i.e. outbound links that are common to two Web sites.

The MPI code below finds the mean number of mutual outlinks, among all pairs of vertices in a graph.

```c
// MPI solution to the mutual outlinks problem

// adjacency matrix m is global at each node, broadcast from node 0

// assumes m is nxn, and number of nodes is < n

// for each node i, check all possible pairing nodes j > i; the various
// nodes work on values of i in a Round Robin fashion, with node k
// handling all i for which i mod nnodes = k

#include <mpi.h>
#include <stdlib.h>

#define MAXLENGTH 10000000

int nnodes, // number of MPI processes
    n, // size of x
    me, // MPI rank of this node
    m[MAXLENGTH], // adjacency matrix
    grandtot; // grand total of all counts of mutuality

// get adjacency matrix, in this case just by simulation
void getm()
{ int i;
   for (i = 0; i < n*n; i++)
      m[i] = rand() % 2;
```

```
27  }
28
29  init(int argc, char **argv)
30  {
31     int i;
32     MPI_Init(&argc,&argv);
33     MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
34     MPI_Comm_rank(MPI_COMM_WORLD,&me);
35     n = atoi(argv[1]);
36     if (me == 0) {
37        getm(); // get the data (app-specific)
38     }
39  }
40
41  void mutlinks()
42  {
43     int i,j,k,tot;
44     MPI_Bcast(m,n*n,MPI_INT,0,MPI_COMM_WORLD);
45     tot = 0;
46     for (i = me; i < n-1; i += nnodes) {
47        for (j = i+1; j < n; j++) {
48           for (k = 0; k < n; k++)
49              tot += m[twod2oned(n,i,k)] * m[twod2oned(n,j,k)];
50        }
51     }
52     MPI_Reduce(&tot,&grandtot,1,MPI_INT,MPI_SUM,0,MPI_COMM_WORLD);
53  }
54
55  // convert 2-D subscript to 1-D
56  int twod2oned(n,i,j)
57  { return n * i + j; }
58
59  int main(int argc,char **argv)
```

```
60  { int i,j;
61    init(argc,argv);
62    if (me == 0 && n < 5) { // check test input
63      for (i = 0; i < n; i++) {
64        for (j = 0; j < n; j++) printf("%d ",m[twod2oned(n,i,j)]);
65        printf("\n");
66      }
67    }
68    mutlinks();
69    if (me == 0) printf("%f\n",((float) grandtot)/(n*(n-1)/2));
70    MPI_Finalize();
71  }
```

8.6.9   The MPI_Barrier()

This implements a barrier for a given communicator. The name of the communicator is the sole argument for the function.

Explicit barriers are less common in message-passing programs than in the shared-memory world.

8.6.10   Creating Communicators

Again, a communicator is a subset (either proper or improper) of all of our nodes. MPI includes a number of functions for use in creating communicators. Some set up a virtual "topology" among the nodes.

For instance, many physics problems consist of solving differential equations in two- or three-dimensional space, via approximation on a grid of points. In two dimensions, groups may consists of rows in the grid.

Here's how we might divide an MPI run into two groups (assumes an even number of MPI processes to begin with):

```
1  MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
2  MPI_Comm_rank(MPI_COMM_WORLD,&me);
3  ...
4  // declare variables to bind to groups
5  MPI_Group worldgroup, subgroup;
6  // declare variable to bind to a communicator
7  MPI_Comm subcomm;
```

```
8    ...
9    int i,startrank,nn2 = nnodes/2;
10   int *subranks = malloc(nn2*sizeof(int));
11   if (me < nn2) start = 0;
12   else start = nn2;
13   for (i = 0; i < nn2; i++)
14      subranks[i] = i + start;
15   // bind the world to a group variable
16   MPI_Comm_group(MPI_COMM_WORLD, &worldgroup);
17   // take worldgroup the nn2 ranks in "subranks" and form group
18   // "subgroup" from them
19   MPI_Group_incl(worldgroup, nn2, subranks, subgroup);
20   // create a communicator for that new group
21   MPI_Comm_create(MPI_COMM_WORLD, subgroup, subcomm);
22   // get my rank in this new group
23   MPI_Group_rank (subgroup, &subme);
```

You would then use **subcomm** instead of MPI_COMM_WORLD whenever you wish to, say, broadcast, only to that group.

8.7   Buffering, Synchrony and Related Issues

As noted several times so far, interprocess communication in parallel systems can be quite expensive in terms of time delay. In this section we will consider some issues which can be extremely important in this regard.

8.7.1   Buffering, Etc.

To understand this point, first consider situations in which MPI is running on some network, under the TCP/IP protocol. Say an MPI program at node A is sending to one at node B.

It is extremely import to keep in mind the levels of abstraction here. The OS's TCP/IP stack is running at the Session, Transport and Network layers of the network. MPI—meaning the MPI internals—is running above the TCP/IP stack, in the Application layers at A and B. And the MPI user-written application could be considered to be running at a "Super-application" layer, since it calls the MPI internals. (From here on, we will refer to the MPI internals as simply "MPI.")

MPI at node A will have set up a TCP/IP socket to B during the user program's call to **MPI_Init()**. The other end of the socket will be a corresponding one at B. This setting up of this socket pair as establishing a **connection** between A and B. When node A calls **MPI_Send()**, MPI will write to

the socket, and the TCP/IP stack will transmit that data to the TCP/IP socket at B. The TCP/IP stack at B will then send whatever bytes come in to MPI at B.

Now, it is important to keep in mind that in TCP/IP the totality of bytes sent by A to B during lifetime of the connection is considered one long message. So for instance if the MPI program at A calls **MPI_Send()** five times, the MPI internals will write to the socket five times, but the bytes from those five messages will not be perceived by the TCP/IP stack at B as five messages, but rather as just one long message (in fact, only part of one long message, since more may be yet to come).

MPI at B continually reads that "long message" and breaks it back into MPI messages, keeping them ready for calls to **MPI_Recv()** from the MPI application program at B. Note carefully that phrase, *keeping them ready*; it refers to the fact that the order in which the MPI application program requests those messages may be different from the order in which they arrive.

On the other hand, looking again at the TCP/IP level, even though all the bytes sent are considered one long message, it will physically be sent out in pieces. These pieces don't correspond to the pieces written to the socket, i.e. the MPI messages. Rather, the breaking into pieces is done for the purpose of **flow control**, meaning that the TCP/IP stack at A will not send data to the one at B if the OS at B has no room for it. The **buffer** space the OS at B has set up for receiving data is limited. As A is sending to B, the TCP layer at B is telling its counterpart at A when A is allowed to send more data.

Think of what happens the MPI application at B calls **MPI_Recv()**, requesting to receive from A, with a certain tag T. Say the first argument is named **x**, i.e. the data to be received is to be deposited at **x**. If MPI sees that it already has a message of tag T, it will have its **MPI_Recv()** function return the message to the caller, i.e. to the MPI application at B. **If no such message has arrived yet, MPI won't return to the caller yet, and thus the caller blocks.**

MPI_Send() can block too. If the platform and MPI implementation is that of the TCP/IP network context described above, then the send call will return when its call to the OS' **write()** (or equivalent, depending on OS) returns, but that could be delayed if the OS' buffer space is full. On the other hand, another implementation could require a positive response from B before allowing the send call to return.

Note that buffering slows everything down. In our TCP scenario above, **MPI_Recv()** at B must copy messages from the OS' buffer space to the MPI application program's program variables, e.g. **x** above. This is definitely a blow to performance. That in fact is why networks developed specially for parallel processing typically include mechanisms to avoid the copying. Infiniband, for example, has a Remote Direct Memory Access capability, meaning that A can write directly to **x** at B. Of course, if

our implementation uses **synchronous** communication, with A's send call not returning until A gets a response from B, we must wait even longer.

Technically, the MPI standard states that **MPI_Send(x,...)** will return only when it is safe for the application program to write over the array which it is using to store its message, i.e. **x**. As we have seen, there are various ways to implement this, with performance implications. Similarly, **MPI_Recv(y,...)** will return only when it is safe to read **y**.

8.7.2 Safety

With **synchronous** communication, deadlock is a real risk. Say A wants to send two messages to B, of types U and V, but that B wants to receive V first. Then A won't even get to send V, because in preparing to send U it must wait for a notice from B that B wants to read U—a notice which will never come, because B sends such a notice for V first. This would not occur if the communication were asynchronous.

But beyond formal deadlock, programs can fail in other ways, even with buffering, as buffer space is always by nature finite. A program can fail if it runs out of buffer space, either at the sender or the receiver. See `www.llnl.gov/computing/tutorials/mpi_performance/samples/unsafe.c` for an example of a test program which demonstrates this on a certain platform, by deliberating overwhelming the buffers at the receiver.

In MPI terminology, asynchronous communication is considered **unsafe**. The program may run fine on most systems, as most systems are buffered, but fail on some systems. Of course, as long as you know your program won't be run in nonbuffered settings, it's fine, and since there is potentially such a performance penalty for doing things synchronously, most people are willing to go ahead with their "unsafe" code.

8.7.3 Living Dangerously

If one is sure that there will be no problems of buffer overflow and so on, one can use variant send and receive calls provided by MPI, such as **MPI_Isend()** and **MPI_Irecv()**. The key difference between them and **MPI_Send()** and **MPI_Recv()** is that they return immediately, and thus are termed **nonblocking**. Your code can go on and do other things, not having to wait.

This does mean that at A you cannot touch the data you are sending until you determine that it has either been buffered somewhere or has reached **x** at B. Similarly, at B you can't use the data at **x** until you determine that it has arrived. Such determinations can be made via **MPI_Wait()**. In other words, you can do your send or receive, then perform some other computations for a while, and

then call **MPI_Wait()** to determine whether you can go on. Or you can call **MPI_Probe()** to ask whether the operation has completed yet.

8.7.4 Safe Exchange Operations

In many applications A and B are swapping data, so both are sending and both are receiving. This too can lead to deadlock. An obvious solution would be, for instance, to have the lower-rank node send first and the higher-rank node receive first.

But a more convenient, safer and possibly faster alternative would be to use MPI's **MPI_Sendrecv()** function. Its prototype is

```
intMPI_Sendrecv_replace(void* buf, int count, MPI_Datatype datatype,
    int dest, int sendtag, int source, int recvtag, MPI_Comm comm,
    MPI_Status *status)
```

Note that the sent and received messages can be of different lengths and can use different tags.

8.8 Use of MPI from Other Languages

MPI is a vehicle for parallelizing C/C++, but some clever people have extended the concept to other languages, such as the cases of Python and R that we treat in Chapters 15 and 9.

8.9 Other MPI Examples in This Book

- The pipelined prime number finder in Chapter 1.
- Bucket sort with sampling, in Section 12.5.

第 9 章　R 并行处理入门

9.1　为什么要在本书中用 R 语言？

在本书的其它章节里，C/C++ 依然是我们的主要语言，但我们也提供很多 R 语言的示例。为什么要用 R 呢？

- R 是最广泛使用的用于统计分析和数据处理的编程语言。在现今这个大数据时代，人民已经开发了相当数量的用于并行计算的 R 扩展包。特别地，**parallel** 扩展包现在已经是 R 基础包的一部分。
- R 语言的广泛使用，从 Google 设置了其内部的 R 语言规范一事就可见一斑[①]。现在 Oracle 也把 R 包含了自己的大数据分析方案中。
- 对于展示各种各样的并行算法，R 非常方便。这点的主要原因在于 R 内置了向量、矩阵和复数类型。

Python 也有很多并行库，比如 **multiprocessing**。关于 Python 的并行话题，我们会在第15章里讨论。

本章的示例会保持尽量简单。但 R 中的并行计算也可以应用到非常庞大而复杂的问题上。在附录B中，有一个 5 分钟的 R 快速入门。阅读时请牢记 R 中 list 结构。

R 中进行并行计算的关键就是——list 结构的操作。许多 R 的并行计算扩展包都非常依赖于 R 中的 list 结构。输入输出的参数和返回值经常都采用 list 的形式。读者可能有兴趣参考一下附录B中的相关内容。

[①]个人角度来讲，我并不喜欢这些代码规范，我更喜欢我自己的。但从 Google 设置自己的 R 语言规范可以看出他们对 R 的重视程度。

9.2   R 和易并行问题（Embarrassing Parallel Problems）

需要注意的是，R 的并行扩展包一般只能处理易并行问题。正如在 2.1节中定义的，这些问题不仅容易并行化，而且信息传递的需求很少[2]。如我们所知，一般只有易并行问题会有很好的表现，但在 R 中情况尤其如此，原因如下。

R 语言的函数式编程的本质意味着，任何对一个向量或矩阵的元素的写入操作，比如

```
1  x[3] <- 8
```

都会重写整个向量或矩阵[3]。虽然有些例外（随着 R 版本更新，例外可能越来越多），但一般来说我们必须承认 R 中并行的向量和矩阵代码代价很高[4]。

对于不易并行的问题，大家应该考虑用 R 调用并行的 C 代码，这点会在9.9 节中讨论。

9.3   一些 R 的并行扩展包

这里我们列举了一些 R 的并行扩展包：

- Message-passing 或 scatter/gather (7.4节)：**Rmpi**、**snow**、**foreach**、**rmr**、**Rhipe**、**multicore**[5]、**rzmq**
- 内存共享：**Rdsm**、**bigmemory**
- GPU：**gputools**、**rgpu**

大家可以从 http://cran.r-project.org/web/views/HighPerformanceComputing.html 找到更加详尽的列表。

从 2.14 版本开始，R 默认包括了由 **snow** 和 **multicore** 构成的 **parallel** 扩展包。（早期版本可能需要分别下载。）正是因为如此，二者都在范围之内。另外，我们也会讨论 **Rdsm/bigmemory** 和 **gputools**。

9.4   安装和载入这些扩展包

安装：
需要注意的是，如果你使用的是 2.14 版或更高版本的 R，你已经安装了 **snow** 和 **multicore**。一

---

[2]后面的要求把很多迭代算法排除在外了，尽管它们很容易并行化。

[3]R 中的元素赋值是一个函数调用，上面这个例子的参数分别为 **x**、3 和 8。

[4]R 中新的引用类（Reference class）可能会对此有所改变。

[5]**multicore** 扩展包运行于多核内存共享的平台之上，但在读写过程中并不共享数据。

般来说，除了 **rgpu**，其它所有扩展包都可以从 R 官方的代码仓库 CRANhttp://cran.r-project.org）下载。这里以 **snow** 为例：

加入你想把它安装在**/a/b/c/** 目录下。最简单的方法就是使用 R 的函数：

```
1  > install.packages("snow","/a/b/c/")
```

这会将 **snow** 安装在**/a/b/c/snow** 目录下。

You'll need to arrange for the directory **/a/b/c** (not **/a/b/c/snow**) to be added to your R library search path. I recommend placing a line

```
1  .libPaths("/a/b/c/")
```

in a file **.Rprofile** in your home directory (this is an R startup file).

In some cases, due to issues such as locations of libraries, you may need to install a CRAN package "by hand." See Section 9.8.1 and 9.8.3 below.

Loading a package:

Call **library()** to load a package. For instance, to load **parallel**, type:

```
1  > library(parallel)
```

9.5 R 中的 snow 扩展包

The real virtue of **snow** is its simplicity. The concept is simple, the implementation is simple, and very little can go wrong. Accordingly, it may be the most popular type of parallel R in use today.

The **snow** package runs directly via network sockets (probably the most common usage, since the user does not have to install anything besides **snow**), or on top of **Rmpi** (R's interface to MPI), PVM or NWS.

It operates under a scatter/gather model (Sec. 7.4).

For instance, just as the ordinary R function **apply()** applies the same function to all rows of a matrix (example below), the **snow** function **parApply()** does that in parallel, across multiple machines; different machines will work on different rows. (Instead of running on several machines, we might one several **snow** clients on one multicore machine.)

9.5.1 Usage

After loading **snow**, by typing

```
1  > library(snow)
```

one sets up a **snow** cluster, by calling the **snow** function **makeCluster()**. The named argument **type** of that function indicates the networking platform, e.g. "MPI" or "SOCK." The last indicates that you wish **snow** to run on TCP/IP sockets that it creates itself, rather than going through MPI etc.

In the examples here, I used "SOCK," on machines named **pc48** and **pc49**, setting up the cluster this way:[⑥]

```
1  > cls <- makeCluster(type="SOCK",c("pc48","pc49"))
```

Note that the above R code sets up **worker nodes** at the machines named **pc48** and **pc49**; these are in addition to the **manager node**, which is the machine on which that R code is executed.

By the way, if you want to make worker nodes on the same machine as the manager (typically on a multicore machine), use **localhost** as the machine name.

There are various other optional arguments. One you may find useful is **outfile**, which records the result of the call in the file **outfile**. This can be helpful for debugging if the call fails.

9.5.2　示例：使用 **parApply()** 进行矩阵向量相乘

To introduce **snow**, consider a simple example of multiplication of a vector by a matrix. We set up a test matrix:

```
1  > a <- matrix(c(1:12),nrow=6)
2  > a
3       [,1] [,2]
4  [1,] 1 7
5  [2,] 2 8
6  [3,] 3 9
7  [4,] 4 10
8  [5,] 5 11
9  [6,] 6 12
```

We will multiply the vector $(1, 1)^T$ (T meaning transpose) by our matrix **a**. In this small example, of course, we would do that directly:

[⑥]If you are on a shared-file system group of machines, try to stick to ones for which the path to R is the same for all, to avoid problems.

```
1  > a %*% c(1,1)
2       [,1]
3  [1,]  8
4  [2,] 10
5  [3,] 12
6  [4,] 14
7  [5,] 16
8  [6,] 18
```

But let's see how we could do it using R's **apply()** function, still in serial form, as it will set the stage for extending to parallel computation.

R's **apply()** function calls a user-specified, scalar-valued function to each of the rows (or each of the columns) of a user-specified matrix. This returns a vector. To use **apply()** for our matrix-times-vector problem here, define a dot product function:

```
1  > dot <- function(x,y) {return(x%*%y)}
```

Now call **apply()**:

```
1  > apply(a,1,dot,c(1,1))
2  [1] 8 10 12 14 16 18
```

This call applies the function **dot()** to each row (indicated by the 1, with 2 meaning column instead of row) of the matrix **a**; a row plays the role of the first argument to **dot()**, and with c(1,1) playing the role of the second argument. In other words, the first call to **dot()** will be

```
1  dot(c(1,7),c(1,1))
```

The **snow** library function **parApply()** then extends **apply()** to parallel computation. Let's use it to parallelize our matrix multiplication, across our the machines in our cluster **cls**:

```
1  > parApply(cls,a,1,dot,c(1,1))
2  [1] 8 10 12 14 16 18
```

What **parApply()** did was to send some of the rows of the matrix to each node, also sending them the function **dot()** and the argument **c(1,1)**. Each node applied **dot()** to each of the rows it was given, and then returned the results to be assembled by the manager node.

R's **apply()** function is normally used in scalar-valued situations, meaning that **f()** in a call **apply(m,i,f)** is scalar-valued. If **f()** is vector-valued, then a matrix will be returned instead of a

vector, with each column of that matrix being the result of calling **f()** on a row or column of **m**. The same holds for **parApply()**.

9.5.3 snow 中的其它函数：clusterApply()、clusterCall() 等

In the last section we introduced the **parApply()** function. Its general call form is

- **parApply():**

  The call

```
1  parApply(cls,m,DIM,f,...)}
```

results in the rows of the matrix **m** parceled out to the various worker nodes of **cls**, at which **f()** will be applied to each row, with optional parameters in the position indicated by the ellipsis. The argument **DIM** is 1 for row operations, 2 for columns.

The return value is a vector (or possibly a matrix, as noted above).

The virtue of **snow** is its simplicity. Thus it does not have a lot of complex functions. But there is certainly more than just **parApply()**. Here are a few more:

- **clusterApply():**

  This function may be the most heavily-used function in **snow**. The call

```
1  clusterApply(cls,individualargs,f,...)}
```

  runs **f()** at each worker node in **cls**. Here **individualargs** is an R list (if it is a vector, it will be converted to a list). When **f()** is called at node i of the cluster, its arguments will be as follows. The first argument will be the ith element of the **individualargs**, i.e. **individualargs[[i]]**. If arguments indicated by the ellipsis are in the call (optional), then these will be passed to **f()** as its second, third and so on arguments.

  If **individualargs** has more elements than the number of nodes in the cluster, then **cls** will be recycled (treating it as a vector), so that most or all nodes will call **f()** on more than element of **individualargs**.

  The return value is an R list, whose i^{th} component is the result of the call to **f()** on the ith element of **individualargs**.

  Typically the list **individualargs** consists of the work to be split up and done in parallel.

- **clusterApplyLB():**

This is a load-balancing form of **clusterApply()**, aimed at addressing the performance issues we discussed on Chapter **??**.

To explain the difference between the two forms of the cluster-apply operation, suppose our cluster consists of 10 nodes, and that we have 25 tasks for them to do (i.e. **individualargs** has length 25). With **clusterApply()**, the following will occur:

– The first 10 tasks will be sent to the workers, one task per worker.

– The manager will wait for all 10 tasks to complete, and then will send out the next 10.

– The manager will wait for these 10 tasks to complete, and then will send out the remaining 5.

– The manager will wait for the results of these 5, and then return the 25 results to the caller.

By contrast, with **clusterApplyLB()**, the event flow will go this way:

– The first 10 tasks will be sent to the workers, one task per worker.

– When some node finishes, the manager will take action right away, sending the 11th task to this node, even though the others aren't done.

– The manager will continue in this fashion, giving each node a new task as soon as the node finishes its old one, until all the tasks are done.

– The manager will then return the 25 results to the caller.

In the language of Chapter **??**, and of Section 4.3.3 of our OpenMP chapter, **clusterApply()** employs a **static** scheduling policy, while **clusterApplyLB()** uses a dynamic one; chunk size is 1.

- **clusterCall():**

  The function **clusterCall(cls,f,...)** sends the function **f()**, and the set of arguments (if any) represented by the ellipsis above to each worker node, where **f()** is evaluated on the arguments. The return value is an R list, with the ith element is the result of the computation at node i in the cluster. (It might seem at first that each node will return the same value, but typically the `f()` will make use of variables special to the node, thus yielding different results.)

- **clusterExport():**

  The function **clusterExport(cls,varlist)** copies the variables whose names appear in the character vector **varlist** to each worker in the cluster **cls**. You can use this, for instance, to avoid constant shipping of large data sets from the master to the workers, at great communications costs. With this function, you are able to ship a quantity just once; you call **clusterExport()**

on the corresponding variables, and then access those variables at worker nodes as (node-specific) globals. Again, the return value is an R list, with the ith element is the result of the computation at node i in the cluster.

By default, the variables to be exported must be global on the manager node.

Note carefully that once you export a variable, say **x**, from the manager to the workers, their copies become independent of the one at the manager (and independent of each other). If one copy changes, that change will not be reflected in the other copies.

- **clusterEvalQ():**

The function **clusterEvalQ(cls,expression)** runs **expression** at each worker node in **cls**.

9.5.4 Example: Parallel Sum

Let's go over one more toy problem, in which we have **snow** do parallel summation. We'll do a simpler version, then a more advanced one.

```
parsum <- function(cls,x) {
  # partition the indices of x among the cluster nodes (nothing
  # is actually sent to them yet)
  xparts <- clusterSplit(cls,x)
  # now send to the nodes and have them sum
  tmp <- clusterApply(cls,xparts,sum)
  # now finish, combing the individual sums into the grand total
  tot <- 0
  for (i in 1:length(tmp)) tot <- tot + tmp[[i]]
  return(tot)
}
```

Let's test it on a two-worker cluster **cls**:

```
> x
[1] 1 2 3 4 5 6 5 12 13
> parsum1(cls,x)
[1] 51
```

Good. Now, how does it work?

The basic idea is to break our vector into chunks, then distribute the chunks to the worker nodes. Each of the latter will sum its chunk, and send the sum back to the manager node. The latter will sum the sums, giving us the grand total as desired.

In order to break our vector **x** into chunks to send to the workers, we'll first turn to the **snow** function **clusterSplit()**. That function inputs an R vector and breaks it into as many chunks as we have worker nodes, just what we want.

For example, with **x** as above on a two-worker cluster, we get

```
> xparts <- clusterSplit(cls,x)
> xparts
[[1]]
[1] 1 2 3 4

[[2]]
[1] 5 6 5 12 13
```

Sure enough, our R list **xparts** has one chunk of **x** in one of its components, and the other chunk of **x** in the other component. These two chunks are now sent to our two worker nodes:

```
> tmp <- clusterApply(cls,xparts,sum)
> tmp
[[1]]
[1] 10

[[2]]
[1] 41
```

Again, **clusterApply()**, like most **snow** functions, returns its results in an R list, which we've assigned to **tmp**. The contents of the latter are

```
> tmp
[[1]]
[1] 10

[[2]]
[1] 41
```

i.e. the sum of each chunk of **x**.

To get the grand total, we can't merely call R's **sum()** function on **tmp**:

```
1 > sum(tmp)
2 Error in sum(tmp) : invalid 'type' (list) of argument
```

This is because **sum()** works on vectors, not lists. So, we just wrote a loop to add everything together:

```
1 tot <- 0
2 for (i in 1:length(tmp)) tot <- tot + tmp[[i]]
```

Note that we need double brackets to access list elements.

We can improve the code a little by replacing the above loop code by a call to R's **Reduce()** function, which works like the reduction operators we saw in Sections 4.3.5 and 8.6.3. (Note, though, that this is a serial operation here, not parallel.) It takes the form **Reduce(f,y)** for a function **f()** and a list **y**, and essentially does

```
1 z <- y[1]
2 for (i in 2:length(y)) z <- f(z,y[i])
```

Using **Reduce()** makes for more compact, readable code, and in some cases may speed up execution (not an issue here, since we'll have only a few items to sum). Moreover, **Reduce()** changes **tmp** from an R list to a vector for us, solving the problem we had above when we tried to apply **sum()** to **tmp** directly.

Here's the new code:

```
1 parsum <- function(cls,x) {
2   xparts <- clusterSplit(cls,x)
3   tmp <- clusterApply(cls,xparts,sum)
4   Reduce(sum,tmp) # implicit return()
5 }
```

Note that in R, absent an explcit **return()** call, the last value computed is returned, in this case the value produced by **Reduce()**.

Reduce() is a very handy function in R in general, and with **snow** in particular. Here's an example in which we combine several matrices into one:

```
1  > Reduce(rbind,list(matrix(5:8,nrow=2),3:4,c(-1,1)))
2       [,1] [,2]
3  [1,] 5 7
4  [2,] 6 8
5  [3,] 3 4
6  [4,] -1 1
```

The **rbind()** functions has two operands, but in the situation above we have three. Calling **Reduce()** solves that problem.

9.5.5　Example: Inversion of Block-Diagonal Matrices

Suppose we have a block-diagonal matrix, such as

$$
\begin{pmatrix}
1 & 2 & 0 & 0 \\
3 & 4 & 0 & 0 \\
0 & 0 & 8 & 1 \\
0 & 0 & 1 & 5
\end{pmatrix}
$$

and we wish to find its inverse. This is an embarrassingly parallel problem: If we have two processes, we simply have one process invert that first 2x2 submatrix, have the second process invert the second 2x2 submatrix, and we then place the inverses back in the same diagonal positions.

Communication costs might not be too bad here, since inversion of an nxn matrix takes $O(n^3)$ time while communication is only $O(n^2)$.

Here we'll discuss **snow** code for inverting block-diagonal matrices.

```
1  # invert a block diagonal matrix m, whose sizes are given in szs;
2  # return value is the inverted matrix
3  bdiaginv <- function(cls,m,szs) {
4     nb <- length(szs) # number of blocks
5     dgs <- list() # will form args for clusterApply()
6     rownums <- getrng(szs)
7     for (i in 1:nb) {
8        rng <- rownums[i,1]:rownums[i,2]
9        dgs[[i]] <- m[rng,rng]
10     }
```

```
11    invs <- clusterApply(cls,dgs,solve)
12    for (i in 1:nb) {
13       rng <- rownums[i,1]:rownums[i,2]
14       m[rng,rng] <- invs[[i]]
15    }
16    m
17 }
18
19 # find row number ranges for the blocks, returned in a # 2-column
20 # matrix; blkszs = block sizes
21 getrng <- function(blkszs) {
22    col2 <- cumsum(blkszs) # cumulative sums function
23    col1 <- col2 - (blkszs-1)
24    cbind(col1,col2) # column bind
25 }
```

Let's test it:

```
1 > m
2      [,1] [,2] [,3] [,4] [,5]
3 [1,] 1 2 0 0 0
4 [2,] 7 8 0 0 0
5 [3,] 0 0 1 2 3
6 [4,] 0 0 2 4 5
7 [5,] 0 0 1 1 1
8 > bdiaginv(cls,m,c(2,3))
9          [,1] [,2] [,3] [,4] [,5]
10 [1,] -1.333333 0.3333333 0 0 0
11 [2,] 1.166667 -0.1666667 0 0 0
12 [3,] 0.000000 0.0000000 1 -1 2
13 [4,] 0.000000 0.0000000 -3 2 -1
14 [5,] 0.000000 0.0000000 2 -1 0
```

Note the **szs** argument here, which contains the sizes of the blocks. Since we had one 2x2 block and a 3x3 one, the sizes were 2 and 3, hence the **c(2,3)** argument in our call.

The use of **clusterApply()** here is similar to our earlier one. The main point in the code is to keep track of the positions of the blocks within the big matrix. To that end, we wrote **getrng()**, which returns the starting and ending row numbers for the various blocks. we use that to set up the argument **dg** to be fed into **clusterApply()**:

```
1  for (i in 1:nb) {
2    rng <- rownums[i,1]:rownums[i,2]
3    dgs[[i]] <- m[rng,rng]
```

Keep in mind that the expression **m[rng,rng]** extracts a subset of the rows and columns of **m**, in this case the ith block.

9.5.6   Example: Mutual Outlinks

Consider the example of Section **??**. We have a network graph of some kind, such as Web links. For any two vertices, say any two Web sites, we might be interested in mutual outlinks, i.e. outbound links that are common to two Web sites.

The **snow** code below finds the mean number of mutual outlinks, among all pairs of sites in a set of Web sites.

```
1  # snow version of mutual links problem
2
3  library(snow)
4
5  mtl <- function(ichunks,m) {
6     n <- ncol(m)
7     matches <- 0
8     for (i in ichunks) {
9        if (i < n) {
10          rowi <- m[i,]
11          matches <- matches +
12            sum(m[(i+1):n,] %*% as.vector(rowi))
13       }
14    }
15    matches
16 }
```

```
17

18  # returns the mean number of mutual outlinks in m, computing on the

19  # cluster cls

20  mutlinks <- function(cls,m) {

21     n <- nrow(m)

22     nc <- length(cls)

23     # determine which worker gets which chunk of i

24     options(warn=-1)

25     ichunks <- split(1:n,1:nc)

26     options(warn=0)

27     counts <- clusterApply(cls,ichunks,mtl,m)

28     do.call(sum,counts) / (n*(n-1)/2)

29  }
```

For each row in **m**, we will count mutual links in all rows below that one. To distribute the work among the worker nodes, we could have a call to **clusterSplit()** along the lines of

```
1  clusterSplit(cls,1:nrow(m))
```

But this would presents a load imbalance problem, discussed in Section **??**. For instance, suppose again we have two worker nodes, and there are 100 rows. If we were to use **clusterSplit()** as in the last section, the first worker would be doing a lot more row comparisons than would the second worker.

One solution to this problem would be to randomize the row numbers before calling **clusterSplit()**. Another approach, taken in our full code above, is to use R's **split()** function.

What does **split()** do? It forms chunks of its first argument, according to "categories" specified in the second. Look at this example:

```
1  > split(2:5,c('a','b'))

2  $a

3  [1] 2 4

4

5  $b

6  [1] 3 5
```

Here the categories are 'a' and 'b'. The **split()** function requires the second argument to be the same length as the first, so it will first **recycle** the second argument to 'a','b','a','b','a'. The split will

take 2,3,4,5 and treat 2 and 4 as being in categort 'a', and 3 and 5 to be category 'b'. The function returns a list accordingly.

Now coming back to our above **snow** example, and again assuming two workers and **m** 100x100, the code

```
1  nc <- length(cls)
2  ichunks <- split(1:n,1:nc)
```

produces a list of two components, with the odd-numbered rows in one component and the evens in the other. Our call,

```
1  counts <- clusterApply(cls,ichunks,mtl,m)
```

then results in good load balance between the two workers.

Note that the call needed includ **m** as an argument (which becomes an argument to **mtl()**). Otherwise the workers would have no **m** to work it. One alternative would have been to use **clusterExport()** to ship **m** to the workers, at which it then would be a global variable accessible by **mtl()**.

By the way, the calls to **options()** tell R not to warn us that it did recycling. It doesn't usually do so, but it will for **split()**.

Then to get the grand total from the output list of individual sums, we could have used **Reduce()** again, but for variety utilized R's **do.call()** function. That function does exactly what its name implies: It will extract the elements of the list **counts**, and then plug them as arguments into **sum()**! (In general, **do.call()** is useful when we wish to call a certain function on a set of arguments whose number won't be known until run time.)

As noted, instead of **split()**, we could have randomized the rows:

```
1  tmp <- clusterSplit(cls,order(runif(nrow(m))))
```

This generates a random number in (0,1) for each row, then finds the order of these numbers. If for instance the third number is the 20th-smallest, element 3 of the output of **order()** will be 20. This amounts to finding a random permutation of the row numbers of **m**.

9.5.7 Example: Transforming an Adjacency Matrix

Here is a **snow** version of the code in Section 4.13. To review, here is the problem:

Say we have a graph with adjacency matrix

$$
\begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}
\tag{9.1}
$$

with row and column numbering starting at 0, not 1. We'd like to transform this to a two-column matrix that displays the links, in this case

$$
\begin{pmatrix}
0 & 1 \\
1 & 0 \\
1 & 3 \\
2 & 1 \\
2 & 3 \\
3 & 0 \\
3 & 1 \\
3 & 2
\end{pmatrix}
\tag{9.2}
$$

For instance, there is a 1 on the far right, second row of the above matrix, meaning that in the graph there is an edge from vertex 1 to vertex 3. This results in the row (1,3) in the transformed matrix seen above.

Here is code to do this computation in **snow**:

```
1  tg <- function(cls,m) {
2    n <- nrow(m)
3    rowschunks <- clusterSplit(cls,1:n) # make chunks of row numbers
4    m1 <- cbind(1:n,m) # prepend col of row numbers to m
5    # now make the chunks of rows themselves
6    tmp <- lapply(rowschunks,function(rchunk) m1[rchunk,])
7    # launch the computation
8    tmp <- clusterApply(cls,tmp,tgonchunk)
9    do.call(rbind,tmp) # combine into one large matrix
10 }
11
12 # a worker works on a chunk of rows
13 tgonchunk <- function(rows) {
```

```
14     # note: matrix space allocation not efficient
15     mat <- NULL
16     nc <- ncol(rows)
17     for (i in 1:nrow(rows)) {
18        row <- rows[i,]
19        rownum <- row[1]
20        for (j in 2:nc) {
21           if (row[j] == 1) {
22              if (is.null(mat)) {
23                 mat <- matrix(c(rownum,j-1),ncol=2)
24              } else
25                 mat <- rbind(mat,c(rownum,j-1))
26           }
27        }
28     }
29     return(mat)
30  }
```

What is new here? First, since we desired the output matrix to be in lexicographical order, we needed a way to keep track of the original indices of the rows. So, we added a column for those numbers to **m**:

```
1  m1 <- cbind(1:n,m) # prepend col of row numbers to m
```

Second, note the use of R's **lapply()** function. Just as **apply()** calls a specified function on each row (or each column) of a matrix, **lapply()** calls a specified function on each element of a list. The output will also be a list.

In our case here, we need to feed the row chunks of **m** into **clusterApply()**, but the latter requires that we do that via a list. We could have done that using a **for** loop, adding row chunks to a list one by one, but it is more compact to use **lapply()**.

In the end, the manager node receives many parts of the new matrix, which must be combined. It's natural to do that with the **rbind()** function, but again we need to overcome the fact that the parts are packaged in an R list. It's handy to use **do.call()** again, though **Reduce()** would have worked too.

Note carefully that although it's natural to use **rbind()** as mentioned in the preceding paragraph,

it's not efficient. This is because each call to **rbind()** causes a new matrix to be allocated, a time-consuming action. It would be better to allocate, say, 50 rows at a time, and fill in the rows as we build the matrix. Whenever we would use up all of a matrix, we would start a new one, and then return all the matrices in a list.

9.5.8 Example: Setting Node IDs and Notification of Cluster Size

Recall that in OpenMP there are functions **omp_get_thread_num()** and **omp_get_num_threads()** that report a thread's ID number and the total number of threads. In MPI, the corresponding functions are **MPI_Comm_rank()** and **MPI_Comm_size()**. It would be nice to have such functions (or such functionality) in **snow**. Here is code for that purpose:

```
# sets a list myinfo as a global variable in the worker nodes in the
# cluster cls, with myinfo$id being the ID number of the worker and
# myinfo$nwrkrs being the number of workers in the cluster; called from
# the manager node
setmyinfo <- function(cls) {
   setmyinfo <- function(i,n) {
      myinfo <<- list(id = i, nwrkrs = n)
   }
   ncls <- length(cls)
   clusterApply(cls,1:ncls,setmyinfo,ncls)
}
```

Yes, R does allow defining a function within a function. Note by the way the use of the superassignment operator, **<<-**, which assigns to the global level.

