Programming on Parallel Machines

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GPU, Multicore, Clusters and More

This book is often revised and updated, latest edition available at http://heather.cs.ucdavis.edu/ matloff/158/PLN/ParProcBook.pdf

Author's Biographical Sketch

Dr. Norm Matloff is a professor of computer science at the University of California at Davis, and was formerly a professor of statistics at that university. He is a former database software developer in Silicon Valley, and has been a statistical consultant for firms such as the Kaiser Permanente Health Plan.

Dr. Matloff was born in Los Angeles, and grew up in East Los Angeles and the San Gabriel Valley. He has a PhD in pure mathematics from UCLA, specializing in probability theory and statistics. He has published numerous papers in computer science and statistics, with current research interests in parallel processing, statistical computing, and regression methodology.

Prof. Matloff is a former appointed member of IFIP Working Group 11.3, an international committee concerned with database software security, established under UNESCO. He was a founding member of the UC Davis Department of Statistics, and participated in the formation of the UCD Computer Science Department as well. He is a recipient of the campuswide Distinguished Teaching Award and Distinguished Public Service Award at UC Davis.

Dr. Matloff is the author of two published textbooks, and of a number of widely-used Web tutorials on computer topics, such as the Linux operating system and the Python programming language. He and Dr. Peter Salzman are authors of *The Art of Debugging with GDB, DDD, and Eclipse*. Prof. Matloff's book on the R programming language, *The Art of R Programming*, was published in 2011. His book, *Parallel Computation for Data Science*, came out in 2015. His current book project, *From Linear Models to Machine Learning: Predictive Insights through R*, will be published in 2016. He is also the author of several open-source textbooks, including *From Algorithms to Z-Scores: Probabilistic and Statistical Modeling in Computer Science* (`http://heather.cs.ucdavis.edu/probstatbook`), and *Programming on Parallel Machines* (`http://heather.cs.ucdavis.edu/~matloff/ParProcBook.pdf`).

About This Book

Why is this book different from all other parallel programming books? It is aimed more on the practical end of things, in that:

- There is very little theoretical content, such as O() analysis, maximum theoretical speedup, PRAMs, directed acyclic graphs (DAGs) and so on.
- Real code is featured throughout.
- We use the main parallel platforms—OpenMP, CUDA and MPI—rather than languages that at this stage are largely experimental or arcane.
- The running *performance* themes—communications latency, memory/network contention, load balancing and so on—are interleaved throughout the book, discussed in the context of specific platforms or applications.
- Considerable attention is paid to techniques for debugging.

The main programming language used is C/C++, but some of the code is in R, which has become the pre-eminent language for data analysis. As a scripting language, R can be used for rapid prototyping. In our case here, it enables me to write examples which are much less less cluttered than they would be in C/C++, thus easier for students to discern the fundamental parallelixation principles involved. For the same reason, it makes it easier for students to write their own parallel code, focusing on those principles. And R has a rich set of parallel libraries.

It is assumed that the student is reasonably adept in programming, and has math background through linear algebra. An appendix reviews the parts of the latter needed for this book. Another appendix presents an overview of various systems issues that arise, such as process scheduling and virtual memory.

It should be note that most of the code examples in the book are NOT optimized. The primary emphasis is on simplicity and clarity of the techniques and languages used. However, there is plenty of discussion on factors that affect speed, such cache coherency issues, network delays, GPU memory structures and so on.

Here's how to get the code files you'll see in this book: The book is set in LaTeX, and the raw **.tex** files are available in `http://heather.cs.ucdavis.edu/~matloff/158/PLN`. Simply download the relevant file (the file names should be clear), then use a text editor to trim to the program code of interest.

In order to illustrate for students the fact that research and teaching (should) enhance each other, I occasionally will make brief references here to some of my research work.

Like all my open source textbooks, this one is **constantly evolving**. I continue to add new topics, new examples and so on, and of course fix bugs and improve the exposition. For that reason, it is better to link to the latest version, which will always be at `http://heather.cs.ucdavis.edu/~matloff/158/PLN/ParProcBook.pdf`, rather than to copy it.

For that reason, feedback is highly appreciated. I wish to thank Stuart Ambler, Matt Butner, Stuart Hansen, Bill Hsu, Sameer Khan, Mikel McDaniel, Richard Minner, Lars Seeman, Marc Sosnick, and Johan Wikström for their comments. I'm also very grateful to Professor Hsu for his making available to me advanced GPU-equipped machines.

You may also be interested in my open source textbook on probability and statistics, at `http://heather.cs.ucdavis.edu/probstatbook`.

Contents

Chapter 1

Introduction to Parallel Processing

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 Platforms

For parallel computing, one must always keep in mind what hardware and software environments we will be working in. Our hardware platforms here will be multicore, GPU and clusters. For software we will use C/C++, OpenMP, MPI, CUDA and R.

1.1.1 Why R?

Many algorithms are just too complex to understand or express easily in C/C++. So, a scripting language will be very handy, and R has good parallelization features (and is a language I use a lot).

Appendix C presents a quick introduction to R.

1.2 Why Use Parallel Systems?

1.2.1 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 hoping 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.

1.2.2 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.

1.2.3 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.

1.2.4 Our Focus Here

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

1.3 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.

1.3.1 Shared-Memory Systems

1.3.1.1 Basic Architecture

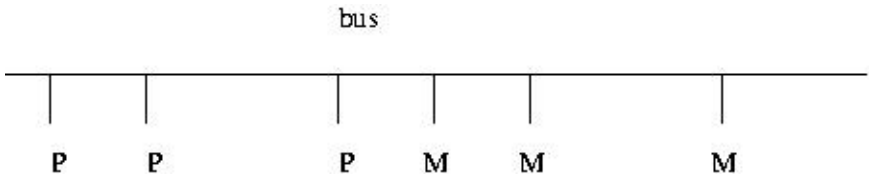
Here many CPUs share the same physical memory. This kind of architecture is sometimes called MIMD, standing for Multiple Instruction (different CPUs are working independently, and thus typically are executing different instructions at any given instant), Multiple Data (different CPUs are generally accessing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

[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.

1.3.1.2 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.

1.3.1.3 Memory Issues Etc.

Consider the SMP figure above.

- 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 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 same 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.

1.3.2 Message-Passing Systems

1.3.2.1 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.

1.3.2.2 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.

1.3.3 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.

1.4 Programmer World Views

1.4.1 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..

1.4.2 Shared-Memory

1.4.2.1 Programmer View

In implementing the matrix-vector multiply example of Section 1.4.1 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

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

and then node 15 were to subsequently execute

```
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.

1.5 Shared Memory Programming

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, 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 A.1 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.

1.5.1 Low-Level Threads Systems: Pthreads

Shared-memory programming is generally done with *threads*. All major OSs offer threads systems, and independent ones have been developed too. One issue, though, is whether one uses threads directly, as with the Pthreads system, or from a higher-level interface such as OpenMP, both of which will be discussed here. Another possibility is to use the threads interface **std::thread** in C++11.

[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.

1.5.1.1 Pthreads Example: Finding Primes

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.

Here is the header file (note the global variables),

```
1  #include <stdio.h>
2  #include <math.h>
3  #include <pthread.h>  // required for threads usage
4
5  #define MAX_N 100000000
6  #define MAX_THREADS 25
7
8  // shared variables
9  int nthreads,  // number of threads (not counting main())
10     n,  // range to check for primeness
11     prime[MAX_N+1],  // in the end, prime[i] = 1 if i prime, else 0
12     nextbase;  // next sieve multiplier to be used
13     // lock for the shared variable nextbase
14     pthread_mutex_t nextbaselock = PTHREAD_MUTEX_INITIALIZER;
15     // ID structs for the threads
16     pthread_t id[MAX_THREADS];
```

and the code:

```
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  // usage:  primesthreads n num_threads
10
11 #include "PrimeThreads.h"
12
13 // "crosses out" all odd multiples of k
14 void crossout(int k)
15 {  int i;
16    for (i = 3; i*k <= n; i += 2)  {
17       prime[i*k] = 0;
18    }
19 }
20
21 // each thread runs this routine
22 void *worker(int tn)  // tn is the thread number (0,1,...)
23 {  int lim,base,
```

```
24          work = 0;  // amount of work done by this thread
25      // no need to check multipliers bigger than sqrt(n)
26      lim = sqrt(n);
27      do  {
28         // get next sieve multiplier, avoiding duplication across threads
29         // lock the lock
30         pthread_mutex_lock(&nextbaselock);
31         base = nextbase;
32         nextbase += 2;
33         // unlock
34         pthread_mutex_unlock(&nextbaselock);
35         if (base <= lim)  {
36            // don't bother crossing out if base known composite
37            if (prime[base])  {
38               crossout(base);
39               work++;  // log work done by this thread
40            }
41         }
42         else return work;
43      } while (1);
44  }
45
46  main(int argc, char **argv)
47  {  int nprimes,  // number of primes found
48          i,work;
49      n = atoi(argv[1]);
50      nthreads = atoi(argv[2]);
51      // mark all even numbers nonprime, and the rest "prime until
52      // shown otherwise"
53      for (i = 3; i <= n; i++)  {
54         if (i%2 == 0) prime[i] = 0;
55         else prime[i] = 1;
56      }
57      nextbase = 3;
58      // get threads started
59      for (i = 0; i < nthreads; i++)  {
60         // this call says create a thread, record its ID in the array
61         // id, and get the thread started executing the function worker(),
62         // passing the argument i to that function
63         pthread_create(&id[i],NULL,worker,i);
64      }
65
66      // wait for all done
67      for (i = 0; i < nthreads; i++)  {
68         // this call says wait until thread number id[i] finishes
69         // execution, and to assign the return value of that thread to our
70         // local variable work here
71         pthread_join(id[i],&work);
72         printf("%d values of base done\n",work);
73      }
```

```
74
75      // report results
76      nprimes = 1;
77      for (i = 3; i <= n; i++)
78         if (prime[i])  {
79            nprimes++;
80         }
81      printf("the number of primes found was %d\n",nprimes);
82
83   }
```

1.5.2 Compiling and Linking

With **gcc**, for instance, we would run

```
gcc -g -o primesthreads PrimesThreads.c -lpthread -lm
```

The reader should be warned that this will produce a number of negative comments from the compiler, as our code above is rather sloppy, not making the proper casts. Argument types in **pthreads** APIs are rather complex, and for readabiiity we have omitted the casts.

1.5.3 The Notion of a "Critical Section"

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 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

```
pthread_mutex_lock(&nextbaselock);
base = nextbase
nextbase += 2
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

```
base = nextbase;
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 a **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:

```
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.

1.5.4 Role of the OS

Let's again ponder the role of the OS here.

The threads are processes, just like any process except that they share memory by default. Thus they are managed by the OS. Now consider the code from above,

```
pthread_create(&id[i],NULL,worker,i);
```

This does create the thread, in the sense that a stack is allocated for it in memory and an entry is added to the OS' process table for the thread. But **that doesn't mean the thread is now actually runnin**

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()**.

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 unblocked.

Finally, keep in mind that although the global 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.

1.5.5 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.

```
(gdb) r 100 2
Starting program: /debug/primes 100 2
[New Thread 16384 (LWP 28653)]
[New Thread 32769 (LWP 28676)]
[New Thread 16386 (LWP 28677)]
[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.

1.6 A Note on Global Variables

Note the global variables in the above code:

```
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

[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.

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.

1.6.1 Higher-Level Threads Programming: OpenMP

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.

1.6.1.1 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;
```

[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.

```
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.

1.6.1.2 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 1.6.1.1.

(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.

```
int *counts;
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 their values upon exit from a parallel block etc., but the workaround does work.

1.6.2 Message Passing

1.6.2.1 Programmer View

Again consider the matrix-vector multiply example of Section 1.4.1. In contrast to the shared-memory case, in the message-passing paradigm all nodes would have separate copies of A, X and Y. Our example in Section 1.4.2.1 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.

1.6.2.2 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.

The program is self-documenting, via the comments.