After this call, any code executed by a worker node can then determine its node number, e.g. in code such as

```
if (myinfo$id == 1) ...
```

Or, we could send code from the manager to be executed on the workers:

```
> setmyinfo(cls)
[[1]]
[[1]]$id
[1] 1
```

```
5
6   [[1]]$nwrkrs
7   [1] 2
8
9
10  [[2]]
11  [[2]]$id
12  [1] 2
13
14  [[2]]$nwrkrs
15  [1] 2
16
17  > clusterEvalQ(cls,myinfo$id)
18  [[1]]
19  [1] 1
20
21  [[2]]
22  [1] 2
```

In that first case, since **clusterApply()** returns a value, it was printed out. In the second case, the call

```
1   clusterEvalQ(cls,myinfo$id)
```

asks each worker to evaluate the expression **myinfo$id**; **clusterEvalQ()** then returns the results of evaluating the expression at each worker node.

9.5.9   Shutting Down a Cluster

Don't forget to stop your clusters before exiting R, by calling **stopCluster(clustername)**.

9.6   The multicore Package

As the name implies, the **multicore** package is used to exploit the power of multicore machines. This might seem odd: Since **snow** can be used on either a (physical) cluster of machines or on a multicore machine, while **multicore** can only be used on the latter, one might wonder what, if anything,

is to be gained by using **multicore**. The answer is that one might gain in performance, as will be explained.

The package's main function, **mclapply()**, is similar in syntax to **snow**'s **clusterApply()**, and similarly parcels tasks out to the various worker nodes.

The worker nodes here, though, are just different processes on the same machine. Say for example you are running **multicore** on a quad-core machine. Calling **mclapply()** will start (a default value of) 4 new invocations of R on your machine, each of which will work on a piece of your application in parallel. Each invocation has exactly the same R variables set up as your original R process did before the call. Thus all the variables are shared initially (note that qualifier), and you as the programmer do not take any special action to transfer variables from the manager node to the worker nodes, quite a contrast to **snow**.

The way all this is accomplished is that **mclapply()** calls your OS' **fork()** function. (It is thus limited to Unix-family OSs, such as Linux and Macs.) The process that is forked is R itself, with one new copy per desired worker node.

The workers thus start with copies of R all sharing whatever variables existed at the time of the fork (including locals in the function that you had call **mclapply()**). Thus your code does not have to copy these variables to the workers, which automatically have access to them. But note carefully that the variables are shared only initially, and a write to one copy is NOT reflected in the other copies (including the original one).

The copying of the initial values of the variables from the manager node to the worker nodes is done on a **copy-on-write** basis, meaning that data isn't copied to a node until (and unless) the node tries to access that data. The granularity is at the virtual memory page level (Section **??**). Again, the OS handles this, not R.

Thus some physical copying does occur eventually, done by the OS, so **multicore** will not have as much advantage over **snow** as one might think. However, there may be some latency-hiding advantage (Section **??**). It may be the case that not all workers need to access some variable at the same time, so one worker might do so while others are doing actual computation.

Note too that, in contrast to **snow**, in which a cluster is set up once per session and then repeatedly reused at each **snow** function call, with **multicore** the worker R processes are set up again from scratch each time a **multicore** function is called.

9.6.1 Example: Transforming an Adjacency Matrix, multicore Version

Same application as in Section 9.5.7, and indeed the function **tgonchunk()** below is just a modified version of what we had in the **snow** code.

The call

```
1  mclapply(starts,tgonchunk,m1,chunksize,mc.cores=ncores)
```

applies the function **tgonchunk()** to every element of the vector **starts** (changed to an R list first), with **m1** and **chunksize** serving as additional arguments to **mclapply()**.

```
1  # transgraph problem, R multicore version
2
3  # arguments:
4  # m: the input matrix
5  # ncores: desired number of cores to use
6  tgmc <- function(m,ncores) {
7     n <- nrow(m)
8     chunksize <- floor(n/ncores)
9     starts <- seq(1,n,chunksize)
10    m1 <- cbind(1:n,m) # prepend col of row numbers to m
11    tmp <- mclapply(starts,tgonchunk,m1,chunksize,mc.cores=ncores)
12    do.call(rbind,tmp)
13 }
14
15 # a worker works on a chunk of rows
16 tgonchunk <- function(start,m1,chunksize) {
17    # note: matrix space allocation not efficient
18    outmat <- NULL
19    end <- start + chunksize - 1
20    nrm <- nrow(m1)
21    if (end > nrm) end <- nrm
22    ncm <- ncol(m1)
23    for (i in start:end) {
24       rownum <- m1[i,1]
25       for (j in 2:ncm) {
```

```
26        if (m1[i,j] == 1) {
27           if (is.null(outmat)) {
28              outmat <- matrix(c(rownum,j-1),ncol=2)
29           } else
30              outmat <- rbind(outmat,c(rownum,j-1))
31        }
32     }
33   }
34   return(outmat)
35 }
```

9.7　Rdsm

My **Rdsm** package can be used as a threads system regardless of whether you are on a NOW or a multicore machine. It is an extension of a similar package I wrote in 2002 for Perl, called PerlDSM. (N. Matloff, PerlDSM: A Distributed Shared Memory System for Perl, *Proceedings of PDPTA 2002*, 2002, 63-68.) The major advantages of **Rdsm** are:

- It uses a shared-memory programming model, which as noted in Section **??**, is commonly considered in the parallel processing community to be clearer than messag-passing.
- It allows full use of R's debugging tools.

Rdsm gives the R programmer a shared memory view, but the objects are not physically shared. Instead, they are stored in a server and accessed through network sockets,[7] thus enabling a threads-like view for R programmers even on NOWs. There is no manager/worker structure here. All of the R processes execute the same code, as peers.

Shared objects in **Rdsm** can be numerical vectors or matrices, via the classes **dsmv** and **dsmm**, or R lists, using the class **dsml**. Communication with the server in the vector and matrix cases is done in binary form for efficiency, while serialization is used for lists. There is as a built-in variable **myinfo** that gives a process' ID number and the total number of processes, analogous to the information obtained in **Rmpi** from the functions **mpi.comm.rank()** and **mpi.comm.size()**.

---

[7]Or, **Rdsm** can be used with the **bigmemory** package, as seen in Section 9.7.3.

To install, again use **install.packages()** as above. There is built-in documentation, but it's best to read through the code **MatMul.R** in the **examples** directory of the **Rdsm** distribution first. It is heavily commented, with the goal of serving as an introduction to the package.

9.7.1 Example: Inversion of Block-Diagonal Matrices

Let's see how the block-diagonal matrix inversion example from Section 9.5.5 can be handled in **Rdsm**.

```
1  # invert a block diagonal matrix m, whose sizes are given in szs; here m
2  # is either an Rdsm or bigmemory shared variable; no return
3  # value--inversion is done in-place; it is assumed that there is one
4  # thread for each block
5
6  bdiaginv <- function(bd,szs) {
7     # get number of rows of bd
8     nrdb <- if(class(bd) == "big.matrix") dim(bd)[1] else bd$size[1]
9     rownums <- getrng(nrdb,szs)
10    myid <- myinfo$myid
11    rng <- rownums[myid,1]:rownums[myid,2]
12    bd[rng,rng] <- solve(bd[rng,rng])
13    barr() # barrier
14 }
15
16 # find row number ranges for the blocks, returned in a 2-column matrix;
17 # matsz = number of rows in matrix, blkszs = block sizes
18 getrng <- function(matsz, blkszs) {
19    nb <- length(blkszs)
20    rwnms <- matrix(nrow=nb,ncol=2)
21    for (i in 1:nb) {
22       # i-th block will be in rows (and cols) i1:i2
23       i1 <- if (i==1) 1 else i2 + 1
24       i2 <- if (i == nb) matsz else i1 + blkszs[i] - 1
25       rwnms[i,] <- c(i1,i2)
```

```
26      }
27      rwnms
28 }
```

The parallel work is basically done in four lines:

```
1 myid <- myinfo$myid
2 rng <- rownums[myid,1]:rownums[myid,2]
3 bd[rng,rng] <- solve(bd[rng,rng])
4 barr() # barrier
```

compared to about 11 lines in the **snow** implementation above. This illustrates the power of the shared-memory programming model over message passing.

9.7.2　Example: Web Probe

In the general programming community, one major class of applications, even on a serial platform, is parallel I/O. Since each I/O operation may take a long time (by CPU standards), it makes sense to do them in parallel if possible. **Rdsm** facilitates doing this in R.

The example below repeatedly cycles through a large list of Web sites, taking measurements on the time to access each one. The data are stored in a shared variable **accesstimes**; the **n** most recent access times are stored. Each **Rdsm** process works on one Web site at a time.

An unusual feature here is that one of the processes immediately exits, returning to the R interactive command line. This allows the user to monitor the data that is being collected. Remember, the shared variables are still accessible to that process. Thus while the other processes are continually adding data to **accesstimes** (and deleted one item for each one added), the user can give commands to the exited process to analyze the data, say with histograms, as the collection progresses.

Note the use of lock/unlock operations here, with the **Rdsm** variables of the same names.

```
1 # if the variable accesstimes is length n, then the Rdsm vector
2 # accesstimes stores the n most recent probed access times, with element
3 # i being the i-th oldest
4
5 # arguments:
6 # sitefile: IPs, one Web site per line
7 # ww: window width, desired length of accesstimes
```

```
8   webprobe <- function(sitefile,ww) {
9     # create shared variables
10    cnewdsm("accesstimes","dsmv","double",rep(0,ww))
11    cnewdsm("naccesstimes","dsmv","double",0)
12    barr() # Rdsm barrier
13    # last thread is intended simply to provide access to humans, who
14    # can do analyses on the data, typing commands, so have it exit this
15    # function and return to the R command prompt
16    # built-in R list myinfo has components to give thread ID number and
17    # overall number of threads
18    if (myinfo$myid == myinfo$nclnt) {
19      print("back to R now")
20      return()
21    } else { # the other processes continually probe the Web:
22      sites <- scan(sitefile,what="") # read from URL file
23      nsites <- length(sites)
24      repeat {
25        # choose random site to probe
26        site <- sites[sample(1:nsites,1)]
27        # now probe it, recording the access time
28        acc <- system.time(system(paste("wget --spider -q",site)))[3]
29        # add to accesstimes, in sliding-window fashion
30        lock("acclock")
31        if (naccesstimes[1] < ww) {
32          naccesstimes[1] <- naccesstimes[1] + 1
33          accesstimes[naccesstimes[1]] <- acc
34        } else {
35          # out with the oldest, in with the newest
36          newvec <- c(accesstimes[-1],acc)
37          accesstimes[] <- newvec
38        }
39        unlock("acclock")
40      }
```

```
41      }
42  }
```

9.7.3　The bigmemory Package

Jay Emerson and Mike Kane developed the **bigmemory** package when I was developing **Rdsm**; neither of us knew about the other.

The **bigmemory** package is not intended to provide a threads environment. Instead, it is used to deal with a hard limit R has: No R object can be larger than $2^{31} - 1$ bytes. This holds even if you have a 64-bit machine with lots of RAM. The **bigmemory** package solves the problem on a multicore machine, by making use of operating system calls to set up shared memory between processes.[8]

In principle, **bigmemory** could be used for threading, but the package includes no infrastructure for this. However, one can use **Rdsm** in conjunction with **bigmemory**, an advantage since the latter is very efficient.

Using **bigmemory** variables in **Rdsm** is quite simple: Instead of calling **cnewdsm()** to create a shared variable, call **newbm()**.

9.8　R with GPUs

The blinding speed of GPUs (for certain problems) is sure to of interest to more and more R users in the coming years.

As of today, the main vehicle for writing GPU code is CUDA, on NVIDIA graphics cards. CUDA is a slight extension of C.

You may need to write your own CUDA code, in which case you need to use the methods of Section 9.9. But in many cases you can get what you need in ready-made form, via the two main packages for GPU programming with R, **gputools** and **rgpu**. Both deal mainly with linear algebra operations. The remainder of this section will deal with these packages.

9.8.1　Installation

Note that, due to issues involving linking to the CUDA libraries, in the cases of these two packages, you probably will *not* be able to install them by merely calling **install.packages()**. The alternative I recommend works as follows:

---

[8]It can also be used on distributed systems, by exploiting OS services to map memory to files.

- Download the package in **.tar.gz** form.

- Unpack the package, producing a directory that we'll call **x**.

- Let's say you wish to install to **/a/b/c**.

- Modify some files within **x**.

- Then run

```
1  R CMD INSTALL -l /a/b/c x
```

Details will be shown in the following sections.

9.8.2   The gputools Package

In installing **gputools**, I downloaded the source from the CRAN R repository site, and unpacked as above. I then removed the subcommand

```
-gencode arch=compute_20,code=sm_20
```

from the file **Makefile.in** in the **src** directory. I also made sure that my shell startup file included my CUDA executable and library paths, **/usr/local/cuda/bin** and **/usr/local/cuda/lib**.

I then ran **R CMD INSTALL** as above. I tested it by trying **gpuLm.fit()**, the **gputools** version of R's regular **lm.fit()**.

The package offers various linear algebra routines, such as matrix multiplication, solution of Ax = b (and thus matrix inversion), and singular value decomposition, as well as some computation-intensive operations such as linear/generalize linear model estimation and hierarchical clustering.

Here for instance is how to find the square of a matrix **m**:

```
1  > m2 <- gpuMatMult(m,m)
```

The **gpuSolve()** function works like the R **solve()**. The call `gpuSolve(a,b)` will solve the linear system ax = b, for a square matrix **a** and vector **b**. If the second argument is missing, then a^{-1} will be returned.

9.8.3   The rgpu Package

In installing **rgpu**, I downloaded the source code from `https://gforge.nbic.nl/frs/?group_id=38` and unpacked as above. I then changed the file **Makefile**, with the modified lines being

```
1  LIBS = -L/usr/lib/nvidia -lcuda -lcudart -lcublas
2  CUDA_INC_PATH ?= /home/matloff/NVIDIA_GPU_Computing_SDK/C/common/inc
3  R_INC_PATH ?= /usr/include/R
```

The first line was needed to pick up **-lcuda**, as with **gputools**. The second line was needed to acquire the file **cutil.h** in the NVIDIA SDK, which I had installed earlier at the location see above.

For the third line, I made a file **z.c** consisting solely of the line

```
1  #include <R.h>
```

and ran

```
1  R CMD SHLIB z.c
```

just to see whether the R include file was.

As of May 2010, the routines in **rgpu** are much less extensive than those of **gputools**. However, one very nice feature of **rgpu** is that one can compute matrix expressions without bringing intermediate results back from the device memory to the host memory, which would be a big slowdown. Here for instance is how to compute the square of the matrix **m**, plus itself:

```
1  > m2m <- evalgpu(m %*% m + m)
```

9.9   Parallelism Via Calling C from R

Parallel R aims to be faster than ordinary R. But even if that aim is achieved, it's still R, and thus potentially slow.

One must always decide how much effort one is willing to devote to optimization. For the fastest code, we should not write in C, but rather in assembly language. Similarly, one must decide whether to stick purely to R, or go to the faster C. If parallel R gives you the speed you need in your application, fine; if not, though, you should consider writing part of your application in C, with the main part still written in R. You may find that placing the parallelism in the C portion of your code is good enough, while retaining the convenience of R for the rest of your code.

9.9.1   Calling C from R

In C, two-dimensional arrays are stored in row-major order, in contrast to R's column-major order. For instance, if we have a 3x4 array, the element in the second row and second column is element number

5 of the array when viewed linearly, since there are three elements in the first column and this is the second element in the second column. Of course, keep in mind that C subscripts begin at 0, rather than at 1 as with R. In writing your C code to be interfaced to R, you must keep these issues in mind.

All the arguments passed from R to C are received by C as pointers. Note that the C function itself must return `void`. Values that we would ordinarily return must in the R/C context be communicated through the function's arguments, such as `result` in our example below.

9.9.2 Example: Extracting Subdiagonals of a Matrix

As an example, here is C code to extract subdiagonals from a square matrix.[9] The code is in a file **sd.c**:

```
// arguments:
// m: a square matrix
// n: number of rows/columns of m
// k: the subdiagonal index--0 for main diagonal, 1 for first
// subdiagonal, 2 for the second, etc.
// result: space for the requested subdiagonal, returned here

void subdiag(double *m, int *n, int *k, double *result)
{
  int nval = *n, kval = *k;
  int stride = nval + 1;
  for (int i = 0, j = kval; i < nval-kval; ++i, j+= stride)
    result[i] = m[j];
}
```

For convenience, you can compile this by rubnning R in a terminal window, which will invoke GCC:

```
% R CMD SHLIB sd.c
gcc -std=gnu99 -I/usr/share/R/include -fpic -g -O2 -c sd.c -o sd.o
gcc -std=gnu99 -shared -o sd.so sd.o -L/usr/lib/R/lib -lR
```

---

[9]I wish to thank my former graduate assistant, Min-Yu Huang, who wrote an earlier version of this function.

Note that here R showed us exactly what it did in invoking GCC. This allows us to do some customization.

But note that this simply produced a dynamic library, **sd.o**, not an executable program. (On Windows this would presumably be a **.dll** file.) So, how is it executed? The answer is that it is loaded into R, using R's **dyn.load()** function. Here is an example:

```
> dyn.load("sd.so")
> m <- rbind(1:5, 6:10, 11:15, 16:20, 21:25)
> k <- 2
> .C("subdiag", as.double(m), as.integer(dim(m)[1]), as.integer(k),
result=double(dim(m)[1]-k))
[[1]]
 [1] 1 6 11 16 21 2 7 12 17 22 3 8 13 18 23 4 9 14 19 24 5 10 15 20 25

[[2]]
[1] 5

[[3]]
[1] 2

$result
[1] 11 17 23
```

Note that we needed to allocate space for `result` in our call, in a variable we've named `result`. The value placed in there by our function is seen above to be correct.

9.9.3　Calling C OpenMP Code from R

Since OpenMP is usable from C, that makes it in turn usable from R. (See Chapter 4 for a detailed discussion of OpenMP.)

The code is compiled and then loaded into R as in Section 9.9, though with the additional step of specifying the `-fopenmp` command-line option in both invocations of GCC (which you run by hand, instead of using **R CMD SHLIB**).

9.9.4   Calling CUDA Code from R

The same principles apply here, but one does have to be careful with libraries and the like.

As before, we want to compile not to an executable file, but to a dynamic library file. Here's how, for the C file **mutlinksforr.cu** presented in the next section, the compile command is

```
pc41:~% nvcc -g -G -I/usr/local/cuda/include -Xcompiler
   "-I/usr/include/R -fpic" -c mutlinksforr.cu -o mutlinks.o -arch=sm_11
pc41:~% nvcc -shared -Xlinker "-L/usr/lib/R/lib -lR"
   -L/usr/local/cuda/lib mutlinks.o -o meanlinks.so
```

The product of this was **meanlinks.so**. I then tested it on R:

```
> dyn.load("meanlinks.so")
> m <- rbind(c(0,1,1,1),c(1,0,0,1),c(1,0,0,1),c(1,1,1,0))
> ma <- rbind(c(0,1,0),c(1,0,0),c(1,0,0))
> .C("meanout",as.integer(m),as.integer(4),mo=double(1))
[[1]]
 [1] 0 1 1 1 1 0 0 1 1 0 0 1 1 1 1 0

[[2]]
[1] 4

$mo
[1] 1.333333

> .C("meanout",as.integer(ma),as.integer(3),mo=double(1))
[[1]]
[1] 0 1 1 1 0 0 0 0 0

[[2]]
[1] 3

$mo
[1] 0.3333333
```

9.9.5　Example: Mutual Outlinks

We again take as our example the mutual-outlinks example from Section **??**. Here is an R/CUDA version:

```
1  // CUDA example: finds mean number of mutual outlinks, among all pairs
2  // of Web sites in our set
3
4  #include <cuda.h>
5  #include <stdio.h>
6
7  // the following is needed to avoid variable name mangling
8  extern "C" void meanout(int *hm, int *nrc, double *meanmut);
9
10 // for a given thread number tn, calculates pair, the (i,j) to be
11 // processed by that thread; for nxn matrix
12 __device__ void findpair(int tn, int n, int *pair)
13 { int sum=0,oldsum=0,i;
14    for(i=0; ;i++) {
15       sum += n - i - 1;
16       if (tn <= sum-1) {
17          pair[0] = i;
18          pair[1] = tn - oldsum + i + 1;
19          return;
20       }
21       oldsum = sum;
22    }
23 }
24
25 // proc1pair() processes one pair of Web sites, i.e. one pair of rows in
26 // the nxn adjacency matrix m; the number of mutual outlinks is added to
27 // tot
28 __global__ void proc1pair(int *m, int *tot, int n)
29 {
```

```
30      // find (i,j) pair to assess for mutuality
31      int pair[2];
32      findpair(threadIdx.x,n,pair);
33      int sum=0;
34      // make sure to account for R being column-major order; R's i-th row
35      // is our i-th column here
36      int startrowa = pair[0],
37          startrowb = pair[1];
38      for (int k = 0; k < n; k++)
39         sum += m[startrowa + n*k] * m[startrowb + n*k];
40      atomicAdd(tot,sum);
41   }
42
43   // meanout() is called from R
44   // hm points to the link matrix, nrc to the matrix size, meanmut to the output
45   void meanout(int *hm, int *nrc, double *meanmut)
46   {
47      int n = *nrc,msize=n*n*sizeof(int);
48      int *dm, // device matrix
49          htot, // host grand total
50          *dtot; // device grand total
51      cudaMalloc((void **)&dm,msize);
52      cudaMemcpy(dm,hm,msize,cudaMemcpyHostToDevice);
53      htot = 0;
54      cudaMalloc((void **)&dtot,sizeof(int));
55      cudaMemcpy(dtot,&htot,sizeof(int),cudaMemcpyHostToDevice);
56      dim3 dimGrid(1,1);
57      int npairs = n*(n-1)/2;
58      dim3 dimBlock(npairs,1,1);
59      proc1pair<<<dimGrid,dimBlock>>>(dm,dtot,n);
60      cudaThreadSynchronize();
61      cudaMemcpy(&htot,dtot,sizeof(int),cudaMemcpyDeviceToHost);
62      *meanmut = htot/double(npairs);
```

```
63      cudaFree(dm);
64      cudaFree(dtot);
65   }
```

The code is hardly optimal. We should, for instance, have more than one thread per block.

9.10   Debugging R Applications

The built-in debugging facilities in R are primitive, but alternatives are available.

9.10.1   Text Editors

However, if you are a Vim editor fan, I've developed a tool that greatly enhances the power of R's debugger. Download **edtdbg** from R's CRAN repository. It's also available for Emacs.

Vitalie Spinu's `ess-tracebug` runs under Emacs. It was modeled roughly on `edtdbg`, but has more Emacs-specific features than does `edtdbg`.

9.10.2   IDEs

I'm personally not a fan of IDEs, but some excellent ones are available.

REvolution Analytics, a firm that offers R consulting and develops souped-up versions of R, offers an IDE for R that includes nice debugging facilities. It is only available on Windows, and even then only for those who have Microsoft Visual Studio.

The developers of StatET, a platform-independent Eclipse-based IDE for R added a debugging tool in May 2011.

The people developing RStudio, another a platform-independent IDE for R, also plan to begin work on a debugger, beginning summer 2011.

9.10.3   The Problem of Lack of a Terminal

Parallel R packages such as **Rmpi**, **snow**, **foreach** and so on do not set up a terminal for each process, thus making it impossible to use R's debugger on the workers. What then can one do to debug apps for those packages? Let's consider **snow** for concreteness.

First, one should debug the underlying single-worker function, such as **mtl()** in our mutual outlinks example in Section 9.5.6. Here one would set up some artificial values of the arguments, and then use R's ordinary debugging facilities.

This may be sufficient. However, the bug may be in the arguments themselves, or in the way we set them up. Then things get more difficult. It's hard to even print out trace information, e.g. values of variables, since **print()** won't work in the worker processes. The **message()** function may work for some of these packages; if not, you may have to resort to using **cat()** to write to a file.

Rdsm allows full debugging, as there is a separate terminal window for each process.

9.10.4   Debugging C Called from R

For parallel R that is implemented via R calls to C code, producing a dynamically-loaded library as in Section 9.9, debugging is a little more involved. First start R under GDB, then load the library to be debugged. At this point, R's interpreter will be looping, anticipating reading an R command from you. Break the loop by hitting ctrl-c, which will put you back into *GDB's* interpreter. Then set a breakpoint at the C function you want to debug, say **subdiag()** in our example above. Finally, tell GDB to continue, and it will then stop in your function! Here's how your session will look:

```
1  $ R -d gdb
2  GNU gdb 6.8-debian
3  ...
4  (gdb) run
5  Starting program: /usr/lib/R/bin/exec/R
6  ...
7  > dyn.load("sd.so")
```

9.11   Other R Examples in This Book

See these examples (some nonparallel):
in Sections 11.5.4, 13.2.1 (nonparallel) and 13.5.1 (nonparallel).

- Parallel Jacobi iteration of linear equations, Section 11.5.4.
- Matrix computation of 1-D FFT, Section 13.2.1 (can paralleliza using parallel matrix multiplication).
- Parallel computation of 2-D FFT, Section 13.4.1.
- Image smoothing, Section 13.5.1.

第 10 章　The Parallel Prefix Problem

An operation that arises in a variety of parallel algorithms is that of *prefix* (or *scan*). In its abstract form, it inputs a sequence of objects $(x_0, ..., x_{n-1})$, and outputs $(s_0, ..., s_{n-1})$, where

$$
\begin{aligned}
s_0 &= x_0, \\
s_1 &= x_0 \otimes x_1, \\
&..., \\
s_{n-1} &= x_0 \otimes x_1 \otimes ... \otimes x_{n-1}
\end{aligned}
\tag{10.1}
$$

where $\otimes$ is some associative operator.

That's pretty abstract. The most concrete example would be that in which $\otimes$ is + and the objects are numbers. The scan of (12,5,13) would then be (12,12+5,12+5+13) = (12,17,30).

This is called an **inclusive** scan, in which x_i is included in s_i. The **exclusive** version of the above example would be (0,12,17).

Prefix scan has become a popular tool in the parallel processing community, applicable in a surprising variety of situations. Various examples will arise in succeeding chapters, but we'll present one in the next section in order to illustrate the versatility of the prefix approach.

10.1　Example: Permutations

Say we have the vector (12,5,13,8,88). Applying the permutation (2,0) would say the old element 0 becomes element 2, the old element 2 becomes element 0, and all the rest stay the same. The result would be (13,5,12,8,88). If we then applied the permutation (1,2,4), it would mean that element 1 goes to position 2, 2 goes to 4, and 4 goes to 1, with everything else staying put. Our new vector would then be (13,88,5,8,12).

This too can be cast in matrix terms, by representing any permutation as a matrix multiplication.

We just apply the permutation to the identity matrix I, and then postmultiply the (row) vector by the matrix. For instance, the matrix corresponding to the permutation (1,2,4) is

$$
\begin{pmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}
\tag{10.2}
$$

so applying (1,2,4) to (12,5,13,8,88) above can be done as

$$
(12, 5, 13, 8, 88)
\begin{pmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}
= (13, 5, 12, 8, 88)
\tag{10.3}
$$

So in terms of (10.1), x_0 would be the identity matrix, x_i for i > 0 would be the ith permutation matrix, and $\otimes$ would be matrix multiplication.

Note, however, that although we've couched the problem in terms of matrix multiplication, these are *sparse* matrices, i.e. have many 0s. Thus a general parallel matrix-multiply routine may not be efficient, and special parallel methods for sparse matrices should be used (Section 11.7).

Note that the above example shows that in finding a scan,

- the elements might be nonscalars
- the associative operator need not be commutative

10.2 General Strategies for Parallel Scan Computation

For the time being, we'll assume we have n threads, i.e. one for each datum. Clearly this condition will often not hold, so we'll extend things later.

We'll describe what is known as a *data parallel* solution to the prefix problem.

Here's the basic idea, say for n = 8:

Step 1:

$$x_1 \quad \leftarrow \quad x_0 + x_1 \tag{10.4}$$

$$x_2 \quad \leftarrow \quad x_1 + x_2 \tag{10.5}$$

$$x_3 \quad \leftarrow \quad x_2 + x_3 \tag{10.6}$$

$$x_4 \quad \leftarrow \quad x_3 + x_4 \tag{10.7}$$

$$x_5 \quad \leftarrow \quad x_4 + x_5 \tag{10.8}$$

$$x_6 \quad \leftarrow \quad x_5 + x_6 \tag{10.9}$$

$$x_7 \quad \leftarrow \quad x_6 + x_7 \tag{10.10}$$

Step 2:

$$x_2 \quad \leftarrow \quad x_0 + x_2 \tag{10.11}$$

$$x_3 \quad \leftarrow \quad x_1 + x_3 \tag{10.12}$$

$$x_4 \quad \leftarrow \quad x_2 + x_4 \tag{10.13}$$

$$x_5 \quad \leftarrow \quad x_3 + x_5 \tag{10.14}$$

$$x_6 \quad \leftarrow \quad x_4 + x_6 \tag{10.15}$$

$$x_7 \quad \leftarrow \quad x_5 + x_7 \tag{10.16}$$

Step 3:

$$x_4 \quad \leftarrow \quad x_0 + x_4 \tag{10.17}$$

$$x_5 \quad \leftarrow \quad x_1 + x_5 \tag{10.18}$$

$$x_6 \quad \leftarrow \quad x_2 + x_6 \tag{10.19}$$

$$x_7 \quad \leftarrow \quad x_3 + x_7 \tag{10.20}$$

In Step 1, we look at elements that are 1 apart, then Step 2 considers the ones that are 2 apart, then 4 for Step 3.

Why does this work? Well, consider how the contents of x_7 evolve over time. Let a_i be the original x_i, i = 0,1,...,n-1. Then here is x_7 after the various steps:

step	contents
1	$a_6 + a_7$
2	$a_4 + a_5 + a_6 + a_7$
3	$a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6 + a_7$

Similarly, after Step 3, the contents of x_7 will be $a_0 + a_1 + a_2 + a_3 + a_4 + a_5 + a_6$ (check it!). So, in the end, the locations of x_i will indeed contain the prefix sums.

For general n, the routing is as follows. At Step i, each x_j is routed both to itself and to $x_{j+2^{i-1}}$, for $j >= 2^{i-1}$. (Some threads, more in each successive step, are idle.)

There will be $log_2 n$ steps, or if n is not a power of 2, case the number of steps is $\lfloor log_2 n \rfloor$.

Note two important points:

- The location x_i appears both as an input and an output in the assignment operations above. In our implementation, we need to take care that the location is not written to before its value is read. One way to do this is to set up an auxiliary array y_i. In odd-numbered steps, the y_i are written to with the x_i as inputs, and vice versa for the even-numbered steps.

- As noted above, as time goes on, more and more threads are idle. Thus load balancing is poor.

- Synchronization at each step incurs overhead in a multicore/multiprocessr setting. (Worse for GPU if multiple blocks are used).

Now, what if n is greater than p, our number of threads? Let Ti denote thread i. The standard approach is that taken in Section 5.10:

```
1  break the array into p blocks
2  parallel for i = 0,...,p-1
3    Ti does scan of block i, resulting in Si
4  form new array G of rightmost elements of each Si
5  do parallel scan of G
6  parallel for i = 1,...,p-1
7    Ti adds Gi to each element of block i
```

For example, say we have the array

```
1  2 25 26 8 50 3 1 11 7 9 29 10
```

and three threads. We break the data into three sections,

2 25 26 8	50 3 1 11	7 9 29 10

and then apply a scan to each section:

2 27 53 61	50 53 54 65	7 16 45 55

But we still don't have the scan of the array overall. That 50, for instance, should be $61+50 = 111$ and the 53 should be $61+53 = 114$. In other words, 61 must be added to that second section, $(50,53,54,65)$, and $61+65 = 126$ must be added to the third section, $(7,16,45,55)$. This then is the last step, yielding

2 27 53 61	111 114 115 126	133 142 171 181

Another possible approach would be make n "fake" threads FTj. Each Ti plays the role of n/p of the FTj. The FTj then do the parallel scan as at the beginning of this section. Key point: Whenever a Ti becomes idle, it is assigned to help other Tk.

10.3   Implementations

The MPI standard actually includes built-in parallel prefix functions, **MPI_Scan()**. A number of choices are offered for $\otimes$, such as maximum, minimum, sum, product etc.

The Thrust library for CUDA or OpenMP includes functions **thrust::inclusive_scan()** and **thrust::exclusive_scan()**.

The CUDPP (CUDA Data Parallel Primitives Library) package contains CUDA functions for sorting and other operations, many of which are based on parallel scan. See `http://gpgpu.org/developer/cudpp` for the library code, and a detailed analysis of optimizing parallel prefix in a GPU context in the book *GPU Gems 3*, available either in bookstores or free online at `http://developer.nvidia.com/object/gpu_gems_home.html`.

10.4   Example: Parallel Prefix, Run-Length Decoding in OpenMP

Here an OpenMP implementation of the approach described at the end of Section 10.2, for addition:

```
1  #include <omp.h>
2
3  // calculates prefix sums sequentially on u, in-place, where u is an
4  // m-element array
5  void seqprfsum(int *u,int m)
6  { int i,s=u[0];
7    for (i = 1; i < m; i++) {
```

```
8       u[i] += s;
9       s = u[i];
10    }
11  }
12
13  // OMP example, calculating prefix sums in parallel on the n-element
14  // array x, in-place; for simplicity, assume that n is divisible by the
15  // number of threads; z is for intermediate storage, an array with length
16  // equal to the number of threads; x and z point to global arrays
17  void parprfsum(int *x, int n, int *z)
18  {
19    #pragma omp parallel
20    { int i,j,me = omp_get_thread_num(),
21         nth = omp_get_num_threads(),
22         chunksize = n / nth,
23         start = me * chunksize;
24      seqprfsum(&x[start],chunksize);
25      #pragma omp barrier
26      #pragma omp single
27      {
28      for (i = 0; i < nth-1; i++)
29        z[i] = x[(i+1)*chunksize - 1];
30      seqprfsum(z,nth-1);
31      }
32      if (me > 0) {
33        for (j = start; j < start + chunksize; j++) {
34          x[j] += z[me - 1];
35        }
36      }
37    }
38  }
```

Here is an example of use: A method for compressing data is to store only repeat counts in *runs*, where the latter means a set of consecutive, identical values. For instance, the sequence 2,2,2,0,0,5,0,0

would be compressed to 3,2,2,0,1,5,2,0, meaning that the data consist of first three 2s, then two 0s, then one 5, and finally two 0s. Note that the compressed version consists of alternating *run counts* and *run values*, respectively 2 and 0 at the end of the above example.

To solve this in OpenMP, we'll first call the above functions to decide where to place the runs in our overall output.

```c
void uncomprle(int *x,int nx,int *tmp,int *y,int *ny)
{
   int i,nx2 = nx/2;
   int z[MAXTHREADS];
   for (i = 0; i < nx2; i++) tmp[i+1] = x[2*i];
   parprfsum(tmp+1,nx2+1,z);
   tmp[0] = 0;
   #pragma omp parallel
   { int j,k;
     int me=omp_get_thread_num();
     #pragma omp for
     for (j = 0; j < nx2; j++) {
       // where to start the j-th run?
       int start = tmp[j];
       // what value is in the run?
       int val = x[2*j+1];
       // how long is the run?
       int nrun = x[2*j];
       for (k = 0; k < nrun; k++)
         y[start+k] = val;
     }
   }
   *ny = tmp[nx2];
}
```

10.5   Example: Run-Length Decompression in Thrust

Here's how we could do the first part of the operation above, i.e. determining where to place the runs in our overall output, in Thrust:

```
#include <stdio.h>
#include <thrust/device_vector.h>
#include <thrust/scan.h>
#include <thrust/sequence.h>
#include <thrust/remove.h>

struct iseven {
   bool operator()(const int i)
   { return (i % 2) == 0;
   }
};

int main()
{ int i;
   int x[12] = {2,3,1,9,3,5,2,6,2,88,1,12};
   int nx = 12;
   thrust::device_vector<int> out(nx);
   thrust::device_vector<int> seq(nx);
   thrust::sequence(seq.begin(),seq.end(),0);
   thrust::device_vector<int> dx(x,x+nx);
   thrust::device_vector<int>::iterator newend =
      thrust::copy_if(dx.begin(),dx.end(),seq.begin(),out.begin(),iseven());
   thrust::inclusive_scan(out.begin(),out.end(),out.begin());
   // "out" should be 2,2+1 = 3,2+1+3=6,...
   thrust::copy(out.begin(), newend,
      std::ostream_iterator<int>(std::cout, " "));
   std::cout << "\n";
}
```

第 11 章 Introduction to Parallel Matrix Operations

11.1 "We're Not in Physicsland Anymore, Toto"

In the early days parallel processing was mostly used in physics problems. Typical problems of interest would be grid computations such as the heat equation, matrix multiplication, matrix inversion (or equivalent operations) and so on. These matrices are not those little 3x3 toys you worked with in your linear algebra class. In parallel processing applications of matrix algebra, our matrices can have thousands of rows and columns, or even larger.

The range of applications of parallel processing is of course far broader today, such as image processing, social networks and data mining. Google employs a number of linear algebra experts, and they deal with matrices with literally millions of rows or columns.

We assume for now that the matrices are **dense**, meaning that most of their entries are nonzero. This is in contrast to **sparse** matrices, with many zeros. Clearly we would use differents type of algorithms for sparse matrices than for dense ones. We'll cover sparse matrices a bit in Section 11.7.

11.2 Partitioned Matrices

Parallel processing of course relies on finding a way to partition the work to be done. In the matrix algorithm case, this is often done by dividing a matrix into blocks (often called **tiles** these days).