```
1  /* MPI sample program; NOT INTENDED TO BE EFFICIENT as a prime
2     finder, either in algorithm or implementation
3
4     MPI (Message Passing Interface) is a popular package using
5     the "message passing" paradigm for communicating between
6     processors in parallel applications; as the name implies,
```

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

```
7     processors communicate by passing messages using "send" and
8     "receive" functions
9
10    finds and reports the number of primes less than or equal to N
11
12    uses a pipeline approach:  node 0 looks at all the odd numbers (i.e.
13    has already done filtering out of multiples of 2) and filters out
14    those that are multiples of 3, passing the rest to node 1; node 1
15    filters out the multiples of 5, passing the rest to node 2; node 2
16    then removes the multiples of 7, and so on; the last node must check
17    whatever is left
18
19    note that we should NOT have a node run through all numbers
20    before passing them on to the next node, since we would then
21    have no parallelism at all; on the other hand, passing on just
22    one number at a time isn't efficient either, due to the high
23    overhead of sending a message if it is a network (tens of
24    microseconds until the first bit reaches the wire, due to
25    software delay); thus efficiency would be greatly improved if
26    each node saved up a chunk of numbers before passing them to
27    the next node */
28
29  #include <mpi.h>  // mandatory
30
31  #define PIPE_MSG 0  // type of message containing a number to be checked
32  #define END_MSG 1  // type of message indicating no more data will be coming
33
34  int NNodes,  // number of nodes in computation
35      N,  // find all primes from 2 to N
36      Me;  // my node number
37  double T1,T2;  // start and finish times
38
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.

1.6.3 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 1.6.2.1 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 1.6.3.1) for the R language is also a scatter/gather operation.

1.6.3.1 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. 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:

```
> library(parallel)
> c2 <- makePSOCKcluster(rep("localhost",2))
> c2
socket cluster with 2 nodes on host  localhost
> mmul
function(cls,u,v) {
   rowgrps <- splitIndices(nrow(u),length(cls))
   grpmul <- function(grp) u[grp,] %*% v
   mout <- clusterApply(cls,rowgrps,grpmul)
   Reduce(c,mout)
}
> a <- matrix(sample(1:50,16,replace=T),ncol=2)
> a
      [,1] [,2]
[1,]   34   41
[2,]   10   28
[3,]   44   23
[4,]    7   29
[5,]    6   24
[6,]   28   29
[7,]   21    1
[8,]   38   30
> b <- c(5,-2)
> b
[1]  5 -2
> a %*% b  # serial multiply
      [,1]
[1,]   88
[2,]   -6
[3,]  174
[4,]  -23
[5,]  -18
[6,]   82
[7,]  103
[8,]  130
> clusterExport(c2,"b")  # send b to workers
> clusterEvalQ(c2,b)  # check that they have it
[[1]]
```

```
39  [1]   5 -2
40
41  [[2]]
42  [1]   5 -2
43
44  > mmul(c2,a,b)  # test our parallel code
45  [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; those R processes may be running on different machines (i.e. a real cluster), or on a multicore machine, or a combination of the two.

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.

```
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:

```
> 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 1.4.1, 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.

```
> splitIndices(12,5)
[[1]]
[1] 1 2 3

[[2]]
[1] 4 5

[[3]]
[1] 6 7

[[4]]
[1] 8 9

[[5]]
[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

```
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 (or a vector, which is promotable to a lists), 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:

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

```
7 }
```

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
[3,]  185
[4,]  113
[5,]   32
[6,]  -50
[7,]  119
[8,]  210
> mmul1(c2,a,b)
[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,

By the way, the function **clusterApply()** has an optional third argument, used to form the actual parameter if the function to be applied has two parameters, e.g.

```
> library(parallel)
> c2 <- makeCluster(2)
> f <- function(x,y) x + y
> clusterApply(c2,list(5,12),f,8)
[[1]]
[1] 13

[[2]]
[1] 20
```

A fourth argument can be added if the function has three arguments, and so on.

1.7 Threads Programming in R: Rdsm

As noted, R features the **parallel** package, composed of its old **snow** and **multicore** packages. The former uses message-passing, while the latter involves a weak version of shared-memory access. For those who prefer a general shared-memory interface, there is Rdsm.

R itself is not threaded. However, Rdsm achieves a quasi-thread interface, involving several invocations of R that act as "rtheads," in that (a) the "threads" do operate independently of each other and (b) they genuinely share memory.

This is achieved via operator overloading. All operators in R are actually functions, e.g.

```
> 1+1
[1] 2
> "+"(1,1)
[1] 2
```

including the [operator for array access. What Rdsm does is redefine that operator to access a location in shared memory.

Rdsm is built on top of the packages **snow** and **bigmemory**; the former atter is used for APIs, and for the distribution of shared-memory keys that address memory locations managed by the latter.

1.7.1 Example: Matrix Multiplication

```
# matrix multiplication; the product u %*% v is
# computed on the snow cluster cls, and written
# in-place in w; w is a big.matrix object

mmulthread <- function(u,v,w) {
   require(parallel)
   # determine which rows this thread will handle
   myidxs <-
      splitIndices(nrow(u),
         myinfo$nwrkrs)[[myinfo$id]]
   # compute this thread's portion of the product
   w[myidxs,] <- u[myidxs,] %*% v[,]
   0  # don't do expensive return of result
}

# test on snow cluster cls
test <- function(cls) {
   # init Rdsm
   mgrinit(cls)
   # set up shared variables a,b,c,
```

```
    mgrmakevar(cls,"a",6,2)
    mgrmakevar(cls,"b",2,6)
    mgrmakevar(cls,"c",6,6)
    # fill in some test data
    a[,] <- 1:12
    b[,] <- rep(1,12)
    # give the threads the function to be run
    clusterExport(cls,"mmulthread")
    # run it
    clusterEvalQ(cls,mmulthread(a,b,c))
    print(c[,])  # not print(c)!
}

> library(parallel)
> c2 <- makeCluster(2)  # 2 threads
> test(c2)
     [,1] [,2] [,3] [,4] [,5] [,6]
[1,]    8    8    8    8    8    8
[2,]   10   10   10   10   10   10
[3,]   12   12   12   12   12   12
[4,]   14   14   14   14   14   14
[5,]   16   16   16   16   16   16
[6,]   18   18   18   18   18   18
```

1.7.2 Example: Maximal Burst in a Time Series

Consider a time series of length n. We may be interested in bursts, periods in which a high average value is sustained. We might stipulate that we look only at periods of length k consecutive points, for a user-specified k. So, we wish to find the period of length k that has the maximal mean value.

Once again, let's leverage the power of R. The **zoo** time series package includes a function **rollmean(w,m)**, which returns all the means of blocks of length k, i.e., what are usually called *moving averages*—just what we need.

Here is the code:

```
# Rdsm code to find max burst in a time series;

# arguments:

#    x:  data vector
#    k:  block size
#    mas:  scratch space, shared, 1 x (length(x)-1)
#    rslts:  2-tuple showing the maximum burst value,
#            and where it starts; shared, 1 x 2

maxburst <- function(x,k,mas,rslts) {
   require(Rdsm)
   require(zoo)
```

```
    # determine this thread's chunk of x
    n <- length(x)
    myidxs <- getidxs(n-k+1)
    myfirst <- myidxs[1]
    mylast <- myidxs[length(myidxs)]
    mas[1,myfirst:mylast] <-
       rollmean(x[myfirst:(mylast+k-1)],k)
    # make sure all threads have written to mas
    barr()
    # one thread must do wrapup, say thread 1
    if (myinfo$id == 1) {
       rslts[1,1] <- which.max(mas[,])
       rslts[1,2] <- mas[1,rslts[1,1]]
    }
}

test <- function(cls) {
    require(Rdsm)
    mgrinit(cls)
    mgrmakevar(cls,"mas",1,9)
    mgrmakevar(cls,"rslts",1,2)
    x <<- c(5,7,6,20,4,14,11,12,15,17)
    clusterExport(cls,"maxburst")
    clusterExport(cls,"x")
    clusterEvalQ(cls,maxburst(x,2,mas,rslts))
    print(rslts[,])  # not print(rslts)!
}
```

Chapter 2

Recurring Performance Issues

Oh no! It's actually slower in parallel!—almost everyone's exclamation the first time they try to parallelize code

The available parallel hardware systems sound wonderful at first. But everyone who uses such systems has had the experience of enthusiastically writing his/her first parallel program, anticipating great speedups, only to find that the parallel code actually runs more slowly than the original nonparallel program.

In this chapter, we highlight some major issues that will pop up throughout the book.

2.1 Communication Bottlenecks

Whether you are on a shared-memory, message-passing or other platform, communication is always a potential bottleneck:

- On a shared-memory system, the threads must contend with each other in communicating with memory. And the problem is exacerbated by cache coherency transactions (Section 3.5.1.
- On a cluster, even a very fast network is very slow compared to CPU speeds.
- GPUs are really fast, but their communication with their CPU hosts is slow. There are also memory contention issues as in ordinary shared-memory systems.

Among other things, communication considerations largely drive the load balancing issue, discussed next.

2.2 Load Balancing

Arguably the most central performance issue is **load balancing,** i.e. keeping all the processors busy as much as possible. This issue arises constantly in any discussion of parallel processing.

A nice, easily understandable example is shown in Chapter 7 of the book, *Multicore Application Programming: for Windows, Linux and Oracle Solaris*, Darryl Gove, 2011, Addison-Wesley. There the author shows code to compute the **Mandelbrot set**, defined as follows.

Start with any number c in the complex plane, and initialize z to 0. Then keep applying the transformation

$$z \leftarrow z^2 + c \tag{2.1}$$

If the resulting sequence remains bounded (say after a certain number of iterations), we say that c belongs to the Mandelbrot set.

Gove has a rectangular grid of points in the plane, and wants to determine whether each point is in the set or not; a simple but time-consuming computation is used for this determination.[1]

Gove sets up two threads, one handling all the points in the left half of the grid and the other handling the right half. He finds that the latter thread is very often idle, while the former thread is usually busy—extremely poor **load balance**. We'll return to this issue in Section 2.4.

2.3 "Embarrassingly Parallel" Applications

The term **embarrassingly parallel** is heard often in talk about parallel programming.

2.3.1 What People Mean by "Embarrassingly Parallel"

Consider a matrix multiplication application, for instance, in which we compute AX for a matrix A and a vector X. One way to parallelize this problem would be to have each processor handle a group of rows of A, multiplying each by X in parallel with the other processors, which are handling other groups of rows. We call the problem embarrassingly parallel, with the word "embarrassing" meaning that the problem is too easy, i.e. there is no intellectual challenge involved. It is pretty obvious that the computation Y = AX can be parallelized very easily by splitting the rows of A into groups.

[1] You can download Gove's code from `http://blogs.sun.com/d/resource/map_src.tar.bz2`. Most relevant is **listing7.64.c**.

By contrast, most parallel sorting algorithms require a great deal of interaction. For instance, consider Mergesort. It breaks the vector to be sorted into two (or more) independent parts, say the left half and right half, which are then sorted in parallel by two processes. So far, this is embarrassingly parallel, at least after the vector is broken in half. But then the two sorted halves must be merged to produce the sorted version of the original vector, and that process is *not* embarrassingly parallel; it can be parallelized, but in a more complex, less obvious manner.

Of course, it's no shame to have an embarrassingly parallel problem! On the contrary, except for showoff academics, having an embarrassingly parallel application is a cause for celebration, as it is easy to program.

In recent years, the term **embarrassingly parallel** has drifted to a somewhat different meaning. Algorithms that are embarrassingly parallel in the above sense of simplicity tend to have very low communication between processes, key to good performance. That latter trait is the center of attention nowadays, so the term **embarrassingly parallel** generally refers to an algorithm with low communication needs.

For that reason, many people would NOT considered even our prime finder example in Section 1.5.1 to be embarrassingly parallel. Yes, it was embarrassingly easy to write, but it has high communication costs, as both its locks and its global array are accessed quite often.

On the other hand, the Mandelbrot computation described in Section 2.2 is truly embarrassingly parallel, in both the old and new sense of the term. There the author Gove just assigned the points on the left to one thread and the rest to the other thread—very simple—and there was no communication between them.

2.3.2 Iterative Algorithms

Many parallel algorithms involve iteration, with a rendezvous of the tasks after each iteration. Within each iteration, the nodes act entirely independently of each other, which makes the problem seem embarrassingly parallel.

But unless the granularity of the problem is coarse, i.e. there is a large amount of work to do in each iteration, the communication overhead will be significant, and the algorithm may not be considered embarrassingly parallel.

2.4 Static (But Possibly Random) Task Assignment Typically Better Than Dynamic

Say an algorithm generates t independent[2] tasks and we have p processors to handle them. In our matrix-times-vector example of Section 1.4.1, say, each row of the matrix might be considered one task. A processor's work would then be to multiply the vector by this processor's assigned rows of the matrix.

How do we decide which tasks should be done by which processors? In **static** assignment, our code would decide at the outset which processors will handle which tasks. The alternative, **dynamic** assignment, would have processors determine their tasks as the computation proceeds.

In the matrix-times-vector example, say we have 10000 rows and 10 processors. In static task assignment, we could pre-assign processor 0 rows 0-999, processor 1 rows 1000-1999 and so on. On the other hand, we could set up a **task farm**, a queue consisting here of the numbers 0-9999. Each time a processor finished handling one row, it would remove the number at the head of the queue, and then process the row with that index.

It would at first seem that dynamic assignment is more efficient, as it is more flexible. However, accessing the task farm, for instance, entails communication costs, which might be very heavy. In this section, we will show that it's typically better to use the static approach, though possibly randomized.[3]

2.4.1 Example: Matrix-Vector Multiply

Consider again the problem of multiplying a vector X by a large matrix A, yielding a vector Y. Say A has 10000 rows and we have 10 threads. Let's look at little closer at the static/dynamic tradeoff outlined above. For concreteness, assume the shared-memory setting.

There are several possibilities here:

- **Method A:** We could simply divide the 10000 rows into chunks of 10000/10 = 1000, and parcel them out to the threads. We would pre-assign thread 0 to work on rows 0-999 of A, thread 1 to work on rows 1000-1999 and so on.

  This is essentially OpenMP's **static** scheduling policy, with default chunk size.[4]

  There would be no communication between the threads this way, but there could be a problem of load imbalance. Say for instance that by chance thread 3 finishes well before the others.

[2] Note the qualifying term.

[3] This is still static, as the randomization is done at the outset, before starting computation.

[4] See Section 4.3.3.

Then it will be idle, as all the work had been pre-allocated.

- **Method B:**

  OpenMP's **dynamic** policy does what the name implies, which can be described as follows (in non-OpenMP terms):

  We would have a shared variable named,say, **nextchunk** similar to **nextbase** in our prime-finding program in Section 1.5.1. Each time a thread would finish a chunk, it would obtain a new chunk to work on, by recording the value of **nextchunk** and incrementing that variable by 1 (all atomically, of course).

  This approach would have better load balance, because the first thread to find there is no work left to do would be idle for at most 100 rows' amount of computation time, rather than 1000 as above. Meanwhile, though, communication would increase, as access to the locks around **nextchunk** would often make one thread wait for another.[5]

- **Method C:** So, Method A above minimizes communication at the possible expense of load balance, while the Method B does the opposite. OpenMP also offers the **guided** policy, which is like **dynamic** except the chunk size decreases over time. In the earlier part of a run, the large chunk size reduces communication, while later the small chunk size avoid load imbalance.

I will now show that in typical settings, the Method A above (or a slight modification) works well. To this end, consider a chunk consisting of m tasks, such as m rows in our matrix example above, with times $T_1, T_2, ..., T_m$. The total time needed to process the chunk is then $T_1 + ..., T_m$.

The T_i can be considered random variables; some tasks take a long time to perform, some take a short time, and so on. As an idealized model, let's treat them as independent and identically distributed random variables. Under that assumption (if you don't have the probability background, follow as best you can), we have that the mean (**expected value**) and variance of total task time are

$$E(T_1 + ..., T_m) = mE(T_1)$$

and

$$Var(T_1 + ..., T_m) = mVar(T_1)$$

[5]Why are we calling it "communication" here? Recall that in shared-memory programming, the threads communicate through shared variables. When one thread increments **nextchunk**, it "communicates" that new value to the other threads by placing it in shared memory where they will see it, and as noted earlier contention among threads to shared memory is a major source of potential slowdown.

Thus

$$\frac{\text{standard deviation of chunk time}}{\text{mean of chunk time}} \sim O\left(\frac{1}{\sqrt{m}}\right)$$

In other words:

- run time for a chunk is essentially constant if m is large, and
- there is essentially no load imbalance in Method A

Since load imbalance was the only drawback to Method A and we now see it's not a problem after all, then Method A is best.

For more details and timing examples, see N. Matloff, "Efficient Parallel R Loops on Long-Latency Platforms," *Proceedings of the 42nd Interface between Statistics and Computer Science*, Rice University, June 2012.[6]

2.4.2 Load Balance, Revisited

But what about the assumptions behind that reasoning? Consider for example the Mandelbrot problem in Section 2.2. There were two threads, thus two chunks, with the tasks for a given chunk being computations for all the points in the chunk's assigned region of the picture.

Gove noted there was fairly strong load imbalance here, and that the *reason* was that most of the Mandelbrot points turned out to be in the left half of the picture! The computation for a given point is iterative, and if a point is not in the set, it tends to take only a few iterations to discover this. That's why the thread handling the right half of the picture was idle so often.

So Method A would not work well here, and upon reflection one can see that the problem was that the tasks within a chunk were not independent, but were instead highly correlated, thus violating our mathematical assumptions above. Of course, before doing the computation, Gove didn't know that it would turn out that most of the set would be in the left half of the picture. But, one could certainly anticipate the correlated nature of the points; if one point is not in the Mandelbrot set, its near neighbors are probably not in it either.

But Method A can still be made to work well, via a simple modification: Simply form the chunks randomly. In the matrix-multiply example above, with 10000 rows and chunk size 1000, do NOT

[6] As noted in the Preface to this book, I occasionally refer here to my research, to illustrate for students the beneficial interaction between teaching and research.

assign the chunks contiguously. Instead, generate a random permutation of the numbers 0,1,...,9999, naming them $i_0, i_1, ..., i_{9999}$. Then assign thread 0 rows $i_0 - i_{999}$, thread 1 rows $i_{1000} - i_{1999}$, etc.

In the Mandelbrot example, we could randomly assign rows of the picture, in the same way, and avoid load imbalance.

So, actually, Method A, or let's call it Method A', will still typically work well.

2.4.3 Example: Mutual Web Outlinks

Here's an example that we'll use at various points in this book:

> **Mutual outlinks in a graph:**
>
> 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. Say we want to find the number of mutual outlinks, averaged over all pairs of Web sites.
>
> Let A be the **adjacency matrix** of the graph. Then the mean of interest would be found as follows:

```
1  sum = 0
2  for i = 0...n-2
3      for j = i+1...n-1
4          count = 0
5          for k = 0...n-1 count += a[i][k] * a[j][k]
6  mean = sum / (n*(n-1)/2)
```

> Say again n = 10000 and we have 10 threads. We should not simply assign work to the threads by dividing up the i loop, with thread 0 taking the cases i = 0,...,999, thread 1 the cases 1000,...,1999 and so on. This would give us a real load balance problem. Thread 8 would have much less work to do than thread 3, say.
>
> We could randomize as discussed earlier, but there is a much better solution: Just pair the rows of A. Thread 0 would handle rows 0,...,499 and 9500,...,9999, thread 1 would handle rows 500,999 and 9000,...,9499 etc. This approach is taken in our OpenMP implementation, Section 4.12.
>
> In other words, Method A still works well.

In the mutual outlinks problem, we have a good idea beforehand as to how much time each task needs, but this may not be true in general. An alternative would be to do *random* pre-assignment of tasks to processors.

On the other hand, if we know beforehand that all of the tasks should take about the same time, we should use static scheduling, as it might yield better cache and virtual memory performance.

2.4.4 Work Stealing

There is another variation to Method A that is of interest today, called **work stealing**. Here a thread that finishes its assigned work and has thus no work left to do will "raid" the work queue of some other thread. This is the approach taken, for example, by the elegant Cilk language. Needless to say, accessing the other work queue is going to be expensive in terms of time and memory contention overhead.

2.4.5 Timing Example

I ran the Mandelbrot example on a shared memory machine with four cores, two threads per core, with the following results for eight threads, on an 8000x8000 grid:

policy	time
static	47.8
dynamic	21.4
guided	29.6
random	15.7

Default values were used for chunk size in the first three cases. I did try other chunk sizes for the **dynamic** policy, but it didn't make much difference. See Section 4.4 for the code.

Needless to say, one shouldn't overly extrapolate from the above timings, but it does illustrate the issues.

2.4.6 Example: Extracting a Submatrix

OpenMP implements the various scheduling algorithms via its **for** pragma, e.g.

```
#pragma omp for schedule(guided)
```

We'll cover this in more detail in Chapter 4, but here is an example of the default, static scheduling with chunk size 1.

```
// creates a new matrix from a group of {\bf nColsSubM}
// consecutive columns of an old one, starting at column
// firstCol} of the old matrix
```

```
#include<omp.h>
#include<stdio.h>
#include<stdlib.h>
#include<string.h>

int onedim(int row, int col, int nCols) { return row * nCols + col; }

int *getCols(int *m, int nRowsM, int nColsM, int firstCol, int nColsSubM) {
   int *subMat;
   #pragma omp parallel
   {  int *startFrom,*startTo;

      #pragma omp single
      subMat = malloc(nRowsM * nColsSubM * sizeof(int));

      #pragma omp for
      for (int row = 0; row < nRowsM; row++) {
         startFrom = m + onedim(row,firstCol,nColsM);
         startTo = subMat + onedim(row,0,nColsSubM);
         memcpy(startTo, startFrom, nColsSubM * sizeof(int));
      }
   }
   return subMat;
}