For example, let

$$A = \left(\begin{array}{ccc} 1 & 5 & 12 \\ 0 & 3 & 6 \\ 4 & 8 & 2 \end{array} \right) \tag{11.1}$$

and

$$B = \begin{pmatrix} 0 & 2 & 5 \\ 0 & 9 & 10 \\ 1 & 1 & 2 \end{pmatrix}, \tag{11.2}$$

so that

$$C = AB = \begin{pmatrix} 12 & 59 & 79 \\ 6 & 33 & 42 \\ 2 & 82 & 104 \end{pmatrix}. \tag{11.3}$$

We could partition A as

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}, \tag{11.4}$$

where

$$A_{00} = \begin{pmatrix} 1 & 5 \\ 0 & 3 \end{pmatrix}, \tag{11.5}$$

$$A_{01} = \begin{pmatrix} 12 \\ 6 \end{pmatrix}, \tag{11.6}$$

$$A_{10} = \begin{pmatrix} 4 & 8 \end{pmatrix} \tag{11.7}$$

and

$$A_{11} = \begin{pmatrix} 2 \end{pmatrix}. \tag{11.8}$$

Similarly we would partition B and C into blocks of a compatible size to A,

$$B = \begin{pmatrix} B_{00} & B_{01} \\ B_{10} & B_{11} \end{pmatrix} \tag{11.9}$$

and

$$C = \begin{pmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{pmatrix}, \tag{11.10}$$

so that for example

$$B_{10} = \left(\begin{array}{cc} 1 & 1 \end{array} \right). \tag{11.11}$$

The key point is that multiplication still works if we pretend that those submatrices are numbers! For example, pretending like that would give the relation

$$C_{00} = A_{00}B_{00} + A_{01}B_{10}, \tag{11.12}$$

which the reader should verify really is correct as matrices, i.e. the computation on the right side really does yield a matrix equal to C_{00}.

11.3　Parallel Matrix Multiplication

Since so many parallel matrix algorithms rely on matrix multiplication, a core issue is how to parallelize that operation.

Let's suppose for the sake of simplicity that each of the matrices to be multiplied is of dimensions n x n. Let p denote the number of "processes," such as shared-memory threads or message-passing nodes.

11.3.1　Message-Passing Case

For concreteness here and in other sections below on message passing, assume we are using MPI.

The obvious plan of attack here is to break the matrices into blocks, and then assign different blocks to different MPI nodes. Assume that $\sqrt{p}$ evenly divides n, and partition each matrix into submatrices of size $n/\sqrt{p}$ x $n/\sqrt{p}$. In other words, each matrix will be divided into m rows and m columns of blocks, where $m = n/\sqrt{p}$.

One of the conditions assumed here is that the matrices A and B are stored in a distributed manner across the nodes. This situation could arise for several reasons:

- The application is such that it is natural for each node to possess only part of A and B.
- One node, say node 0, originally contains all of A and B, but in order to conserve communication time, it sends each node only parts of those matrices.
- The entire matrix would not fit in the available memory at the individual nodes.

As you'll see, the algorithms then have the nodes passing blocks among themselves.

Fox's Algorithm

Consider the node that has the responsibility of calculating block (i,j) of the product C, which it calculates as

$$A_{i0}B_{0j} + A_{i1}B_{1j} + ... + A_{ii}B_{ij} + ... + A_{i,m-1}B_{m-1,j} \tag{11.13}$$

Rearrange this with A_{ii} first:

$$A_{ii}B_{ij} + A_{i,i+1}B_{,i+1j} + ... + A_{i,m-1}B_{m-1,j} + A_{i0}B_{0j} + A_{i1}B_{1j} + ... + A_{i,i-1}B_{i-1,j} \tag{11.14}$$

Written more compactly, this is

$$\sum_{k=0}^{m-1} A_{i,(i+k)mod\ m}B_{(i+k)mod\ m,j} \tag{11.15}$$

In other words, start with the A_{ii} term, then go across row i of A, wrapping back up to the left end when you reach the right end. The order of summation in this rearrangement will be the actual order of computation. It's similar for B, in column j.

The algorithm is then as follows. The node which is handling the computation of C_{ij} does this (in parallel with the other nodes which are working with their own values of i and j):

```
1  iup = i+1 mod m;
2  idown = i-1 mod m;
3  for (k = 0; k < m; k++) {
4     km = (i+k) mod m;
5     broadcast(A[i,km]) to all nodes handling row i of C;
6     C[i,j] = C[i,j] + A[i,km]*B[km,j]
7     send B[km,j] to the node handling C[idown,j]
8     receive new B[km+1 mod m,j] from the node handling C[iup,j]
9  }
```

The main idea is to have the various computational nodes repeatedly exchange submatrices with each other, timed so that a node receives the submatrix it needs for its computation "just in time."

This is Fox's algorithm. Cannon's algorithm is similar, except that it does cyclical rotation in both rows and columns, compared to Fox's rotation only in columns but broadcast within rows.

The algorithm can be adapted in the obvious way to nonsquare matrices, etc.

Performance Issues

Note that in MPI we would probably want to implement this algorithm using communicators. For example, this would make broadcasting within a block row more convenient and efficient.

Note too that there is a lot of opportunity here to overlap computation and communication, which is the best way to solve the communication problem. For instance, we can do the broadcast above at the same time as we do the computation.

Obviously this algorithm is best suited to settings in which we have PEs in a mesh topology. This includes hypercubes, though one needs to be a little more careful about communications costs there.

11.3.2   Shared-Memory Case

Example: Matrix Multiply in OpenMP

Since a matrix multiplication in serial form consists of nested loops, a natural way to parallelize the operation in OpenMP is through the **for** pragma, e.g.

```
1  #pragma omp parallel for
2  for (i = 0; i < ncolsa; i++)
3    for (j = 0; i < nrowsb; j++) {
4      sum = 0;
5      for (k = 0; i < ncolsa; i++)
6        sum += a[i][k] * b[k][j];
7    }
```

This would parallelize the outer loop, and we could do so at deeper nesting levels if profitable.

Example: Matrix Multiply in CUDA

Given that CUDA tends to work better if we use a large number of threads, a natural choice is for each thread to compute one element of the product, like this:

```
1  __global__ void matmul(float *ma,float *mb,float *mc,int nrowsa,
2    int ncolsa,int ncolsb, float *total)
3  { int k,i,j; float sum;
4    // find i,j according to thread and block ID
5    sum = 0;
```

```
6    for (k = 0; k < ncolsa; k++)
7        sum += a[i*ncolsa+k] * b[k*ncols+j];
8    *total = sum;
9  }
```

This should produce a good speedup. But we can do even better, much much better.

The CUBLAS package includes very finely-tuned algorithms for matrix multiplication. The CUBLAS source code is not public, though, so in order to get an idea of how such tuning might be done, let's look at Prof. Richard Edgar's algorithm, which makes use of shared memory. (Actually, this may be what CUBLAS uses.)

```
1  __global__ void MultiplyOptimise(const float *A, const float *B, float *C) {
2    // Extract block and thread numbers
3    int bx = blockIdx.x; int by = blockIdx.y;
4    int tx = threadIdx.x; int ty = threadIdx.y;
5
6    // Index of first A sub-matrix processed by this block
7    int aBegin = dc_wA * BLOCK_SIZE * by;
8    // Index of last A sub-matrix
9    int aEnd = aBegin + dc_wA - 1;
10   // Stepsize of A sub-matrices
11   int aStep = BLOCK_SIZE;
12   // Index of first B sub-matrix
13   // processed by this block
14   int bBegin = BLOCK_SIZE * bx;
15   // Stepsize for B sub-matrices
16   int bStep = BLOCK_SIZE * dc_wB;
17   // Accumulator for this thread
18   float Csub = 0;
19   for(int a = aBegin, b = bBegin; a <= aEnd; a += aStep, b+= bStep) {
20     // Shared memory for sub-matrices
21     __shared__ float As[BLOCK_SIZE][BLOCK_SIZE];
22     __shared__ float Bs[BLOCK_SIZE][BLOCK_SIZE];
23     // Load matrices from global memory into shared memory
24     // Each thread loads one element of each sub-matrix
```

```
25       As[ty][tx] = A[a + (dc_wA * ty) + tx];
26       Bs[ty][tx] = B[b + (dc_wB * ty) + tx];
27       // Synchronise to make sure load is complete
28       __syncthreads();
29       // Perform multiplication on sub-matrices
30       // Each thread computes one element of the C sub-matrix
31       for( int k = 0; k < BLOCK_SIZE; k++ ) {
32          Csub += As[ty][k] * Bs[k][tx];
33       }
34      // Synchronise again
35      __syncthreads();
36     }
37     // Write the C sub-matrix back to global memory
38     // Each thread writes one element
39     int c = (dc_wB * BLOCK_SIZE * by) + (BLOCK_SIZE*bx);
40     C[c + (dc_wB*ty) + tx] = Csub;
41 }
```

Here are the relevant portions of the calling code, including defined constants giving the number of columns ("width") of the multiplier matrix and the number of rows ("height") of the multiplicand:

```
1  #define BLOCK_SIZE 16
2  ...
3  __constant__ int dc_wA;
4  __constant__ int dc_wB;
5  ...
6  // Sizes must be multiples of BLOCK_SIZE
7  dim3 threads(BLOCK_SIZE,BLOCK_SIZE);
8  dim3 grid(wB/BLOCK_SIZE,hA/BLOCK_SIZE);
9  MultiplySimple<<<grid,threads>>>(d_A, d_B, d_C);
10  ...
```

(Note the alternative way to configure threads, using the functions **threads()** and **grid()**.)

Here the the term "block" in the defined value **BLOCK_SIZE** refers both to blocks of threads and the partitioning of matrices. In other words, a thread block consists of 256 threads, to be thought of as a 16x16 "array" of threads, and each matrix is partitioned into submatrices of size 16x16.

In addition, in terms of grid configuration, there is again a one-to-one correspondence between thread blocks and submatrices. Each submatrix of the product matrix C will correspond to, and will be computed by, one block in the grid.

We are computing the matrix product C = AB. Denote the elements of A by a_{ij} for the element in row i, column j, and do the same for B and C. Row-major storage is used.

Each thread will compute one element of C, i.e. one c_{ij}. It will do so in the usual way, by multiplying column j of B by row i of A. However, the key issue is how this is done in concert with the other threads, and the timing of what portions of A and B are in shared memory at various times.

Concerning the latter, note the code

```
1   for(int a = aBegin, b = bBegin; a <= aEnd; a += aStep, b+= bStep) {
2       // Shared memory for sub-matrices
3       __shared__ float As[BLOCK_SIZE][BLOCK_SIZE];
4       __shared__ float Bs[BLOCK_SIZE][BLOCK_SIZE];
5       // Load matrices from global memory into shared memory
6       // Each thread loads one element of each sub-matrix
7       As[ty][tx] = A[a + (dc_wA * ty) + tx];
8       Bs[ty][tx] = B[b + (dc_wB * ty) + tx];
```

Here we loop across a row of submatrices of A, and a column of submatrices of B, calculating one submatrix of C. In each iteration of the loop, we bring into shared memory a new submatrix of A and a new one of B. Note how even this copying from device global memory to device shared memory is shared among the threads.

As an example, suppose

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 7 & 8 & 9 & 10 & 11 & 12 \end{pmatrix} \tag{11.16}$$

and

$$
B = \begin{pmatrix}
1 & 2 & 3 & 4 \\
5 & 6 & 7 & 8 \\
9 & 10 & 11 & 12 \\
13 & 14 & 15 & 16 \\
17 & 18 & 19 & 20 \\
21 & 22 & 23 & 24
\end{pmatrix}
\tag{11.17}
$$

Further suppose that **BLOCK_SIZE** is 2. That's too small for good efficiency—giving only four threads per block rather than 256—but it's good for the purposes of illustration.

Let's see what happens when we compute C_{00}, the 2x2 submatrix of C's upper-left corner. Due to the fact that partitioned matrices multiply "just like numbers," we have

$$
\begin{align}
C_{00} &= A_{00}B_{00} + A_{01}B_{10} + A_{02}B_{20} \tag{11.18} \\
&= \begin{pmatrix} 1 & 2 \\ 7 & 8 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 5 & 6 \end{pmatrix} + ... \tag{11.19}
\end{align}
$$

Now, all this will be handled by thread block number (0,0), i.e. the block whose X and Y "coordinates" are both 0. In the first iteration of the loop, A_{11} and B_{11} are copied to shared memory for that block, then in the next iteration, A_{12} and B_{21} are brought in, and so on.

Consider what is happening with thread number (1,0) within that block. Remember, its ultimate goal is to compute c_{21} (adjusting for the fact that in math, matrix subscripts start at 1). In the first iteration, this thread is computing

$$
\begin{pmatrix} 1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 5 \end{pmatrix} = 11
\tag{11.20}
$$

It saves that 11 in its running total **Csub**, eventually writing it to the corresponding element of C:

```
1  int c = (dc_wB * BLOCK_SIZE * by) + (BLOCK_SIZE*bx);
2  C[c + (dc_wB*ty) + tx] = Csub;
```

Professor Edgar found that use of shared device memory resulted a huge improvement, extending the original speedup of 20X to 500X!

11.3.3 R Snow

Section 1.3.4 showed how to parallelize a matrix-vector product computation in **snow**, by breaking the matrix rows into chunks, and then exploiting the tiling properties of matrices. Computation of matrix-matrix products can be done in the same way.

11.3.4 R Interfaces to GPUs

The most widely used of these is probability the **gputools** library. It includes various matrix routines, including **gpuMatMult()** for matrix multiplication.

11.4 Finding Powers of Matrices

In some applications, we are interested not just in multiplying two matrices, but rather in multiplying a matrix by itself, many times.

11.4.1 Example: Graph Connectedness

Let n denote the number of vertices in the graph. As before, define the graph's **adjacency matrix** A to be the n x n matrix whose element (i,j) is equal to 1 if there is an edge connecting vertices i an j (i.e. i and j are "adjacent"), and 0 otherwise.

Our ultimate goal here will be to compute the corresponding **reachability matrix** $R^{(k)}$ has its (i,j) element equal to 1 if there is some path from i to j taking k or fewer steps, and 0 otherwise. (Note that the notation "(k)" here is a superscript, not an exponent.) We would especially like to compute R, whose elements indicate whether one can *ever* reach one vertex starting at another. In particular, we may be interested in determining whether the graph is **connected**, meaning that every vertex eventually leads to every other vertex.

Toward that end, consider the matrix

$$
\begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}
\tag{11.21}
$$

Let's take our row/column numbering convention to start at 1, not 0.

Let's ask the question, Can we get from vertex 3 to vertex 1 in two steps? The answer is yes; indeed, there are two such paths:

$$3 \to 2 \to 1 \tag{11.22}$$

$$3 \to 4 \to 1 \tag{11.23}$$

If we were to answer this kind of question systematically, say for the number of two-step paths from i to j, we would evaluate the following boolean expression:

$$p(i \to 1 \to j) + p(i \to 2 \to j) + p(i \to 3 \to j) + p(i \to 4 \to j) \tag{11.24}$$

where $p()$ is equal to 1 if the postulated path exists, 0 if not.

But observe that

$$p(i \to k \to j) = a_{ik} \cdot a_{kj} \tag{11.25}$$

Thus the number of paths for a general $n \times n$ matrix A from vertex i to vertex j is

$$\sum_{i=1}^{n} a_{ik} \cdot a_{kj} \tag{11.26}$$

But this is the the (i,j) element of A^2! Moreover, this says that $R^{(2)} = b(A^2)$, where **b()** changes nonzero elements of a matrix to 1s, and retains the original 0s.

In general:

Theorem 1 *Suppose A is the adjacency matrix A for a graph. Then*

(a) The number of r-step paths from i to j is the (i,j) element of A^r.

(b)

$$R^{(k)} = b(A^k) \tag{11.27}$$

(c) Since the longest possible distinct path has length n-1, we have that the graph is connected if and only if each of the matrices $R^{(1)}, ..., R^{(n-1)}$ has all of its off-diagonal elements equal to 1.

*(d) Suppose the graph is undirected. Then **cycles** are possible, so we can keep coming back to a vertex. Thus the graph is connected if and only if some matrix among $R^{(1)}, ..., R^{(n-1)}$ has all of its off-diagonal elements equal to 1.*

So, the original graph connectivity problem reduces to a matrix problem. And (d) is especially interesting, as it means that if we do manage to find some $R^{(k)}$ that consists of all 1s (off the diagonal), our computation is done.

11.4.2   Example: Fibonacci Numbers

The basic problem is well known: Find the Fibonacci numbers f_n, where

$$f_0 = f_1 = 1 \tag{11.28}$$

and

$$f_n = f_{n-1} + f_{n-2}, \ n > 1 \tag{11.29}$$

The point is that (11.29) can be couched in matrix terms as

$$\begin{pmatrix} f_{n+1} \\ f_n \end{pmatrix} = A \begin{pmatrix} f_n \\ f_{n-1} \end{pmatrix} \tag{11.30}$$

where

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{11.31}$$

Given the initial conditions (11.28) and (11.30), we have

$$\begin{pmatrix} f_{n+1} \\ f_n \end{pmatrix} = A^{n-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{11.32}$$

In other words, our problem reduces to one of finding the powers $A, A^2, ..., A^{n-1}$.

11.4.3   Example: Matrix Inversion

Many applications make use of A^{-1} for an n x n square matrix A. In many cases, it is not computed directly, but here we address methods for direct computation.

We could use the methods of Section 11.5 to find matrix inverses, but there is alos a power series method.

Recall that for numbers x that are smaller than 1 in absolute value,

$$\frac{1}{1-x} = 1 + x + x^2 + ... \tag{11.33}$$

In algebraic terms, this would be that for an n x n matrix C,

$$(I - C)^{-1} = I + C + C^2 + ... \tag{11.34}$$

This can be shown to converge if

$$\max_{i,j} |c_{ij}| < 1 \tag{11.35}$$

To invert our matrix A, then, we can set C = I - A, giving us

$$A^{-1} = (I - C)^{-1} = I + C + C^2 + ... = I + (I - A) + (I - A)^2 + ... \tag{11.36}$$

To meet the convergence condition, we could set $\tilde{A} = dA$, where d is small enough so that (11.35) holds for $I - \tilde{A}$. This will be possible, if all the elements of A are nonnegative. We then find the inverse of dA, and in the end multiply by d to get the inverse of A.

11.4.4   Parallel Computation

So, how can we speed up the computation of matrix powers?

First, there is an important trick, useable even in the nonparallel case. Suppose we need to find only a single power, say A^{32}. We could do 31 multiplications. But a much faster approach would be to first calculate A^2, then square that result to get A^4, then square it to get A^8 and so on. That would get us A^{32} by applying a matrix multiplication algorithm only five times, instead of 31.

Now what if we need to find all powers, in certain range? Of course we can use the methods of Section 11.3, but actually we can do a bit better on some platforms, by exploiting the fact that both the multiplier and multiplicand are the same matrix, as follows:

Consider a situation in which we are using MPI, CUDA or **snow**, and we do matrix multiplication by some fixed tiling, say that of Section 11.3.3. Then instead of having the workers return their section of the product to the manager, just *keep those sections at the workers*. Because they are always multiplying by the same matrix, they can reuse that data, eliminating the large overhead of repeatedly shipping it back and forth between the manager and the workers.

11.5   Solving Systems of Linear Equations

Suppose we have a system of equations

$$a_{i0}x_0 + ... + a_{i,n-1}x_{n-1} = b_i, i = 0, 1, ..., n - 1, \tag{11.37}$$

where the x_i are the unknowns to be solved for.

As you know, this system can be represented compactly as

$$Ax = b, \tag{11.38}$$

where A is n x n and x and b is n x 1.

11.5.1   Gaussian Elimination

Form the n x (n+1) matrix C = (A | b) by appending the column vector b to the right of A. (It may be advantageous to add padding on the right of b.)

Then we work on the rows of C, with the pseudocode for the sequential case in the most basic version being

```
1   for ii = 0 to n-1
2     divide row ii by c[i][i]
3     for r = 0 to n-1, r != i
4       replace row r by row r - c[r][ii] times row ii
```

In the divide operation in the above pseudocode, c_{ii} might be 0, or close to 0. In that case, a **pivoting** operation is performed (not shown in the pseudocode): that row is first swapped with another one further down.

This transforms C to **reduced row echelon form**, in which A is now the identity matrix I and b is now our solution vector x.

A variation is to transform only to **row echelon form**. This means that C ends up in upper triangular form, with all the elements c_{ij} with $i > j$ being 0, and with all diagonal elements being equal to 1. Here is the pseudocode:

```
1   for ii = 0 to n-1
2     divide row ii by c[i][i]
3     for r = ii+1 to n-1 // vacuous if r = n-1
```

```
4        replace row r by row r - c[r][ii] times row ii
```

This corresponds to a new set of equations,

$$
\begin{aligned}
c_{00}x_0 + c_{11}x_1 + c_{22}x_2 + ... + c_{0,n-1}x_{n-1} &= b_0 \\
c_{11}x_1 + c_{22}x_2 + ... + c_{1,n-1}x_{n-1} &= b_1 \\
c_{22}x_2 + ... + c_{2,n-1}x_{n-1} &= b_2 \\
... \\
c_{n-1,n-1}x_{n-1} &= b_{n-1}
\end{aligned}
$$

We then find the x_i via **back substitution**:

```
1  x[n-1] = b[n-1] / c[n-1,n-1]
2  for i = n-2 downto 0
3    x[i] = (b[i] - c[i][n-1] * x[n-1] - ... - c[i][i+1] * x[i+1]) / c[i][i]
```

11.5.2 Example: Gaussian Elimination in CUDA

Here's CUDA code for the reduced row echelon form version, suitable for a not-extremely-large matrix:

```
1  // linear index for matrix element at row i, column j, in an m-column
2  // matrix
3  __device__ int onedim(int i,int j,int m) {return i*m+j;}
4
5  // replace u by c* u; vector of length m
6  __device__ void cvec(float *u, int m, float c)
7  { for (int i = 0; i < m; i++) u[i] = c * u[i]; }
8
9  // multiply the vector u of length m by the constant c (not changing u)
10 // and add the result to v
11 __device__ void vplscu(float *u, float *v, int m, float c)
12 { for (int i = 0; i < m; i++) v[i] += c * u[i]; }
13
14 // copy the vector u of length m to v
```

```
15  __device__ void cpuv(float *u, float *v, int m)
16  { for (int i = 0; i < m; i++) v[i] = u[i]; }
17
18  // solve matrix equation Ax = b; straight Gaussian elimination, no
19  // pivoting etc.; the matrix ab is (A|b), n rows; ab is destroyed, with
20  // x placed in the last column; one block, with thread i handling row i
21  __global__ void gauss(float *ab, int n)
22  { int i,n1=n+1,abii,abme;
23    extern __shared__ float iirow[];
24    int me = threadIdx.x;
25    for (i = 0; i < n; i++) {
26      if (i == me) {
27        abii = onedim(i,i,n1);
28        cvec(&ab[abii],n1-i,1/ab[abii]);
29        cpuv(&ab[abii],iirow,n1-i);
30      }
31      __syncthreads();
32      if (i != me) {
33        abme = onedim(me,i,n1);
34        vplscu(iirow,&ab[abme],n1-i,-ab[abme]);
35      }
36      __syncthreads();
37    }
38  }
```

Here we have one thread for each row, and are using just one block, so as to avoid interblock synchronization problems and to easily use shared memory. Concerning the latter, note that since the pivot row, **iirow**, is read many times, it makes sense to put it in shared memory.

Needless to say, the restriction to one block is quite significant. With a 512-thread limit per block, this would limit us to 512x512 matrices. But it's even worse than that—if shared memory is only 4K in size, in single precision that would mean something like 30x30 matrices! We could go to multiple blocks, at the cost of incurring synchronization delays coming from repeated kernel calls.

In a row echelon version of the code, we could have dynamic assignment of rows to threads, but still would eventually have load balancing issues.

11.5.3   The Jacobi Algorithm

One can rewrite (11.37) as

$$x_i = \frac{1}{a_{ii}}[b_i - (a_{i0}x_0 + ... + a_{i,i-1}x_{i-1} + a_{i,i+1}x_{i+1} + ... + a_{i,n-1}x_{n-1})], i = 0, 1, ..., n - 1. \qquad (11.39)$$

This suggests a natural iterative algorithm for solving the equations. We start with our guess being, say, $x_i = b_i$ for all i. At our k^{th} iteration, we find our $(k+1)^{st}$ guess by plugging in our k^{th} guess into the right-hand side of (11.39). We keep iterating until the difference between successive guesses is small enough to indicate convergence.

This algorithm is guaranteed to converge if each diagonal element of A is larger in absolute value than the sum of the absolute values of the other elements in its row.

Parallelization of this algorithm is easy: Just assign each process to handle a section of $x = (x_0, x_1, ..., x_{n-1})$. Note that this means that each process must make sure that all other processes get the new value of its section after every iteration.

Note too that in matrix terms (11.39) can be expressed as

$$x^{(k+1)} = D^{-1}(b - Ox^{(k)}) \qquad (11.40)$$

where D is the diagonal matrix consisting of the diagonal elements of A (so its inverse is just the diagonal matrix consisting of the reciprocals of those elements), O is the square matrix obtained by replacing A's diagonal elements by 0s, and $x^{(i)}$ is our guess for x in the ith iteration. This reduces the problem to one of matrix multiplication, and thus we can parallelize the Jacobi algorithm by utilizing a method for doing parallel matrix multiplication.

11.5.4   Example: OpenMP Implementation of the Jacobi Algorithm

OpenMP code for Jacobi is straightforward:

```
#include <omp.h>

// partitions s..e into nc chunks, placing the ith in first and last (i
// = 0,...,nc-1)
void chunker(int s, int e, int nc, int i, int *first, int *last)
{ int chunksize = (e-s+1) / nc;
  *first = s + i * chunksize;
```

```
8      if (i < nc-1) *last = *first + chunksize - 1;
9      else *last = e;
10  }
11
12  // returns the "dot product" of vectors u and v
13  float innerprod(float *u, float *v, int n)
14  { float sum = 0.0; int i;
15      for (i = 0; i < n; i++)
16         sum += u[i] * v[i];
17      return sum;
18  }
19
20  // solves AX = Y, A nxn; stops iteration when total change is < n*eps
21  void jacobi(float *a, float *x, float *y, int n, float eps)
22  {
23      float *oldx = malloc(n*sizeof(float));
24      float se;
25      #pragma omp parallel
26      { int i;
27         int thn = omp_get_thread_num();
28         int nth = omp_get_num_threads();
29         int first,last;
30         chunker(0,n-1,nth,thn,&first,&last);
31         for (i = first; i <= last; i++) oldx[i] = x[i] = 1.0;
32         float tmp;
33         while (1) {
34            for (i = first; i <= last; i++) {
35               tmp = innerprod(&a[n*i],oldx,n);
36               tmp -= a[n*i+i] * oldx[i];
37               x[i] = (y[i] - tmp) / a[n*i+i];
38            }
39            #pragma omp barrier
40            #pragma omp for reduction(+:se)
```

```
41        for (i = first; i <= last; i++)
42           se += abs(x[i]-oldx[i]);
43        #pragma omp barrier
44        if (se < n*eps) break;
45        for (i = first; i <= last; i++)
46           oldx[i] = x[i];
47     }
48   }
49 }
```

Note the use of the OpenMP **reduction** clause.

11.5.5   Example: R/gputools Implementation of Jacobi

Here's the R code, using **gputools**:

```
1  library(gputools)
2
3  jcb <- function(a,b,eps) {
4    n <- length(b)
5    d <- diag(a) # a vector, not a matrix
6    tmp <- diag(d) # a matrix, not a vector
7    o <- a - diag(d)
8    di <- 1/d
9    x <- b # initial guess, could be better
10   repeat {
11     oldx <- x
12     tmp <- gpumatmult(o,x)
13     tmp <- b - tmp
14     x <- di * tmp # elementwise multiplication
15     if (sum(abs(x-oldx)) < n * eps) return(x)
16   }
17 }
```

11.6   Eigenvalues and Eigenvectors

With the popularity of document search (Web search, text mining etc.), eigenanalysis has become much more broadly used. Given the size of the problems, again parallel computation is needed. This can become quite involved, with many complicated methods having been developed.

11.6.1   The Power Method

One of the simplest methods is the **power method**. Consider an nxn matrix A, with eigenvalues $\lambda_1, ..., \lambda_n$, where the labeling is such that $|\lambda_1| \geq |\lambda_2| \geq ... \geq |\lambda_n|$. We'll assume here that A is a symmetric matrix, which it is for instance in statistical applications (Section 14.4). That implies that the eigenvalues of A are real, and that the eigenvectors are orthogonal to each other.

Start with some nonzero vector x, and define the kth iterate by

$$x^{(k)} = \frac{A^k x}{\| A^k x \|} \tag{11.41}$$

Under mild conditions, $x^{(k)}$ converges to an eigenvector v_1 corresponding to λ_1. Moreover, the quantities $(Ax^{(k)})' x^{(k)}$ converge to λ_1.

This method is reportedly used in Google's PageRank algorithm, which is only concerned with the largest eigenvalue/eigenvector. But what if you want more?

Consider now the matrix

$$B = A - \lambda_1 v_1 v_1' \tag{11.42}$$

where we've now scaled v_1 to have length 1.

Then

$$
\begin{aligned}
Bv_1 &= Av_1 - \lambda_1 v1(v_1' v_1) & (11.43)\\
&= \lambda_1 v_1 - \lambda_1 v1(1) & (11.44)\\
&= 0 & (11.45)
\end{aligned}
$$

and for $i > 0$,

$$
\begin{aligned}
Bv_i &= Av_i - \lambda_1 v1(v_1'v_i) & (11.46) \\
&= \lambda_i v_i - \lambda_1 v1(0) & (11.47) \\
&= \lambda_i v_i & (11.48)
\end{aligned}
$$

In other words, the eigenvalues of B are $\lambda_2, ..., \lambda_n, 0$. So we can now apply the same procedure to B to get λ_2 and v_2, and iterate for the rest.

11.6.2 Parallel Computation

To use the power method in parallel, note that this is again a situation in which we wish to compute powers of matrices. However, there is also scaling involved, as seen in (11.41). We may wish to try the "log method" of Section 11.4, with scaling done occasionally.

The CULA library for CUDA, mentioned earlier, includes routines for finding the **singular value decomposition** of a matrix, thus providing the eigenvectors.[①] The R package **gputools** has an interface to the SVD routine in CULA.

11.7   Sparse Matrices

As mentioned earlier, in many parallel processing applications of linear algebra, the matrices can be huge, even having millions of rows or columns. However, in many such cases, most of the matrix consists of 0s. In an effort to save memory, one can store such matrices in compressed form, storing only the nonzero elements.

Sparse matrices roughly fall into two categories. In the first category, the matrices all have 0s at the same known positions. For instance, in **tridiagonal** matrices, the only nonzero elements are either on the diagonal or on subdiagonals just below or above the diagonal, and all other elements are guaranteed to be 0, such as

$$
\begin{pmatrix}
2 & 0 & 0 & 0 & 0 \\
1 & 1 & 8 & 0 & 0 \\
0 & 1 & 5 & 8 & 0 \\
0 & 0 & 0 & 8 & 8 \\
0 & 0 & 0 & 3 & 5
\end{pmatrix}
\tag{11.49}
$$

[①]The term *singular value* is a synonym for *eigenvalue*.

Code to deal with such matrices can then access the nonzero elements based on this knowledge.

In the second category, each matrix that our code handles will typically have its nonzero matrices in different, "random," positions. A number of methods have been developed for storing amorphous sparse matrices, such as the Compressed Sparse Row format, which we'll code in this C **struct**, representing an mxn matrix A, with k nonzero entries:

```
1  struct {
2    int m,n; // numbers of rows and columns of A
3    float *avals; // the nonzero values of A, in row-major order; length k
4    int *cols; // avals[i] is in column cols[i] in A; length k
5    int *rowplaces; // rowplaces[i] is the index in avals for the 1st
6                    // nonzero element of row i in A (but last element
7                    // is k); length m+1
8  }
```

For the matrix in (11.49) (if we were not to exploit its tridiagonal nature, and just treat it as amorphous):

- **m,n:** 5,5
- **avals:** 2,1,1,8,1,5,8,8,8,3,5
- **cols:** 0,0,1,2,1,2,3,3,4,3,4
- **rowplaces:** 0,2,4,6,9,11

For instance, look at the 4 in **rowplaces**. It's at position 2 in that array, so it says that element 4 in **avals**—the third 1—is the first nonzero element in row 2 of A. Look at the matrix, and you'll see this is true.

Parallelizing operations for sparse matrices can be done in the usual manner, e.g. breaking the rows of A into chunks. Note, though, that there could be a load-balance issue, again addressable in ways we've used before.

11.8 Libraries

Of course, remember that CUDA provides some excellent matrix-operation routines, in CUBLAS. There is also the CUSP library for sparse matrices (i.e. those with a lot of 0s). Note too the CULA library (not developed by NVIDIA, but using CUDA).

More general (i.e. non-CUDA) parallel libraries for linear algebra include ScalaPACK and PLA-PACK.

第 12 章 Introduction to Parallel Sorting

Sorting is one of the most common operations in parallel processing applications. For example, it is central to many parallel database operations, and important in areas such as image processing, statistical methodology and so on. A number of different types of parallel sorting schemes have been developed. Here we look at some of these schemes.

12.1 Quicksort

You are probably familiar with the idea of quicksort: First break the original array into a "small-element" pile and a "large-element" pile, by comparing to a **pivot** element. In a naive implementation, the first element of the array serves as the pivot, but better performance can be obtained by taking, say, the median of the first three elements. Then "recurse" on each of the two piles, and then string the results back together again.

This is an example of the **divide and conquer** approach seen in so many serial algorithms. It is easily parallelized (though load-balancing issues may arise). Here, for instance, we might assign one pile to one thread and the other pile to another thread.

Suppose the array to be sorted is named **x**, and consists of **n** elements.

12.1.1 The Separation Process

A major issue is how we separate the data into piles.

In a naive implementation, the piles would be put into new arrays, but this is bad in two senses: It wastes memory space, and wastes time, since much copying of arrays needs to be done. A better implementation places the two piles back into the original array **x**. The following C code does that.

The function **separate()** is intended to be used in a recursive quicksort operation. It operates on **x[l]** through **x[h]**, a subarray of **x** that itself may have been formed at an earlier stage of the recursion.

It forms two piles from those elements, and placing the piles back in the same region **x[l]** through **x[h]**. It also has a return value, showing where the first pile ends.

```
int separate(int l, int h)
{  int ref,i,j,k,tmp;
   ref = x[h]; i = l-1; j = h;
   do  {
      do i++; while (x[i] < ref && i < h);
      do j--; while (x[j] > ref && j > l);
      tmp = x[i];  x[i] = x[j];  x[j] = tmp;
   } while (j > i);
   x[j] = x[i];  x[i] = x[h];  x[h] = tmp;
   return i;
}
```

The function **separate()** rearranges the subarray, returning a value **m**, so that:

- **x[l]** through **x[m-1]** are less than **x[m]**,

- **x[m+1]** through **x[h]** are greater than **x[m]**, and

- **x[m]** is in its "final resting place," meaning that **x[m]** will never move again for the remainder of the sorting process. (Another way of saying this is that the current **x[m]** is the **m**-th smallest of all the original **x[i]**, **i** = 0,1,...,**n**-1.)

By the way, **x[l]** through **x[m-1]** will also be in their final resting places as a group. They may be exchanging places with each other from now on, but they will never again leave the range **i** though **m-1** within the **x** array as a whole. A similar statement holds for **x[m+1]** through **x[n-1]**.

Another approach is to do a prefix scan. As an illustration, consider the array

$$28 \quad 35 \quad 12 \quad 5 \quad 13 \quad 6 \quad 8 \quad 10 \quad 168 \tag{12.1}$$

We'll take the first element, 28, as the pivot, and form a new array of 1s and 0s, where 1 means "less than the pivot":

28 35 12 5 13 6 48 10 168
 0   0   1 1   1 1   0   1   0

Now form the prefix scan (Chapter 10) of that second array, with respect to addition. It will be an *exclusive* scan (Section 10.3). This gives us

28 35 12 5 13 6 48 10 168
 0   0   1 1   1 1   0   1   0
 0   0   0 1   2 3   3   4   4

Now, the key point is that for every element 1 in that second row, the corresponding element in the

third row shows where the first-row element should be placed under the separation operation! Here's why:

The elements 12, 5, 13, 6 and 10 should go in the first pile, which in an in-place separation would means indices 0, 1, 2, 3, and 4. Well, as you can see above, these are precisely the values shown in the third row for 12, 5, 13, 6 and 10, all of which have 1s in the second row.

The pivot, 28, then should immediately follow that low pile, i.e. it should be placed at index 5.

We can simply place the high pile at the remaining indicies, 6 through 8 (though we'll do it more systematically below).

In general for an array of length k, we:

- form the second row of 1s and 0s indicating < pivot

- form the third row, the exclusive prefix scan

- for each 1 in the second row, place the corresponding element in row 1 into the spot indicated by row 3

- place the pivot in the place indicated by 1 plus m, the largest value in row 3

- form row 4, equal to (0,1,...,k-1) minus row 3 plus m

- for each 0 in the second row, place the corresponding element in row 1 into the spot indicated by row 4

Note that this operation, using scan, could be used an an alternative to the **separate()** function above. But it could be done in parallel; more on this below.

12.1.2 Example: OpenMP Quicksort

Here is OpenMP code which performs quicksort in the shared-memory paradigm (adapted from code in the OpenMP Source Code Repository, `http://www.pcg.ull.es/ompscr/`):

```
1   void qs(int *x, int l, int h)
2   {  int newl[2], newh[2], i, m;
3      m = separate(x,l,h);
4      newl[0] = l;  newh[0] = m-1;
5      newl[1] = m+1;  newh[1] = h;
6      #pragma omp parallel
7      {
8         #pragma omp for nowait
9         for (i = 0; i < 2; i++)
10           qs(newl[i],newh[i]);
11     }
12  }
```

Note the **nowait** clause. Since different threads are operating on different portions of the array, they need not be synchronized.