int main() {
   // intended as a 4x3 matrix
   int z[12] = {5,12,13,6,2,22,15,3,1,2,3,4};
   omp_set_num_threads(2);
   // extract the last 2 cols; should be
   // 12 13
   // 2 22
   // 3 1
   // 3 4
   int *outM = getCols(z,4,3,1,2);
   for (int i = 0; i < 4; i++) {
      printf("%d %d\n",outM[2*i],outM[2*i+1]);
   }
}
```

2.5 Latency and Bandwidth

We've been speaking of communications delays so far as being monolithic, but they are actually (at least) two-dimensional. The key measures are **latency** and **bandwidth**:

- Latency is the time it takes for one bit to travel for source to destination, e.g. from a CPU

to memory in a shared memory system, or from one computer to another in a cluster.

- Bandwidth is the number of bits per unit time that can be input into the communications channel. This can be affected by factors such as bus width in a shared memory system and number of parallel network paths in a message passing system, and also by the speed of the links.

It's helpful to think of a bridge, with toll booths at its entrance. Latency is the time needed for one car to get from one end of the bridge to the other. Bandwidth is the number of cars that can enter the bridge per unit time. We can reduce latency by increasing the speed limit, and can increase bandwidth by improving the speed by which toll takers can collect tolls, and increasing the number of toll booths.

Latency hiding:

One way of dealing with long latencies is known as **latency hiding**. The idea is to do a long-latency operation in parallel with something else.

For example, GPUs tend to have very long memory access times, but this is solved by having many pending memory accesses at the same time. During the latency of some accesses, earlier ones that have now completed can now be acted upon (Section 5.4.3.2).

2.6 Relative Merits: Performance of Shared-Memory Vs. Message-Passing

My own preference is shared-memory, but there are pros and cons to each paradigm.

It is generally believed in the parallel processing community that the shared-memory paradigm produces code that is easier to write, debug and maintain than message-passing. See for instance R. Chandra, *Parallel Programming in OpenMP*, MKP, 2001, pp.10ff (especially Table 1.1), and M. Hess *et al*, Experiences Using OpenMP Based on Compiler Directive Software DSM on a PC Cluster, in *OpenMP Shared Memory Parallel Programming: International Workshop on OpenMP Applications and Tools*, Michael Voss (ed.), Springer, 2003, p.216.

On the other hand, in some cases message-passing can produce faster code. Consider the Odd/Even Transposition Sort algorithm, for instance. Here pairs of processes repeatedly swap sorted arrays with each other. In a shared-memory setting, this might produce a bottleneck at the shared memory, slowing down the code. Of course, the obvious solution is that if you are using a shared-memory machine, you should just choose some other sorting algorithm, one tailored to the shared-memory setting.

There used to be a belief that message-passing was more **scalable**, i.e. amenable to very large

systems. However, GPU has demonstrated that one can achieve extremely good scalability with shared-memory.

As will be seen, though, GPU is hardly a panacea. Where, then, are people to get access to large-scale parallel systems? Most people do not (currently) have access to large-scale multicore machines, while most do have access to large-scale message-passing machines, say in cloud computing venues. Thus message-passing plays a role even for those of us who preferred the shared-memory paradigm.

Also, hybrid systems are common, in which a number of shared-memory systems are tied together by, say, MPI.

2.7 Memory Allocation Issues

Many algorithms require large amounts of memory for intermediate storage of data. It may be prohibitive to allocate this memory statically, i.e. at compile time. Yet dynamic allocation, say via **malloc()** or C++'s **new** (which probably produces a call to **malloc() anyway**, is very expensive in time.

Using large amounts of memory also can be a major source of overhead due to cache misses and page faults.

One way to avoid **malloc()**, of course, is to set up static arrays whenever possible.

There are no magic solutions here. One must simply be aware of the problem, and tweak one's code accordingly, say by adjusting calls to **malloc()** so that one achieves a balance between allocating too much memory and making too many calls.

2.8 Issues Particular to Shared-Memory Systems

This topic is covered in detail in Chapter 3, but is so important that the main points should be mentioned here.

- Memory is typically divided into **banks**. If more than one thread attempts to access the same bank at the same time, that effectively serializes the program.
- There is typically a cache at each processor. Keeping the contents of these caches consistent with each other, and with the memory itself, adds a lot of overhead, causing slowdown.

In both cases, awareness of these issues should impact how you write your code.

See Sections 3.2 and 3.5.

Chapter 3

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 A.3.1.

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

```
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 same 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 += localsum  // critical section
```

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 += localsum
```

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.

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

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.

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:

```
1 struct {
2    char name[25];
3    float salary;
4    float yrs;
5 } 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:

```
1 struct {
2    char name[100];
3    float salary[100];
4    float yrs[100];
5 }
```

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.

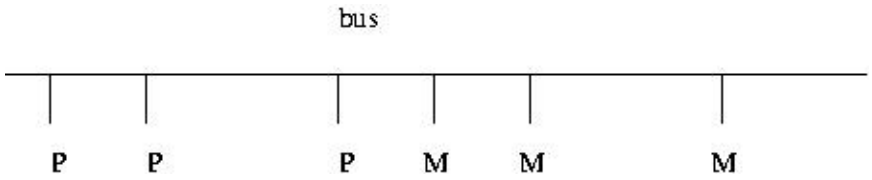
```
1
2 // routines to initialize, read and write
3 // padded versions of a matrix of floats;
4 // the matrix is nominally mxn, but its
5 // rows will be padded on the right ends,
6 // so as to enable a stride of s down each
7 // column; it is assumed that s >= n
```

```
 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:



Here and below:

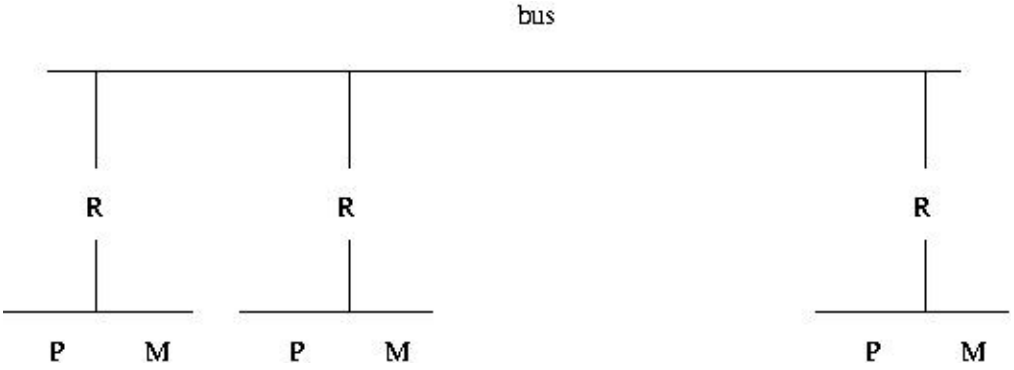
- The Ps are processors, e.g. off-the-shelf chips such as Pentiums.
- The Ms are **memory modules**. These are physically separate objects, e.g. separate boards of memory chips. It is typical that there will be the same number of Ms as Ps.
- To make sure only one P uses the bus at a time, standard bus 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:



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.)

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

[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.

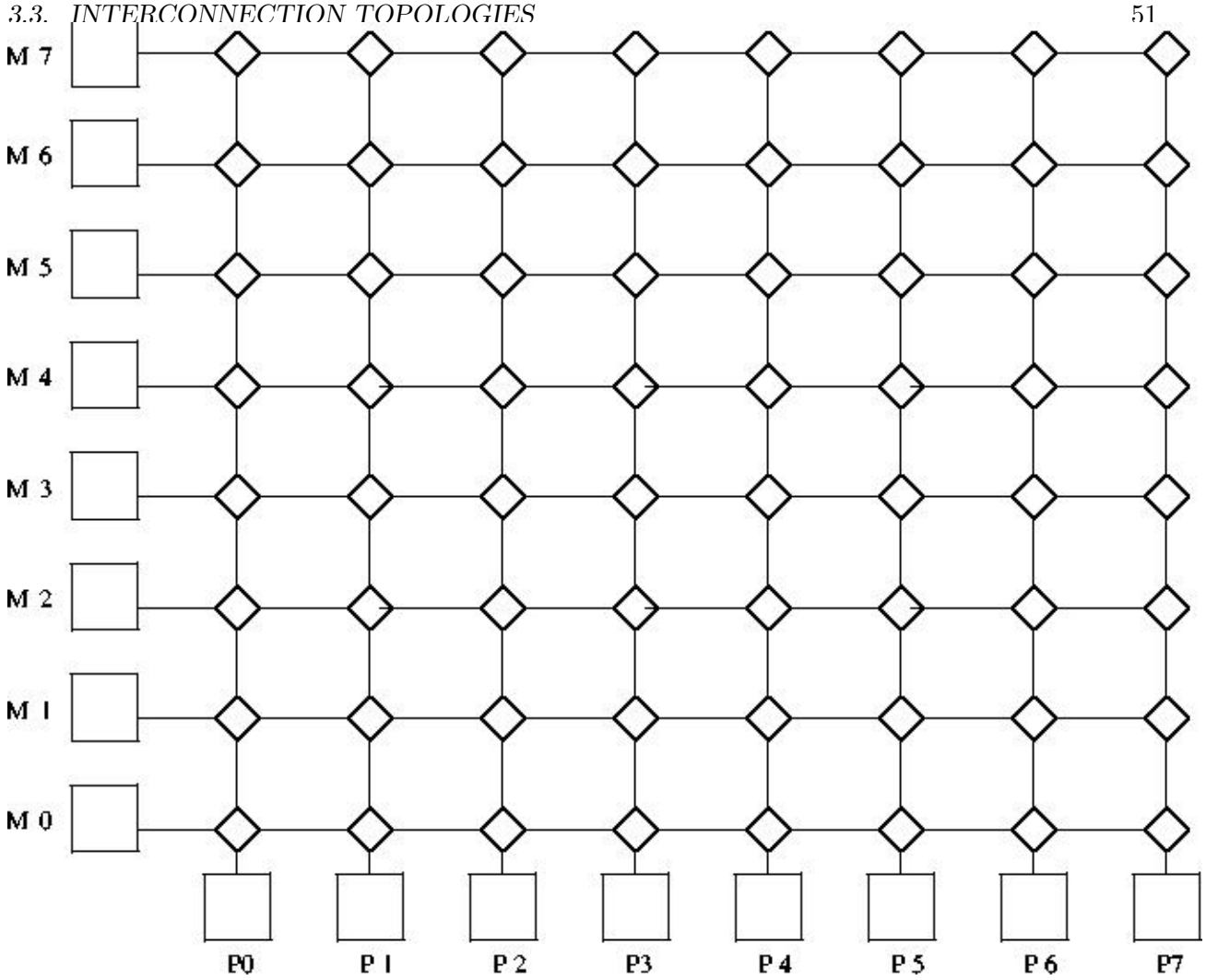
of the memory hardware structure, i.e. the interleaving.

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.

3.3.3.1 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.

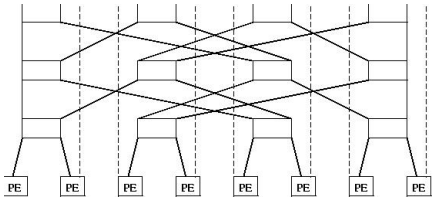
There could also be a return network of the same type, with this one being memory → processor, to return the result of the read requests.[3]

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.

3.3.3.2 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

[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.

its right-hand 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

[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.

figure 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 not 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 same 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:

```
copy L to R
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:

```
TRY:  TAS R,L
      JNZ TRY
  C:  ...   ; start of critical section
      ...
      ...   ; end of critical section
      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.

3.4.1.1 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,

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

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 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 instance, say we are maintaining some global count, **total**. Instead of

```
pthread_mutex_lock(&totlock);
total ++;
pthread_mutex_unlock(&totlock);
```

we could do

```
lock inc total
```

without software locks!

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

```
    movl $lockvar, %ebx  # copy the address of lockvar to EBX
    movl $1, %ecx
top:
    movl $0, %eax
    lock cmpxchg (%ebx), %ecx
    jz top  # else leave the loop and enter the critical section
```

The operation CMPXCHG ("compare and exchange") has EAX as an unnamed operand. The instruction basically does (here *source* is ECX, *destination* is **lockvar**, and *c()* means "contents of")

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

The LOCK prefix locks the bus for the entire duration of the instruction. Note that the ADD instruction involves two memory transactions. Consider

```
lock addl $3, x
```

which adds 3 to the memory location named **x**. There is one bus transaction needed to read the old value of **x**, and a second one to write the new, incremented value back to **x**. 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 compared to using software locks.

3.4.1.2 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

```
LOCK(K);
Y = ++X
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.

And even better, we could allow other increments than 1.

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

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

The C code above would compile to, say,

```
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

```
X++;
```

operation (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.

But the key is that this is all done in an atomic manner.

3.5 Cache Issues

If you need a review of cache memories or don't have background in that area at all, read Section A.2.1 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?

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

The answer of course is that eventually L will 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 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 other 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

[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.

1, P6 also sends an invalidate signal to all the other caches. So, when P5 tries its execution of the TAS again, it 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

```
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.)

On the other hand, if **Sum** is the *only* word in the block that we access here, when the cache block is finally sent to other caches, the entire block must be sent under the invalidate, say 512 bytes. If we perform the above summation operation fewer than 512/8 times, the update protocol will do less global memory writing, thus tying up the bus less.

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 positive feature in terms of cache coherency, because it makes broadcast 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.

[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.

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 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 not 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:

[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.

present state	event	newstate
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.

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.

That's a hardware example. On the software level, compilers typically will store a program variable x in a register rather than in the memory location the compiler has chosen for that variable. Register access is fast, so this makes sense, but the compiler must produce code so that eventually the value of x is written to memory, so that other processors can use it.

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 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

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

[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.

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.

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

3.11.1 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

```
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

```
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 A.2.2 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**:

```
int Y,*P;
...
...
P = &Y;
...
```

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.

Similarly, each SDSM system must decide between sequential consistency, release consistency etc.

[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.

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.

3.11.2 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
11 // pointer to shared variable
12 float *x;  // array to be sorted
```

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

```
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 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.

[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.

[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.

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.

3.12 Barrier Implementation

Recall that a **barrier** is program code[26] 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, e.g. **pthread_barrier_wait()**. 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.

[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.

[26] 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.

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 (which is the main place barriers are used). 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         pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
5  } ;
6
7  Barrier(struct BarrStruct *PB)
8  {  pthread_mutex_lock(&PB->Lock);
9     PB->Count++;
10    pthread_mutex_unlock(&PB->Lock);
11    while (PB->Count < PB->NNodes) ;
12 }
```

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.