Recall that another implementation, using the **task** directive, was given earlier in Section 4.5.

In both of these implementations, we used the function **separate()** defined above. So, different threads apply different separation operations to different subarrays. An alternative would be to place the parallelism in the separation operation itself, using the parallel algorithms for prefix scan in Chapter 10.

12.1.3　Hyperquicksort

This algorithm was originally developed for hypercubes, but can be used on any message-passing system having a power of 2 for the number of nodes.[①]

It is assumed that at the beginning each PE contains some chunk of the array to be sorted. After sorting, each PE will contain some chunk of the <u>sorted</u> array, meaning that:

- each chunk is itself in sorted form
- for all cases of $i < j$, the elements at PE i are less than the elements at PE j

If the sorted array itself were our end, rather than our means to something else, we could now collect it at some node, say node 0. If, as is more likely, the sorting is merely an intermediate step in a larger distributed computation, we may just leave the chunks at the nodes and go to the next phase of work.

Say we are on a d-cube. The intuition behind the algorithm is quite simple:

```
1  for i = d downto 1
2      for each i-cube:
3          root of the i-cube broadcasts its median to all in the i-cube,
4              to serve as pivot
5          consider the two (i-1)-subcubes of this i-cube
6          each pair of partners in the (i-1)-subcubes exchanges data:
7              low-numbered PE gives its partner its data larger than pivot
8              high-numbered PE gives its partner its data smaller than pivot
```

To avoid deadlock, have the lower-numbered partner send then receive, and vice versa for the higher-numbered one. Better, in MPI, use **MPI_SendRcv()**.

After the first iteration, all elements in the lower (d-1)-cube are less than all elements in higher (d-1)-cube. After d such steps, the array will be sorted.

[①]See Chapter 7 for definitions of hypercube terms.

12.2 Mergesorts

12.2.1 Sequential Form

In its serial form, mergesort has the following pseudocode:

```
1  // initially called with l = 0 and h = n-1, where n is the length of the
2  // array and is assumed here to be a power of 2
3  void seqmergesort(int *x, int l, int h)
4  {  seqmergesort(x,0,h/2-1);
5     seqmergesort(x,h/2,h);
6     merge(x,l,h);
7  }
```

The function **merge()** should be done in-place, i.e. without using an auxiliary array. It basically codes the operation shown in pseudocode for the message-passing case in Section 12.2.3.

12.2.2 Shared-Memory Mergesort

This is similar to the patterns for shared-memory quicksort in Section 12.1.2 above.

12.2.3 Message Passing Mergesort on a Tree Topology

First, we organize the processing nodes into a binary tree. This is simply from the point of view of the software, rather than a physical grouping of the nodes. We will assume, though, that the number of nodes is one less than a power of 2.

To illustrate the plan, say we have seven nodes in all. We could label node 0 as the root of the tree, label nodes 1 and 2 to be its two children, label nodes 3 and 4 to be node 1's children, and finally label nodes 5 and 6 to be node 2's children.

It is assumed that the array to be sorted is initially distributed in the leaf nodes (recall a similar situation for hyperquicksort), i.e. nodes 3-6 in the above example. The algorithm works best if there are approximately the same number of array elements in the various leaves.

In the first stage of the algorithm, each leaf node applies a regular sequential sort to its current holdings. Then each node begins sending its now-sorted array elements to its parent, one at a time, in ascending numerical order.

Each nonleaf node then will merge the lists handed to it by its two children. Eventually the root node will have the entire sorted array. Specifically, each nonleaf node does the following:

```
1  do
2     if my left-child datum < my right-child datum
```

```
3       pass my left-child datum to my parent
4    else
5       pass my right-child datum to my parent
6  until receive the "no more data" signal from both children
```

There is quite a load balancing issue here. On the one hand, due to network latency and the like, one may get better performance if each node accumulates a chunk of data before sending to the parent, rather than sending just one datum at a time. Otherwise, "upstream" nodes will frequently have no work to do.

On the other hand, the larger the chunk size, the earlier the leaf nodes will have no work to do. So for any particular platform, there will be some optimal chunk size, which would need to be determined by experimentation.

12.2.4   Compare-Exchange Operations

These are key to many sorting algorithms.

A **compare-exchange**, also known as **compare-split**, simply means in English, "Let's pool our data, and then I'll take the lower half and you take the upper half." Each node executes the following pseudocode:

```
1  send all my data to partner
2  receive all my partner's data
3  if I have a lower id than my partner
4     I keep the lower half of the pooled data
5  else
6     I keep the upper half of the pooled data
```

12.2.5   Bitonic Mergesort

Definition: A sequence $(a_0, a_1, .., a_{k-1})$ is called **bitonic** if either of the following conditions holds:

(a) The sequence is first nondecreasing then nonincreasing, meaning that for some r

$$(a_0 \leq a_1 \leq ... \leq a_r \geq a_{r+1} \geq a_{n-1})$$

(b) The sequence can be converted to the form in (a) by rotation, i.e. by moving the last k elements from the right end to the left end, for some k.

As an example of (b), the sequence (3,8,12,15,14,5,1,2) can be rotated rightward by two element positions to form (1,2,3,8,12,15,14,5). Or we could just rotate by one element, moving the 2 to forming (2,3,8,12,15,14,5,1).

Note that the definition includes the cases in which the sequence is purely nondecreasing (r = n-1) or purely nonincreasing (r = 0).

Also included are "V-shape" sequences, in which the numbers first decrease then increase, such as (12,5,2,8,20). By (b), these can be rotated to form (a), with (12,5,2,8,20) being rotated to form (2,8,20,12,5), an "A-shape" sequence.

(For convenience, from here on I will use the terms *increasing* and *decreasing* instead of *nonincreasing* and *nondecreasing*.)

Suppose we have bitonic sequence $(a_0, a_1, .., a_{k-1})$, where k is a power of 2. Rearrange the sequence by doing compare-exchange operations between a_i and $a_{n/2+i}$), i = 0,1,...,n/2-1. Then it is not hard to prove that the new $(a_0, a_1, .., a_{k/2-1})$ and $(a_{k/2}, a_{k/2+1}, .., a_{k-1})$ are bitonic, and every element of that first subarray is less than or equal to every element in the second one.

So, we have set things up for yet another divide-and-conquer attack:

```
// x is bitonic of length n, n a power of 2
void sortbitonic(int *x, int n)
{  do the pairwise compare-exchange operations
   if (n > 2) {
      sortbitonic(x,n/2);
      sortbitonic(x+n/2,n/2);
   }
}
```

This can be parallelized in the same ways we saw for Quicksort earlier.

So much for sorting bitonic sequences. But what about general sequences?

We can proceed as follows, using our function **sortbitonic()** above:

1. For each i = 0,2,4,...,n-2:

    - Each of the pairs (a_i, a_{i+1}), i = 0,2,...,n-2 is bitonic, since *any* 2-element array is bitonic!
    - Apply **sortbitonic()** to (a_i, a_{i+1}). In this case, we are simply doing a compare-exchange.
    - If i/2 is odd, reverse the pair, so that this pair and the pair immediately preceding it now form a 4-element bitonic sequence.

2. For each i = 0,4,8,...,n-4:

    - Apply **sortbitonic()** to $(a_i, a_{i+1}, a_{i+2}, a_{i+3})$.
    - If i/4 is odd, reverse the quartet, so that this quartet and the quartet immediately preceding it now form an 8-element bitonic sequence.

3. Keep building in this manner, until get to a single sorted n-element list.

There are many ways to parallelize this. In the hypercube case, the algorithm consists of doing compare-exchange operations with all neighbors, pretty much in the same pattern as hyperquicksort.

12.3　The Bubble Sort and Its Cousins

12.3.1　The Much-Maligned Bubble Sort

Recall the **bubble sort**:

```
void bubblesort(int *x, int n)
{  for i = n-1 downto 1
      for j = 0 to i
         compare-exchange(x,i,j,n)
}
```

Here the function **compare-exchange()** is as in Section 12.2.4 above. In the context here, it boils down to

```
if x[i] > x[j]
   swap x[i] and x[j]
```

In the first **i** iteration, the largest element "bubbles" all the way to the right end of the array. In the second iteration, the second-largest element bubbles to the next-to-right-end position, and so on.

You learned in your algorithms class that this is a very inefficient algorithm—when used serially. But it's actually rather usable in parallel systems.

For example, in the shared-memory setting, suppose we have one thread for each value of **i**. Then those threads can work in parallel, as long as a thread with a larger value of **i** does not overtake a thread with a smaller **i**, where "overtake" means working on a larger **j** value.

Once again, it probably pays to chunk the data. In this case, **compare-exchange()** fully takes on the meaning it had in Section 12.2.4.

12.3.2　A Popular Variant: Odd-Even Transposition

A popular variant of this is the **odd-even transposition sort**. The pseudocode for a shared-memory version is:

```
// the argument "me" is this thread's ID
void oddevensort(int *x, int n, int me)
{  for i = 1 to n
      if i is odd
```

```
5              if me is even
6                 compare-exchange(x,me,me+1,n)
7              else  // me is odd
8                 compare-exchange(x,me,me-1,n)
9           else  // i is even
10             if me is even
11                compare-exchange(x,me,me-1,n)
12             else  // me is odd
13                compare-exchange(x,me,me+1,n)
```

If the second or third argument of **compare-exchange()** is less than 0 or greater than **n**-1, the function has no action.

This looks a bit complicated, but all it's saying is that, from the point of view of an even-numbered element of **x**, it trades with its right neighbor during odd phases of the procedure and with its left neighbor during even phases.

Again, this is usually much more effective if done in chunks.

12.3.3   Example: CUDA Implementation of Odd/Even Transposition Sort

```
1   #include <stdio.h>
2   #include <stdlib.h>
3   #include <cuda.h>
4
5   // compare and swap; copies from the f to t, swapping f[i] and
6   // f[j] if the higher-index value is smaller; it is required that i < j
7   __device__ void cas(int *f,int *t,int i,int j, int n, int me)
8   {
9      if (i < 0 || j >= n) return;
10     if (me == i) {
11        if (f[i] > f[j]) t[me] = f[j];
12        else t[me] = f[i];
13     } else {  // me == j
14        if (f[i] > f[j]) t[me] = f[i];
15        else t[me] = f[j];
16     }
17  }
18
19  // does one iteration of the sort
20  __global__ void oekern(int *da, int *daaux, int n, int iter)
21  { int bix = blockIdx.x;  // block number within grid
22     if (iter % 2) {
23        if (bix % 2) cas(da,daaux,bix-1,bix,n,bix);
24        else cas(da,daaux,bix,bix+1,n,bix);
25     } else {
```

```
26          if (bix % 2) cas(da,daaux,bix,bix+1,n,bix);
27          else cas(da,daaux,bix-1,bix,n,bix);
28      }
29  }
30
31  // sorts the array ha, length n, using odd/even transp. sort;
32  // kept simple for illustration, no optimization
33  void oddeven(int *ha, int n)
34  {
35      int *da;
36      int dasize = n * sizeof(int);
37      cudaMalloc((void **)&da,dasize);
38      cudaMemcpy(da,ha,dasize,cudaMemcpyHostToDevice);
39      // the array daaux will serve as "scratch space"
40      int *daaux;
41      cudaMalloc((void **)&daaux,dasize);
42      dim3 dimGrid(n,1);
43      dim3 dimBlock(1,1,1);
44      int *tmp;
45      for (int iter = 1; iter <= n; iter++) {
46          oekern<<<dimGrid,dimBlock>>>(da,daaux,n,iter);
47          cudaThreadSynchronize();
48          if (iter < n) {
49              // swap pointers
50              tmp = da;
51              da = daaux;
52              daaux = tmp;
53          } else
54              cudaMemcpy(ha,daaux,dasize,cudaMemcpyDeviceToHost);
55      }
56  }
```

Recall that in CUDA code, separate blocks of threads cannot synchronize with each other. Unless we deal with just a single block, this necessitates limiting the kernel to a single iteration of the algorithm, so that as iterations progress, execution alternates between the device and the host.

Moreover, we do not take advantage of shared memory. One possible solution would be to use **___syncthreads()** within each block for most of the compare-and-exchange operations, and then having the host take care of the operations on the boundaries between blocks.

12.4   Shearsort

In some contexts, our hardware consists of a two-dimensional mesh of PEs. A number of methods have been developed for such settings, one of the most well known being Shearsort, developed by Sen,

Shamir and the eponymous Isaac Scherson of UC Irvine. Again, the data is assumed to be initially distributed among the PEs. Here is the pseudocode:

```
for i = 1 to ceiling(log2(n)) + 1
    if i is odd
        sort each even row in descending order
        sort each odd row in ascending order
    else
        sort each column is ascending order
```

At the end, the numbers are sorted in a "snakelike" manner.

For example:

6	12
5	9

6	12
9	5

6	5
9	12

5	6 ↓
12	← 9

No matter what kind of system we have, a natural domain decomposition for this problem would be for each process to be responsible for a group of rows. There then is the question about what to do during the even-numbered iterations, in which column operations are done. This can be handled via a parallel matrix transpose operation. In MPI, the function **MPI_Alltoall()** may be useful.

12.5 Bucket Sort with Sampling

For concreteness, suppose we are using MPI on message-passing hardware, say with 10 PEs. As usual in such a setting, suppose our data is initially distributed among the PEs.

Suppose we knew that our array to be sorted is a random sample from the uniform distribution on (0,1). In other words, about 20% of our array will be in (0,0.2), 38% will be in (0.45,0.83) and so on.

What we could do is assign PE0 to the interval (0,0.1), PE1 to (0.1,0.2) etc. Each PE would look at its local data, and distribute it to the other PEs according to this interval scheme. Then each PE would do a local sort.

In general, we don't know what distribution our data comes from. We solve this problem by

doing sampling. In our example here, each PE would sample some of its local data, and send the sample to PE0. From all of these samples, PE0 would find the decile values, i.e. 10th percentile, 20th percentile,..., 90th percentile. These values, called **splitters** would then be broadcast to all the PEs, and they would then distribute their local data to the other PEs according to these intervals.

OpenMP code for this was given in Section 1.3.2. Here is similar MPI code below (various improvements could be made, e.g. with broadcast):

```
// bucket sort, bin boundaries known in advance

// node 0 is manager, all else worker nodes; node 0 sends full data, bin
// boundaries to all worker nodes; i-th worker node extracts data for
// bin i-1, sorts it, sends sorted chunk back to node 0; node 0 places
// sorted results back in original array

// not claimed efficient; e.g. could be better to have manager place
// items into bins

#include <mpi.h>

#define MAX_N 100000 // max size of original data array
#define MAX_NPROCS 100 // max number of MPI processes
#define DATA_MSG 0 // manager sending original data
#define BDRIES_MSG 0 // manager sending bin boundaries
#define CHUNKS_MSG 2 // workers sending their sorted chunks

int nnodes, //
    n, // size of full array
    me, // my node number
    fulldata[MAX_N],
    tmp[MAX_N],
    nbdries, // number of bin boundaries
    counts[MAX_NPROCS];
float bdries[MAX_NPROCS-2]; // bin boundaries

```

```
28  int debug,debugme;

29

30  init(int argc, char **argv)
31  {
32     int i;
33     debug = atoi(argv[3]);
34     debugme = atoi(argv[4]);
35     MPI_Init(&argc,&argv);
36     MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
37     MPI_Comm_rank(MPI_COMM_WORLD,&me);
38     nbdries = nnodes - 2;
39     n = atoi(argv[1]);
40     int k = atoi(argv[2]); // for random # gen
41     // generate random data for test purposes
42     for (i = 0; i < n; i++) fulldata[i] = rand() % k;
43     // generate bin boundaries for test purposes
44     for (i = 0; i < nbdries; i++) {
45        bdries[i] = i * (k+1) / ((float) nnodes);
46     }
47  }

48

49  void managernode()
50  {
51     MPI_Status status;
52     int i;
53     int lenchunk; // length of a chunk received from a worker
54     // send full data, bin boundaries to workers
55     for (i = 1; i < nnodes; i++) {
56        MPI_Send(fulldata,n,MPI_INT,i,DATA_MSG,MPI_COMM_WORLD);
57        MPI_Send(bdries,nbdries,MPI_FLOAT,i,BDRIES_MSG,MPI_COMM_WORLD);
58     }
59     // collect sorted chunks from workers, place them in their proper
60     // positions within the original array
```

```
61    int currposition = 0;
62    for (i = 1; i < nnodes; i++) {
63       MPI_Recv(tmp,MAX_N,MPI_INT,i,CHUNKS_MSG,MPI_COMM_WORLD,&status);
64       MPI_Get_count(&status,MPI_INT,&lenchunk);
65       memcpy(fulldata+currposition,tmp,lenchunk*sizeof(int));
66       currposition += lenchunk;
67    }
68    if (n < 25) {
69       for (i = 0; i < n; i++) printf("%d ",fulldata[i]);
70       printf("\n");
71    }
72 }
73
74 // adds xi to the part array, increments npart, the length of part
75 void grab(int xi, int *part, int *npart)
76 {
77    part[*npart] = xi;
78    *npart += 1;
79 }
80
81 int cmpints(int *u, int *v)
82 { if (*u < *v) return -1;
83    if (*u > *v) return 1;
84    return 0;
85 }
86
87 void getandsortmychunk(int *tmp, int n, int *chunk, int *lenchunk)
88 {
89    int i,count = 0;
90    int workernumber = me - 1;
91       if (me == debugme) while (debug) ;
92    for (i = 0; i < n; i++) {
93       if (workernumber == 0) {
```

```
 94          if (tmp[i] <= bdries[0]) grab(tmp[i],chunk,&count);
 95       }
 96       else if (workernumber < nbdries-1) {
 97          if (tmp[i] > bdries[workernumber-1] &&
 98             tmp[i] <= bdries[workernumber]) grab(tmp[i],chunk,&count);
 99       } else
100          if (tmp[i] > bdries[nbdries-1]) grab(tmp[i],chunk,&count);
101    }
102    qsort(chunk,count,sizeof(int),cmpints);
103    *lenchunk = count;
104 }
105
106 void workernode()
107 {
108    int n,fulldata[MAX_N], // size and storage of full data
109        chunk[MAX_N],
110        lenchunk,
111        nbdries; // number of bin boundaries
112    float bdries[MAX_NPROCS-1]; // bin boundaries
113    MPI_Status status;
114    MPI_Recv(fulldata,MAX_N,MPI_INT,0,DATA_MSG,MPI_COMM_WORLD,&status);
115    MPI_Get_count(&status,MPI_INT,&n);
116    MPI_Recv(bdries,MAX_NPROCS-2,MPI_FLOAT,0,BDRIES_MSG,MPI_COMM_WORLD,&status);
117    MPI_Get_count(&status,MPI_FLOAT,&nbdries);
118    getandsortmychunk(fulldata,n,chunk,&lenchunk);
119    MPI_Send(chunk,lenchunk,MPI_INT,0,CHUNKS_MSG,MPI_COMM_WORLD);
120 }
121
122 int main(int argc,char **argv)
123 {
124    int i;
125    init(argc,argv);
126    if (me == 0) managernode();
```

```
127    else workernode();
128    MPI_Finalize();
129  }
```

12.6 Radix Sort

The radix sort is essentially a special case of a bucket sort. If we have 16 threads, say, we could determine a datum's bucket by its lower 4 bits. As long as our data is uniformly distributed under the mod 16 operation, we would not need to do any sampling.

The CUDPP GPU library uses a radix sort. The buckets are formed one bit at a time, using segmented scan as above.

12.7 Enumeration Sort

This one is really simple. Take for instance the array (12,5,13,18,6). There are 2 elements less than 12, so in the end, it should go in position 2 of the sorted array, (5,6,12,13,18).

Say we wish to sort **x**, which for convenience we assume contains no tied values. Then the pseudocode for this algorithm, placing the results in **y**, is

```
1  for all i in 0...n-1:
2      count = 0
3      elt = x[i]
4      for all j in 0...n-1:
5         if x[j] < elt then count++
6      y[count] = elt
```

The outer (or inner) loop is easily parallelized.

第 13 章 Parallel Computation for Audio and Image Processing

Mathematical computations involving images can become quite intensive, and thus parallel methods are of great interest. Here we will be primarily interested in methods involving **Fourier** analysis.

13.1 General Principles

13.1.1 One-Dimensional Fourier Series

A sound **wave form** graphs volume of the sound against time. Here, for instance, is the wave form for a vibrating reed:[1]
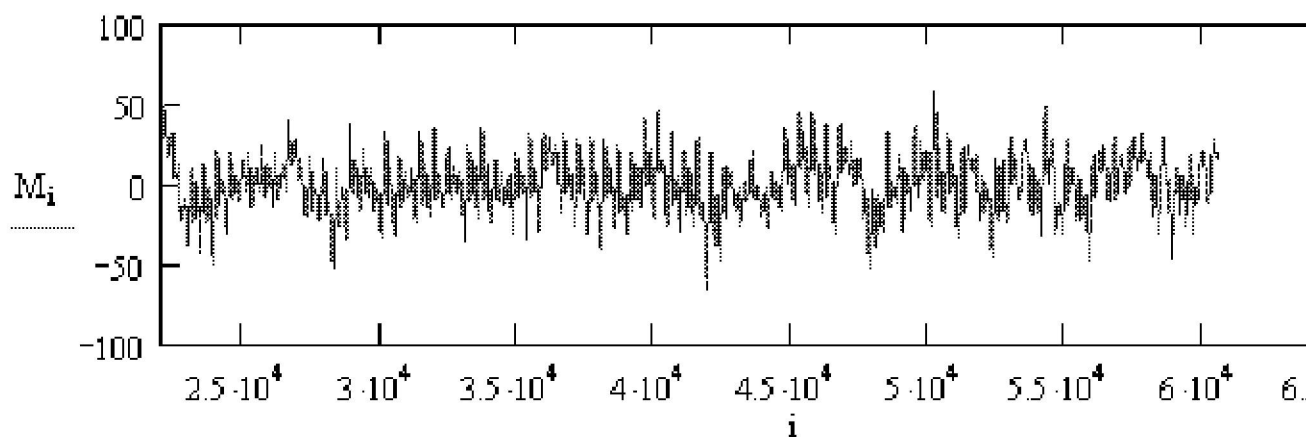
Recall that we say a function of time g(t) is **periodic** ("repeating," in our casual wording above)

---

[1]Reproduced here by permission of Prof. Peter Hamburger, Indiana-Purdue University, Fort Wayne. See http://www.ipfw.edu/math/Workshop/PBC.html

with period T if if g(u+T) = g(u) for all u. The **fundamental frequency** of g() is then defined to be the number of periods per unit time,

$$f_0 = \frac{1}{T} \tag{13.1}$$

Recall also from calculus that we can write a function g(t) (not necessarily periodic) as a Taylor series, which is an "infinite polynomial":

$$g(t) = \sum_{n=0}^{\infty} c_n t^n. \tag{13.2}$$

The specific values of the c_n may be derived by differentiating both sides of (13.2) and evaluating at t = 0, yielding

$$c_n = \frac{g^{(n)}(0)}{n!}, \tag{13.3}$$

where $g^{(j)}$ denotes the ith derivative of g().

For instance, for e^t,

$$e^t = \sum_{n=0}^{\infty} \frac{1}{n!} t^n \tag{13.4}$$

In the case of a repeating function, it is more convenient to use another kind of series representation, an "infinite trig polynomial," called a **Fourier series**. This is just a fancy name for a weighted sum of sines and cosines of different frequencies. More precisely, we can write any repeating function g(t) with period T and fundamental frequency f_0 as

$$g(t) = \sum_{n=0}^{\infty} a_n \cos(2\pi n f_0 t) + \sum_{n=1}^{\infty} b_n \sin(2\pi n f_0 t) \tag{13.5}$$

for some set of weights a_n and b_n. Here, instead of having a weighted sum of terms

$$1, \ t, \ t^2, \ t^3, \ ... \tag{13.6}$$

as in a Taylor series, we have a weighted sum of terms

$$1, \ \cos(2\pi f_0 t), \ \cos(4\pi f_0 t), \ \cos(6\pi f_0 t), \ ... \tag{13.7}$$

and of similar sine terms. Note that the frequencies $n f_0$, in those sines and cosines are integer multiples of the fundamental frequency of x, f_0, called **harmonics**.

The weights a_n and b_n, n = 0, 1, 2, ... are called the **frequency spectrum** of g(). The coefficients are calculated as follows:[2]

$$a_0 = \frac{1}{T} \int_0^T g(t) \ dt \tag{13.8}$$

$$a_n = \frac{2}{T} \int_0^T g(t) \ cos(2\pi n f_0 t) \ dt \tag{13.9}$$

$$b_n = \frac{2}{T} \int_0^T g(t) \ sin(2\pi n f_0 t) \ dt \tag{13.10}$$

By analyzing these weights, we can do things like machine-based voice recognition (distinguishing one person's voice from another) and speech recognition (determining what a person is saying). If for example one person's voice is higher-pitched than that of another, the first person's weights will be concentrated more on the higher-frequency sines and cosines than will the weights of the second.

Since g(t) is a graph of loudness against time, this representation of the sound is called the **time domain**. When we find the Fourier series of the sound, the set of weights a_n and b_n is said to be a representation of the sound in the **frequency domain**. One can recover the original time-domain representation from that of the frequency domain, and vice versa, as seen in Equations (13.8), (13.9), (13.10) and (13.5).

In other words, the transformations between the two domains are inverses of each other, and there is a one-to-one correspondence between them. Every g() corresponds to a unique set of weights and vice versa.

Now here is the frequency-domain version of the reed sound:

---

[2]The get an idea as to how these formulas arise, see Section 13.9. But for now, if you integrate both sides of (13.5), you will at least verify that the formulas below do work.
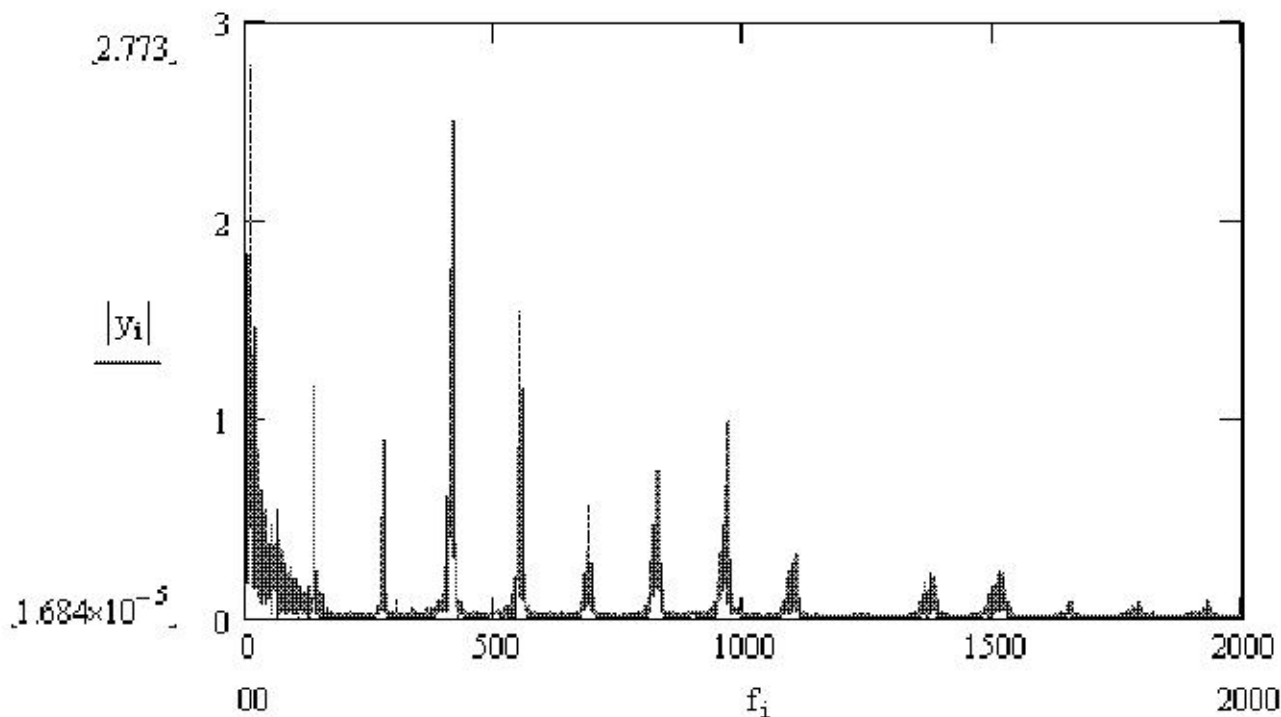
Note that this graph is very "spiky." In other words, even though the reed's waveform includes all frequencies, most of the power of the signal is at a few frequencies which arise from the physical properties of the reed.

Fourier series are often expressed in terms of complex numbers, making use of the relation

$$e^{i\theta} = \cos(\theta) + i\ \sin(\theta),\tag{13.11}$$

where $i = \sqrt{-1}$.[3]

The complex form of (13.5) is

$$g(t) = \sum_{j=-\infty}^{\infty} c_j e^{2\pi i j \frac{t}{T}}.\tag{13.12}$$

The c_j are now generally complex numbers. They are functions of the a_j and b_j, and thus form the frequency spectrum.

---

[3]There is basically no physical interpretation of complex numbers. Instead, they are just mathematical abstractions. However, they are highly useful abstractions, with the complex form of Fourier series, beginning with (13.12), being a case in point.

It is not assumed that you know complex variables well. All that is required is knowledge of how to add, subtract, multiply and divide, and the definition of $|c|$ for complex c.

Equation (13.12) has a simpler, more compact form than (13.5). Do you now see why I referred to Fourier series as trig polynomials? The series (13.12) involves the jth powers of $e^{2\pi\frac{t}{T}}$.

13.1.2 Two-Dimensional Fourier Series

Let's now move from sounds to images. Just as we were taking time to be a continuous variable above, for the time being we are taking the position within an image to be continuous too; this is equivalent to having infinitely many pixels. Here g() is a function of two variables, g(u,v), where u and v are the horizontal and vertical coordinates of a point in the image, with g(u,v) being the intensity of the image at that point. If it is a gray-scale image, the intensity is whiteness of the image at that point, typically with 0 being pure black and 255 being pure white. If it is a color image, a typical graphics format is to store three intensity values at a point, one for each of red, green and blue. The various colors come from combining three colors at various intensities.

The terminology changes a bit. Our original data is now referred to as being in the **spatial domain**, rather than the time domain. But the Fourier series coefficients are still said to be in the frequency domain.

13.2 Discrete Fourier Transforms

In sound and image applications, we seldom if ever know the exact form of the repeating function g(). All we have is a **sampling** from g(), i.e. we only have values of g(t) for a set of discrete values of t.

In the sound example above, a typical sampling rate is 8000 samples per second.[4] So, we may have g(0), g(0.000125), g(0.000250), g(0.000375), and so on. In the image case, we sample the image pixel by pixel.

Integrals like (13.8) now change to sums.

13.2.1 One-Dimensional Data

Let $X = (x_0, ..., x_{n-1})$ denote the sampled values, i.e. the time-domain representation of g() based on our sample data. These are interpreted as data from one period of g(), with the period being n and the fundamental frequency being 1/n. The frequency-domain representation will also consist of n numbers, $c_0, ..., c_{n-1}$, defined as follows:

---

[4]See Section 13.10 for the reasons behind this.

$$c_k = \frac{1}{n} \sum_{j=0}^{n-1} x_j e^{-2\pi ijk/n} = \frac{1}{n} \sum_{j=0}^{n-1} x_j q^{jk} \tag{13.13}$$

where

$$q = e^{-2\pi i/n} \tag{13.14}$$

again with $i = \sqrt{-1}$. The array C of complex numbers c_k is called the **discrete Fourier transform** (DFT) of X. Note that (13.13) is basically a discrete analog of (13.9) and (13.10).

Note that instead of having infinitely many frequencies, we only have n of them, i.e. the n original data points x_j map to n frequency weights c_k.[5]

The quantity q is a nth root of 1:

$$q^n = e^{-2\pi i} = \cos(-2\pi) + i\sin(-2\pi) = 1 \tag{13.15}$$

Equation (13.13) can be written as

$$C = \frac{1}{n} AX, \tag{13.16}$$

where X is the vector x_j and

$$A = \begin{pmatrix} 1 & 1 & 1 & ... & 1 \\ 1 & q & q^2 & ... & q^{n-1} \\ ... & ... & ... & ... & ... \\ 1 & q^{n-1} & q^{2(n-1)} & ... & q^{(n-1)(n-1)} \end{pmatrix} \tag{13.17}$$

Here's R code to calculate A:

```
1  makeamat <- function(n,u)  {
2     m <- matrix(nrow=n,ncol=n)
3     for (i in 1:n) {
4        for (j in i:n) {
5           if (i == j) {
6              m[i,i] <- u^((i-1)^2)
7           }
8           else {
9              m[i,j] <- u^((i-1)*(j-1))
10             m[j,i] <- m[i,j]
```

[5] Actually, in the case of x_j real, which occurs with sound data, we really get only n/2 frequencies. The weight of the frequences after k = n/2 turn out to be the **conjugates** of those before n/2, where the conjugate of a+bi is defined to be a-bi.

```
11          }
12        }
13      }
14    m
15  }
```

13.2.2 Inversion

As in the continuous case, the DFT is a one-to-one transformation. so we can recover each domain from the other. The details are important:

The matrix A in (13.17) is a special case of **Vandermonde** matrices, known to be invertible. In fact, if we think of that matrix as a function of q, A(q), then it turns out that

$$[A(q)]^{-1} = \frac{1}{n} A(\frac{1}{q}) \tag{13.18}$$

Thus (13.16) becomes

$$X = n[A(q)]^{-1}C = A(\frac{1}{q})C \tag{13.19}$$

In nonmatrix terms:

$$x_j = \sum_{k=0}^{n-1} c_k e^{2\pi ijk/n} = \sum_{k=0}^{n-1} c_k q^{-jk} \tag{13.20}$$

Equation (13.20) is basically a discrete analog of (13.5).

Alternate Formulation

Equation (13.16) has a factor 1/n while (13.19) doesn't. In order to achieve symmetry, some authors of material on DFT opt to define the DFT and its inverse with $1/\sqrt{n}$ in (13.13) instead of 1/n, and by adding a factor $1/\sqrt{n}$ in (13.20). They then include a factor $1/\sqrt{n}$ in (13.17), with the result that $[A(q)]^{-1} = A(1/q)$. Thus everything simplifies.

Other formulations are possible. For instance, the R **fft()** routine's documentation says it's "unnormalized," meaning that there is neither a $1/n$ nor a $1/\sqrt{n}$ in (13.20). When using a DFT routine, be sure to determine what it assumes about these constant factors.

13.2.3　Two-Dimensional Data

The spectrum numbers c_{rs} are double-subscripted, like the original data x_{uv}, the latter being the pixel intensity in row u, column v of the image, u = 0,1,...,n-1, v = 0,1,...,m-1. Equation (13.13) becomes

$$c_{rs} = \frac{1}{n}\frac{1}{m}\sum_{j=0}^{n-1}\sum_{k=0}^{m-1} x_{jk}e^{-2\pi i(\frac{jr}{n}+\frac{ks}{m})} \tag{13.21}$$

where r = 0,1,...,n-1, s = 0,1,...,m-1.

Its inverse is

$$x_{rs} = \sum_{j=0}^{n-1}\sum_{k=0}^{m-1} c_{jk}e^{2\pi i(\frac{jr}{n}+\frac{ks}{m})} \tag{13.22}$$

13.3　Parallel Computation of Discrete Fourier Transforms

13.3.1　The Fast Fourier Transform

Speedy computation of a discrete Fourier transform was developed by Cooley and Tukey in their famous Fast Fourier Transform (FFT), which takes a "divide and conquer" approach:

Equation (13.13) can be rewritten as

$$c_k = \frac{1}{n}\left[\sum_{j=0}^{m-1} x_{2j}q^{2jk} + \sum_{j=0}^{m-1} x_{2j+1}q^{(2j+1)k},\right] \tag{13.23}$$

where $m = n/2$.

After some algebraic manipulation, this becomes

$$c_k = \frac{1}{2}\left[\frac{1}{m}\sum_{j=0}^{m-1} x_{2j}z^{jk} + q^k\frac{1}{m}\sum_{j=0}^{m-1} x_{2j+1}z^{jk}\right] \tag{13.24}$$

where $z = e^{-2\pi i/m}$.

A look at Equation (13.24) shows that the two sums within the brackets have the same form as Equation (13.13). In other words, Equation (13.24) shows how we can compute an n-point FFT from two $\frac{n}{2}$-point FFTs. That means that a DFT can be computed recursively, cutting the sample size in half at each recursive step.

In a shared-memory setting such as OpenMP, we could implement this recursive algorithm in the manners of Quicksort in Chapter 12.

In a message-passing setting, again because this is a divide-and-conquer algorithm, we can use the pattern of Hyperquicksort, also in Chapter 12.

Some digital signal processing chips implement this in hardware, with a special interconnection network to implement this algorithm.

13.3.2   A Matrix Approach

The matrix form of (13.13) is

$$C = \frac{1}{n} A X \tag{13.25}$$

where A is n x n. Element (j,k) of A is q^{jk}, while element j of X is x_j. This formulation of the problem then naturally leads one to use parallel methods for matrix multiplication, as in Chapter 11.

Divide-and-conquer tends not to work too well in shared-memory settings, because after some point, fewer and fewer threads will have work to do. Thus this matrix formulation is quite valuable.