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:

```
1  struct BarrStruct {
2     int NNodes, // number of threads participating in the barrier
3         Count[2], // number of threads that have hit the barrier so far
4         pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
5  } ;
6
7  Barrier(struct BarrStruct *PB)
8  {  int Par,OldCount;
9     Par = PB->EvenOdd;
10    pthread_mutex_lock(&PB->Lock);
11    OldCount = PB->Count[Par]++;
12    if (OldCount == PB->NNodes-1)  {
13       PB->Count[Par] = 0;
14       PB->EvenOdd = 1 - Par;
15       pthread_mutex_unlock(&PB->Lock);
16    }
17    else {
18       pthread_mutex_unlock(&PB->Lock);
19       while (PB->Count[Par] > 0) ;
20    }
21 }
```

3.12.4 Refinements

3.12.4.1 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:

```
1  struct BarrStruct {
2     int NNodes, // number of threads participating in the barrier
3         Count[2], // number of threads that have hit the barrier so far
4         pthread_mutex_t Lock = PTHREAD_MUTEX_INITIALIZER;
5         pthread_cond_t CV = PTHREAD_COND_INITIALIZER;
6  } ;
7
8  Barrier(struct BarrStruct *PB)
9  {  int Par,I;
10    Par = PB->EvenOdd;
11    pthread_mutex_lock(&PB->Lock);
12    PB->Count[Par]++;
13    if (PB->Count < PB->NNodes)
14       pthread_cond_wait(&PB->CV,&PB->Lock);
15    else  {
16       PB->Count[Par] = 0;
17       PB->EvenOdd = 1 - Par;
18       for (I = 0; I < PB->NNodes-1; I++)
19          pthread_cond_signal(&PB->CV);
20    }
21    pthread_mutex_unlock(&PB->Lock);
22 }
```

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.

3.12.4.2 Parallelizing the Barrier Operation

3.12.4.2.1 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 i^{th} level (starting with the root as level 0) with consist of 2^i parallel barriers, each one representing $n/2^i$ threads.

3.12.4.2.2 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 **ReachedBarrier**. 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 k^{th} 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.

Chapter 4

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

```
#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 from 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

```
   // parallel
   dowork();
   // 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

```
void dowork()
{
   #pragma omp parallel
   {  int startv,endv,  // start, end vertices for this thread
          step,  // whole procedure goes nv steps
          mymv,  // vertex which attains that value
          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:

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

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

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

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

4.2.3 Scope Issues

Note carefully that in

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

[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.

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,

```
#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.:

```
#pragma omp single
{  nth = omp_get_num_threads();
   if (nv % nth != 0) {
      printf("nv must be divisible by nth\n");
      exit(1);
   }
   chunk = nv/nth;
   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.

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

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.

```
#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.

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

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:

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

```
    }
}
```

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.

```
#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.

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

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

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

Here **static** is still a keyword but **chunk**, specifying the chunk size, 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**, e.g.

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

As discussed in Section 2.4, 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 2.4, I showed that these would seldom be necessary or desirable; having each thread handle a single chunk would be best.

See Section 2.4 for a timing example.

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.

```
1 #include <omp.h>
2
3 // translate from 2-D to 1-D indices
4 int onedim(int n,int i,int j) {  return n * i + j;  }
5
```

```
 6  void transp(int *m, int n)
 7  {
 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

```
int z,myz=0;
...
#pragma omp for private(myz)
for (i = 0; i < n; i++)  myz += x[i];
#pragma omp critical
{ 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.

4.4 Example: Mandelbrot Set

Here's the code for the timings in Section 2.4.5:

```
1 // compile with -D, e.g.
```

[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.

```
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 2.2. Here RC is the random chunk method discussed in Section 2.4.

4.5 The Task Directive

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 queue. 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

```
if (firstcall == 1) {
   #pragma omp single nowait
   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

```
part = separate(z,zstart,zend);
#pragma omp task
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 eventually."

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.

```
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.

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

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

The eligible operators are:

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

Here is an example. The code in Section 4.12 includes an instance of this pragma:

```
for (i = me; i < n; i += nth) {
   mysum += procpairs(i);
}
#pragma omp atomic
tot += mysum;
#pragma omp barrier
```

The compiler produces the following code from that snippet:[4]

```
movl    n(%rip), %eax
cmpl    %eax, -8(%rbp)
jl      .L22
movl    -12(%rbp), %eax
lock addl       %eax, tot(%rip)
call    GOMP_barrier
jmp     .L24
```

Recall that in (Unix-family) Intel assembly language, a percent sign indicates a CPU register, e.g. the EAX register.

The first couple of lines are part of the compiled version of the **for** loop, comparing **i** to **n** and jumping to the top of the look if **i** is still less than **n**.

The **movl** then fills the EAX register with **mysum**, which the compiler has apparently assigned to the location 12 bytes above the place in memory pointed to by the RBP register. The instructions

```
lock addl       %eax, tot(%rip)
```

atomically adds **mysum** to **tot**.

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

[4] This can be obtained by compiling with **gcc** with the **-S** option, producing a **.s** file.

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:

```
#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:

```
#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 2.2 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://www.hpcs.cs.tsukuba.ac.jp/omni-compiler/`). To compile an OpenMP program in **x.c** and create an executable file **x**, run

  ```
  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

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

- GCC, version 4.2 or later:[5] Compile **x.c** via

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

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

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

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

```
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 1.5.5 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 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 functoin 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 for a function f() that is continuous
5  // and strictly monotonic; f() is known to be negative
6  // at a, positive at b; thus f() has a root in (a,b)
7
8  // strategy: in each iteration, the current
9  // interval is split into nth equal parts,
10 // and each thread checks its subinterval
11 // for a sign change of f(); if one is
12 // found, this subinterval becomes the
13 // new current interval; the current guess
14 // for the root is the left endpoint of the
15 // current interval
16
17 // of course, this approach is useful in
18 // parallel only if f() is very expensive
19 // to evaluate
20
21 // for simplicity, assumes that no endpoint
22 // of a subinterval will ever exactly
23 // coincide with a root
```

```
24
25 float root(float(*f)(float),
26    float inita, float initb, int niters) {
27    float curra = inita;
28    float currb = initb;
29    #pragma omp parallel
30    {
31       int nth = omp_get_num_threads();
32       int me = omp_get_thread_num();
33       int iter;
34       for (iter = 0; iter < niters; iter++) {
35          #pragma omp barrier
36          float subintwidth =
37             (currb - curra) / nth;
38          float myleft =
39             curra + me * subintwidth;
40          float myright = myleft + subintwidth;
41          // only one thread will find its interval contains the root, so
42          // don't need anything lik #pragma omp critical here
43          if ((*f)(myleft) < 0 &&
44              (*f)(myright) > 0) {
45             curra = myleft;
46             currb = myright;
47          }
48       }
49    }
50    return curra;
51 }
52
53 float testf(float x) {
54    return pow(x-2.1,3);
55 }
56
57 int main(int argc, char **argv)
58 {  printf("%f\n",root(testf,-4.1,4.1,1000));  }
```

4.12 Example: Mutual Outlinks

Consider the example of Section 2.4.3. 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 2.4.3.

```
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
30       // that equal 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 Example: Finding the Maximal Burst in a Time Series

Consider a time series of length n, in the context of our example in Section **??**, but with a modified goal, to find the period of at least k consecutive time points that has the maximal mean value.

Denote our time series by $x_1, x_2, ..., x_n$. Consider checking for bursts that begin at x_i. We could check for bursts of length $k, k+1, ..., n-i+1$, i.e. about $n-i-k$ different cases. Since i itself can take on $O(n)$ values, the time complexity of this application is, for fixed k and varying n, $O(n^2)$. This growth rate in n suggests that this is a good candidate for parallelization.

For convenience, the code will assume that the time series values of nonnegative.

```
1  // OpenMP example program, Burst.c; burst() finds period of
2  // highest burst of activity in a time series
3
4  #include <omp.h>
5  #include <stdio.h>
6  #include <stdlib.h>
7
8  // arguments for burst()
9
10 //    inputs:
11 //       x:  the time series, assumed nonnegative
12 //       nx:  length of x
13 //       k:  shortest period of interest
14 //    outputs:
15 //       startmax, endmax:  pointers to indices of the maximal-burst period
16 //       maxval:  pointer to maximal burst value
17
18 // finds the mean of the block between y[s] and y[e]
19 double mean(double *y, int s, int e) {
20    int i; double tot = 0;
21    for (i = s; i <= e; i++) tot += y[i];
22    return tot / (e - s + 1);
23 }
24
25 void burst(double *x, int nx, int k,
26    int *startmax, int *endmax, double *maxval)
27    {
28    int nth;  // number of threads
29    #pragma omp parallel
30    {  int perstart, // period start
31           perlen,  // period length
```

```
32            perend, // perlen end
33            pl1; // perlen - 1
34        // best found by this thread so far
35        int mystartmax, myendmax; // locations
36        double mymaxval; // value
37        // scratch variable
38        double xbar;
39        int me; // ID for this thread
40        #pragma omp single
41        {
42            nth = omp_get_num_threads();
43        }
44        me = omp_get_thread_num();
45        mymaxval = -1;
46        #pragma omp for
47        for (perstart = 0; perstart <= nx-k; perstart++) {
48           for (perlen = k; perlen <= nx - perstart; perlen++) {
49              perend = perstart+perlen-1;
50              if (perlen == k)
51                 xbar = mean(x,perstart,perend);
52              else {
53                 // update the old mean
54                 pl1 = perlen - 1;
55                 xbar = (pl1 * xbar + x[perend]) / perlen;
56              }
57              if (xbar > mymaxval) {
58                 mymaxval = xbar;
59                 mystartmax = perstart;
60                 myendmax = perend;
61              }
62           }
63        }
64        #pragma omp critical
65        {
66           if (mymaxval > *maxval) {
67              *maxval = mymaxval;
68              *startmax = mystartmax;
69              *endmax = myendmax;
70           }
71        }
72     }
73  }
74
75  // here's our test code
76
77  int main(int argc, char **argv)
78  {
79     int startmax, endmax;
80     double maxval;
81     double *x;
```

```
82      int k = atoi(argv[1]);
83      int i,nx;
84      nx = atoi(argv[2]);  // length of x
85      x = malloc(nx*sizeof(double));
86      for (i = 0; i < nx; i++) x[i] = rand() / (double) RAND_MAX;
87      double startime,endtime;
88      startime = omp_get_wtime();
89      // parallel
90      burst(x,nx,k,&startmax,&endmax,&maxval);
91      // back to single thread
92      endtime = omp_get_wtime();
93      printf("elapsed time: %f\n",endtime-startime);
94      printf("%d %d %f\n",startmax,endmax,maxval);
95      if (nx < 25) {
96         for (i = 0; i < nx; i++) printf("%f ",x[i]);
97         printf("\n");
98      }
99  }
```

4.15 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

4.16 Other Examples of OpenMP Code in This Book

There are additional OpenMP examples in later sections of this book, such as:[6]

- sampling bucket sort, Section 1.6.1.1
- parallel prefix sum/run-length decoding, Section 10.3.

[6] 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`

- matrix multiplication, Section 11.3.2.1.
- 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

Chapter 5

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 hardware, 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. The same is true for another language, OpenACC. These languages are 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, Kepler, Pascal and so on. Unless otherwise stated, all statements here refer to Tesla, keeping things at the basic level.

5.2 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.

5.3 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.

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

  Of course, "will run on the device" means that the compiler will general machine code for the device's architecture.

  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.
- A "call" to a kernel is somewhat more than a simply call in C. Consider the code above,

  ```
  dim3 dimGrid(n,1);
  dim3 dimBlock(1,1,1);
  find1elt<<<dimGrid,dimBlock>>>(dm,drs,n);
  ```

  The first two statements set up the desired number of blocks per grid and the number of threads per block. The "call" then transmits this information to the GPU along with the ordinary arguments **dm** etc.

  Due to the GPU's heritage in physics, one has the option of making the grid look "two dimensional" to the programmer, and likewise make each block look "three dimensional." This is just a programming convenience, which we will not pursue here.
- 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

  ```
  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

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

[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.