13.3.3   Parallelizing Computation of the Inverse Transform

The form of the DFT (13.13) and its inverse (13.20) are very similar. For example, the inverse transform is again of a matrix form as in (13.25); even the new matrix looks a lot like the old one.[6]

Thus the methods mentioned above, e.g. FFT and the matrix approach, apply to calculation of the inverse transforms too.

13.3.4   Parallelizing Computation of the Two-Dimensional Transform

Regroup (13.21) as:

$$c_{rs} = \frac{1}{n} \sum_{j=0}^{n-1} \left(\frac{1}{m} \sum_{k=0}^{m-1} x_{jk} e^{-2\pi i \left(\frac{ks}{m} \right)} \right) e^{-2\pi i \left(\frac{jr}{n} \right)} \tag{13.26}$$

$$= \frac{1}{n} \sum_{j=0}^{n-1} y_{js} e^{-2\pi i \left(\frac{jr}{n} \right)} \tag{13.27}$$

---

[6]In fact, one can obtain the new matrix easily from the old, as explained in Section 13.9.

Note that y_{js}, i.e. the expression between the large parentheses, is the sth component of the DFT of the jth row of our data. And hey, the last expression (13.27) above is in the same form as (13.13)! Of course, this means we are taking the DFT of the spectral coefficients rather than observed data, but numbers are numbers.

In other words: To get the two-dimensional DFT of our data, we first get the one-dimensional DFTs of each row of the data, place these in rows, and then find the DFTs of each column. This property is called **separability**.

This certainly opens possibilities for parallelization. Each thread (shared memory case) or node (message passing case) could handle groups of rows of the original data, and in the second stage each thread could handle columns.

Or, we could interchange rows and columns in this process, i.e. put the j sum inside and k sum outside in the above derivation.

13.4 Available FFT Software

13.4.1 R

As of now, R only offers serial computation, through its function **fft()**. It works on both one- and two-dimensional (or more) data. If its argument **inverse** is set to TRUE, it will find the inverse.

Parallel computation of a two-dimensional transform can be easily accomplished by using **fft()** together with the approach in Section 13.3.4 and one of the packages for parallel R in Chapter 9. Here's how to do it in **snow**:

```
1  parfft2 <- function(cls,m) {
2    tmp <- parApply(cls,m,1,fft)
3    parApply(cls,tmp,1,fft)
4  }
```

Recall that when **parApply()** is called with a vector-valued function argument, the output from row i of the input matrix is placed in *column* i of the output matrix. Thus in the second call above, we used rows (argument 1) instead of columns.

13.4.2 CUFFT

Remember that CUDA includes some excellent FFT routines, in CUFFT.

13.4.3   FFTW

FFTW ("Fastest Fourier Transform in the West") is available for free download at `http://www.fftw.org`. It includes versions callable from OpenMP and MPI.

13.5   Applications to Image Processing

In image processing, there are a number of different operations which we wish to perform. We will consider two of them here.

13.5.1   Smoothing

An image may be too "rough." There may be some pixels which are noise, accidental values that don't fit smoothly with the neighboring points in the image.

One way to smooth things out would be to replace each pixel intensity value[7] by the mean or median among the pixels neighbors. These could be the four immediate neighbors if just a little smoothing is needed, or we could go further out for a higher amount of smoothing. There are many variants of this.

But another way would be to apply a **low-pass filter** to the DFT of our image. This means that after we compute the DFT, we simply delete the higher harmonics, i.e. set c_{rs} to 0 for the larger values of r and s. We then take the inverse transform back to the spatial domain. Remember, the sine and cosine functions of higher harmonics are "wigglier," so you can see that all this will have the effect of removing some of the wiggliness in our image—exactly what we wanted.

We can control the amount of smoothing by the number of harmonics we remove.

The term *low-pass filter* obviously alludes to the fact that the low frequencies "pass" through the filter but the high frequencies are blocked. Since we've removed the high-oscillatory components, the effect is a smoother image.[8]

To do smoothing in parallel, if we just average neighbors, this is easily parallelized. If we try a low-pass filter, then we use the parallelization methods shown here earlier.

13.5.2   Example: Audio Smoothing in R

Below is code to do smoothing on sound. It inputs a sound sequence **snd**, and performs low-pass filtering, setting to 0 all DFT terms having *k* greater than `maxidx` in (13.13).

---

[7]Remember, there may be three intensity values per pixel, for red, green and blue.

[8]Note that we may do more smoothing in some parts of the image than in others.

```
1  p <- function(snd,maxidx) {
2      four <- fft(snd)
3      n <- length(four)
4      newfour <- c(four[1:maxidx],rep(0,n-maxidx))
5      return(Re(fft(newfour,inverse=T)/n))
6  }
```

Here the **Re()** function extracts the real part of a complex number.

13.5.3　Edge Detection

In computer vision applications, we need to have a machine-automated way to deduce which pixels in an image form an edge of an object.

Again, edge-detection can be done in primitive ways. Since an edge is a place in the image in which there is a sharp change in the intensities at the pixels, we can calculate slopes of the intensities, in the horizontal and vertical directions. (This is really calculating the approximate values of the partial derivatives in those directions.)

But the Fourier approach would be to apply a high-pass filter. Since an edge is a set of pixels which are abruptly different from their neighbors, we want to keep the high-frequency components and block out the low ones.

Again, this means first taking the Fourier transform of the original, then deleting the low-frequency terms, then taking the inverse transform to go back to the spatial domain.

Below we have "before and after" pictures, first of original data and then the picture after an edge-detection process has been applied.[9]

---

[9]These pictures are courtesy of Bill Green of the Robotics Laboratory at Drexel University. In this case he is using a Sobel process instead of Fourier analysis, but the result would have been similar for the latter. See his Web tutorial at `www.pages.drexel.edu/` `~weg22/edge.html`, including the original pictures, which may not show up well in our printed book here.

The second picture looks like a charcoal sketch! But it was derived mathematically from the original picture, using edge-detection methods.

Note that edge detection methods also may be used to determine where sounds ("ah," "ee") begin and end in speech-recognition applications. In the image case, edge detection is useful for face recognition, etc.

Parallelization here is similar to that of the smoothing case.

13.6   R Access to Sound and Image Files

In order to apply these transformations to sound and image files, you need to extract the actual data from the files. The formats are usually pretty complex. You can do this easily using the R **tuneR** and **pixmap** libraries.

After extracting the data, you can apply the transformations, then transform back to the time/spatial domain, and replace the data component of the original class.

13.7   Keeping the Pixel Intensities in the Proper Range

Normally pixel intensities are stored as integers between 0 and 255, inclusive. With many of the operations mentioned above, both Fourier-based and otherwise, we can get negative intensity values, or values higher than 255. We may wish to discard the negative values and scale down the positive ones so that most or all are smaller than 256.

Furthermore, even if most or all of our values are in the range 0 to 255, they may be near 0, i.e. too faint. If so, we may wish to multiply them by a constant.

13.8　Does the Function g() Really Have to Be Repeating?

It is clear that in the case of a vibrating reed, our loudness function g(t) really is periodic. What about other cases?

A graph of your voice would look "locally periodic." One difference would be that the graph would exhibit more change through time as you make various sounds in speaking, compared to the one repeating sound for the reed. Even in this case, though, your voice *is* repeating within short time intervals, each interval corresponding to a different sound. If you say the word *eye*, for instance, you make an "ah" sound and then an "ee" sound. The graph of your voice would show one repeating pattern during the time you are saying "ah," and another repeating pattern during the time you are saying "ee." So, even for voices, we do have repeating patterns over short time intervals.

On the other hand, in the image case, the function may be nearly constant for long distances (horizontally or vertically), so a local periodicity argument doesn't seem to work there.

The fact is, though, that it really doesn't matter in the applications we are considering here. Even though mathematically our work here has tacitly assumed that our image is duplicated infinitely times (horizontally and vertically),[10] we don't care about this. We just want to get a measure of "wiggliness," and fitting linear combinations of trig functions does this for us.

13.9　Vector Space Issues (optional section)

The theory of Fourier series (and of other similar transforms), relies on vector spaces. It actually is helpful to look at some of that here. Let's first discuss the derivation of (13.13).

Define X and C as in Section 13.2. X's components are real, but it is also a member of the vector space V of all n-component arrays of complex numbers.

For any complex number a+bi, define its **conjugate**, $\overline{a+bi} = a - bi$. Note that

$$\overline{e^{i\theta}} = \cos\theta - i\sin\theta == \cos(-\theta) + i\sin(-\theta) = e^{-i\theta} \tag{13.28}$$

Define an inner product ("dot product"),

$$[u, w] = \frac{1}{n}\sum_{j=0}^{n-1} u_j \bar{w}_j. \tag{13.29}$$

Define

---

[10] And in the case of the cosine transform, implicitly we are assuming that the image flips itself on every adjacent copy of the image, first right-side up, then upside-own, then right-side up again, etc.

$$v_h = (1, q^{-h}, q^{-2h}, ..., q^{-(n-1)h}), h = 0, 1, ..., n - 1. \tag{13.30}$$

Then it turns out that the v_h form an orthonormal basis for V.[1] For example, to show orthnogonality, observe that for $r \neq s$

$$
\begin{aligned}
[v_r, v_s] &= \frac{1}{n} \sum_{j=0}^{n-1} v_{rj} \overline{v_{sj}} & (13.31) \\
&= \frac{1}{n} \sum_{j=0} q^{j(-r+s)} & (13.32) \\
&= \frac{1 - q^{(-r+s)n}}{n(1 - q)} & (13.33) \\
&= 0, & (13.34)
\end{aligned}
$$

due to the identity $1 + y + y^2 + ... + y^k = \frac{1-y^{k+1}}{1-y}$ and the fact that $q^n = 1$. In the case r = s, the above computation shows that $[v_r, v_s] = 1$.

The DFT of X, which we called C, can be considered the "coordinates" of X in V, relative to this orthonormal basis. The kth coordinate is then $[X, v_k]$, which by definition is (13.13).

The fact that we have an orthonormal basis for V here means that the matrix A/n in (13.25) is an orthogonal matrix. For real numbers, this means that this matrix's inverse is its transpose. In the complex case, instead of a straight transpose, we do a conjugate transpose, $B = \overline{A/n}^t$, where t means transpose. So, B is the inverse of A/n. In other words, in (13.25), we can easily get back to X from C, via

$$X = BC = \frac{1}{n} \bar{A}^t C. \tag{13.35}$$

It's really the same for the nondiscrete case. Here the vector space consists of all the possible periodic functions g() (with reasonable conditions placed regarding continuity etc.) forms the vector space, and the sine and cosine functions form an orthonormal basis. The a_n and b_n are then the "coordinates" of g() when the latter is viewed as an element of that space.

---

[1] Recall that this means that these vectors are orthogonal to each other, and have length 1, and that they span V.

13.10 Bandwidth: How to Read the *San Francisco Chronicle* Business Page (optional section)

The popular press, especially business or technical sections, often uses the term **bandwidth**. What does this mean?

Any transmission medium has a natural range $[f_{min}, f_{max}]$ of frequencies that it can handle well. For example, an ordinary voice-grade telephone line can do a good job of transmitting signals of frequencies in the range 0 Hz to 4000 Hz, where "Hz" means cycles per second. Signals of frequencies outside this range suffer fade in strength, i.e are **attenuated**, as they pass through the phone line.[12]

We call the frequency interval [0,4000] the **effective bandwidth** (or just the **bandwidth**) of the phone line.

In addition to the bandwidth of a **medium**, we also speak of the bandwidth of a **signal**. For instance, although your voice is a mixture of many different frequencies, represented in the Fourier series for your voice's waveform, the really low and really high frequency components, outside the range [340,3400], have very low power, i.e. their a_n and b_n coefficients are small. Most of the power of your voice signal is in that range of frequencies, which we would call the effective bandwidth of your voice waveform. This is also the reason why digitized speech is sampled at the rate of 8,000 samples per second. A famous theorem, due to Nyquist, shows that the sampling rate should be double the maximum frequency. Here the number 3,400 is "rounded up" to 4,000, and after doubling we get 8,000.

Obviously, in order for your voice to be heard well on the other end of your phone connection, the bandwidth of the phone line must be at least as broad as that of your voice signal, and that is the case.

However, the phone line's bandwidth is not much broader than that of your voice signal. So, some of the frequencies in your voice will fade out before they reach the other person, and thus some degree of distortion will occur. It is common, for example, for the letter 'f' spoken on one end to be mis-heard as 's'on the other end. This also explains why your voice sounds a little different on the phone than in person. Still, most frequencies are reproduced well and phone conversations work well.

We often use the term "bandwidth" to literally refer to width, i.e. the width of the interval $[f_{min}, f_{max}]$.

There is huge variation in bandwidth among transmission media. As we have seen, phone lines have bandwidth intervals covering values on the order of 10^3. For optical fibers, these numbers are more on the order of 10^{15}.

The radio and TV frequency ranges are large also, which is why, for example, we can have many

---

[12]And in fact will probably be deliberately filtered out.

AM radio stations in a given city. The AM frequency range is divided into subranges, called **channels**. The width of these channels is on the order of the 4000 we need for a voice conversation. That means that the transmitter at a station needs to shift its content, which is something like in the [0,4000] range, to its channel range. It does that by multiplying its content times a sine wave of frequency equal to the center of the channel. If one applies a few trig identities, one finds that the product signal falls into the proper channel!

Accordingly, an optical fiber could also carry many simultaneous phone conversations.

Bandwidth also determines how fast we can set digital bits. Think of sending the sequence 10101010... If we graph this over time, we get a "squarewave" shape. Since it is repeating, it has a Fourier series. What happends if we double the bit rate? We get the same graph, only horizontally compressed by a factor of two. The effect of this on this graph's Fourier series is that, for example, our former a_3 will now be our new a_6, i.e. the $2\pi \cdot 3f_0$ frequency cosine wave component of the graph now has the double the old frequency, i.e. is now $2\pi \cdot 6f_0$. That in turn means that the effective bandwidth of our 10101010... signal has doubled too.

In other words: To send high bit rates, we need media with large bandwidths.

第 14 章 Parallel Computation in Statistics/Data Mining

How did the word *statistics* get supplanted by *data mining*? In a word, it is a matter of scale.

In the old days of statistics, a data set of 300 observations on 3 or 4 variables was considered large. Today, the widespread use of computers and the Web yield data sets with numbers of observations that are easily in the tens of thousands range, and in a number of cases even tens of millions. The numbers of variables can also be in the thousands or more.

In addition, the methods have become much more combinatorial in nature. In a classification problem, for instance, the old discriminant analysis involved only matrix computation, whereas a nearest-neighbor analysis requires far more computer cycles to complete.

In short, this calls for parallel methods of computation.

14.1 Itemset Analysis

14.1.1 What Is It?

The term **data mining** is a buzzword, but all it means is the process of finding relationships among a set of variables. In other words, it would seem to simply be a good old-fashioned statistics problem.

Well, in fact it *is* simply a statistics problem—but writ large, as mentioned earlier.

Major, Major Warning: With so many variables, the chances of picking up spurious relations between variables is large. And although many books and tutorials on data mining will at least pay lip service to this issue (referring to it as **overfitting**), they don't emphasize it enough.[1]

---

[1] Some writers recommend splitting one's data into a **training set**, which is used to discover relationships, and a **validation set**, which is used to confirm those relationships. It's a good idea, but overfitting can still occur even with this precaution.

Putting the overfitting problem aside, though, by now the reader's reaction should be, "This calls for parallel processing," and he/she is correct. Here we'll look at parallelizing a particular problem, called **itemset analysis**, the most famous example of which is the **market basket problem**:

14.1.2 The Market Basket Problem

Consider an online bookstore that has records of every sale on the store's site. Those sales may be represented as a matrix S, whose (i,j)th element S_{ij} is equal to either 1 or 0, depending on whether the ith sale included book j, i = 0,1,...,s-1, j = 0,1,...,t-1. So each row of S represents one sale, with the 1s in that row showing which titles were bought. Each column of S represents one book title, with the 1s showing which sales transactions included that book.

Let's denote the entire line of book titles by $T_0, ..., T_{b-1}$. An **itemset** is just a subset of this. A **frequent** itemset is one which appears in many of sales transactions. But there is more to it than that. The store wants to choose some books for special ads, of the form "We see you bought books X and Y. We think you may be interested in Z."

Though we are using marketing as a running example here (which is the typical way that this subject is introduced), we will usually just refer to "items" instead of books, and to "database records" rather than sales transactions.

We have the following terminology:

- An **association rule** $I \to J$ is simply an ordered pair of disjoint itemsets I and J.

- The **support** of an an association rule $I \to J$ is the proportion of records which include both I and J.

- The **confidence** of an association rule $I \to J$ is the proportion of records which include J, *among those records which include I*.

Note that in probability terms, the support is basically P(I and J) while the confidence is P(J|I). If the confidence is high in the book example, it means that buyers of the books in set I also tend to buy those in J. But this information is not very useful if the support is low, because it means that the combination occurs so rarely that it may not be worth our time to deal with it.

So, the user—let's call him/her the "data miner"—will first set thresholds for support and confidence, and then set out to find all association rules for which support and confidence exceed their respective thresholds.

14.1.3 Serial Algorithms

Various algorithms have been developed to find frequent itemsets and association rules. The most famous one for the former task is the **Apriori** algorithm. Even it has many forms. We will discuss one of the simplest forms here.

The algorithm is basically a breadth-first tree search. At the root we find the frequent 1-item itemsets. In the online bookstore, for instance, this would mean finding all individual books that appear in at least r of our sales transaction records, where r is our threshold.

At the second level, we find the frequent 2-item itemsets, e.g. all pairs of books that appear in at least r sales records, and so on. After we finish with level i, we then generate new candidate itemsets of size i+1 from the frequent itemsets we found of size i.

The key point in the latter operation is that if an itemset is not frequent, i.e. has support less than the threshold, then adding further items to it will make it even less frequent. That itemset is then pruned from the tree, and the branch ends.

Here is the pseudocode:

set F_1 to the set of 1-item itemsets whose support exceeds the threshold
for i = 2 to b
    $F_i = \phi$
    for each I in F_{i-1}
        for each K in F_1
            $Q = I \cup K$
            if support(Q) exceeds support threshold
                add Q to F_i
    if F_i is empty break
return $\cup_i F_i$

In other words, we are building up the itemsets of size i from those of size i-1, adding all possible choices of one element to each of the latter.

Again, there are many refinements of this, which shave off work to be done and thus increase speed. For example, we should avoid checking the same itemsets twice, e.g. first {1,2} then {2,1}. This can be accomplished by keeping itemsets in lexicographical order. We will not pursue any refinements here.

14.1.4   Parallelizing the Apriori Algorithm

Clearly there is lots of opportunity for parallelizing the serial algorithm above. Both of the inner **for** loops can be parallelized in straightforward ways; they are "embarrassingly parallel." There are of course critical sections to worry about in the shared-memory setting, and in the message-passing setting one must designate a manager node in which to store the F_i.

However, as more and more refinements are made in the serial algorithm, then the parallelism in this algorithm become less and less "embarrassing." And things become more challenging if the storage needs of the F_i, and of their associated "accounting materials" such as a directory showing the current tree structure (done via hash trees), become greater than what can be stored in the memory of one node, say in the message-passing case.

In other words, parallelizing the market basket problem can be very challenging. The interested reader is referred to the considerable literature which has developed on this topic.

14.2   Probability Density Estimation

Let X denote some quantity of interest in a given population, say people's heights. Technically, the **probability density function** of X, typically denoted by f, is a function on the real line with the following properties:

- $f(t) \geq 0$ for all t
- for any $r < s$,

$$P(r < X < s) = \int_r^s f(t) \ dt \tag{14.1}$$

(Note that this implies that f integrates to 1.)

This seems abstract, but it's really very simple: Say we have data on X, n sample values $X_1, ..., X_n$, and we plot a histogram from this data. Then *f is what the histogram is estimating.* If we have more and more data, the histogram gets closer and closer to the true f.[2]

So, how do we estimate f, and how do we use parallel computing to reduce the time needed?

---

[2]The histogram must be scaled to have total area 1. Most statistical programs have options for this.

14.2.1   Kernel-Based Density Estimation

Histogram computation breaks the real down into intervals, and then counts how many X_i fall into each interval. This is fine as a crude method, but one can do better.

No matter what the interval width is, the histogram will consist of a bunch of rectanges, rather than a smooth curve. This problem basically stems from a lack of weighting on the data.

For example, suppose we are estimating f(25.8), and suppose our histogram interval is [24.0,26.0], with 54 points falling into that interval. Intuitively, we can do better if we give the points closer to 25.8 more weight.

One way to do this is called **kernel-based** density estimation, which for instance in R is handled by the function **density()**.

We need a set of weights, more precisely a weight function k, called the **kernel**. Any nonnegative function which integrates to 1—i.e. a density function in its own right—will work. Typically k is taken to be the Gaussian or normal density function,

$$k(u) = \frac{1}{\sqrt{2\pi}} e^{-0.5u^2} \tag{14.2}$$

Our estimator is then

$$\widehat{f}(t) = \frac{1}{nh} \sum_{i=1}^{n} k\left(\frac{t - X_i}{h}\right) \tag{14.3}$$

In statistics, it is customary to use the $\widehat{}$ symbol (pronounced "hat") to mean "estimate of." Here $\widehat{f}$ means the estimate of f.

Note carefully that we are estimating an entire function! There are infinitely many possible values of t, thus infinitely many values of f(t) to be estimated. This is reflected in (14.3), as $\widehat{f}(t)$ does indeed give a (potentially) different value for each t.

Here h, called the *bandwidth*, is playing a role analogous to the interval width in the case of histograms. We must choose the value of h, just like for a histogram we must choose the bin width.[3]

Again, this looks very abstract, but all it is doing is assigning weights to the data. Consider our example above in which we wish to estimate f(25.8), i.e. t = 25.8 and suppose we choose h to be 6.0. If say, X_{88} is 1209.1, very far as away from 25.8, we don't want this data point to have much weight in our estimation of f(25.8). Well, it won't have much weight at all, because the quantity

$$u = \frac{25.8 - 88}{6} \tag{14.4}$$

---

[3]Some statistical programs will choose default values, based on theory.

will be very large, and (14.2) will be tiny, as u will be way, way out in the left tail.

Now, keep all this in perspective. In the end, we will be plotting a curve, *just like we do with a histogram.* We simply have a more sophiticated way to do this than plotting a histogram. Following are the graphs generated first by the histogram method, then by the kernel method, on the same data:

Histogram of x

density.default(x = x)
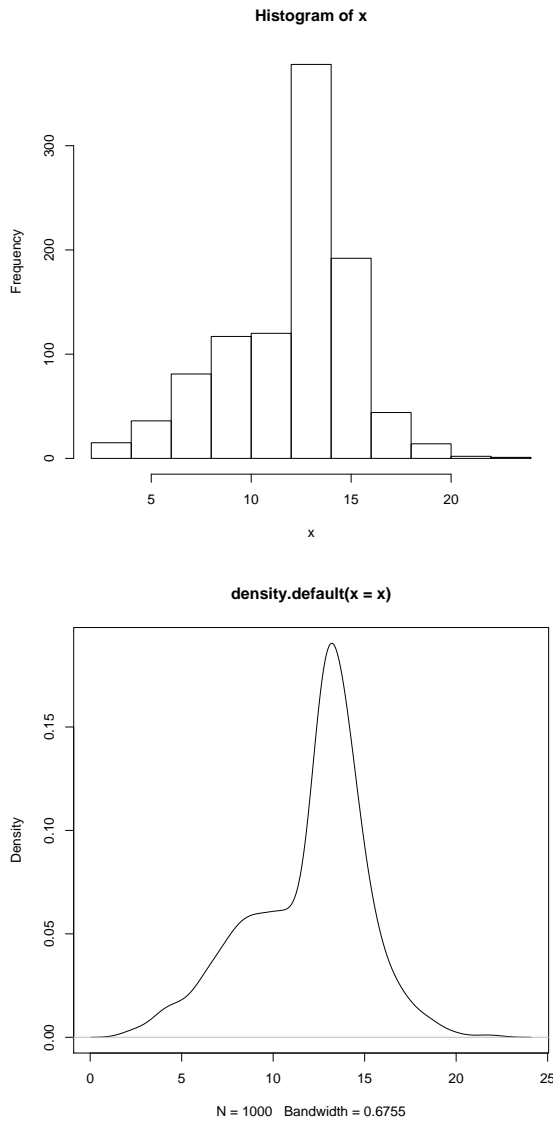
There are many ways to parallelize this computation, such as:

- Remember, we are going to compute (14.3) for many values of t. So, we can just have each process compute a block of those values.

- We may wish to try several different values of h, just as we might try several different interval widths for a histogram. We could have each process compute using its own values of h.

- It can be shown that (14.3) has the form of something called a **convolution**. The theory of convolution would take us too far afield,[④] but this fact is useful here, as the Fourier transform of a convolution can be shown to be the product of the Fourier transforms of the two convolved components.[⑤] In other words, *this reduces the problem to that of parallelizing Fourier transforms*—something we know how to do, from Chapter 13.

14.2.2 Histogram Computation for Images

In image processing, histograms are used to find tallies of how many pixels there are of each intensity. (Note that there is thus no interval width issue, as there is a separate "interval" value for each possible intensity level.) The serial pseudocode is:

```
1  for i = 1,...,numintenslevels:
2      count = 0
3      for row = 1,...,numrows:
4        for col = 1,...,numcols:
5            if image[row][col] == i: count++
6      hist[i] = count
```

On the surface, this is certainly an "embarrassingly parallel" problem. In OpenMP, for instance, we might have each thread handle a block of rows of the image, i.e. parallelize the **for row** loop. In CUDA, we might have each thread handle an individual pixel, thus parallelizing the nested **for row/col** loops.

---

④

If you've seen the term before and are curious as to how this is a convolution, read on:

Write (14.3) as

$$\widehat{f}(t) = \sum_{i=1}^{n} \frac{1}{h} k \left(\frac{t - X_i}{h} \right) \cdot \frac{1}{n} \tag{14.5}$$

Now consider two artificial random variables U and V, created just for the purpose of facilitating computation, defined as follows.

The random variable U takes on the values ih with probability $g \cdot \frac{1}{h} k(i)$, i = -c,-c+1,...,0,1,...,c for some value of c that we choose to cover most of the area under k, with g chosen so that the probabilities sum to 1. The random variable V takes on the values $X_1, ..., X_n$ (considered fixed here), with probability 1/n each. U and V are set to be independent.

Then (g times) (14.5) becomes P(U+V=t), exactly what convolution is about, the probability mass function (or density, in the continuous case) of a random variable arising as the sum of two independent nonnegative random variables.

⑤ Again, if you have some background in probability and have see characteristic functions, this fact comes from the fact that the characteristic function of the sum of two independent random variables is equal to the product of the characteristic functions of the two variables.

However, to make this go fast is a challenge, say in CUDA, due to issues of what to store in shared memory, when to swap it out, etc. A very nice account of fine-tuning this computation in CUDA is given in *Histogram Calculation in CUDA*, by Victor Podlozhnyuk of NVIDIA, 2007, `http://developer.download.nvidia.com/compute/cuda/1_1/Website/projects/histogram256/doc/histogram.pdf`. The actual code is at `http://developer.download.nvidia.com/compute/cuda/sdk/website/Data-Parallel_Algorithms.html#histogram`. A summary follows:

(Much of the research into understand Podlozhnyuk's algorithm was done by UC Davis graduate student Spencer Mathews.)

Podlozhnyuk's overall plan is to have the threads compute subhistograms for various chunks of the image, then merge the subhistograms to create the histogram for the entire data set. Each thread will handle 1/k of the image's pixels, where k is the total number of threads in the grid, i.e. across all blocks.

In Podlozhnyuk's first cut at the problem, he maintains a separate subhistogram for each thread. He calls this version of the code **histogram64**. The name stems from the fact that only 64 intensity levels are used, i.e. the more significant 6 bits of each pixel's data byte. The reason for this restriction will be discussed later.

Each thread will store its subhistogram as an array of bytes; the count of pixels that a thread finds to have intensity i will be stored in the ith byte of this array. Considering the content of a byte as an unsigned number, that means that each thread can process only 255 pixels.

The subhistograms will be stored together in a two-dimensional array, the jth being the subhistogram for thread j. Since the subhistograms are accessed repeatedly, we want to store this two-dimensional array in shared memory. (Since each pixel will be read only once, there would be no value in storing it in shared memory, so it is in global memory.)

The main concern is bank conflicts. As the various threads in a block write to the two-dimensional array, they may collide with each other, i.e. try to write to different locations within the same bank. But Podlozhnyuk devised a clever way to stagger the accesses, so that in fact there are no bank conflicts at all.

In the end, the many subhistograms within a block must be merged, and those merged counts must in turn be merged across all blocks. The former operation is done again by careful ordering to avoid any bank conflicts, and then the latter is done **atomicAdd()**.

Now, why does **histogram64** tabulate image intensities at only 6-bit granularity? It's simply a matter of resource limitations. Podlozhnyuk notes that NVIDIA says that for best efficiency, there should be between 128 and 256 threads per block. He takes the middle ground, 192. With 16K of

shared memory per block, 16K/192 works out to about 85 bytes per thread. That eliminates computing a histogram for the full 8-bit image data, with 256 intensity levels, which would require 256 bytes for each thread.

Accordingly, Podlozhnyuk offers **histogram256**, which refines the process, by having one subhistogram per warp, instead of per thread. This allows the full 8-bit data, 256 levels, to be tabulated, one word devoted to each count, rather than just one byte. A subhistogram is now a table, 256 rows by 32 columns (one column for each thread in the warp), with each table entry being 4 bytes (1 byte is not sufficient, as 32 threads are tabulating with it).

14.3   Clustering

Suppose you have data consisting of (X,Y) pairs, which when plotted look like this:
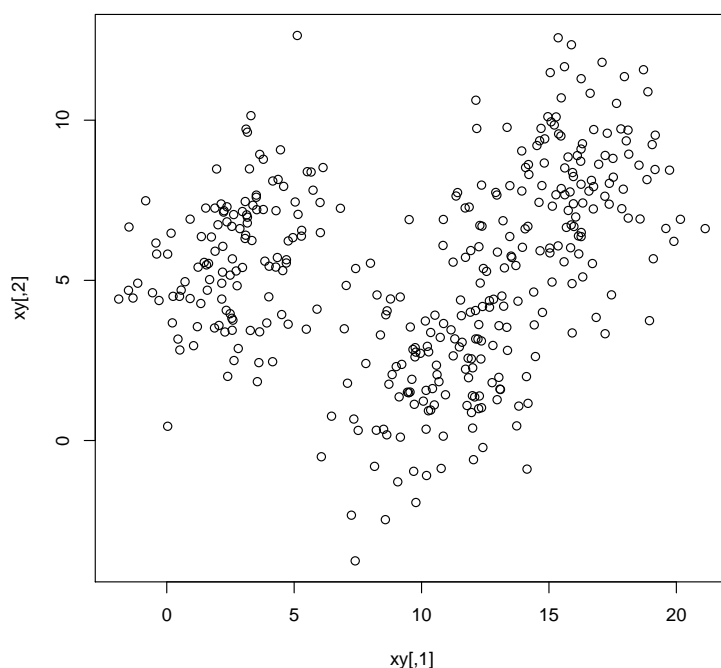
It looks like there may be two or three groups here. What clustering algorithms do is to form groups, both their number and their membership, i.e. which data points belong to which groups. (Note carefully that *there is no "correct" answer here. This is merely an exploratory data analysis tool.*)

Clustering is used is many diverse fields. For instance, it is used in image processing for segmentation and edge detection.

Here we have to two variables, say people's heights and weights. In general we have many variables, say p of them, so whatever clustering we find will be in p-dimensional space. No, we can't picture it very easily of p is larger than (or even equal to) 3, but we can at least identify membership, i.e. John and Mary are in group 1, Jenny is in group 2, etc. We may derive some insight from this.

There are many, many types of clustering algorithms. Here we will discuss the famous **k-means** algorithm, developed by Prof. Jim MacQueen of the UCLA business school.

The method couldn't be simpler. Choose k, the number of groups you want to form, and then run this:

```
1   # form initial groups from the first k data points (or choose randomly)
2   for i = 1,...,k:
3      group[i] = (x[i],y[i])
4      center[i] = (x[i],y[i])
5   do:
6      for j = 1,...,n:
7         find the closest center[i] to (x[j],y[j])
8         cl[j] = the i you got in the previous line
9      for i = 1,...,k:
10        group[i] = all (x[j],y[j]) such that cl[j] = i
11        center[i] = average of all (x,y) in group[i]
12   until group memberships do not change from one iteration to the next
```

Definitions of terms:

- *Closest* means in p-dimensional space, with the usual Euclidean distance: The distance from $(a_1, ..., a_p)$ to $(b_1, ..., b_p)$ is

$$\sqrt{(b_1 - a_1)^2 + ... + (b_p - a_p)^2} \qquad (14.6)$$

Other distance definitions could be used too, of course.

- The *center* of a group is its **centroid**, which is a fancy name for taking the average value in each component of the data points in the group. If p = 2, for example, the center consists of the point whose X coordinate is the average X value among members of the group, and whose Y coordinate is the average Y value in the group.

14.3.1 Example: k-Means Clustering in R

In terms of parallelization, again we have an embarrassingly parallel problem. Here's **snow** code for it:

```r
# snow version of k-means clustering problem

# returns distances from x to each vector in y;
# here x is a single vector and y is a bunch of them
#
# define distance between 2 points to be the sum of the absolute values
# of their componentwise differences; e.g. distance between (5,4.2) and
# (3,5.6) is 2 + 1.4 = 3.4
dst <- function(x,y) {
    tmpmat <- matrix(abs(x-y),byrow=T,ncol=length(x)) # note recycling
    rowSums(tmpmat)
}

# will check this worker's mchunk matrix against currctrs, the current
# centers of the groups, returning a matrix; row j of the matrix will
# consist of the vector sum of the points in mchunk closest to j-th
# current center, and the count of such points
findnewgrps <- function(currctrs) {
    ngrps <- nrow(currctrs)
    spacedim <- ncol(currctrs) # what dimension space are we in?
    # set up the return matrix
    sumcounts <- matrix(rep(0,ngrps*(spacedim+1)),nrow=ngrps)
    for (i in 1:nrow(mchunk)) {
        dsts <- dst(mchunk[i,],t(currctrs))
        j <- which.min(dsts)
        sumcounts[j,] <- sumcounts[j,] + c(mchunk[i,],1)
    }
    sumcounts
}
```

```
30
31  parkm <- function(cls,m,niters,initcenters) {
32     n <- nrow(m)
33     spacedim <- ncol(m) # what dimension space are we in?
34     # determine which worker gets which chunk of rows of m
35     options(warn=-1)
36     ichunks <- split(1:n,1:length(cls))
37     options(warn=0)
38     # form row chunks
39     mchunks <- lapply(ichunks,function(ichunk) m[ichunk,])
40     mcf <- function(mchunk) mchunk <<- mchunk
41     # send row chunks to workers; each chunk will be a global variable at
42     # the worker, named mchunk
43     invisible(clusterApply(cls,mchunks,mcf))
44     # send dst() to workers
45     clusterExport(cls,"dst")
46     # start iterations
47     centers <- initcenters
48     for (i in 1:niters) {
49        sumcounts <- clusterCall(cls,findnewgrps,centers)
50        tmp <- Reduce("+",sumcounts)
51        centers <- tmp[,1:spacedim] / tmp[,spacedim+1]
52        # if a group is empty, let's set its center to 0s
53        centers[is.nan(centers)] <- 0
54     }
55     centers
56  }
```

14.4 Principal Component Analysis (PCA)

Consider data consisting of (X,Y) pairs as we saw in Section 14.3. Suppose X and Y are highly correlated with each other. Then for some constants c and d,

$$Y \approx c + dX \tag{14.7}$$

Then in a sense there is really just one random variable here, as the second is nearly equal to some linear combination of the first. The second provides us with almost no new information, once we have the first. In other words, even though the vector (X,Y) roams in *two*-dimensional space, it usually sticks close to a *one*-dimensional object, namely the line (14.7).

Now think again of p variables. It may be the case that there exist r < p variables, consisting of linear combinations of the p variables, that carry most of the information of the full set of p variables. If r is much less than p, we would prefer to work with those r variables. In data mining, this is called **dimension reduction**.

It can be shown that we can find these r variables by finding the r eigenvectors corresponding to the r largest eigenvalues of a certain matrix. So again we have a matrix formulation, and thus parallelizing the problem can be done easily by using methods for parallel matrix operations. We discussed parallel eigenvector algorithms in Section 11.6.

14.5　Monte Carlo Simulation

Monte Carlo simulation is typically (though not always) used to find probabilistic quantities such as probabilities and expected values. Consider a simple example problem:

> An urn contains blue, yellow and green marbles, in numbers 5, 12 and 13, respectively. We choose 6 marbles at random. What is the probability that we get more yellow marbles than than green and more green than blue?

We could find the approximate answer by simulation:

```
1  count = 0
2  for i = 1,...,n
3     simulate drawing 6 marbles
4     if yellows > greens > blues then count = count + 1
5  calculate approximate probability as count/n
```

The larger n is, the more accurate will be our approximate probability.

At first glance, this problem seems quite embarrassingly parallel. Say we are on a shared memory machine running 10 threads and wish to have n = 100000. Then we simply have each of our threads run the above code with n = 10000, and then average our 10 results.

The trouble with this, though, is that it assumes that the random numbers used by each thread are independent of the others. A naive approach, say by calling **random()** in the C library, will not achieve such independence. With some random number libraries, in fact, you'll get the same stream for each thread, certainly not what you want.

A number of techniques have been developed for generating parallel independent random number streams. We will not pursue the technical details here, but will give links to code for them.

- The NVIDIA CUDA SDK includes a parallel random number generator, the Mersenne Twister. The CURAND library has more.
- RngStream can be used with, for example, OpenMP and MPI.
- SPRNG is aimed at MPI, but apparently usable in shared memory settings as well. Rsprng is an R interface to SPRNG.
- OpenMP: An OpenMP version of the Mersenne Twister is available at `http://www.pgroup.com/lit/articles/insider/v2n2a4.htm`. Other parallel random number generators for OpenMP are available via a Web search.

There are many, many more.

第 15 章　Parallel Python Threads and Multiprocessing Modules

(Francis Hsu contributed sections of this chapter.)

There are a number of ways to write parallel Python code.[①]

15.1　The Python Threads and Multiprocessing Modules

Python's thread system builds on the underlying OS threads. They are thus pre-emptible. Note, though, that Python adds its own threads manager on top of the OS thread system; see Section 15.1.3.

15.1.1　Python Threads Modules

Python threads are accessible via two modules, **thread.py** and **threading.py**. The former is more primitive, thus easier to learn from, and we will start with it.

The `thread` Module

The example here involves a client/server pair.[②] As you'll see from reading the comments at the start of the files, the program does nothing useful, but is a simple illustration of the principles. We set up two invocations of the client; they keep sending letters to the server; the server concatenates all the letters it receives.

[①]This chapter is shared by two of my open source books: `http://heather.cs.ucdavis.edu/~matloff/158/PLN/ParProcBook.pdf` and `http://heather.cs.ucdavis.edu/~matloff/Python/PLN/FastLanePython.pdf`. If you wish to more about the topics covered in the book other than the one you are now reading, please check the other!

[②]It is preferable here that the reader be familiar with basic network programming. See my tutorial at `http://heather.cs.ucdavis.edu/~matloff/Python/PLN/FastLanePython.pdf`. However, the comments preceding the various network calls would probably be enough for a reader without background in networks to follow what is going on.

Only the server needs to be threaded. It will have one thread for each client.

Here is the client code, **clnt.py**:

```
1    # simple illustration of thread module
2
3    # two clients connect to server; each client repeatedly sends a letter,
4    # stored in the variable k, which the server appends to a global string
5    # v, and reports v to the client; k = '' means the client is dropping
6    # out; when all clients are gone, server prints the final string v
7
8    # this is the client; usage is
9
10   #     python clnt.py server_address port_number
11
12   import socket  # networking module
13   import sys
14
15   # create Internet TCP socket
16   s = socket.socket(socket.AF_INET, socket.SOCK_STREAM)
17
18   host = sys.argv[1]  # server address
19   port = int(sys.argv[2])  # server port
20
21   # connect to server
22   s.connect((host, port))
23
24   while(1):
25      # get letter
26      k = raw_input('enter a letter:')
27      s.send(k)  # send k to server
28      # if stop signal, then leave loop
29      if k == '': break
30      v = s.recv(1024)  # receive v from server (up to 1024 bytes)
31      print v
32
33   s.close() # close socket
```

And here is the server, **srvr.py**:

```
1    # simple illustration of thread module
2
3    # multiple clients connect to server; each client repeatedly sends a
4    # letter k, which the server adds to a global string v and echos back
5    # to the client; k = '' means the client is dropping out; when all
6    # clients are gone, server prints final value of v
7
8    # this is the server
```

```
 9
10   import socket  # networking module
11   import sys
12
13   import thread
14
15   # note the globals v and nclnt, and their supporting locks, which are
16   #     also global; the standard method of communication between threads is
17   #     via globals
18
19   # function for thread to serve a particular client, c
20   def serveclient(c):
21      global v,nclnt,vlock,nclntlock
22      while 1:
23         # receive letter from c, if it is still connected
24         k = c.recv(1)
25         if k == '': break
26         # concatenate v with k in an atomic manner, i.e. with protection
27         #    by locks
28         vlock.acquire()
29         v += k
30         vlock.release()
31         # send new v back to client
32         c.send(v)
33      c.close()
34      nclntlock.acquire()
35      nclnt -= 1
36      nclntlock.release()
37
38   # set up Internet TCP socket
39   lstn = socket.socket(socket.AF_INET, socket.SOCK_STREAM)
40
41   port = int(sys.argv[1])  # server port number
42   # bind lstn socket to this port
43   lstn.bind(('', port))
44   # start listening for contacts from clients (at most 2 at a time)
45   lstn.listen(5)
46
47   # initialize concatenated string, v
48   v = ''
49   # set up a lock to guard v
50   vlock = thread.allocate_lock()
51
52   # nclnt will be the number of clients still connected
53   nclnt = 2
54   # set up a lock to guard nclnt
55   nclntlock = thread.allocate_lock()
```

```
56
57    # accept calls from the clients
58    for i in range(nclnt):
59       # wait for call, then get a new socket to use for this client,
60       #   and get the client's address/port tuple (though not used)
61       (clnt,ap) = lstn.accept()
62       # start thread for this client, with serveclient() as the thread's
63       #   function, with parameter clnt; note that parameter set must be
64       #   a tuple; in this case, the tuple is of length 1, so a comma is
65       #   needed
66       thread.start_new_thread(serveclient,(clnt,))
67
68    # shut down the server socket, since it's not needed anymore
69    lstn.close()
70
71    # wait for both threads to finish
72    while nclnt > 0: pass
73
74    print 'the final value of v is', v
```

Make absolutely sure to run the programs before proceeding further.[3] Here is how to do this:

I'll refer to the machine on which you run the server as **a.b.c**, and the two client machines as **u.v.w** and **x.y.z**.[4] First, on the server machine, type

```
python srvr.py 2000
```

and then on each of the client machines type

```
python clnt.py a.b.c 2000
```

(You may need to try another port than 2000, anything above 1023.)

Input letters into both clients, in a rather random pattern, typing some on one client, then on the other, then on the first, etc. Then finally hit Enter without typing a letter to one of the clients to end the session for that client, type a few more characters in the other client, and then end that session too.

The reason for threading the server is that the inputs from the clients will come in at unpredictable times. At any given time, the server doesn't know which client will send input next, and thus doesn't

---

[3]You can get them from the **.tex** source file for this tutorial, located wherever your picked up the **.pdf** version.

[4]You could in fact run all of them on the same machine, with address name **localhost** or something like that, but it would be better on separate machines.

know on which client to call **recv()**. One way to solve this problem is by having threads, which run "simultaneously" and thus give the server the ability to read from whichever client has sent data.[5].

So, let's see the technical details. We start with the "main" program.[6]

```
1  vlock = thread.allocate_lock()
```

Here we set up a **lock variable** which guards **v**. We will explain later why this is needed. Note that in order to use this function and others we needed to import the **thread** module.

```
1  nclnt = 2
2  nclntlock = thread.allocate_lock()
```

We will need a mechanism to insure that the "main" program, which also counts as a thread, will be passive until both application threads have finished. The variable **nclnt** will serve this purpose. It will be a count of how many clients are still connected. The "main" program will monitor this, and wrap things up later when the count reaches 0.

```
1  thread.start_new_thread(serveclient,(clnt,))
```

Having accepted a a client connection, the server sets up a thread for serving it, via **thread.start__new__thread** The first argument is the name of the application function which the thread will run, in this case **serveclient()**. The second argument is a tuple consisting of the set of arguments for that application function. As noted in the comment, this set is expressed as a tuple, and since in this case our tuple has only one component, we use a comma to signal the Python interpreter that this is a tuple.

So, here we are telling Python's threads system to call our function **serveclient()**, supplying that function with the argument **clnt**. The thread becomes "active" immediately, but this does not mean that it starts executing right away. All that happens is that the threads manager adds this new thread to its list of threads, and marks its current state as Run, as opposed to being in a Sleep state, waiting for some event.

By the way, this gives us a chance to show how clean and elegant Python's threads interface is compared to what one would need in C/C++. For example, in **pthreads**, the function analogous to **thread.start__new__thread()** has the signature

```
1  pthread_create (pthread_t *thread_id, const pthread_attr_t *attributes,
2      void *(*thread_function)(void *), void *arguments);
```

---

[5] Another solution is to use nonblocking I/O. See this example in that context in `http://heather.cs.ucdavis.edu/~matloff/Python/PyNet.pdf`

[6] Just as you should write the main program first, you should read it first too, for the same reasons.

What a mess! For instance, look at the types in that third argument: A pointer to a function whose argument is pointer to `void` and whose value is a pointer to `void` (all of which would have to be `cast` when called). It's such a pleasure to work in Python, where we don't have to be bothered by low-level things like that.

Now consider our statement

```
while nclnt > 0: pass
```

The statement says that as long as at least one client is still active, do nothing. Sounds simple, and it is, but you should consider what is really happening here.

Remember, the three threads—the two client threads, and the "main" one—will take turns executing, with each turn lasting a brief period of time. Each time "main" gets a turn, it will loop repeatedly on this line. But all that empty looping in "main" is wasted time. What we would really like is a way to prevent the "main" function from getting a turn at all until the two clients are gone. There are ways to do this which you will see later, but we have chosen to remain simple for now.

Now consider the function **serveclient()**. Any thread executing this function will deal with only one particular client, the one corresponding to the connection **c** (an argument to the function). So this **while** loop does nothing but read from that particular client. If the client has not sent anything, the thread will block on the line

```
k = c.recv(1)
```

This thread will then be marked as being in Sleep state by the thread manager, thus allowing the other client thread a chance to run. If neither client thread can run, then the "main" thread keeps getting turns. When a user at one of the clients finally types a letter, the corresponding thread unblocks, i.e. the threads manager changes its state to Run, so that it will soon resume execution.

Next comes the most important code for the purpose of this tutorial:

```
vlock.acquire()
v += k
vlock.release()
```

Here we are worried about a **race condition**. Suppose for example **v** is currently 'abx', and Client 0 sends **k** equal to 'g'. The concern is that this thread's turn might end in the middle of that addition to **v**, say right after the Python interpreter had formed 'abxg' but before that value was written back to **v**. This could be a big problem. The next thread might get to the same statement, take **v**, still equal to 'abx', and append, say, 'w', making **v** equal to 'abxw'. Then when the first thread gets its

next turn, it would finish its interrupted action, and set **v** to 'abxg'—which would mean that the 'w' from the other thread would be lost.

All of this hinges on whether the operation

```
1  v += k
```

is interruptible. Could a thread's turn end somewhere in the midst of the execution of this statement? If not, we say that the operation is **atomic**. If the operation were atomic, we would not need the lock/unlock operations surrounding the above statement. I did this, using the methods described in Section 15.1.3, and it appears to me that the above statement is *not* atomic.

Moreover, it's safer not to take a chance, especially since Python compilers could vary or the virtual machine could change; after all, we would like our Python source code to work even if the machine changes.

So, we need the lock/unlock operations:

```
1  vlock.acquire()
2  v += k
3  vlock.release()
```

The lock, **vlock** here, can only be held by one thread at a time. When a thread executes this statement, the Python interpreter will check to see whether the lock is locked or unlocked right now. In the latter case, the interpreter will lock the lock and the thread will continue, and will execute the statement which updates **v**. It will then release the lock, i.e. the lock will go back to unlocked state.

If on the other hand, when a thread executes **acquire()** on this lock when it is locked, i.e. held by some other thread, its turn will end and the interpreter will mark this thread as being in Sleep state, waiting for the lock to be unlocked. When whichever thread currently holds the lock unlocks it, the interpreter will change the blocked thread from Sleep state to Run state.

Note that if our threads were non-preemptive, we would not need these locks.

Note also the crucial role being played by the global nature of **v**. Global variables are used to communicate between threads. In fact, recall that this is one of the reasons that threads are so popular—easy access to global variables. Thus the dogma so often taught in beginning programming courses that global variables must be avoided is wrong; on the contrary, there are many situations in which globals are necessary and natural.[7]

The same race-condition issues apply to the code

```
1  nclntlock.acquire()
2  nclnt -= 1
3  nclntlock.release()
```

---

[7] I think that dogma is presented in a far too extreme manner anyway. See `http://heather.cs.ucdavis.edu/~matloff/globals.html`.

Following is a Python program that finds prime numbers using threads. Note carefully that it is not claimed to be efficient at all (it may well run more slowly than a serial version); it is merely an illustration of the concepts. Note too that we are again using the simple **thread** module, rather than **threading**.

```python
#!/usr/bin/env python

import sys
import math
import thread

def dowork(tn):  # thread number tn
    global n,prime,nexti,nextilock,nstarted,nstartedlock,donelock
    donelock[tn].acquire()
    nstartedlock.acquire()
    nstarted += 1
    nstartedlock.release()
    lim = math.sqrt(n)
    nk = 0
    while 1:
        nextilock.acquire()
        k = nexti
        nexti += 1
        nextilock.release()
        if k > lim: break
        nk += 1
        if prime[k]:
            r = n / k
            for i in range(2,r+1):
                prime[i*k] = 0
    print 'thread', tn, 'exiting; processed', nk, 'values of k'
    donelock[tn].release()

def main():
    global n,prime,nexti,nextilock,nstarted,nstartedlock,donelock
    n = int(sys.argv[1])
    prime = (n+1) * [1]
    nthreads = int(sys.argv[2])
    nstarted = 0
    nexti = 2
    nextilock = thread.allocate_lock()
    nstartedlock = thread.allocate_lock()
    donelock = []
    for i in range(nthreads):
        d = thread.allocate_lock()
        donelock.append(d)
```

```
42          thread.start_new_thread(dowork,(i,))
43      while nstarted < nthreads: pass
44      for i in range(nthreads):
45          donelock[i].acquire()
46      print 'there are', reduce(lambda x,y: x+y, prime) - 2, 'primes'
47
48  if __name__ == '__main__':
49       main()
```

So, let's see how the code works.

The algorithm is the famous Sieve of Erathosthenes: We list all the numbers from 2 to **n**, then cross out all multiples of 2 (except 2), then cross out all multiples of 3 (except 3), and so on. The numbers which get crossed out are composite, so the ones which remain at the end are prime.

Line 32: We set up an array **prime**, which is what we will be "crossing out." The value 1 means "not crossed out," so we start everything at 1. (Note how Python makes this easy to do, using list "multiplication.")

Line 33: Here we get the number of desired threads from the command line.

Line 34: The variable **nstarted** will show how many threads have already started. This will be used later, in Lines 43-45, in determining when the **main()** thread exits. Since the various threads will be writing this variable, we need to protect it with a lock, on Line 37.

Lines 35-36: The variable **nexti** will say which value we should do "crossing out" by next. If this is, say, 17, then it means our next task is to cross out all multiples of 17 (except 17). Again we need to protect it with a lock.

Lines 39-42: We create the threads here. The function executed by the threads is named **dowork()**. We also create locks in an array **donelock**, which again will be used later on as a mechanism for determining when **main()** exits (Line 44-45).

Lines 43-45: There is a lot to discuss here.

To start, recall that in **srvr.py**, our example in Section 15.1.1, we didn't want the main thread to exit until the child threads were done.[8] So, Line 50 was a **busy wait**, repeatedly doing nothing (**pass**). That's a waste of time—each time the main thread gets a turn to run, it repeatedly executes **pass** until its turn is over.

Here in our primes program, a premature exit by **main()** result in printing out wrong answers. On the other hand, we don't want **main()** to engage in a wasteful busy wait. We could use **join()** from **threading.Thread** for this purpose, to be discussed later, but here we take a different tack: We set

---

[8]The effect of the main thread ending earlier would depend on the underlying OS. On some platforms, exit of the parent may terminate the child threads, but on other platforms the children continue on their own.

up a list of locks, one for each thread, in a list **donelock**. Each thread initially acquires its lock (Line 9), and releases it when the thread finishes its work (Lin 27). Meanwhile, **main()** has been waiting to acquire those locks (Line 45). So, when the threads finish, **main()** will move on to Line 46 and print out the program's results.

But there is a subtle problem (threaded programming is notorious for subtle problems), in that there is no guarantee that a thread will execute Line 9 before **main()** executes Line 45. That's why we have a busy wait in Line 43, to make sure all the threads acquire their locks before **main()** does. Of course, we're trying to avoid busy waits, but this one is quick.

Line 13: We need not check any "crosser-outers" that are larger than $\sqrt{n}$.

Lines 15-25: We keep trying "crosser-outers" until we reach that limit (Line 20). Note the need to use the lock in Lines 16-19. In Line 22, we check the potential "crosser-outer" for primeness; if we have previously crossed it out, we would just be doing duplicate work if we used this **k** as a "crosser-outer."

Here's one more example, a type of Web crawler. This one continually monitors the access time of the Web, by repeatedly accessing a list of "representative" Web sites, say the top 100. What's really different about this program, though, is that we've reserved one thread for human interaction. The person can, whenever he/she desires, find for instance the mean of recent access times.

```python
import sys
import time
import os
import thread

class glbls:
    acctimes = []  # access times
    acclock = thread.allocate_lock()  # lock to guard access time data
    nextprobe = 0  # index of next site to probe
    nextprobelock = thread.allocate_lock()  # lock to guard access time data
    sites = open(sys.argv[1]).readlines()  # the sites to monitor
    ww = int(sys.argv[2])  # window width

def probe(me):
    if me > 0:
        while 1:
            # determine what site to probe next
            glbls.nextprobelock.acquire()
            i = glbls.nextprobe
            i1 = i + 1
            if i1 >= len(glbls.sites): i1 = 0
            glbls.nextprobe = i1
            glbls.nextprobelock.release()
            # do probe
```

```
25            t1 = time.time()
26            os.system('wget --spider -q '+glbls.sites[i1])
27            t2 = time.time()
28            accesstime = t2 - t1
29            glbls.acclock.acquire()
30            # list full yet?
31            if len(glbls.acctimes) < glbls.ww:
32                glbls.acctimes.append(accesstime)
33            else:
34                glbls.acctimes = glbls.acctimes[1:] + [accesstime]
35            glbls.acclock.release()
36        else:
37           while 1:
38               rsp = raw_input('monitor: ')
39               if rsp == 'mean': print mean(glbls.acctimes)
40               elif rsp == 'median': print median(glbls.acctimes)
41               elif rsp == 'all': print all(glbls.acctimes)
42
43  def mean(x):
44      return sum(x)/len(x)
45
46  def median(x):
47      y = x
48      y.sort()
49      return y[len(y)/2]   # a little sloppy
50
51  def all(x):
52      return x
53
54  def main():
55      nthr = int(sys.argv[3])   # number of threads
56      for thr in range(nthr):
57          thread.start_new_thread(probe,(thr,))
58      while 1: continue
59
60  if __name__ == '__main__':
61      main()
62
```

The `threading` Module

The program below treats the same network client/server application considered in Section 15.1.1, but with the more sophisticated **threading** module. The client program stays the same, since it didn't involve threads in the first place. Here is the new server code:

```
1   # simple illustration of threading module
2
3   # multiple clients connect to server; each client repeatedly sends a
4   # value k, which the server adds to a global string v and echos back
5   # to the client; k = '' means the client is dropping out; when all
6   # clients are gone, server prints final value of v
7
8   # this is the server
9
10  import socket  # networking module
11  import sys
12  import threading
13
14  # class for threads, subclassed from threading.Thread class
15  class srvr(threading.Thread):
16     # v and vlock are now class variables
17     v = ''
18     vlock = threading.Lock()
19     id = 0  # I want to give an ID number to each thread, starting at 0
20     def __init__(self,clntsock):
21        # invoke constructor of parent class
22        threading.Thread.__init__(self)
23        # add instance variables
24        self.myid = srvr.id
25        srvr.id += 1
26        self.myclntsock = clntsock
27     # this function is what the thread actually runs; the required name
28     #   is run(); threading.Thread.start() calls threading.Thread.run(),
29     #   which is always overridden, as we are doing here
30     def run(self):
31        while 1:
32           # receive letter from client, if it is still connected
33           k = self.myclntsock.recv(1)
34           if k == '': break
35           # update v in an atomic manner
36           srvr.vlock.acquire()
37           srvr.v += k
38           srvr.vlock.release()
39           # send new v back to client
40           self.myclntsock.send(srvr.v)
41        self.myclntsock.close()
42
43  # set up Internet TCP socket
44  lstn = socket.socket(socket.AF_INET, socket.SOCK_STREAM)
45  port = int(sys.argv[1])  # server port number
46  # bind lstn socket to this port
47  lstn.bind(('', port))
```

```
48  # start listening for contacts from clients (at most 2 at a time)
49  lstn.listen(5)
50
51  nclnt = int(sys.argv[2])  # number of clients
52
53  mythreads = []  # list of all the threads
54  # accept calls from the clients
55  for i in range(nclnt):
56      # wait for call, then get a new socket to use for this client,
57      #    and get the client's address/port tuple (though not used)
58      (clnt,ap) = lstn.accept()
59      # make a new instance of the class srvr
60      s = srvr(clnt)
61      # keep a list all threads
62      mythreads.append(s)
63      # threading.Thread.start calls threading.Thread.run(), which we
64      #    overrode in our definition of the class srvr
65      s.start()
66
67  # shut down the server socket, since it's not needed anymore
68  lstn.close()
69
70  # wait for all threads to finish
71  for s in mythreads:
72      s.join()
73
74  print 'the final value of v is', srvr.v
```

Again, let's look at the main data structure first:

```
1  class srvr(threading.Thread):
```

The **threading** module contains a class **Thread**, any instance of which represents one thread. A typical application will subclass this class, for two reasons. First, we will probably have some application-specific variables or methods to be used. Second, the class **Thread** has a member method **run()** which is meant to be overridden, as you will see below.

Consistent with OOP philosophy, we might as well put the old globals in as class variables:

```
1  v = ''
2  vlock = threading.Lock()
```

Note that class variable code is executed immediately upon execution of the program, as opposed to when the first object of this class is created. So, the lock is created right away.

```
1  id = 0
```

This is to set up ID numbers for each of the threads. We don't use them here, but they might be useful in debugging or in future enhancement of the code.

```
def __init__(self,clntsock):
    ...
    self.myclntsock = clntsock

# ``main'' program
...
    (clnt,ap) = lstn.accept()
    s = srvr(clnt)
```

The "main" program, in creating an object of this class for the client, will pass as an argument the socket for that client. We then store it as a member variable for the object.

```
def run(self):
    ...
```

As noted earlier, the **Thread** class contains a member method **run()**. This is a dummy, to be overridden with the application-specific function to be run by the thread. It is invoked by the method **Thread.start()**, called here in the main program. As you can see above, it is pretty much the same as the previous code in Section 15.1.1 which used the **thread** module, adapted to the class environment.

One thing that is quite different in this program is the way we end it:

```
for s in mythreads:
    s.join()
```

The **join()** method in the class **Thread** blocks until the given thread exits. (The threads manager puts the main thread in Sleep state, and when the given thread exits, the manager changes that state to Run.) The overall effect of this loop, then, is that the main program will wait at that point until all the threads are done. They "join" the main program. This is a much cleaner approach than what we used earlier, and it is also more efficient, since the main program will not be given any turns in which it wastes time looping around doing nothing, as in the program in Section 15.1.1 in the line

```
while nclnt > 0: pass
```

Here we maintained our own list of threads. However, we could also get one via the call **threading.enumerate()**. If placed after the **for** loop in our server code above, for instance as

```
print threading.enumerate()
```

we would get output like

```
1  [<_MainThread(MainThread, started)>, <srvr(Thread-1, started)>,
2  <srvr(Thread-2, started)>]
```

Here's another example, which finds and counts prime numbers, again not assumed to be efficient:

```
1   #!/usr/bin/env python
2
3   # prime number counter, based on Python threading class
4
5   # usage:  python PrimeThreading.py n nthreads
6   #   where we wish the count of the number of primes from 2 to n, and to
7   #   use nthreads to do the work
8
9   # uses Sieve of Erathosthenes:  write out all numbers from 2 to n, then
10  # cross out all the multiples of 2, then of 3, then of 5, etc., up to
11  # sqrt(n); what's left at the end are the primes
12
13  import sys
14  import math
15  import threading
16
17  class prmfinder(threading.Thread):
18     n = int(sys.argv[1])
19     nthreads = int(sys.argv[2])
20     thrdlist = []  # list of all instances of this class
21     prime = (n+1) * [1]  # 1 means assumed prime, until find otherwise
22     nextk = 2  # next value to try crossing out with
23     nextklock = threading.Lock()
24     def __init__(self,id):
25        threading.Thread.__init__(self)
26        self.myid = id
27     def run(self):
28        lim = math.sqrt(prmfinder.n)
29        nk = 0  # count of k's done by this thread, to assess load balance
30        while 1:
31           # find next value to cross out with
32           prmfinder.nextklock.acquire()
33           k = prmfinder.nextk
34           prmfinder.nextk += 1
35           prmfinder.nextklock.release()
36           if k > lim: break
37           nk += 1  # increment workload data
38           if prmfinder.prime[k]:  # now cross out
39              r = prmfinder.n / k
40              for i in range(2,r+1):
41                 prmfinder.prime[i*k] = 0
42        print 'thread', self.myid, 'exiting; processed', nk, 'values of k'
```

```
43
44   def main():
45      for i in range(prmfinder.nthreads):
46         pf = prmfinder(i)  # create thread i
47         prmfinder.thrdlist.append(pf)
48         pf.start()
49      for thrd in prmfinder.thrdlist: thrd.join()
50      print 'there are', reduce(lambda x,y: x+y, prmfinder.prime) - 2, 'primes'
51
52   if __name__ == '__main__':
53       main()
```

15.1.2 Condition Variables

General Ideas

We saw in the last section that **threading.Thread.join()** avoids the need for wasteful looping in **main()**, while the latter is waiting for the other threads to finish. In fact, it is very common in threaded programs to have situations in which one thread needs to wait for something to occur in another thread. Again, in such situations we would not want the waiting thread to engage in wasteful looping.

The solution to this problem is **condition variables**. As the name implies, these are variables used by code to wait for a certain condition to occur. Most threads systems include provisions for these, and Python's **threading** package is no exception.

The **pthreads** package, for instance, has a type **pthread_cond** for such variables, and has functions such as **pthread_cond_wait()**, which a thread calls to wait for an event to occur, and **pthread_cond_signal()**, which another thread calls to announce that the event now has occurred.

But as is typical with Python in so many things, it is easier for us to use condition variables in Python than in C. At the first level, there is the class **threading.Condition**, which corresponds well to the condition variables available in most threads systems. However, at this level condition variables are rather cumbersome to use, as not only do we need to set up condition variables but we also need to set up extra locks to guard them. This is necessary in any threading system, but it is a nuisance to deal with.

So, Python offers a higher-level class, **threading.Event**, which is just a wrapper for **threading.Condition**, but which does all the condition lock operations behind the scenes, alleviating the programmer of having to do this work.

Other `threading` Classes

The function **Event.set()** "wakes" all threads that are waiting for the given event. That didn't matter in our example above, since only one thread (**main()**) would ever be waiting at a time in that example. But in more general applications, we sometimes want to wake only one thread instead of all of them. For this, we can revert to working at the level of **threading.Condition** instead of **threading.Event**. There we have a choice between using **notify()** or **notifyAll()**.

The latter is actually what is called internally by **Event.set()**. But **notify()** instructs the threads manager to wake just one of the waiting threads (we don't know which one).

The class **threading.Semaphore** offers semaphore operations. Other classes of advanced interest are **threading.RLock** and **threading.Timer**.

15.1.3   Threads Internals

The thread manager acts like a "mini-operating system." Just like a real OS maintains a table of processes, a thread system's thread manager maintains a table of threads. When one thread gives up the CPU, or has its turn pre-empted (see below), the thread manager looks in the table for another thread to activate. Whichever thread is activated will then resume execution where it had left off, i.e. where its last turn ended.

Just as a process is either in Run state or Sleep state, the same is true for a thread. A thread is either ready to be given a turn to run, or is waiting for some event. The thread manager will keep track of these states, decide which thread to run when another has lost its turn, etc.

Kernel-Level Thread Managers

Here each thread really is a process, and for example will show up on Unix systems when one runs the appropriate **ps** process-list command, say **ps axH**. The threads manager is then the OS.

The different threads set up by a given application program take turns running, among all the other processes.

This kind of thread system is is used in the Unix **pthreads** system, as well as in Windows threads.

User-Level Thread Managers

User-level thread systems are "private" to the application. Running the **ps** command on a Unix system will show only the original application running, not all the threads it creates. Here the threads are not pre-empted; on the contrary, a given thread will continue to run until it voluntarily gives up

control of the CPU, either by calling some "yield" function or by calling a function by which it requests a wait for some event to occur.[9]

A typical example of a user-level thread system is **pth**.

Comparison

Kernel-level threads have the advantage that they can be used on multiprocessor systems, thus achieving true parallelism between threads. This is a major advantage.

On the other hand, in my opinion user-level threads also have a major advantage in that they allow one to produce code which is much easier to write, is easier to debug, and is cleaner and clearer. This in turn stems from the non-preemptive nature of user-level threads; application programs written in this manner typically are not cluttered up with lots of lock/unlock calls (details on these below), which are needed in the pre-emptive case.

The Python Thread Manager

Python "piggybacks" on top of the OS' underlying threads system. A Python thread is a real OS thread. If a Python program has three threads, for instance, there will be three entries in the **ps** output.

However, Python's thread manager imposes further structure on top of the OS threads. It keeps track of how long a thread has been executing, in terms of the number of Python **byte code** instructions that have executed.[10] When that reaches a certain number, by default 100, the thread's turn ends. In other words, the turn can be pre-empted either by the hardware timer and the OS, or when the interpreter sees that the thread has executed 100 byte code instructions.[11]

The GIL

In the case of CPython (but not Jython or Iron Python), there is a global interpreter lock, the famous (or infamous) GIL. It is set up to ensure that only one thread runs at a time, in order to facilitate easy garbage collection.

Suppose we have a C program with three threads, which I'll call X, Y and Z. Say currently Y is running. After 30 milliseconds (or whatever the quantum size has been set to by the OS), Y will be interrupted by the timer, and the OS will start some other process. Say the latter, which I'll call Q, is

---

[9]In typical user-level thread systems, an external event, such as an I/O operation or a signal, will also also cause the current thread to relinquish the CPU.

[10]This is the "machine language" for the Python virtual machine.

[11]The author thanks Alex Martelli for a helpful clarification.

a different, unrelated program. Eventually Q's turn will end too, and let's say that the OS then gives X a turn. From the point of view of our X/Y/Z program, i.e. ignoring Q, control has passed from Y to X. The key point is that the point within Y at which that event occurs is random (with respect to where Y is at the time), based on the time of the hardware interrupt.

By contrast, say my Python program has three threads, U, V and W. Say V is running. The hardware timer will go off at a random time, and again Q might be given a turn, *but* definitely neither U nor W will be given a turn, because the Python interpreter had earlier made a call to the OS which makes U and W wait for the GIL to become unlocked.

Let's look at this a little closer. The key point to note is that the Python interpreter itself is threaded, say using **pthreads**. For instance, in our X/Y/Z example above, when you ran **ps axH**, you would see three Python processes/threads. I just tried that on my program **thsvr.py**, which creates two threads, with a command-line argument of 2000 for that program. Here is the relevant portion of the output of **ps axH**:

```
1  28145 pts/5    Rl     0:09 python thsvr.py 2000
2  28145 pts/5    Sl     0:00 python thsvr.py 2000
3  28145 pts/5    Sl     0:00 python thsvr.py 2000
```

What has happened is the Python interpreter has spawned two child threads, one for each of my threads in **thsvr.py**, in addition to the interpreter's original thread, which runs my **main()**. Let's call those threads UP, VP and WP. Again, these are the threads that the OS sees, while U, V and W are the threads that I see—or think I see, since they are just virtual.

The GIL is a **pthreads** lock. Say V is now running. Again, what that actually means on my real machine is that VP is running. VP keeps track of how long V has been executing, in terms of the number of Python **byte code** instructions that have executed. When that reaches a certain number, by default 100, UP will release the GIL by calling **pthread_mutex_unlock()** or something similar.

The OS then says, "Oh, were any threads waiting for that lock?" It then basically gives a turn to UP or WP (we can't predict which), which then means that from my point of view U or W starts, say U. Then VP and WP are still in Sleep state, and thus so are my V and W.

So you can see that it is the Python interpreter, not the hardware timer, that is determining how long a thread's turn runs, relative to the other threads in my program. Again, Q might run too, but within this Python program there will be no control passing from V to U or W simply because the timer went off; such a control change will only occur when the Python interpreter wants it to. This will be either after the 100 byte code instructions or when U reaches an I/O operation or other wait-event operation.

So, the bottom line is that while Python uses the underlying OS threads system as its base, it superimposes further structure in terms of transfer of control between threads.

Most importantly, the presence of the GIL means that two Python threads (spawned from the same program) cannot run at the same time—*even on a multicore machine.* This has been the subject of great controversy.

Implications for Randomness and Need for Locks

I mentioned in Section 15.1.3 that non-pre-emptive threading is nice because one can avoid the code clutter of locking and unlocking (details of lock/unlock below). Since, barring I/O issues, a thread working on the same data would seem to always yield control at exactly the same point (i.e. at 100 byte code instruction boundaries), Python would seem to be deterministic and non-pre-emptive. However, it will not quite be so simple.

First of all, there is the issue of I/O, which adds randomness. There may also be randomness in how the OS chooses the first thread to be run, which could affect computation order and so on.

Finally, there is the question of atomicity in Python operations: The interpreter will treat any Python virtual machine instruction as indivisible, thus not needing locks in that case. But the bottom line will be that unless you know the virtual machine well, you should use locks at all times.

15.1.4   The `multiprocessing` Module

CPython's GIL is the subject of much controversy. As we saw in Section 15.1.3, it prevents running true parallel applications when using the **thread** or **threading** modules.

That might not seem to be too severe a restriction—after all if you really need the speed, you probably won't use a scripting language in the first place. But a number of people took the point of view that, given that they have decided to use Python no matter what, they would like to get the best speed subject to that restriction. So, there was much grumbling about the GIL.

Thus, later the **multiprocessing** module was developed, which enables true parallel processing with Python on a multiprocore machine, with an interface very close to that of the **threading** module.

Moreover, one can run a program across machines! In other words, the **multiprocessing** module allows to run several threads not only on the different cores of one machine, but on many machines at once, in cooperation in the same manner that threads cooperate on one machine. By the way, this idea is similar to something I did for Perl some years ago (PerlDSM: A Distributed Shared Memory System for Perl. *Proceedings of PDPTA 2002*, 63-68), and for which I did in R as a package **Rdsm** some time later. We will not cover the cross-machine case here.

So, let's go to our first example, a simulation application that will find the probability of getting a total of exactly k dots when we roll n dice:

```python
# dice probability finder, based on Python multiprocessing class

# usage:  python DiceProb.py n k nreps nthreads
#   where we wish to find the probability of getting a total of k dots
#   when we roll n dice; we'll use nreps total repetitions of the
#   simulation, dividing those repetitions among nthreads threads

import sys
import random
from multiprocessing import Process, Lock, Value

class glbls:  # globals, other than shared
    n = int(sys.argv[1])
    k = int(sys.argv[2])
    nreps = int(sys.argv[3])
    nthreads = int(sys.argv[4])
    thrdlist = []  # list of all instances of this class

def worker(id,tot,totlock):
    mynreps = glbls.nreps/glbls.nthreads
    r = random.Random()  # set up random number generator
    count = 0  # number of times get total of k
    for i in range(mynreps):
        if rolldice(r) == glbls.k:
            count += 1
    totlock.acquire()
    tot.value += count
    totlock.release()
    # check for load balance
    print 'thread', id, 'exiting; total was', count

def rolldice(r):
    ndots = 0
    for roll in range(glbls.n):
        dots = r.randint(1,6)
        ndots += dots
    return ndots

def main():
    tot = Value('i',0)
    totlock = Lock()
    for i in range(glbls.nthreads):
        pr = Process(target=worker, args=(i,tot,totlock))
        glbls.thrdlist.append(pr)
```

```
45        pr.start()
46     for thrd in glbls.thrdlist: thrd.join()
47     # adjust for truncation, in case nthreads doesn't divide nreps evenly
48     actualnreps = glbls.nreps/glbls.nthreads * glbls.nthreads
49     print 'the probability is',float(tot.value)/actualnreps
50
51 if __name__ == '__main__':
52     main()
```

As in any simulation, the longer one runs it, the better the accuracy is likely to be. Here we run the simulation **nreps** times, but divide those repetitions among the threads. This is an example of an "embarrassingly parallel" application, so we should get a good speedup (not shown here).

So, how does it work? The general structure looks similar to that of the Python **threading** module, using **Process()** to create a create a thread, **start()** to get it running, **Lock()** to create a lock, **acquire()** and **release()** to lock and unlock a lock, and so on.

The main difference, though, is that globals are not automatically shared. Instead, shared variables must be created using **Value** for a scalar and **Array** for an array. Unlike Python in general, here one must specify a data type, 'i' for integer and 'd' for double (floating-point). (One can use **Namespace** to create more complex types, at some cost in performance.) One also specifies the initial value of the variable. One must pass these variables explicitly to the functions to be run by the threads, in our case above the function **worker()**. Note carefully that the shared variables are still accessed syntactically as if they were globals.