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

```
__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 in the above rowsums example) 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:

  ```
  cudaThreadSynchronize();
  ```

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

  ```
  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

  ```
  __syncthreads();
  ```

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

- 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

```
for (int k = 0; k < n; k++)
   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:

```
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.

5.4 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.

5.4.1 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 groups of threads within 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 basic word size is 32 bits. Newer devices are capable of double precision, etc., e.g. by declaring say,

```
float2 x;  // 64 bits
```

5.4.2 Thread Operation

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

5.4.2.1 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 5.4.4.

5.4.2.2 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 somewhat 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.)

5.4.2.3 "OS in Hardware"

Each SM runs the threads on a timesharing basis, just like an operating system (OS). This timesharing 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 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. Each warp has its own set of registers, so a context switch does very little saving and restoring of context, 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, where coarser granularity is generally needed.

5.4.3 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.

5.4.3.1 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[2]	no

In prose form:

- Shared memory: This memory is partitioned among all blocks in an SM. All threads in a block have access to this block's portion of the shared memory on that SM (but not access

to the shared memory of other blocks). Access is very fast, both in terms of latency and bandwidth, 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, 16K bytes per SM on the lower models, 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. Note that the term *shared* only refers to the fact that it is shared among threads in the same block.

- 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 5.4.3.2.

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.[3]

(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, the current instruction first running in one half-warp and then in the other. From the point of view of the programmer, the issue of half-warps is not important.)

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

[3] Again, newer devices can relax this requirement somewhat; see Sec. 5.17.

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:

```
1  #include <stdio.h>
2  #include <stdlib.h>
3  #include <cuda.h>
4
5  // CUDA example:  illustrates kernel-allocated shared memory; does
6  // nothing useful, just copying an array from host to device global,
7  // then to device shared, doubling it there, then copying back to device
8  // global then host
9
10 __global__ void doubleit(int *dv, int n)
11 {  extern __shared__ int sv[];
12    int me = threadIdx.x;
13    // threads share in copying dv to sv, with each thread copying one
14    // element
15    sv[me] = dv[me];
16    sv[me] = 2 * sv[me];
17    dv[me] = sv[me];
18 }
19
20 int main(int argc, char **argv)
21 {
22     int n = atoi(argv[1]);  // number of matrix rows/cols
23     int *hv, // host array
24         *dv; // device array
25     int vsize = n * sizeof(int);  // size of array in bytes
26     // allocate space for host array
27     hv = (int *) malloc(vsize);
28     // fill test array with consecutive integers
29     int t = 0,i;
30     for (i = 0; i < n; i++)
31        hv[i] = t++;
```

```
32      // allocate space for device array
33      cudaMalloc((void **)&dv, vsize);
34      // copy host array to device array
35      cudaMemcpy(dv,hv,vsize,cudaMemcpyHostToDevice);
36      // set up parameters for threads structure
37      dim3 dimGrid(1,1);
38      dim3 dimBlock(n,1,1);  // all n threads in the same block
39      // invoke the kernel; third argument is amount of shared memory
40      doubleit<<<dimGrid,dimBlock,vsize>>>(dv,n);
41      // wait for kernel to finish
42      cudaThreadSynchronize();
43      // copy row array from device to host
44      cudaMemcpy(hv,dv,vsize,cudaMemcpyDeviceToHost);
45      // check results
46      if (n < 10) for(int i=0; i<n; i++) printf("%d\n",hv[i]);
47      // clean up
48      free(hv);
49      cudaFree(dv);
50  }
```

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

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

but actually allocated during the kernel invocation

```
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.:

  ```
  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.

5.4.3.2 Global-Memory Performance Issues

As noted, the latency (Section 2.5) 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 2.5) 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).

5.4.3.3 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.

5.4.3.4 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.

5.4.3.5 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

```
int z[20],i;
...
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

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

  For example:

```
__constant__ int x;  // not contained in any function

// host code
int y = 3;
cudaMemcpyToSymbol("x",&y,sizeof(int));
...

// device code
int z;
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:

```
/ host code
for 1 to number of iterations
   set Constant array x
   call kernel (do scatter op)
   cudaThreadSynchronize()
   do gather op, using kernel results to form new x

// device code
use x together with thread-specific data
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.

5.4.4 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. in OpenMP by calling **omp_get_thread_num()**, 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

```
dim3 dimGrid(n,1);
dim3 dimBlock(1,1,1);
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. (As noted earlier, this is just an example, very inefficient but simple for introductory purposes.)

  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

$$A_{11} = \begin{pmatrix} 2 \end{pmatrix}. \tag{5.6}$$

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.

5.4.5 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:[4]

- You don't have access to the C library (the library consists of host machine language, after all). There are special versions of math functions, however, e.g. **__sin()**.
- No stack. Functions are essentially inlined, rather than their calls being handled by pushes onto a stack.
- No pointers to functions.

5.5 Synchronization, Within and Between Blocks

As mentioned, a barrier for the threads in the same block is available by calling **__syncthreads()**. Note carefully that if one thread writes a variable to memory (of whatever kind) 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

```
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.

[4] As noted, the statements below apply to the Tesla series.

As with compare-and-exchange operations on other machines, we can use it to implement locks, e.g.[5]

```
__device__ void lock(int* lockVar) {
  while (atomicCAS(lockVar, 0, 1) != 0) { ; }
}

__device__ void unlock(int* lockVar) {
  atomicExch(lockVar, 0);
}
```

Use **-arch=sm_11** when compiling, e.g.

```
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, thus enabling the use of **__syncthreads()**. 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 GPU.

If you use multiple blocks, though, your only feasible options for synchronization are to either use the global atomic operations or 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 5.4.3.5.

5.6 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.

[5] Modeled on *http://cs.umw.edu/ finlayson/class/fall14/cpsc425/notes/22-cuda-sync.html.*

- 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 use of shared memory, larger block size may be the better, so as to have more shared memory available per block. . On the other hand, the larger the block size, the longer the time it will take for barrier synchronization.
- 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. This argues for a larger block size.
- 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. This argues for a smaller block size, and/or a judicious arrangement of code on the programmer's part.
- 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.

5.7 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.[6]

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

```
$ nvcc -g -G x.cu
```

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_g5aa4f47938af8276f08074d0html`.

Here's a simple program to check some of the properties of device 0:

```
1  #include<cuda.h>
2  #include <stdio.h>
3
4  int main()
5  {
6     cudaDeviceProp Props;
7     cudaGetDeviceProperties( &Props,0);
8
9     printf("shared mem: %d)\n", Props.sharedMemPerBlock);
10    printf("max threads/block: %d\n",Props.maxThreadsPerBlock);
11    printf("max blocks: %d\n",Props.maxGridSize[0]);
12    printf("total Const mem: %d\n",Props.totalConstMem);
13 }
```

[6] It might be in **/sbin**.

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.

5.8 Example: Improving the Row Sums Program

The issues involving coalescing in Section 5.4.3.2 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):

```
pc5:~/CUDA% time rs 20000
2.585u 1.753s 0:04.54 95.3%     0+0k 7104+0io 54pf+0w
pc5:~/CUDA% time cs 20000
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?

```
pc5:~/CUDA% time csc 20000
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.[7]

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.

[7]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 considerations.

5.9 Example: Finding the Mean Number of Mutual Outlinks

As in Sections 2.4.3 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         // need to find my thread number among the totality of all
13         // threads in all blocks
14         me = blockIdx.x * blockDim.x + threadIdx.x;
15     int i,j,k,sum = 0;
16     for (i = me; i < n; i += totth) {  // do various rows i
17        for (j = i+1; j < n; j++) {  // do all rows j > i
18           for (k = 0; k < n; k++)
19              sum += m[n*i+k] * m[n*j+k];
20        }
21     }
22     atomicAdd(tot,sum);
23 }
24
25 int main(int argc, char **argv)
26 {  int n = atoi(argv[1]),  // number of vertices
27         nblk = atoi(argv[2]);  // number of blocks
28     int *hm, // host matrix
29         *dm, // device matrix
30         htot, // host grand total
31         *dtot; // device grand total
32     int msize = n * n * sizeof(int);  // size of matrix in bytes
33     // allocate space for host matrix
34     hm = (int *) malloc(msize);
35     // as a test, fill matrix with random 1s and 0s
36     int i,j;
37     for (i = 0; i < n; i++) {
38        hm[n*i+i] = 0;
39        for (j = 0; j < n; j++) {
40           if (j != i) hm[i*n+j] = rand() % 2;
41        }
42     }
```