Here's the prime number-finding program from before, now using **multiprocessing**:

```
1  #!/usr/bin/env python
2
3  # prime number counter, based on Python multiprocessing class
4
5  # usage:  python PrimeThreading.py n nthreads
6  #   where we wish the count of the number of primes from 2 to n, and to
7  #   use nthreads to do the work
8
9  # uses Sieve of Erathosthenes:  write out all numbers from 2 to n, then
10 # cross out all the multiples of 2, then of 3, then of 5, etc., up to
11 # sqrt(n); what's left at the end are the primes
12
13 import sys
14 import math
15 from multiprocessing import Process, Lock, Array, Value
16
17 class glbls:  # globals, other than shared
18    n = int(sys.argv[1])
```

```
19      nthreads = int(sys.argv[2])
20      thrdlist = []  # list of all instances of this class
21
22  def prmfinder(id,prm,nxtk,nxtklock):
23      lim = math.sqrt(glbls.n)
24      nk = 0  # count of k's done by this thread, to assess load balance
25      while 1:
26          # find next value to cross out with
27          nxtklock.acquire()
28          k = nxtk.value
29          nxtk.value = nxtk.value + 1
30          nxtklock.release()
31          if k > lim: break
32          nk += 1  # increment workload data
33          if prm[k]:  # now cross out
34              r = glbls.n / k
35              for i in range(2,r+1):
36                  prm[i*k] = 0
37      print 'thread', id, 'exiting; processed', nk, 'values of k'
38
39  def main():
40      prime = Array('i',(glbls.n+1) * [1])  # 1 means prime, until find otherwise
41      nextk = Value('i',2)  # next value to try crossing out with
42      nextklock = Lock()
43      for i in range(glbls.nthreads):
44          pf = Process(target=prmfinder, args=(i,prime,nextk,nextklock))
45          glbls.thrdlist.append(pf)
46          pf.start()
47      for thrd in glbls.thrdlist: thrd.join()
48      print 'there are', reduce(lambda x,y: x+y, prime) - 2, 'primes'
49
50  if __name__ == '__main__':
51      main()
```

The main new item in this example is use of **Array()**.

One can use the **Pool** class to create a set of threads, rather than doing so "by hand" in a loop as above. You can start them with various initial values for the threads using **Pool.map()**, which works similarly to Python's ordinary **map()** function.

The **multiprocessing** documentation warns that shared items may be costly, and suggests using **Queue** and **Pipe** where possible. We will cover the former in the next section. Note, though, that in general it's difficult to get much speedup (or difficult even to avoid slowdown!) with non-"embarrassingly parallel" applications.

15.1.5   The `Queue` Module for Threads and Multiprocessing

Threaded applications often have some sort of work queue data structure. When a thread becomes free, it will pick up work to do from the queue. When a thread creates a task, it will add that task to the queue.

Clearly one needs to guard the queue with locks. But Python provides the **Queue** module to take care of all the lock creation, locking and unlocking, and so on. This means we don't have to bother with it, and the code will probably be faster.

Queue is implemented for both **threading** and **multiprocessing**, in almost identical forms. This is good, because the documentation for **multiprocessing** is rather sketchy, so you can turn to the docs for **threading** for more details.

The function **put()** in Queue adds an element to the end of the queue, while **get()** will remove the head of the queue, again without the programmer having to worry about race conditions.

Note that **get()** will block if the queue is currently empty. An alternative is to call it with **block=False**, within a **try/except** construct. One can also set timeout periods.

Here once again is the prime number example, this time done with **Queue**:

```
1   #!/usr/bin/env python
2
3   # prime number counter, based on Python multiprocessing class with
4   # Queue
5
6   # usage:  python PrimeThreading.py n nthreads
7   #   where we wish the count of the number of primes from 2 to n, and to
8   #   use nthreads to do the work
9
10  # uses Sieve of Erathosthenes:  write out all numbers from 2 to n, then
11  # cross out all the multiples of 2, then of 3, then of 5, etc., up to
12  # sqrt(n); what's left at the end are the primes
13
14  import sys
15  import math
16  from multiprocessing import Process, Array, Queue
17
18  class glbls:  # globals, other than shared
19     n = int(sys.argv[1])
20     nthreads = int(sys.argv[2])
21     thrdlist = []  # list of all instances of this class
22
23  def prmfinder(id,prm,nxtk):
24     nk = 0  # count of k's done by this thread, to assess load balance
25     while 1:
```

```
26        # find next value to cross out with
27        try: k = nxtk.get(False)
28        except: break
29        nk += 1  # increment workload data
30        if prm[k]:  # now cross out
31           r = glbls.n / k
32           for i in range(2,r+1):
33              prm[i*k] = 0
34     print 'thread', id, 'exiting; processed', nk, 'values of k'
35
36  def main():
37     prime = Array('i',(glbls.n+1) * [1])  # 1 means prime, until find otherwise
38     nextk = Queue()  # next value to try crossing out with
39     lim = int(math.sqrt(glbls.n)) + 1  # fill the queue with 2...sqrt(n)
40     for i in range(2,lim): nextk.put(i)
41     for i in range(glbls.nthreads):
42        pf = Process(target=prmfinder, args=(i,prime,nextk))
43        glbls.thrdlist.append(pf)
44        pf.start()
45     for thrd in glbls.thrdlist: thrd.join()
46     print 'there are', reduce(lambda x,y: x+y, prime) - 2, 'primes'
47
48  if __name__ == '__main__':
49      main()
```

The way **Queue** is used here is to put all the possible "crosser-outers," obtained in the variable **nextk** in the previous versions of this code, into a queue at the outset. One then uses `get()` to pick up work from the queue. Look Ma, no locks!

Below is an example of queues in an in-place quicksort. (Again, the reader is warned that this is just an example, not claimed to be efficient.)

The work items in the queue are a bit more involved here. They have the form **(i,j,k)**, with the first two elements of this tuple meaning that the given array chunk corresponds to indices **i** through **j** of **x**, the original array to be sorted. In other words, whichever thread picks up this chunk of work will have the responsibility of handling that particular section of **x**.

Quicksort, of course, works by repeatedly splitting the original array into smaller and more numerous chunks. Here a thread will split its chunk, taking the lower half for itself to sort, but placing the upper half into the queue, to be available for other chunks that have not been assigned any work yet. I've written the algorithm so that as soon as all threads have gotten some work to do, no more splitting will occur. That's where the value of **k** comes in. It tells us the split number of this chunk. If it's equal to **nthreads-1**, this thread won't split the chunk.

```
1  # Quicksort and test code, based on Python multiprocessing class and
```

```
2    # Queue
3
4    # code is incomplete, as some special cases such as empty subarrays
5    # need to be accounted for
6
7    # usage:  python QSort.py n nthreads
8    #   where we wish to test the sort on a random list of n items,
9    #   using nthreads to do the work
10
11   import sys
12   import random
13   from multiprocessing import Process, Array, Queue
14
15   class glbls:  # globals, other than shared
16       nthreads = int(sys.argv[2])
17       thrdlist = []  # list of all instances of this class
18       r = random.Random(9876543)
19
20   def sortworker(id,x,q):
21       chunkinfo = q.get()
22       i = chunkinfo[0]
23       j = chunkinfo[1]
24       k = chunkinfo[2]
25       if k < glbls.nthreads - 1:  # need more splitting?
26           splitpt = separate(x,i,j)
27           q.put((splitpt+1,j,k+1))
28           # now, what do I sort?
29           rightend = splitpt + 1
30       else: rightend = j
31       tmp = x[i:(rightend+1)]  # need copy, as Array type has no sort() method
32       tmp.sort()
33       x[i:(rightend+1)] = tmp
34
35   def separate(xc, low, high):  # common algorithm; see Wikipedia
36       pivot = xc[low]  # would be better to take, e.g., median of 1st 3 elts
37       (xc[low],xc[high]) = (xc[high],xc[low])
38       last = low
39       for i in range(low,high):
40           if xc[i] <= pivot:
41               (xc[last],xc[i]) = (xc[i],xc[last])
42               last += 1
43       (xc[last],xc[high]) = (xc[high],xc[last])
44       return last
45
46   def main():
47       tmp = []
48       n = int(sys.argv[1])
```

```
49      for i in range(n): tmp.append(glbls.r.uniform(0,1))
50      x = Array('d',tmp)
51      # work items have form (i,j,k), meaning that the given array chunk
52      # corresponds to indices i through j of x, and that this is the kth
53      # chunk that has been created, x being the 0th
54      q = Queue()  # work queue
55      q.put((0,n-1,0))
56      for i in range(glbls.nthreads):
57         p = Process(target=sortworker, args=(i,x,q))
58         glbls.thrdlist.append(p)
59         p.start()
60      for thrd in glbls.thrdlist: thrd.join()
61      if n < 25: print x[:]
62
63  if __name__ == '__main__':
64       main()
```

15.1.6   Debugging Threaded and Multiprocessing Python Programs

Debugging is always tough with parallel programs, including threads programs. It's especially difficult with pre-emptive threads; those accustomed to debugging non-threads programs find it rather jarring to see sudden changes of context while single-stepping through code. Tracking down the cause of deadlocks can be very hard. (Often just getting a threads program to end properly is a challenge.)

Another problem which sometimes occurs is that if you issue a "next" command in your debugging tool, you may end up inside the internal threads code. In such cases, use a "continue" command or something like that to extricate yourself.

Unfortunately, as of April 2010, I know of no debugging tool that works with **multiprocessing**. However, one can do well with **thread** and **threading**.

15.2   Using Python with MPI

(**Important note**: As of April 2010, a much more widely used Python/MPI interface is MPI4Py. It works similarly to what is described here.)

A number of interfaces of Python to MPI have been developed.[12] A well-known example is pyMPI, developed by a PhD graduate in computer science in UCD, Patrick Miller.

One writes one's pyMPI code, say in **x.py**, by calling pyMPI versions of the usual MPI routines. To run the code, one then runs MPI on the program **pyMPI** with **x.py** as a command-line argument.

---

[12]If you are not familiar with Python, I have a quick tutorial at `http://heather.cs.ucdavis.edu/~matloff/python.html`.

Python is a very elegant language, and pyMPI does a nice job of elegantly interfacing to MPI. Following is a rendition of Quicksort in pyMPI. Don't worry if you haven't worked in Python before; the "non-C-like" Python constructs are explained in comments at the end of the code.

```
1   # a type of quicksort; break array x (actually a Python "list") into
2   # p quicksort-style piles, based # on comparison with the first p-1
3   # elements of x, where p is the number # of MPI nodes; the nodes sort
4   # their piles, then return them to node 0, # which strings them all
5   # together into the final sorted array
6
7   import mpi  # load pyMPI module
8
9   # makes npls quicksort-style piles
10  def makepiles(x,npls):
11      pivot = x[:npls]  # we'll use the first npls elements of x as pivots,
12                        # i.e. we'll compare all other elements of x to these
13      pivot.sort()  # sort() is a member function of the Python list class
14      pls = []  # initialize piles list to empty
15      lp = len(pivot)  # length of the pivot array
16      # pls will be a list of lists, with the i-th list in pls storing the
17      # i-th pile; the i-th pile will start with ID i (to enable
18      # identification later on) and pivot[i]
19      for i in range(lp):  # i = 0,1,...lp-1
20          pls.append([i,pivot[i]])  # build up array via append() member function
21      pls.append([lp])
22      for xi in x[npls:]:  # now place each element in the rest of x into
23                          # its proper pile
24          for j in range(lp):  # j = 0,1,...,lp-1
25              if xi <= pivot[j]:
26                  pls[j].append(xi)
27                  break
28              elif j == lp-1: pls[lp].append(xi)
29      return pls
30
31  def main():
32      if mpi.rank == 0:  # analog of calling MPI_Rank()
33          x = [12,5,13,61,9,6,20,1]  # small test case
34          # divide x into piles to be disbursed to the various nodes
35          pls = makepiles(x,mpi.size)
36      else:  # all other nodes set their x and pls to empty
37          x = []
38          pls = []
39      mychunk = mpi.scatter(pls)  # node 0 (not an explicit argument) disburses
40                                  # pls to the nodes, each of which receives
41                                  # its chunk in its mychunk
42      newchunk = []  # will become sorted version of mychunk
```

```
43    for pile in mychunk:
44        # I need to sort my chunk but most remove the ID first
45        plnum = pile.pop(0)  # ID
46        pile.sort()
47        # restore ID
48        newchunk.append([plnum]+pile)  # the + is array concatenation
49     # now everyone sends their newchunk lists, which node 0 (again an
50     # implied argument) gathers together into haveitall
51     haveitall = mpi.gather(newchunk)
52     if mpi.rank == 0:
53        haveitall.sort()
54        # string all the piles together
55        sortedx = [z for q in haveitall for z in q[1:]]
56        print sortedx
57
58  # common idiom for launching a Python program
59  if __name__ == '__main__': main()
```

Some examples of use of other MPI functions:

```
1  mpi.send(mesgstring,destnodenumber)
2  (message,status) = mpi.recv()  # receive from anyone
3  print message
4  (message,status) = mpi.recv(3)  # receive only from node 3
5  (message,status) = mpi.recv(3,ZMSG)  # receive only message type ZMSG,
6                                       # only from node 3
7  (message,status) = mpi.recv(tag=ZMSG)  # receive from anyone, but
8                                         # only message type ZMSG
```

15.2.1   Using PDB to Debug Threaded Programs

Using PDB is a bit more complex when threads are involved. One cannot, for instance, simply do something like this:

```
1  pdb.py buggyprog.py
```

because the child threads will not inherit the PDB process from the main thread. You can still run PDB in the latter, but will not be able to set breakpoints in threads.

What you can do, though, is invoke PDB from *within* the function which is run by the thread, by calling **pdb.set_trace()** at one or more points within the code:

```
1  import pdb
2  pdb.set_trace()
```

In essence, those become breakpoints.

For example, in our program **srvr.py** in Section 15.1.1, we could add a PDB call at the beginning of the loop in **serveclient()**:

```
1  while 1:
2     import pdb
3     pdb.set_trace()
4     # receive letter from client, if it is still connected
5     k = c.recv(1)
6     if k == '': break
```

You then run the program directly through the Python interpreter as usual, NOT through PDB, but then the program suddenly moves into debugging mode on its own. At that point, one can then step through the code using the **n** or **s** commands, query the values of variables, etc.

PDB's **c** ("continue") command still works. Can one still use the **b** command to set additional breakpoints? Yes, but it might be only on a one-time basis, depending on the context. A breakpoint might work only once, due to a scope problem. Leaving the scope where we invoked PDB causes removal of the trace object. Thus I suggested setting up the trace inside the loop above.

Of course, you can get fancier, e.g. setting up "conditional breakpoints," something like:

```
1  debugflag = int(sys.argv[1])
2  ...
3  if debugflag == 1:
4     import pdb
5     pdb.set_trace()
```

Then, the debugger would run only if you asked for it on the command line. Or, you could have multiple **debugflag** variables, for activating/deactivating breakpoints at various places in the code.

Moreover, once you get the (Pdb) prompt, you could set/reset those flags, thus also activating/deactivating breakpoints.

Note that local variables which were set before invoking PDB, including parameters, are not accessible to PDB.

Make sure to insert code to maintain an ID number for each thread. This really helps when debugging.

15.2.2 RPDB2 and Winpdb

The Winpdb debugger (`www.digitalpeers.com/pythondebugger/`),[13] is very good. Among other things, it can be used to debug threaded code, curses-based code and so on, which many debuggers

---

[13] No, it's not just for Microsoft Windows machines, in spite of the name.

can't. Winpdb is a GUI front end to the text-based RPDB2, which is in the same package. I have a tutorial on both at `http://heather.cs.ucdavis.edu/~matloff/winpdb.html`.

Another very promising debugger that handles threads is PYDB, by Rocky Bernstein (not to be confused with an earlier debugger of the same name). You can obtain it from `http://code.google.com/p/pydbgr/` or the older version at `http://bashdb.sourceforge.net/pydb/`. Invoke it on your code **x.py** by typing

```
$ pydb --threading x.py your_command_line_args_for_x
```

附录 A   Review of Matrix Algebra

This book assumes the reader has had a course in linear algebra (or has self-studied it, always the better approach). This appendix is intended as a review of basic matrix algebra, or a quick treatment for those lacking this background.

A.1   Terminology and Notation

A **matrix** is a rectangular array of numbers. A **vector** is a matrix with only one row (a **row vector** or only one column (a **column vector**).

The expression, "the (i,j) element of a matrix," will mean its element in row i, column j.

Please note the following conventions:

- Capital letters, e.g. A and X, will be used to denote matrices and vectors.

- Lower-case letters with subscripts, e.g. $a_{2,15}$ and x_8, will be used to denote their elements.

- Capital letters with subscripts, e.g. A_{13}, will be used to denote submatrices and subvectors.

If A is a **square** matrix, i.e. one with equal numbers n of rows and columns, then its **diagonal** elements are a_{ii}, i = 1,...,n.

A square matrix is called **upper-triangular** if $a_{ij} = 0$ whenever $i > j$, with a corresponding definition for **lower-triangular** matrices.

The **norm** (or **length**) of an n-element vector **X** is

$$\parallel X \parallel = \sqrt{\sum_{i=1}^{n} x_i^2} \tag{A.1}$$

A.1.1 Matrix Addition and Multiplication

- For two matrices have the same numbers of rows and same numbers of columns, addition is defined elementwise, e.g.

$$\begin{pmatrix} 1 & 5 \\ 0 & 3 \\ 4 & 8 \end{pmatrix} + \begin{pmatrix} 6 & 2 \\ 0 & 1 \\ 4 & 0 \end{pmatrix} = \begin{pmatrix} 7 & 7 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \tag{A.2}$$

- Multiplication of a matrix by a **scalar**, i.e. a number, is also defined elementwise, e.g.

$$0.4 \begin{pmatrix} 7 & 7 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} = \begin{pmatrix} 2.8 & 2.8 \\ 0 & 1.6 \\ 3.2 & 3.2 \end{pmatrix} \tag{A.3}$$

- The **inner product** or **dot product** of equal-length vectors X and Y is defined to be

$$\sum_{k=1}^{n} x_k y_k \tag{A.4}$$

- The product of matrices A and B is defined if the number of rows of B equals the number of columns of A (A and B are said to be **conformable**). In that case, the (i,j) element of the product C is defined to be

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{A.5}$$

For instance,

$$\begin{pmatrix} 7 & 6 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \begin{pmatrix} 1 & 6 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} 19 & 66 \\ 8 & 16 \\ 24 & 80 \end{pmatrix} \tag{A.6}$$

It is helpful to visualize c_{ij} as the inner product of row i of A and column j of B, e.g. as shown in bold face here:

$$\begin{pmatrix} \mathbf{7} & \mathbf{6} \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \begin{pmatrix} \mathbf{1} & 6 \\ \mathbf{2} & 4 \end{pmatrix} = \begin{pmatrix} \mathbf{7} & 70 \\ 8 & 16 \\ 8 & 80 \end{pmatrix} \tag{A.7}$$

- Matrix multiplicatin is associative and distributive, but in general not commutative:

$$A(BC) = (AB)C \tag{A.8}$$

$$A(B + C) = AB + AC \tag{A.9}$$

$$AB \neq BA \tag{A.10}$$

A.2   Matrix Transpose

- The transpose of a matrix A, denoted A' or A^T, is obtained by exchanging the rows and columns of A, e.g.

$$\begin{pmatrix} 7 & 70 \\ 8 & 16 \\ 8 & 80 \end{pmatrix}' = \begin{pmatrix} 7 & 8 & 8 \\ 70 & 16 & 80 \end{pmatrix} \tag{A.11}$$

- If A + B is defined, then

$$(A + B)' = A' + B' \tag{A.12}$$

- If A and B are conformable, then

$$(AB)' = B'A' \tag{A.13}$$

A.3   Linear Independence

Equal-length vectors $X_1,...,X_k$ are said to be **linearly independent** if it is impossible for

$$a_1X_1 + ... + a_kX_k = 0 \tag{A.14}$$

unless all the a_i are 0.

A.4   Determinants

Let A be an nxn matrix. The definition of the determinant of A, det(A), involves an abstract formula featuring permutations. It will be omitted here, in favor of the following computational method.

Let $A_{-(i,j)}$ denote the submatrix of A obtained by deleting its ith row and j^{th} column. Then the determinant can be computed recursively across the kth row of A as

$$det(A) = \sum_{m=1}^{n} (-1)^{k+m} det(A_{-(k,m)}) \tag{A.15}$$

where

$$det \begin{pmatrix} s & t \\ u & v \end{pmatrix} = sv - tu \tag{A.16}$$

Generally, determinants are mainly of theoretical importance, but they often can clarify one's understanding of concepts.

A.5   Matrix Inverse

- The **identity** matrix I of size n has 1s in all of its diagonal elements but 0s in all off-diagonal elements. It has the property that AI = A and IA = A whenever those products are defined.

- The A is a square matrix and AB = I, then B is said to be the **inverse** of A, denoted A^{-1}. Then BA = I will hold as well.

- A^{-1} exists if and only if its rows (or columns) are linearly independent.

- A^{-1} exists if and only if $det(A) \neq 0$.

- If A and B are square, conformable and invertible, then AB is also invertible, and

$$(AB)^{-1} = B^{-1}A^{-1} \tag{A.17}$$

A matrix U is said to be **orthogonal** if its rows each have norm 1 and are orthogonal to each other, i.e. their inner product is 0. U thus has the property that $UU' = I$ i.e. $U^{-1} = U$.

The inverse of a triangular matrix is easily obtain by something called **back substitution**.

Typically one does not compute matrix inverses directly. A common alternative is the **QR decomposition**: For a matrix A, matrices Q and R are calculated so that A = QR, where Q is an orthogonal matrix and R is upper-triangular.

If A is square and inveritble, A^{-1} is easily found:

$$A^{-1} = (QR)^{-1} = R^{-1}Q' \tag{A.18}$$

Again, though, in some cases A is part of a more complex system, and the inverse is not explicitly computed.

A.6   Eigenvalues and Eigenvectors

Let A be a square matrix.[1]

- A scalar λ and a nonzero vector X that satisfy

$$AX = \lambda X \tag{A.19}$$

  are called an **eigenvalue** and **eigenvector** of A, respectively.

- If A is symmetric and real, then it is **diagonalizable**, i.e there exists an orthogonal matrix U such that

$$U'AU = D \tag{A.20}$$

  for a diagonal matrix D. The elements of D are the eigenvalues of A, and the columns of U are the eigenvectors of A.

A.7   Matrix Algebra in R

The R programming language has extensive facilities for matrix algebra, introduced here.

Note first that R matrix subscripts, like those of vectors, begin at 1, rather than 0 as in C/C++. For instance:

```
> m <- rbind(3:4,c(1,8))
> m
     [,1] [,2]
[1,] 3 4
[2,] 1 8
```

---

[1]For nonsquare matrices, the discussion here would generalize to the topic of **singular value decomposition**.

```
6  > m[2,2]
7  [1] 8
```

Next, it is important to know that R uses column-major order, i.e. its elements are stored in memory column-by-column. In the case of the matrix **m** above, for instance, the element 1 will be the second one in the internal memory storage of **m**, while the 8 will be the fourth.

This is also reflected in how R "inputs" data when a matrix is constructed, e.g.

```
1  > d <- matrix(c(1,-1,0,0,3,8),nrow=2)
2  > d
3       [,1] [,2] [,3]
4  [1,] 1 0 3
5  [2,] -1 0 8
```

The R matrix type is a special case of vectors:

```
1  > d[5] # 5th element, i.e. row 1, column 3
2  [1] 3
```

A linear algebra vector can be formed as an R vector, or as a one-row or one-column matrix. If you use it in a matrix product, R will usually be able to figure out whether you mean it to be a row or a column.

```
1  > # constructing matrices
2  > a <- rbind(1:3,10:12)
3  > a
4       [,1] [,2] [,3]
5  [1,] 1 2 3
6  [2,] 10 11 12
7  > b <- matrix(1:9,ncol=3)
8  > b
9       [,1] [,2] [,3]
10 [1,] 1 4 7
11 [2,] 2 5 8
12 [3,] 3 6 9
13 # multiplication, addition etc.
14 > c <- a %*% b
```

```
15  > c
16       [,1] [,2] [,3]
17  [1,] 14 32 50
18  [2,] 68 167 266
19  > c + matrix(c(1,-1,0,0,3,8),nrow=2) # 2 different c's!
20       [,1] [,2] [,3]
21  [1,] 15 32 53
22  [2,] 67 167 274
23  > c %*% c(1,5,6)
24       [,1]
25  [1,] 474
26  [2,] 2499
27  > t(a) # matrix transpose
28       [,1] [,2]
29  [1,] 1 10
30  [2,] 2 11
31  [3,] 3 12
32  > # matrix inverse
33  > u <- matrix(runif(9),nrow=3)
34  > u
35             [,1]       [,2]      [,3]
36  [1,] 0.08446154 0.86335270 0.6962092
37  [2,] 0.31174324 0.35352138 0.7310355
38  [3,] 0.56182226 0.02375487 0.2950227
39  > uinv <- solve(u)
40  > uinv
41             [,1]      [,2]      [,3]
42  [1,] 0.5818482 -1.594123 2.576995
43  [2,] 2.1333965 -2.451237 1.039415
44  [3,] -1.2798127 3.233115 -1.601586
45  > u %*% uinv # check, but note roundoff error
46              [,1] [,2] [,3]
47  [1,] 1.000000e+00 -1.680513e-16 -2.283330e-16
```

```
48  [2,] 6.651580e-17 1.000000e+00 4.412703e-17
49  [3,] 2.287667e-17 -3.539920e-17 1.000000e+00
50  > # eigenvalues and eigenvectors
51  > eigen(u)
52  $values
53  [1] 1.2456220+0.0000000i -0.2563082+0.2329172i -0.2563082-0.2329172i
54
55  $vectors
56               [,1] [,2] [,3]
57  [1,] -0.6901599+0i -0.6537478+0.0000000i -0.6537478+0.0000000i
58  [2,] -0.5874584+0i -0.1989163-0.3827132i -0.1989163+0.3827132i
59  [3,] -0.4225778+0i 0.5666579+0.2558820i 0.5666579-0.2558820i
60  > # diagonal matrices (off-diagonals 0)
61  > diag(3)
62       [,1] [,2] [,3]
63  [1,] 1 0 0
64  [2,] 0 1 0
65  [3,] 0 0 1
66  > diag((c(5,12,13)))
67       [,1] [,2] [,3]
68  [1,] 5 0 0
69  [2,] 0 12 0
70  [3,] 0 0 13
71  > m
72       [,1] [,2] [,3]
73  [1,] 5 6 7
74  [2,] 10 11 12
75  > diag(m) <- c(8,88)
76  > m
77       [,1] [,2] [,3]
78  [1,] 8 6 7
79  [2,] 10 88 12
```

附录 B R Quick Start

Here we present a quick introduction to the R data/statistical programming language. Further learning resources are listed at `http://heather.cs.ucdavis.edu/~/matloff/r.html`.

R syntax is similar to that of C. It is object-oriented (in the sense of encapsulation, polymorphism and everything being an object) and is a functional language (i.e. almost no side effects, every action is a function call, etc.).

B.1 Correspondences

aspect	C/C++	R
assignment	=	<- (or =)
array terminology	array	vector, matrix, array
subscripts	start at 0	start at 1
array notation	m[2][3]	m[2,3]
2-D array storage	row-major order	column-major order
mixed container	struct, members accessed by .	list, members acessed by $ or [[ ]]
return mechanism	return	return() or last value computed
primitive types	int, float, double, char, bool	integer, float, double, character, logica
logical values	true, false	TRUE, FALSE (abbreviated T, F)
mechanism for combining modules	include, link	library()
run method	batch	interactive, batch

B.2 Starting R

To invoke R, just type "R" into a terminal window. On a Windows machine, you probably have an R icon to click.

If you prefer to run from an IDE, you may wish to consider ESS for Emacs, StatET for Eclipse or RStudio, all open source. ESS is the favorite among the "hard core coder" types, while the colorful, easy-to-use, RStudio is a big general crowd pleaser. If you are already an Eclipse user, StatET will be just what you need.

R is normally run in interactive mode, with > as the prompt. Among other things, that makes it easy to try little experiments to learn from; remember my slogan, "When in doubt, try it out!"

B.3 First Sample Programming Session

Below is a commented R session, to introduce the concepts. I had a text editor open in another window, constantly changing my code, then loading it via R's **source()** command. The original contents of the file **odd.R** were:

```
1  oddcount <- function(x) {
2     k <- 0 # assign 0 to k
3     for (n in x) {
4        if (n %% 2 == 1) k <- k+1 # %% is the modulo operator
5     }
6     return(k)
7  }
```

By the way, we could have written that last statement as simply

```
1     k
```

because the last computed value of an R function is returned automatically.

The R session is shown below. You may wish to type it yourself as you go along, trying little experiments of your own along the way.[1]

```
1  > source("odd.R") # load code from the given file
2  > ls() # what objects do we have?
```

---

[1] The source code for this file is at `http://heather.cs.ucdavis.edu/~matloff/MiscPLN/R5MinIntro.tex`. You can download the file, and copy/paste the text from there.

```
3  [1] "oddcount"
4  > # what kind of object is oddcount (well, we already know)?
5  > class(oddcount)
6  [1] "function"
7  > # while in interactive mode, and not inside a function, can print
8  > # any object by typing its name; otherwise use print(), e.g. print(x+y)
9  > oddcount # a function is an object, so can print it
10 function(x) {
11    k <- 0 # assign 0 to k
12    for (n in x) {
13       if (n %% 2 == 1) k <- k+1 # %% is the modulo operator
14    }
15    return(k)
16 }
17
18 > # let's test oddcount(), but look at some properties of vectors first
19 > y <- c(5,12,13,8,88) # c() is the concatenate function
20 > y
21 [1] 5 12 13 8 88
22 > y[2] # R subscripts begin at 1, not 0
23 [1] 12
24 > y[2:4] # extract elements 2, 3 and 4 of y
25 [1] 12 13 8
26 > y[c(1,3:5)] # elements 1, 3, 4 and 5
27 [1] 5 13 8 88
28 > oddcount(y) # should report 2 odd numbers
29 [1] 2
30
31 > # change code (in the other window) to vectorize the count operation,
32 > # for much faster execution
33 > source("odd.R")
34 > oddcount
35 function(x) {
```

```
36     x1 <- (x %% 2 == 1) # x1 now a vector of TRUEs and FALSEs
37     x2 <- x[x1] # x2 now has the elements of x that were TRUE in x1
38     return(length(x2))
39  }
40
41  > # try it on subset of y, elements 2 through 3
42  > oddcount(y[2:3])
43  [1] 1
44  > # try it on subset of y, elements 2, 4 and 5
45  > oddcount(y[c(2,4,5)])
46  [1] 0
47
48  > # further compactify the code
49  > source("odd.R")
50  > oddcount
51  function(x) {
52     length(x[x %% 2 == 1]) # last value computed is auto returned
53  }
54  > oddcount(y) # test it
55  [1] 2
56
57  # and even more compactification, making use of the fact that TRUE and
58  # FALSE are treated as 1 and 0
59  > oddcount <- function(x) sum(x %% 2 == 1)
60  # make sure you understand the steps that that involves: x is a vector,
61  # and thus x %% 2 is a new vector, the result of applying the mod 2
62  # operation to every element of x; then x %% 2 == 1 applies the == 1
63  # operation to each element of that result, yielding a new vector of TRUE
64  # and FALSE values; sum() then adds them (as 1s and 0s)
65
66  # we can also determine which elements are odd
67  > which(y %% 2 == 1)
68  [1] 1 3
```

```
69
70  > # now have ftn return odd count AND the odd numbers themselves, using
71  > # the R list type
72  > source("odd.R")
73  > oddcount
74  function(x) {
75     x1 <- x[x %% 2 == 1]
76     return(list(odds=x1, numodds=length(x1)))
77  }
78  > # R's list type can contain any type; components delineated by $
79  > oddcount(y)
80  $odds
81  [1] 5 13
82
83  $numodds
84  [1] 2
85
86  > ocy <- oddcount(y) # save the output in ocy, which will be a list
87  > ocy
88  $odds
89  [1] 5 13
90
91  $numodds
92  [1] 2
93
94  > ocy$odds
95  [1] 5 13
96  > ocy[[1]] # can get list elements using [[ ]] instead of $
97  [1] 5 13
98  > ocy[[2]]
99  [1] 2
```

Note that the function of the R function **function()** is to produce functions! Thus assignment is used. For example, here is what **odd.R** looked like at the end of the above session:

```
1 oddcount <- function(x) {
2    x1 <- x[x %% 2 == 1]
3    return(list(odds=x1, numodds=length(x1)))
4 }
```

We created some code, and then used **function()** to create a function object, which we assigned to **oddcount**.

Note that we eventually **vectorized** our function **oddcount()**. This means taking advantage of the vector-based, functional language nature of R, exploiting R's built-in functions instead of loops. This changes the venue from interpreted R to C level, with a potentially large increase in speed. For example:

```
1 > x <- runif(1000000) # 1000000 random numbers from the interval (0,1)
2 > system.time(sum(x))
3    user system elapsed
4   0.008 0.000 0.006
5 > system.time({s <- 0; for (i in 1:1000000) s <- s + x[i]})
6    user system elapsed
7   2.776 0.004 2.859
```

B.4   Second Sample Programming Session

A matrix is a special case of a vector, with added class attributes, the numbers of rows and columns.

```
1 > # "rowbind() function combines rows of matrices; there's a cbind() too
2 > m1 <- rbind(1:2,c(5,8))
3 > m1
4     [,1] [,2]
5 [1,] 1 2
6 [2,] 5 8
7 > rbind(m1,c(6,-1))
8     [,1] [,2]
9 [1,] 1 2
10 [2,] 5 8
```

```
11  [3,] 6 -1

12

13  > # form matrix from 1,2,3,4,5,6, in 2 rows; R uses column-major storage

14  > m2 <- matrix(1:6,nrow=2)

15  > m2

16       [,1] [,2] [,3]

17  [1,] 1 3 5

18  [2,] 2 4 6

19  > ncol(m2)

20  [1] 3

21  > nrow(m2)

22  [1] 2

23  > m2[2,3] # extract element in row 2, col 3

24  [1] 6

25  # get submatrix of m2, cols 2 and 3, any row

26  > m3 <- m2[,2:3]

27  > m3

28       [,1] [,2]

29  [1,] 3 5

30  [2,] 4 6

31

32  > m1 * m3 # elementwise multiplication

33       [,1] [,2]

34  [1,] 3 10

35  [2,] 20 48

36  > 2.5 * m3 # scalar multiplication (but see below)

37       [,1] [,2]

38  [1,] 7.5 12.5

39  [2,] 10.0 15.0

40  > m1 %*% m3 # linear algebra matrix multiplication

41       [,1] [,2]

42  [1,] 11 17

43  [2,] 47 73
```

```
44
45  > # matrices are special cases of vectors, so can treat them as vectors
46  > sum(m1)
47  [1] 16
48  > ifelse(m2 %%3 == 1,0,m2) # (see below)
49       [,1] [,2] [,3]
50  [1,] 0 3 5
51  [2,] 2 0 6
```

The "scalar multiplication" above is not quite what you may think, even though the result may be. Here's why:

In R, scalars don't really exist; they are just one-element vectors. However, R usually uses **recycling**, i.e. replication, to make vector sizes match. In the example above in which we evaluated the express 2.5 * m3, the number 2.5 was recycled to the matrix

$$
\begin{pmatrix} 2.5 & 2.5 \\ 2.5 & 2.5 \end{pmatrix} \tag{B.1}
$$

in order to conform with **m3** for (elementwise) multiplication.

The **ifelse()** function is another example of vectorization. Its call has the form

```
1  ifelse(boolean vectorexpression1, vectorexpression2, vectorexpression3)
```

All three vector expressions must be the same length, though R will lengthen some via recycling. The action will be to return a vector of the same length (and if matrices are involved, then the result also has the same shape). Each element of the result will be set to its corresponding element in **vectorexpression2** or **vectorexpression3**, depending on whether the corresponding element in **vectorexpression1** is TRUE or FALSE.

In our example above,

```
1  > ifelse(m2 %%3 == 1,0,m2) # (see below)
```

the expression m2 %%3 == 1 evaluated to the boolean matrix

$$
\begin{pmatrix} T & F & F \\ F & T & F \end{pmatrix} \tag{B.2}
$$

(TRUE and FALSE may be abbreviated to T and F.)

The 0 was recycled to the matrix

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{(B.3)}$$

while **vectorexpression3**, **m2**, evaluated to itself.

B.5 Third Sample Programming Session

This time, we focus on vectors and matrices.

```
> m <- rbind(1:3,c(5,12,13)) # "row bind," combine rows
> m
     [,1] [,2] [,3]
[1,] 1 2 3
[2,] 5 12 13
> t(m) # transpose
     [,1] [,2]
[1,] 1 5
[2,] 2 12
[3,] 3 13
> ma <- m[,1:2]
> ma
     [,1] [,2]
[1,] 1 2
[2,] 5 12
> rep(1,2) # "repeat," make multiple copies
[1] 1 1
> ma %*% rep(1,2) # matrix multiply
     [,1]
[1,] 3
[2,] 17
> solve(ma,c(3,17)) # solve linear system
[1] 1 1
> solve(ma) # matrix inverse
     [,1] [,2]
```

```
26  [1,] 6.0 -1.0
27  [2,] -2.5 0.5
```

B.6   The R List Type

The R **list** type is, after vectors, the most important R construct. A list is like a vector, except that the components are generally of mixed types.

B.6.1   The Basics

Here is example usage:

```
1  > g <- list(x = 4:6, s = "abc")
2  > g
3  $x
4  [1] 4 5 6
5
6  $s
7  [1] "abc"
8
9  > g$x # can reference by component name
10 [1] 4 5 6
11 > g$s
12 [1] "abc"
13 > g[[1]] # can reference by index, but note double brackets
14 [1] 4 5 6
15 > g[[2]]
16 [1] "abc"
17 > for (i in 1:length(g)) print(g[[i]])
18 [1] 4 5 6
19 [1] "abc"
```

B.6.2   The Reduce() Function

One often needs to combine elements of a list in some way. One approach to this is to use **Reduce()**:

```
> x <- list(4:6,c(1,6,8))
> x
[[1]]
[1] 4 5 6

[[2]]
[1] 1 6 8

> sum(x)
Error in sum(x) : invalid 'type' (list) of argument
> Reduce(sum,x)
[1] 30
```

Here **Reduce()** cumulatively applied R's **sum()** to **x**. Of course, you can use it with functions you write yourself too.