```
43      // allocate space for device matrix
44      cudaMalloc((void **)&dm,msize);
45      // copy host matrix to device matrix
46      cudaMemcpy(dm,hm,msize,cudaMemcpyHostToDevice);
47      htot = 0;
48      // set up device total and initialize it
49      cudaMalloc((void **)&dtot,sizeof(int));
50      cudaMemcpy(dtot,&htot,sizeof(int),cudaMemcpyHostToDevice);
51      // set up parameters for threads structure
52      dim3 dimGrid(nblk,1);
53      dim3 dimBlock(192,1,1);
54      // invoke the kernel
55      procpairs<<<dimGrid,dimBlock>>>(dm,dtot,n);
56      // wait for kernel to finish
57      cudaThreadSynchronize();
58      // copy total from device to host
59      cudaMemcpy(&htot,dtot,sizeof(int),cudaMemcpyDeviceToHost);
60      // check results
61      if (n <= 15) {
62         for (i = 0; i < n; i++) {
63            for (j = 0; j < n; j++)
64               printf("%d ",hm[n*i+j]);
65            printf("\n");
66         }
67      }
68      printf("mean = %f\n",htot/float((n*(n-1))/2));
69      // clean up
70      free(hm);
71      cudaFree(dm);
72      cudaFree(dtot);
73  }
```

Again we've used the method in Section 2.4.3 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.

5.10 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, and an inefficient use of the
14 // GPU in any case
15
16 // initialize sprimes, 1s for the odds, 0s for the evens; see sieve()
17 // for the nature of the arguments
18 __device__ void initsp(int *sprimes, int n, int nth, int me)
19 {
20    int chunk,startsetsp,endsetsp,val,i;
21    sprimes[2] = 1;
22    // determine sprimes chunk for this thread to init
23    chunk = (n-1) / nth;
24    startsetsp = 2 + me*chunk;
25    if (me < nth-1) endsetsp = startsetsp + chunk - 1;
26    else endsetsp = n;
27    // now do the init
28    val = startsetsp % 2;
29    for (i = startsetsp; i <= endsetsp; i++) {
30       sprimes[i] = val;
31       val = 1 - val;
32    }
33    // make sure sprimes up to date for all
34    __syncthreads();
35 }
36
37 // copy sprimes back to device global memory; see sieve() for the nature
38 // of the arguments
39 __device__ void cpytoglb(int *dprimes, int *sprimes, int n, int nth, int me)
40 {
41    int startcpy,endcpy,chunk,i;
42    chunk = (n-1) / nth;
43    startcpy = 2 + me*chunk;
44    if (me < nth-1) endcpy = startcpy + chunk - 1;
45    else endcpy = n;
46    for (i = startcpy; i <= endcpy; i++) dprimes[i] = sprimes[i];
47    __syncthreads();
48 }
49
50 // finds primes from 2 to n, storing the information in dprimes, with
51 // dprimes[i] being 1 if i is prime, 0 if composite; nth is the number
52 // of threads (threadDim somehow not recognized)
53 __global__ void sieve(int *dprimes, int n, int nth)
54 {
55    extern __shared__ int sprimes[];
56    int me = threadIdx.x;
```

```
57      int nth1 = nth - 1;
58      // initialize sprimes array, 1s for odds, 0 for evens
59      initsp(sprimes,n,nth,me);
60      // "cross out" multiples of various numbers m, with each thread doing
61      // a chunk of m's; always check first to determine whether m has
62      // already been found to be composite; finish when m*m > n
63      int maxmult,m,startmult,endmult,chunk,i;
64      for (m = 3; m*m <= n; m++) {
65         if (sprimes[m] != 0) {
66            // find largest multiple of m that is <= n
67            maxmult = n / m;
68            // now partition 2,3,...,maxmult among the threads
69            chunk = (maxmult - 1) / nth;
70            startmult = 2 + me*chunk;
71            if (me < nth1) endmult = startmult + chunk - 1;
72            else endmult = maxmult;
73         }
74         // OK, cross out my chunk
75         for (i = startmult; i <= endmult; i++) sprimes[i*m] = 0;
76      }
77      __syncthreads();
78      // copy back to device global memory for return to host
79      cpytoglb(dprimes,sprimes,n,nth,me);
80  }
81
82  int main(int argc, char **argv)
83  {
84      int n = atoi(argv[1]),  // will find primes among 1,...,n
85          nth = atoi(argv[2]);  // number of threads
86      int *hprimes,  // host primes list
87          *dprimes;  // device primes list
88      int psize = (n+1) * sizeof(int);  // size of primes lists in bytes
89      // allocate space for host list
90      hprimes = (int *) malloc(psize);
91      // allocate space for device list
92      cudaMalloc((void **)&dprimes,psize);
93      dim3 dimGrid(1,1);
94      dim3 dimBlock(nth,1,1);
95      // invoke the kernel, including a request to allocate shared memory
96      sieve<<<dimGrid,dimBlock,psize>>>(dprimes,n,nth);
97      // check whether we asked for too much shared memory
98      cudaError_t err = cudaGetLastError();
99      if(err != cudaSuccess) printf("%s\n",cudaGetErrorString(err));
100     // wait for kernel to finish
101     cudaThreadSynchronize();
102     // copy list from device to host
103     cudaMemcpy(hprimes,dprimes,psize,cudaMemcpyDeviceToHost);
104     // check results
105     if (n <= 1000) for(int i=2; i<=n; i++)
106        if (hprimes[i] == 1) printf("%d\n",i);
```

```
107       // clean up
108       free(hprimes);
109       cudaFree(dprimes);
110    }
```

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 1.4.2.1, 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.

Also, it is quite important to note that in this simple version, we are using only one block, thus only one SM, thus only a fraction of the GPU. This would have to be remedied for the best performance.

5.11 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 10.)

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; note disclaimers above.

```
1  // for this simple illustration, it is assumed that the code runs in
2  // just one block, and that the number of threads evenly divides n
3
4  // improvements that could be made:
5  //    1. change to multiple blocks, to try to use all SMs
6  //    2. possibly use shared memory
7  //    3. have each thread work on staggered elements of dx, rather than
8  //       on contiguous ones, to get more efficient bank access
9
10 #include <cuda.h>
11 #include <stdio.h>
12
13 __global__ void cumulker(int *dx, int n)
14 {
15    int me = threadIdx.x;
16    int csize  = n / blockDim.x;
17    int start = me * csize;
18    int i,j,base;
19    for (i = 1; i < csize; i++) {
20       j = start + i;
21       dx[j] = dx[j-1] + dx[j];
22    }
23    __syncthreads();
24    if (me > 0) {
25       base = 0;
26       for (j = 0; j < me; j++)
27          base += dx[(j+1)*csize-1];
28    }
29    if (me > 0) {
30       for (i = start; i < start + csize; i++)
31          dx[i] += base;
32    }
33 }
34
35
36 int main(int argc, char **argv)
37 {
38     int n = atoi(argv[1]),  // length of array
39         nth = atoi(argv[2]);  // number of threads
40     int *ha,  // host array
```

```
41          *da,  // device array
42          nint = n * sizeof(int);
43      ha = (int *) malloc(nint);
44      // test example
45      for (int i = 0; i < n; i++) ha[i] = i*i % 5;
46      if (n < 100) for(int i=0; i<n; i++) printf("%d ",ha[i]);
47      printf("\n");
48      cudaMalloc((void **)&da,nint);
49      cudaMemcpy(da,ha,nint,cudaMemcpyHostToDevice);
50      dim3 dimGrid(1,1);
51      dim3 dimBlock(n/nth,1,1);
52      cumulker<<<dimGrid,dimBlock>>>(da,n);
53      cudaThreadSynchronize();
54      cudaMemcpy(ha,da,nint,cudaMemcpyDeviceToHost);
55      if (n < 100) for(int i=0; i<n; i++) printf("%d ",ha[i]);
56      printf("\n");
57      free(ha);
58      cudaFree(da);
59  }
```

5.12 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 5.11 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 5.10 is less clear, and probably quite dependent on whether we are using the more advanced GPUs, which feature at least some L1 cache space.

5.13 Example: Transforming an Adjacency Matrix

Below is a CUDA version of the code in Section 4.13. Note that in this code, there are two kernel calls.

```
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 // tgkernel1() finds the number of 1s to be handled by a thread, used
23 // to determine where in the output matrix a thread writes its portion
24
25 // arguments:
26 //    dadjm:  the adjacency matrix (NOT assumed symmetric), 1 for edge, 0
27 //            otherwise; note: matrix is overwritten by the function
28 //    n:  number of rows and columns of adjm
29 //    dcounts:  output array, counts of 1s
30
31 __global__ void tgkernel1(int *dadjm, int n, int *dcounts)
32 {  int tot1s,j;
33    // need to find my thread number among the totality of all
34    // threads in all blocks
35    int me = blockDim.x * blockIdx.x + threadIdx.x;
36    tot1s = 0;
37    for (j = 0; j < n; j++) {
38       if (dadjm[n*me+j] == 1) {
39          dadjm[n*me+tot1s++] = j;
40       }
41    dcounts[me] = tot1s;
42    }
43 }
44
45 // tgkernel2() has the given thread write its rows into the output
46 // matrix
47
48 __global__ void tgkernel2(int *dadjm, int n,
49    int *dcounts, int *dstarts, int *doutm)
50 {  int outrow,num1si,j;
51    int me = blockDim.x * blockIdx.x + threadIdx.x;
52    // fill in this thread's portion of doutm
53    outrow = dstarts[me];
54    num1si = dcounts[me];
```

```
55      if (num1si > 0) {
56         for (j = 0; j < num1si; j++) {
57            doutm[2*outrow+2*j] = me;
58            doutm[2*outrow+2*j+1] = dadjm[n*me+j];
59        }
60      }
61  }
62
63  // replaces counts by cumulative counts
64  void cumulcounts(int *c, int *s, int n)
65  {  int i;
66     s[0] = 0;
67     for (i = 1; i < n; i++) {
68        s[i] = s[i-1] + c[i-1];
69     }
70  }
71
72  int *transgraph(int *hadjm, int n, int *nout, int gsize, int bsize)
73  {  int *dadjm;  // device adjacency matrix
74     int *houtm;  // host output matrix
75     int *doutm;  // device output matrix
76     int *hcounts;  // host counts vector
77     int *dcounts;  // device counts vector
78     int *hstarts;  // host starts vector
79     int *dstarts;  // device starts vector
80     hcounts = (int *) malloc(n*sizeof(int));
81     hstarts = (int *) malloc(n*sizeof(int));
82     cudaMalloc((void **)&dadjm,n*n*sizeof(int));
83     cudaMalloc((void **)&dcounts,n*sizeof(int));
84     cudaMalloc((void **)&dstarts,n*sizeof(int));
85     houtm = (int *) malloc(n*n*sizeof(int));
86     cudaMalloc((void **)&doutm,n*n*sizeof(int));
87     cudaMemcpy(dadjm,hadjm,n*n*sizeof(int),cudaMemcpyHostToDevice);
88     dim3 dimGrid(gsize,1);
89     dim3 dimBlock(bsize,1,1);
90     // calculate counts and starts first
91     tgkernel1<<<dimGrid,dimBlock>>>(dadjm,n,dcounts);
92     cudaMemcpy(hcounts,dcounts,n*sizeof(int),cudaMemcpyDeviceToHost);
93     cumulcounts(hcounts,hstarts,n);
94     *nout = hstarts[n-1] + hcounts[n-1];
95     cudaMemcpy(dstarts,hstarts,n*sizeof(int),cudaMemcpyHostToDevice);
96     tgkernel2<<<dimGrid,dimBlock>>>(dadjm,n,dcounts,dstarts,doutm);
97     cudaMemcpy(houtm,doutm,2*(*nout)*sizeof(int),cudaMemcpyDeviceToHost);
98     free(hcounts);
99     free(hstarts);
100    cudaFree(dadjm);
101    cudaFree(dcounts);
102    cudaFree(dstarts);
103    return houtm;
104 }
```

```
105
106 int main(int argc, char **argv)
107 {  int i,j;
108    int *adjm;  // host adjacency matrix
109    int *outm;  // host output matrix
110    int n = atoi(argv[1]);
111    int gsize = atoi(argv[2]);
112    int bsize = atoi(argv[3]);
113    int nout;
114    adjm = (int *) malloc(n*n*sizeof(int));
115    for (i = 0; i < n; i++)
116       for (j = 0; j < n; j++)
117          if (i == j) adjm[n*i+j] = 0;
118          else adjm[n*i+j] = rand() % 2;
119    if (n < 10) {
120       printf("adjacency matrix: \n");
121       for (i = 0; i < n; i++) {
122          for (j = 0; j < n; j++) printf("%d ",adjm[n*i+j]);
123          printf("\n");
124       }
125    }
126
127    struct timespec bgn,nd;
128    clock_gettime(CLOCK_REALTIME, &bgn);
129
130    outm = transgraph(adjm,n,&nout,gsize,bsize);
131    printf("num rows in out matrix = %d\n",nout);
132    if (nout < 50) {
133       printf("out matrix: \n");
134       for (i = 0; i < nout; i++)
135          printf("%d %d\n",outm[2*i],outm[2*i+1]);
136    }
137
138    clock_gettime(CLOCK_REALTIME, &nd);
139    printf("%f\n",timediff(bgn,nd));
140 }
```

5.14 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

```
cudaError_t err = cudaGetLastError();
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 (Section 5.18.1) returns a potential error code, of type **cublasStatus**, not checked here.

5.15 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 constants, GPU registers may be used to implement the array in the unrolled loop.

For example, the loop

```
for (i = 0; i < 2; i++ {
   sum += x[i];
   sum2 += x[i]*x[i];
}
```

could be unrolled to

```
sum += x[1];
sum2 += x[1]*x[1];
sum += x[2];
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:

```
#pragma unroll k
```

suggest to the compiler a k-fold unrolling. Setting k = 1 will instruct the compiler *not* to unroll.

5.16 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.

5.17 Newer Generations

NVIDIA continues to makes advances in its GPUs. Many of the advances are of the "bigger and faster than before" type. However, two newer features are more for programmer convenience than speed.

5.17.1 True Caching

Shared memory is in essence a programmer-managed cache, but now on-chip memory can be apportioned to both shared memory and a true cache. This makes less work for the programmer, at a possible cost of reduced performance.

5.17.2 Unified Memory

One of the most significant aspects of GPU programming is writing code to move data back and forth between the CPU memory and the GPU memory. Under the Unified Memory, one can declare some data in one's code to be *managed*, and CUDA will automatically move the data to the proper processor, be it CPU or GPU.