Continuing the above example:

```
> Reduce(c,x)
[1] 4 5 6 1 6 8
```

B.6.3   S3 Classes

R is an object-oriented (and functional) language. It features two types of classes, S3 and S4. I'll introduce S3 here.

An S3 object is simply a list, with a class name added as an *attribute*:

```
> j <- list(name="Joe", salary=55000, union=T)
> class(j) <- "employee"
> m <- list(name="Joe", salary=55000, union=F)
> class(m) <- "employee"
```

So now we have two objects of a class we've chosen to name **"employee"**. Note the quotation marks.

We can write class *generic functions*:

```
1  > print.employee <- function(wrkr) {
2  + cat(wrkr$name,"\n")
3  + cat("salary",wrkr$salary,"\n")
4  + cat("union member",wrkr$union,"\n")
5  + }
6  > print(j)
7  Joe
8  salary 55000
9  union member TRUE
10 > j
11 Joe
12 salary 55000
13 union member TRUE
```

What just happened? Well, **print()** in R is a *generic* function, meaning that it is just a placeholder for a function specific to a given class. When we printed **j** above, the R interpreter searched for a function **print.employee()**, which we had indeed created, and that is what was executed. Lacking this, R would have used the print function for R lists, as before:

```
1  > rm(print.employee) # remove the function, to see what happens with print
2  > j
3  $name
4  [1] "Joe"
5
6  $salary
7  [1] 55000
8
9  $union
10 [1] TRUE
11
12 attr(,"class")
```

```
13  [1] "employee"
```

B.6.4 Handy Utilities

R functions written by others, e.g. in base R or in the CRAN repository for user-contributed code, often return values which are class objects. It is common, for instance, to have lists within lists. In many cases these objects are quite intricate, and not thoroughly documented. In order to explore the contents of an object—even one you write yourself—here are some handy utilities:

- **names()**: Returns the names of a list.
- **str()**: Shows the first few elements of each component.
- **summary()**: General function. The author of a class **x** can write a version specific to **x**, i.e. **summary.x()**, to print out the important parts; otherwise the default will print some bare-bones information.

For example:

```
1  > z <- list(a = runif(50), b = list(u=sample(1:100,25), v="blue sky"))
2  > z
3  $a
4   [1] 0.301676229 0.679918518 0.208713522 0.510032893 0.405027042
5  0.412388038
6   [7] 0.900498062 0.119936222 0.154996457 0.251126218 0.928304164
7  0.979945937
8  [13] 0.902377363 0.941813898 0.027964137 0.992137908 0.207571134
9  0.049504986
10 [19] 0.092011899 0.564024424 0.247162004 0.730086786 0.530251779
11 0.562163986
12 [25] 0.360718988 0.392522242 0.830468427 0.883086752 0.009853107
13 0.148819125
14 [31] 0.381143870 0.027740959 0.173798926 0.338813042 0.371025885
15 0.417984331
16 [37] 0.777219084 0.588650413 0.916212011 0.181104510 0.377617399
17 0.856198893
18 [43] 0.629269146 0.921698394 0.878412398 0.771662408 0.595483477
```

```
19   0.940457376
20   [49] 0.228829858 0.700500359
21
22   $b
23   $b$u
24    [1] 33 67 32 76 29 3 42 54 97 41 57 87 36 92 81 31 78 12 85 73 26 44
25   86 40 43
26
27   $b$v
28   [1] "blue sky"
29   > names(z)
30   [1] "a" "b"
31   > str(z)
32   List of 2
33    $ a: num [1:50] 0.302 0.68 0.209 0.51 0.405 ...
34    $ b:List of 2
35     ..$ u: int [1:25] 33 67 32 76 29 3 42 54 97 41 ...
36     ..$ v: chr "blue sky"
37   > names(z$b)
38   [1] "u" "v"
39   > summary(z)
40     Length Class Mode
41   a 50 -none- numeric
42   b 2 -none- list
```

B.7　Data Frames

Another workhorse in R is the *data frame.* A data frame works in many ways like a matrix, but differs from a matrix in that it can mix data of different modes. One column may consist of integers, while another can consist of character strings and so on. Within a column, though, all elements must be of the same mode, and all columns must have the same length.

We might have a 4-column data frame on people, for instance, with columns for height, weight, age and name—3 numeric columns and 1 character string column.

Technically, a data frame is an R list, with one list element per column; each column is a vector. Thus columns can be referred to by name, using the **$** symbol as with all lists, or by column number, as with matrices. The matrix **a[i,j]** notation for the element of **a** in row **i**, column **j**, applies to data frames. So do the **rbind()** and **cbind()** functions, and various other matrix operations, such as filtering.

Here is an example using the dataset **airquality**, built in to R for illustration purposes. You can learn about the data through R's online help, i.e.

```
> ?airquality
```

Let's try a few operations:

```
> names(airquality)
[1] "Ozone" "Solar.R" "Wind" "Temp" "Month" "Day"
> head(airquality) # look at the first few rows
  Ozone Solar.R Wind Temp Month Day
1 41 190 7.4 67 5 1
2 36 118 8.0 72 5 2
3 12 149 12.6 74 5 3
4 18 313 11.5 62 5 4
5 NA NA 14.3 56 5 5
6 28 NA 14.9 66 5 6
> airquality[5,3] # temp on the 5th day
[1] 14.3
> airquality$Wind[3] # same
[1] 12.6
> nrow(airquality) # number of days observed
[1] 153
> ncol(airquality) # number of variables
[1] 6
> airquality$Celsius <- (5/9) * (airquality[,4] - 32) # new variable
> names(airquality)
[1] "Ozone" "Solar.R" "Wind" "Temp" "Month" "Day" "Celsius"
> ncol(airquality)
[1] 7
> airquality[1:3,]
```

```
25    Ozone Solar.R Wind Temp Month Day Celsius
26  1 41 190 7.4 67 5 1 19.44444
27  2 36 118 8.0 72 5 2 22.22222
28  3 12 149 12.6 74 5 3 23.33333
29  > aqjune <- airquality[airquality$Month == 6,] # filter op
30  > nrow(aqjune)
31  [1] 30
32  > mean(aqjune$Temp)
33  [1] 79.1
34  > write.table(aqjune,"AQJune") # write data frame to file
35  > aqj <- read.table("AQJune",header=T) # read it in
```

B.8   Graphics

R excels at graphics, offering a rich set of capabilities, from beginning to advanced. In addition to the functions in base R, extensive graphics packages are available, such as **lattice** and **ggplot2**.

One point of confusion for beginninners involves saving an R graph that is currently displayed on the screen to a file. Here is a function for this, which I include in my R startup file, **.Rprofile**, in my home directory:

```
1  pr2file
2  function (filename)
3  {
4      origdev <- dev.cur()
5      parts <- strsplit(filename, ".", fixed = TRUE)
6      nparts <- length(parts[[1]])
7      suff <- parts[[1]][nparts]
8      if (suff == "pdf") {
9          pdf(filename)
10     }
11     else if (suff == "png") {
12         png(filename)
13     }
14     else jpeg(filename)
```

```
15      devnum <- dev.cur()
16      dev.set(origdev)
17      dev.copy(which = devnum)
18      dev.set(devnum)
19      dev.off()
20      dev.set(origdev)
21  }
```

The code, which I won't go into here, mostly involves manipulation of various R graphics devices. I've set it up so that you can save to a file of type either PDF, PNG or JPEG, implied by the file name you give.

B.9   Other Sources for Learning R

There are tons of resources for R on the Web. You may wish to start with the links at `http://heather.cs.ucdavis.edu/~matloff/r.html`.

B.10   Online Help

R's **help()** function, which can be invoked also with a question mark, gives short descriptions of the R functions. For example, typing

```
1  > ?rep
```

will give you a description of R's **rep()** function.

An especially nice feature of R is its **example()** function, which gives nice examples of whatever function you wish to query. For instance, typing

```
1  > example(wireframe())
```

will show examples—R code and resulting pictures—of **wireframe()**, one of R's 3-dimensional graphics functions.

B.11   Debugging in R

The internal debugging tool in R, **debug()**, is usable but rather primitive. Here are some alternatives:

- The RStudio IDE has a built-in debugging tool.

- The StatET IDE for R on Eclipse has a nice debugging tool. Works on all major platforms, but can be tricky to install.

- My own debugging tool, **debugR**, is extensive and easy to install, but for the time being is limited to Linux, Mac and other Unix-family systems. See *http://heather.cs.ucdavis.edu/debugR.html*.

B.12　Complex Numbers

If you have need for complex numbers, R does handle them. Here is a sample of use of the main functions of interest:

```
> za <- complex(real=2,imaginary=3.5)
> za
[1] 2+3.5i
> zb <- complex(real=1,imaginary=-5)
> zb
[1] 1-5i
> za * zb
[1] 19.5-6.5i
> Re(za)
[1] 2
> Im(za)
[1] 3.5
> za^2
[1] -8.25+14i
> abs(za)
[1] 4.031129
> exp(complex(real=0,imaginary=pi/4))
[1] 0.7071068+0.7071068i
> cos(pi/4)
[1] 0.7071068
> sin(pi/4)
[1] 0.7071068
```

Note that operations with complex-valued vectors and matrices work as usual; there are no special complex functions.

B.13   Further Reading

For further information about R as a programming language, there is my book, *The Art of R Programming: a Tour of Statistical Software Design*, NSP, 2011.

For R's statistical functions, a plethora of excellent books is available. such as *The R Book* (2nd Ed.), Michael Crowley, Wiley, 2012. I also very much like *R in a Nutshell* (2nd Ed.), Joseph Adler, O'Reilly, 2012.

附录 C   Introduction to Python

NOTE: This document is the first part of my open source book on Python, `http://heather.cs.ucdavis.edu/~matloff/Python/PLN/FastLanePython.pdf`. Go there for further information.

So, let's get started with programming right away.

C.1   A 5-Minute Introductory Example

C.1.1   Example Program Code

Here is a simple, quick example. Suppose I wish to find the value of

$$g(x) = \frac{x}{1 - x^2}$$

for x = 0.0, 0.1, ..., 0.9. I could find these numbers by placing the following code,

```
1  for i in range(10):
2      x = 0.1*i
3      print x
4      print x/(1-x*x)
```

in a file, say **fme.py**, and then running the program by typing

```
1  python fme.py
```

at the command-line prompt. The output will look like this:

```
1  0.0
2  0.0
3  0.1
4  0.10101010101
5  0.2
6  0.208333333333
7  0.3
```

```
 8   0.32967032967
 9   0.4
10   0.47619047619
11   0.5
12   0.666666666667
13   0.6
14   0.9375
15   0.7
16   1.37254901961
17   0.8
18   2.22222222222
19   0.9
20   4.73684210526
```

C.1.2   Python Lists

How does the program work? First, Python's **range()** function is an example of the use of **lists**, i.e. Python arrays,[①] even though not quite explicitly. Lists are absolutely fundamental to Python, so watch out in what follows for instances of the word "list"; resist the temptation to treat it as the English word "list," instead always thinking about the Python construct **list**.

Python's **range()** function returns a list of consecutive integers, in this case the list [0,1,2,3,4,5,6,7,8,9]. Note that this is official Python notation for lists—a sequence of objects (these could be all kinds of things, not necessarily numbers), separated by commas and enclosed by brackets.

C.1.3   Loops

So, the **for** statement above is equivalent to:

```
1   for i in [0,1,2,3,4,5,6,7,8,9]:
```

As you can guess, this will result in 10 iterations of the loop, with **i** first being 0, then 1, etc. The code

```
1   for i in [2,3,6]:
```

would give us three iterations, with **i** taking on the values 2, 3 and 6.

Python has a **while** construct too (though not an **until**).

[①] I loosely speak of them as "arrays" here, but as you will see, they are more flexible than arrays in C/C++.

On the other hand, true arrays can be accessed more quickly. In C/C++, the ith element of an array **X** is i words past the beginning of the array, so we can go right to it. This is not possible with Python lists, so the latter are slower to access. The NumPy add-on package for Python offers true arrays.

There is also a **break** statement like that of C/C++, used to leave loops "prematurely." For example:

```
1  x = 5
2  while 1:
3     x += 1
4     if x == 8:
5        print x
6        break
```

Also very useful is the **continue** statement, which instructs the Python interpreter to skip the remainder of the current iteration of a loop. For instance, running the code

```
1  sum = 0
2  for i in [5,12,13]:
3     if i < 10: continue
4     sum += i
5  print sum
```

prints out 12+13, i.e. 25.

The **pass** statement is a "no-op," doing nothing.

C.1.4   Python Block Definition

Now focus your attention on that inoccuous-looking colon at the end of the **for** line above, which defines the start of a block. Unlike languages like C/C++ or even Perl, which use braces to define blocks, Python uses a combination of a colon and indenting to define a block. I am using the colon to say to the Python interpreter,

> Hi, Python interpreter, how are you? I just wanted to let you know, by inserting this colon, that a block begins on the next line. I've indented that line, and the two lines following it, further right than the current line, in order to tell you those three lines form a block.

I chose 3-space indenting, but the amount wouldn't matter as long as I am consistent. If for example I were to write[②]

```
1  for i in range(10):
2     print 0.1*i
3        print g(0.1*i)
```

[②]Here **g()** is a function I defined earlier, not shown.

the Python interpreter would give me an error message, telling me that I have a syntax error.[③] I am only allowed to indent further-right within a given block if I have a sub-block within that block, e.g.

```
1  for i in range(10):
2     if i%2 == 1:
3        print 0.1*i
4        print g(0.1*i)
```

Here I am printing out only the cases in which the variable **i** is an odd number; % is the "mod" operator as in C/C++.

Again, note the colon at the end of the **if** line, and the fact that the two **print** lines are indented further right than the **if** line.

Note also that, again unlike C/C++/Perl, there are no semicolons at the end of Python source code statements. A new line means a new statement. If you need a very long line, you can use the backslash character for continuation, e.g.

```
1  x = y + \
2       z
```

Most of the usual C operators are in Python, including the relational ones such as the **==** seen here. The **0x** notation for hex is there, as is the FORTRAN ****** for exponentiation.

Also, the **if** construct can be paired with **else** as usual, and you can abbreviate **else if** as **elif**.

```
1  >> def f(x):
2  ...     if x > 0: return 1
3  ...     else: return 0
4  ...
5  >>> f(2)
6  1
7  >>> f(-1)
8  0
```

The boolean operators are **and**, **or** and **not**.

You'll see examples as we move along.

By the way, watch out for Python statements like **print a or b or c**, in which the first true (i.e. nonzero) expression is printed and the others ignored; this is a common Python idiom.

[③]Keep this in mind. New Python users are often baffled by a syntax error arising in this situation.

C.1.5   Python Also Offers an Interactive Mode

A really nice feature of Python is its ability to run in interactive mode. You usually won't do this, but it's a great way to do a quick tryout of some feature, to really see how it works. Whenever you're not sure whether something works, your motto should be, "When in doubt, try it out!", and interactive mode makes this quick and easy.

We'll also be doing a lot of that in this tutorial, with interactive mode being an easy way to do a quick illustration of a feature.

Instead of executing this program from the command line in **batch** mode as we did above, we could enter and run the code in **interactive** mode:

```
% python
>>> for i in range(10):
...     x = 0.1*i
...     print x
...     print x/(1-x*x)
...
0.0
0.0
0.1
0.10101010101
0.2
0.208333333333
0.3
0.32967032967
0.4
0.47619047619
0.5
0.666666666667
0.6
0.9375
0.7
1.37254901961
0.8
2.22222222222
0.9
4.73684210526
>>>
```

Here I started Python, and it gave me its >>> interactive prompt. Then I just started typing in the code, line by line. Whenever I was inside a block, it gave me a special prompt, "...", for that

purpose. When I typed a blank line at the end of my code, the Python interpreter realized I was done, and ran the code.[④]

While in interactive mode, one can go up and down the command history by using the arrow keys, thus saving typing.

To exit interactive Python, hit ctrl-d.

Automatic printing: By the way, in interactive mode, just referencing or producing an object, or even an expression, without assigning it, will cause its value to print out, even without a **print** statement. For example:

```
>>> for i in range(4):
...     3*i
...
0
3
6
9
```

Again, this is true for general objects, not just expressions, e.g.:

```
>>> open('x')
<open file 'x', mode 'r' at 0xb7eaf3c8>
```

Here we opened the file **x**, which produces a file object. Since we did not assign to a variable, say **f**, for reference later in the code, i.e. we did not do the more typical

```
f = open('x')
```

the object was printed out. We'd get that same information this way:

```
>>> f = open('x')
>>> f
<open file 'x', mode 'r' at 0xb7f2a3c8>
```

C.1.6   Python As a Calculator

Among other things, this means you can use Python as a quick calculator (which I do a lot). If for example I needed to know what 5% above $88.88 is, I could type

---

[④]Interactive mode allows us to execute only single Python statements or evaluate single Python expressions. In our case here, we typed in and executed a single **for** statement. Interactive mode is not designed for us to type in an entire program. Technically we could work around this by beginning with something like "if 1:", making our program one large **if** statement, but of course it would not be convenient to type in a long program anyway.

```
1  % python
2  >>> 1.05*88.88
3  93.323999999999998
```

Among other things, one can do quick conversions between decimal and hex:

```
1  >>> 0x12
2  18
3  >>> hex(18)
4  '0x12'
```

If I need math functions, I must **import** the Python math library first. This is analogous to what we do in C/C++, where we must have a **#include** line for the library in our source code and must link in the machine code for the library.

We must refer to imported functions in the context of the library, in this case the math library. For example, the functions **sqrt()** and **sin()** must be prefixed by **math**:[5]

```
1  >>> import math
2  >>> math.sqrt(88)
3  9.3808315196468595
4  >>> math.sin(2.5)
5  0.59847214410395655
```

C.2　A 10-Minute Introductory Example

C.2.1　Example Program Code

This program reads a text file, specified on the command line, and prints out the number of lines and words in the file:

```
1  # reads in the text file whose name is specified on the command line,
2  # and reports the number of lines and words
3
4  import sys
5
6  def checkline():
7      global l
8      global wordcount
9      w = l.split()
10     wordcount += len(w)
11
```

---

[5] A method for avoiding the prefix is shown in Sec. **??**.

```
12   wordcount = 0
13   f = open(sys.argv[1])
14   flines = f.readlines()
15   linecount = len(flines)
16   for l in flines:
17       checkline()
18   print linecount, wordcount
```

Say for example the program is in the file **tme.py**, and we have a text file **x** with contents

```
1
2    This is an
3    example of a
4    text file.
5
```

(There are five lines in all, the first and last of which are blank.)

If we run this program on this file, the result is:

```
1    python tme.py x
2    5 8
```

On the surface, the layout of the code here looks like that of a C/C++ program: First an **import** statement, analogous to **#include** (with the corresponding linking at compile time) as stated above; second the definition of a function; and then the "main" program. This is basically a good way to look at it, but keep in mind that the Python interpreter will execute everything in order, starting at the top. In executing the **import** statement, for instance, that might actually result in some code being executed, if the module being imported has some free-standing code rather than just function definitions. More on this later. Execution of the **def** statement won't execute any code for now, but the act of defining the function is considered execution.

Here are some features in this program which were not in the first example:

- use of command-line arguments
- file-manipulation mechanisms
- more on lists
- function definition
- library importation
- introduction to scope

I will discuss these features in the next few sections.

C.2.2　Command-Line Arguments

First, let's explain **sys.argv**. Python includes a **module** (i.e. library) named **sys**, one of whose member variables is **argv**. The latter is a Python list, analogous to **argv** in C/C++.[⑥] Element 0 of the list is the script name, in this case **tme.py**, and so on, just as in C/C++. In our example here, in which we run our program on the file **x**, **sys.argv[1]** will be the string 'x' (strings in Python are generally specified with single quote marks). Since **sys** is not loaded automatically, we needed the **import** line.

Both in C/C++ and Python, those command-line arguments are of course strings. If those strings are supposed to represent numbers, we could convert them. If we had, say, an integer argument, in C/C++ we would do the conversion using **atoi()**; in Python, we'd use **int()**. For floating-point, in Python we'd use **float()**.[⑦]

C.2.3　Introduction to File Manipulation

The function **open()** is similar to the one in C/C++. Our line

```
1  f = open(sys.argv[1])
```

created an object of **file** class, and assigned it to **f** .

The **readlines()** function of the **file** class returns a list (keep in mind, "list" is an official Python term) consisting of the lines in the file. Each line is a string, and that string is one element of the list. Since the file here consisted of five lines, the value returned by calling **readlines()** is the five-element list

```
1  ['','This is an','example of a','text file','']
```

(Though not visible here, there is an end-of-line character in each string.)

C.2.4　Lack of Declaration

Variables are not declared in Python. A variable is created when the first assignment to it is executed. For example, in the program **tme.py** above, the variable **flines** does not exist until the statement

```
1  flines = f.readlines()
```

[⑥]There is no need for an analog of **argc**, though. Python, being an object-oriented language, treats lists as objects, The length of a list is thus incorporated into that object. So, if we need to know the number of elements in **argv**, we can get it via **len(argv)**.

[⑦]In C/C++, we could use **atof()** if it were available, or **sscanf()**.

is executed.

By the way, a variable which has not been assigned a value yet, such as **wordcount** at first above, has the value **None**. And this can be assigned to a variable, tested for in an **if** statement, etc.

C.2.5   Locals Vs. Globals

Python does not really have global variables in the sense of C/C++, in which the scope of a variable is an entire program. We will discuss this further in Section **??**, but for now assume our source code consists of just a single **.py** file; in that case, Python does have global variables pretty much like in C/C++ (though with important differences).

Python tries to infer the scope of a variable from its position in the code. If a function includes any code which assigns to a variable, then that variable is assumed to be local, unless we use the **global** keyword. So, in the code for **checkline()**, Python would assume that **l** and **wordcount** are local to **checkline()** if we had not specified **global**.

Use of global variables simplifies the presentation here, and I personally believe that the unctuous criticism of global variables is unwarranted. (See `http://heather.cs.ucdavis.edu/~matloff/globals.html`.) In fact, in one of the major types of programming, **threads**, use of globals is basically *mandatory*.

You may wish, however, to at least group together all your globals into a class, as I do. See Appendix **??**.

C.2.6   A Couple of Built-In Functions

The function **len()** returns the number of elements in a list. In the **tme.py** example above, we used this to find the number of lines in the file, since **readlines()** returned a list in which each element consisted of one line of the file.

The method **split()** is a member of the **string** class.[8] It splits a string into a list of words, for example.[9] So, for instance, in **checkline()** when **l** is 'This is an' then the list **w** will be equal to ['This','is','an']. (In the case of the first line, which is blank, **w** will be equal to the empty list, [].)

---

[8] Member functions of classes are referred to as **methods**.

[9] The default is to use blank characters as the splitting criterion, but other characters or strings can be used.

C.3   Types of Variables/Values

As is typical in scripting languages, type in the sense of C/C++ **int** or **float** is not declared in Python. However, the Python interpreter does internally keep track of the type of all objects. Thus Python variables don't have types, but their values do. In other words, a variable **X** might be bound to (i.e. point to) an integer in one place in your program and then be rebound to a class instance at another point.

Python's types include notions of scalars, **sequences** (lists or **tuples**) and dictionaries (associative arrays, discussed in Sec. C.6), classes, function, etc.

C.4   String Versus Numerical Values

Unlike Perl, Python does distinguish between numbers and their string representations. The functions **eval()** and **str()** can be used to convert back and forth. For example:

```
1  >>> 2 + '1.5'
2  Traceback (most recent call last):
3    File "<stdin>", line 1, in ?
4  TypeError: unsupported operand type(s) for +: 'int' and 'str'
5  >>> 2 + eval('1.5')
6  3.5
7  >>> str(2 + eval('1.5'))
8  '3.5'
```

There are also **int()** to convert from strings to integers, and **float()**, to convert from strings to floating-point values:

```
1  >>> n = int('32')
2  >>> n
3  32
4  >>> x = float('5.28')
5  >>> x
6  5.2800000000000002
```

See also Section C.5.3.

C.5   Sequences

Lists are actually special cases of **sequences**, which are all array-like but with some differences. Note though, the commonalities; all of the following (some to be explained below) apply to any sequence type:

- the use of brackets to denote individual elements (e.g. **x[i]**)
- the built-in **len()** function to give the number of elements in the sequence[①]
- **slicing** operations, i.e. the extraction of subsequences
- use of **+** and ***** operators for concatenation and replication

C.5.1 Lists (Quasi-Arrays)

As stated earlier, lists are denoted by brackets and commas. For instance, the statement

```
x = [4,5,12]
```

would set **x** to the specified 3-element array.

Lists may grow dynamically, using the **list** class' **append()** or **extend()** functions. For example, if after the abovfe statement we were to execute

```
x.append(-2)
```

x would now be equal to [4,5,12,-2].

A number of other operations are available for lists, a few of which are illustrated in the following code:

```
>>> x = [5,12,13,200]
>>> x
[5, 12, 13, 200]
>>> x.append(-2)
>>> x
[5, 12, 13, 200, -2]
>>> del x[2]
>>> x
[5, 12, 200, -2]
>>> z = x[1:3]  # array "slicing": elements 1 through 3-1 = 2
>>> z
[12, 200]
>>> yy = [3,4,5,12,13]
>>> yy[3:]  # all elements starting with index 3
[12, 13]
>>> yy[:3]  # all elements up to but excluding index 3
[3, 4, 5]
>>> yy[-1]  # means "1 item from the right end"
13
>>> x.insert(2,28)  # insert 28 at position 2
```

[①]This function is applicable to dictionaries too.

```
21  >>> x
22  [5, 12, 28, 200, -2]
23  >>> 28 in x  # tests for membership; 1 for true, 0 for false
24  1
25  >>> 13 in x
26  0
27  >>> x.index(28)  # finds the index within the list of the given value
28  2
29  >>> x.remove(200)  # different from "delete," since it's indexed by value
30  >>> x
31  [5, 12, 28, -2]
32  >>> w = x + [1,"ghi"]  # concatenation of two or more lists
33  >>> w
34  [5, 12, 28, -2, 1, 'ghi']
35  >>> qz = 3*[1,2,3]  # list replication
36  >>> qz
37  [1, 2, 3, 1, 2, 3, 1, 2, 3]
38  >>> x = [1,2,3]
39  >>> x.extend([4,5])
40  >>> x
41  [1, 2, 3, 4, 5]
42  >>> y = x.pop(0)  # deletes and returns 0th element
43  >>> y
44  1
45  >>> x
46  [2, 3, 4, 5]
47  >>> t = [5,12,13]
48  >>> t.reverse()
49  >>> t
50  [13, 12, 5]
```

We also saw the **in** operator in an earlier example, used in a **for** loop.

A list could include mixed elements of different types, including other lists themselves.

The Python idiom includes a number of common "Python tricks" involving sequences, e.g. the following quick, elegant way to swap two variables **x** and **y**:

```
1  >>> x = 5
2  >>> y = 12
3  >>> [x,y] = [y,x]
4  >>> x
5  12
6  >>> y
7  5
```

Multidimensional lists can be implemented as lists of lists. For example:

```
1  >>> x = []
2  >>> x.append([1,2])
3  >>> x
4  [[1, 2]]
5  >>> x.append([3,4])
6  >>> x
7  [[1, 2], [3, 4]]
8  >>> x[1][1]
9  4
```

But be careful! Look what can go wrong:

```
1  >>> x = 4*[0]
2  >>> y = 4*[x]
3  >>> y
4  [[0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0]]
5  >>> y[0][2]
6  0
7  >>> y[0][2] = 1
8  >>> y
9  [[0, 0, 1, 0], [0, 0, 1, 0], [0, 0, 1, 0], [0, 0, 1, 0]]
```

The problem is that that assignment to **y** was really a list of four references to the same thing (**x**). When the object pointed to by **x** changed, then all four rows of **y** changed.

The Python Wikibook (`http://en.wikibooks.org/wiki/Python_Programming/Lists`) suggests a solution, in the form of **list comprehensions**, which we cover in Section **??**:

```
1  >>> z = [[0]*4 for i in range(5)]
2  >>> z
3  [[0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0]]
4  >>> z[0][2] = 1
5  >>> z
6  [[0, 0, 1, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0], [0, 0, 0, 0]]
```

C.5.2   Tuples

Tuples are like lists, but are **immutable**, i.e. unchangeable. They are enclosed by parentheses or nothing at all, rather than brackets. The parentheses are mandatory if there is an ambiguity without them, e.g. in function arguments. A comma must be used in the case of empty or single tuple, e.g. **(,)** and **(5,)**.

The same operations can be used, except those which would change the tuple. So for example

```
1  x = (1,2,'abc')
2  print x[1]  # prints 2
```

```
3  print len(x)  # prints 3
4  x.pop()  # illegal, due to immutability
```

A nice function is **zip()**, which strings together corresponding components of several lists, producing tuples, e.g.

```
1  >>> zip([1,2],['a','b'],[168,168])
2  [(1, 'a', 168), (2, 'b', 168)]
```

C.5.3 Strings

Strings are essentially tuples of character elements. But they are quoted instead of surrounded by parentheses, and have more flexibility than tuples of character elements would have.

Strings As Turbocharged Tuples

Let's see some examples of string operations:

```
1   >>> x = 'abcde'
2   >>> x[2]
3   'c'
4   >>> x[2] = 'q'  # illegal, since strings are immmutable
5   Traceback (most recent call last):
6     File "<stdin>", line 1, in ?
7   TypeError: object doesn't support item assignment
8   >>> x = x[0:2] + 'q' + x[3:5]
9   >>> x
10  'abqde'
```

(You may wonder why that last assignment

```
1  >>> x = x[0:2] + 'q' + x[3:5]
```

does not violate immmutability. The reason is that **x** is really a pointer, and we are simply pointing it to a new string created from old ones. See Section **??**.)

As noted, strings are more than simply tuples of characters:

```
1  >>> x.index('d')  # as expected
2  3
3  >>> 'd' in x  # as expected
4  1
5  >>> x.index('de')  # pleasant surprise
6  3
```

As can be seen, the **index()** function from the **str** class has been overloaded, making it more flexible.

There are many other handy functions in the **str** class. For example, we saw the **split()** function earlier. The opposite of this function is **join()**. One applies it to a string, with a sequence of strings as an argument. The result is the concatenation of the strings in the sequence, with the original string between each of them:[1]

```
1  >>> '---'.join(['abc','de','xyz'])
2  'abc---de---xyz'
3  >>> q = '\n'.join(('abc','de','xyz'))
4  >>> q
5  'abc\nde\nxyz'
6  >>> print q
7  abc
8  de
9  xyz
```

Here are some more:

```
1   >>> x = 'abc'
2   >>> x.upper()
3   'ABC'
4   >>> 'abc'.upper()
5   'ABC'
6   >>> 'abc'.center(5) # center the string within a 5-character set
7   ' abc '
8   >>> 'abc de f'.replace(' ','+')
9   'abc+de+f'
10  >>> x = 'abc123'
11  >>> x.find('c1')  # find index of first occurrence of 'c1' in x
12  2
13  >>> x.find('3')
14  5
15  >>> x.find('1a')
16  -1
```

A very rich set of functions for string manipulation is also available in the **re** ("regular expression") module.

The **str** class is built-in for newer versions of Python. With an older version, you will need a statement

```
1  import string
```

---

[1]The example here shows the "new" usage of **join()**, now that string methods are built-in to Python. See discussion of "new" versus "old" below.

That latter class does still exist, and the newer **str** class does not quite duplicate it.

Formatted String Manipulation

String manipulation is useful in lots of settings, one of which is in conjunction with Python's **print** command. For example,

```
1  print "the factors of 15 are %d and %d" % (3,5)
```

prints out

```
1  the factors of 15 are 3 and 5
```

The **%d** of course is the integer format familiar from C/C++.

But actually, the above action is a string issue, not a print issue. Let's see why. In

```
1  print "the factors of 15 are %d and %d" % (3,5)
```

the portion

```
1  "the factors of 15 are %d and %d" % (3,5)
```

is a string operation, producing a new string; the **print** simply prints that new string.

For example:

```
1  >>> x = "%d years old" % 12
```

The variable **x** now is the string '12 years old'.

This is another very common idiom, quite powerful.[12]

Note the importance above of writing '(3,5)' rather than '3,5'. In the latter case, the **%** operator would think that its operand was merely 3, whereas it needs a 2-element tuple. Recall that parentheses enclosing a tuple can be omitted as long as there is no ambiguity, but that is not the case here.

C.6   Dictionaries (Hashes)

Dictionaries are **associative arrays**. The technical meaning of this will be discussed below, but from a pure programming point of view, this means that one can set up arrays with non-integer indices. The statement

```
1  x = {'abc':12,'sailing':'away'}
```

---

[12]Some C/C++ programmers might recognize the similarity to **sprintf()** from the C library.

sets **x** to what amounts to a 2-element array with **x['abc']** being 12 and **x['sailing']** equal to 'away'. We say that **'abc'** and **'sailing'** are **keys**, and 12 and 'away' are **values**. Keys can be any immmutable object, i.e. numbers, tuples or strings.[☺] Use of tuples as keys is quite common in Python applications, and you should keep in mind that this valuable tool is available.

Internally, **x** here would be stored as a 4-element array, and the execution of a statement like

```
w = x['sailing']
```

would require the Python interpreter to search through that array for the key 'sailing'. A linear search would be slow, so internal storage is organized as a hash table. This is why Perl's analog of Python's dictionary concept is actually called a **hash**.

Here are examples of usage of some of the member functions of the **dictionary** class:

```
>>> x = {'abc':12,'sailing':'away'}
>>> x['abc']
12
>>> y = x.keys()
>>> y
['abc', 'sailing']
>>> z = x.values()
>>> z
[12, 'away']
x['uv'] = 2
>>> x
{'abc': 12, 'uv': 2, 'sailing': 'away'}
```

Note how we added a new element to **x** near the end.

The keys need not be tuples. For example:

```
>>> x
{'abc': 12, 'uv': 2, 'sailing': 'away'}
>>> f = open('z')
>>> x[f] = 88
>>> x
{<open file 'z', mode 'r' at 0xb7e6f338>: 88, 'abc': 12, 'uv': 2, 'sailing': 'away'}
```

Deletion of an element from a dictionary can be done via **pop()**, e.g.

```
>>> x.pop('abc')
12
>>> x
{<open file 'x', mode 'r' at 0xb7e6f338>: 88, 'uv': 2, 'sailing': 'away'}
```

[☺]Now one sees a reason why Python distinguishes between tuples and lists. Allowing mutable keys would be an implementation nightmare, and probably lead to error-prone programming.

The **in** operator works on dictionary keys, e.g.

```
1  >>> x = {'abc': 12, 'uv': 2, 'sailing': 'away'}
2  >>> 'uv' in x
3  True
4  >>> 2 in x
5  False
```

C.7 Extended Example: Computing Final Grades

```
1   # computes and records final grades
2
3   # input line format:
4
5   #    name and misc. info, e.g. class level
6   #    Final Report grade
7   #    Midterm grade
8   #    Quiz grades
9   #    Homework grades
10
11  # comment lines, beginning with #, are ignored for computation but are
12  # printed out; thus various notes can be put in comment lines; e.g.
13  # notes on missed or makeup exams
14
15  # usage:
16
17  #   python FinalGrades.py input_file nq nqd nh wts
18
19  #     where there are nq Quizzes, the lowest nqd of which will be
20  #     deleted; nh Homework assignments; and wts is the set of weights
21  #     for Final Report, Midterm, Quizzes and Homework
22
23  # outputs to stdout the input file with final course grades appended;
24  # the latter are numerical only, allowing for personal inspection of
25  # "close" cases, etc.
26
27  import sys
28
29  def convertltr(lg):  # converts letter grade lg to 4-point-scale
30      if lg == 'F': return 0
31      base = lg[0]
32      olg = ord(base)
33      if len(lg) > 2 or olg < ord('A') or olg > ord('D'):
34          print lg, 'is not a letter grade'
35          sys.exit(1)
36      grade = 4 - (olg-ord('A'))
```

```python
37      if len(lg) == 2:
38          if lg[1] == '+': grade += 0.3
39          elif lg[1] == '-': grade -= 0.3
40          else:
41              print lg, 'is not a letter grade'
42              sys.exit(1)
43      return grade
44
45  def avg(x,ndrop):
46      tmp = []
47      for xi in x: tmp.append(convertltr(xi))
48      tmp.sort()
49      tmp = tmp[ndrop:]
50      return float(sum(tmp))/len(tmp)
51
52  def main():
53      infile = open(sys.argv[1])
54      nq = int(sys.argv[2])
55      nqd = int(sys.argv[3])
56      nh = int(sys.argv[4])
57      wts = []
58      for i in range(4): wts.append(float(sys.argv[5+i]))
59      for line in infile.readlines():
60          toks = line.split()
61          if toks[0] != '#':
62              lw = len(toks)
63              startpos = lw - nq - nh - 3
64              # Final Report
65              frgrade = convertltr(toks[startpos])
66              # Midterm letter grade (skip over numerical grade)
67              mtgrade = convertltr(toks[startpos+2])
68              startquizzes = startpos + 3
69              qgrade = avg(toks[startquizzes:startquizzes+nq],nqd)
70              starthomework = startquizzes + nq
71              hgrade = avg(toks[starthomework:starthomework+nh],0)
72              coursegrade = 0.0
73              coursegrade += wts[0] * frgrade
74              coursegrade += wts[1] * mtgrade
75              coursegrade += wts[2] * qgrade
76              coursegrade += wts[3] * hgrade
77              print line[:len(line)-1], coursegrade
78          else:
79              print line[:len(line)-1]
80
81  main()
```