Say for instance a vector **x** is the subject of both CPU and GPU code. If when the CPU code executes **x** is not in CPU memory, the Unified Memory system will copy it from the GPU memory, transparently to the programmer.

Starting with the Pascal model series, there is hardware assist for this, using something similar to virtual memory page tables.

Again, this is for the convenience of the programmer. Hand coding of the memory-to-memory transfers may be much more efficient.

5.18 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.

5.18.1 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.

5.18.1.1 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/lib64 RowSumsCB.c -lcublas
```

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:

```
1  #include <stdio.h>
2  #include <cublas.h>  // required include
3
4  int main(int argc, char **argv)
5  {
6     int n = atoi(argv[1]);  // number of matrix rows/cols
7     float *hm, // host matrix
8           *hrs, // host rowsums vector
9           *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

```
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

```
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 device. 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

```
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:

```
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, this constant multiplication is not actually performed, which we could have specificed 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.

5.18.2 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.

5.18.3 CUFFT

CUFFT does for the Fast Fourier Transform what CUBLAS does for linear algebra, i.e. it provides CUDA-optimized FFT routines.

5.19 Other CUDA Examples in This Book

There are additional CUDA examples in later sections of this book. These include:[8]

- Prof. Richard Edgar's matrix-multiply code, optimized for use of shared memory, Section 11.3.2.2.
- 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.

[8] 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`

Chapter 6

Introduction to Thrust Programming

In the spirit of CUBLAS (Section 5.18.1) 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, which often produces faster code than OpenMP.

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 \
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>
```

[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]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.

```
 8 #include <cstdlib>
 9
10 int rand16()  // generate random integers mod 16
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 — we can save *state*. So, we might create several callable structs, all having the same code but with different values of their member variables. (There are no member variables in this example, but the examples below do have them.)

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

```
thrust::transform(dv.begin(),dv.end()-1,
        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. Again, the key is that we are creating an object in that case to **finddiff()**.

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

```
thrust::device_vector<int>::iterator newend =
```

```
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:

```
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,

```
nvcc -c SortForC.cu
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:

```
g++ -g -mcmodel=medium -fopenmp -lgomp \
   -DTHRUST_DEVICE_SYSTEM=THRUST_DEVICE_SYSTEM_OMP \
   -I/home/matloff/Thrust SortForC.cpp -o sort.o -c
g++ -g -mcmodel=medium TestSort.cpp sort.o -fopenmp -lgomp
% a.out
5
8
12
13
88
```

And for the CUDA case:

```
nvcc SortForC.cu -c -o sfc.o
gcc -g TestSort.c sfc.o -L/usr/local/cuda/lib -lcudart
% a.out
5
8
12
13
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 some 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, and store in increm
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    // copy x to device
31    thrust::device_vector<int> dx(x,x+n);
32    // sort on the device
33    thrust::sort(dx.begin(),dx.end());
34    // set up stencil seq for copy_if(), filled with 0,1,2,...
35    thrust::device_vector<int> seq(n);
36    thrust::sequence(seq.begin(),seq.end(),0);
37    // set up output vector
38    thrust::device_vector<int> out(n);
39    int incr = atoi(argv[1]);  // k
40    // for each i in seq, call ismultk() on this i, and if get a true
41    // result, put dx[i] into out; newend marks (1 past) end of out
42    thrust::device_vector<int>::iterator newend =
43       thrust::copy_if(dx.begin(),dx.end(),seq.begin(),out.begin(),
44          ismultk(incr));
45    thrust::copy(out.begin(), newend,
46       std::ostream_iterator<int>(std::cout, " "));
47    std::cout << "\n";
48 }
```

The **sequence()** function simply generates an array consisting of 0,1,2,...,n-1. Note that **this is typically used because Thrust has no direct parallel loop facilities.**

Here is a good way to think of the function **copy_if()**:

> In the call **thrust::copy_if(a.begin(),a.end(),b.begin(),c.begin(), callable_struct(args))**, think of the "copy" part as referring to the vector **a**, and the "if" part as referring to **b**. So, the call is saying copy the parts of **a** that satisfy the conditions specified by **b** and the callable struct, and place the results in **c**.

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,

```
thrust::copy_if(dx.begin(),dx.end(),seq,out,ismultk(incr));
```

That is then used to set a member variable in the struct:

```
const int increm;  // k in above comments
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,

```
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

```
bool operator()(const int i)
{  return i != 0 && (i % increm) == 0;
}
```

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.

Consider again the code,

```
thrust::copy_if(dx.begin(),dx.end(),seq,out,ismultk(incr));
```

We might write this as

```
bool (*ismk)(int) = ismultk(incr));
thrust::copy_if(dx.begin(),dx.end(),seq,out,ismk;
```

This highlights the fact that the original call, **ismultk(incr)** is actually *creating* a function, after which we pass a pointer to that function to **thrust::copy_if()**

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:

```
int *wd;
...
```

```
wd = thrust::raw_pointer_cast(&w[0]);
...
{  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

```
int *dz;
...
cudaMalloc(&dz,100*sizeof(int));
...
thrust::device_ptr<int> tz(dz);
...
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    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."

The point of converting to the raw array here was to enable the use of ordinary array subscripting, rather than Thrust iterators.

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  }
```

You might think that, having one of the scatter/gather operations available might make the other redundant, but it's handy to have both, because one might be copying between two vectors of different sizes. Say for instance the source vector is larger than the destination one. Then only some elements from the source will be copied, so a scatter operation won't work, as it would require all source elements to be mapped. Thus a gather is useful. The opposite would be true if the destination vector is larger.

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

```
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
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;
```

[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.

```
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 5.13. To review, here is the problem:

Say we have a graph with adjacency matrix

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \tag{6.1}$$

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

```
thrust::counting_iterator<int> seqb(0);
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()**:

```
thrust::transform(ones.begin(),newend,seq2b,
   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

```
terminate called after throwing an instance of 'std::bad_alloc'
  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

```
thrust::device_vector<int> seq(n);
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

```
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 10.6

Chapter 7

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 hardward for connection to its "neighbor" processors.

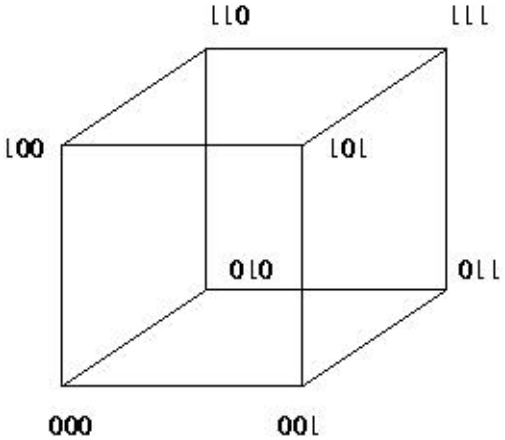
Hypercubes proved to be too expensive for the type of performance they could achieve, and the market was small anyway. Thus they are not common today, but they are still important, both for historical reasons (in the computer field, old techniques are often recycled decades later), and because the algorithms 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 ith 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)-

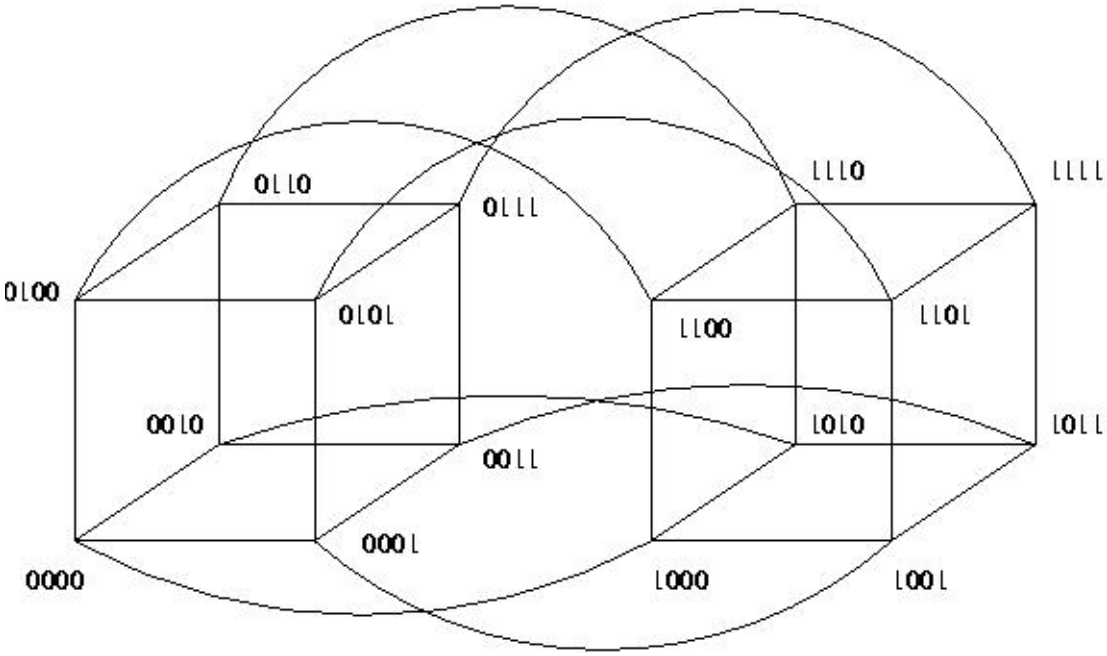
[1]Note that we number the digits from right to left, with the rightmost digit being digit 0.

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.

(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.

[2]Note that this is indeed an i-dimensional cube, because the last i digits are free to vary.

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.

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 non-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.

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

[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*.

MPI applications. R's **snow** package, which will be discussed in Section **??**, is based entirely on scatter/gather, as is MapReduce, to be discussed below.

Chapter 8

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 1.6.2.2, 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

8.3.3.1 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.

8.3.3.2 MPI_Comm_size() and MPI_Comm_rank()

In our function **init()** above, note the calls

```
MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
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**.

8.3.3.3 MPI_Send()

To see how MPI's basic send function works, consider our line above,

```
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

```
#define MYMIN_MSG 0
```

Receive calls, described in the next section, can ask to receive only messages of a certain type.

COMM_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**.

8.3.3.4 MPI_Recv()

Let's now look at the arguments for a basic receive:

```
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**.

COMM_WORLD: Group name.

status: Recall our line

```
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 ",no0s[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

```
% 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

```
(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

```
for (i = 1; i < nnodes; i++)
   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

```
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

```
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,

```
MPI_Reduce(mymin,overallmin,1,MPI_2INT,MPI_MINLOC,0,MPI_COMM_WORLD);
MPI_Bcast(overallmin,1,MPI_2INT,0,MPI_COMM_WORLD);
```

could be replaced by

```
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

```
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):

```
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

```
MPI_Scatter(oh, lenchunk, MPI_INT, ohchunk, lenchunk, MPI_INT, 0,
   MPI_COMM_WORLD);
```

means

> Node 0 will break up the array **oh** of type MPI_INT into chunks of length **lenchunk**, sending the i^{th} 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(MPLCOMM_WORLD,&nnodes);
24      MPI_Comm_rank(MPLCOMM_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,MPLCOMM_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,MPLCOMM_WORLD);
50      MPI_Bcast(maxvals,nnodes,MPI_INT,0,MPLCOMM_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,MPLCOMM_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 2.4.3. 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.

```
1  // MPI solution to the mutual outlinks problem
2
3  // adjacency matrix m is global at each node, broadcast from node 0
4
5  // assumes m is nxn, and number of nodes is < n
6
7  // for each node i, check all possible pairing nodes j > i; the various
8  // nodes work on values of i in a Round Robin fashion, with node k
9  // handling all i for which i mod nnodes = k
10
11 #include <mpi.h>
12 #include <stdlib.h>
13
14 #define MAXLENGTH 10000000
15
16 int nnodes,  // number of MPI processes
17     n,  // size of x
18     me,  // MPI rank of this node
19     m[MAXLENGTH],  // adjacency matrix
20     grandtot;  // grand total of all counts of mutuality
21
22 // get adjacency matrix, in this case just by simulation
23 void getm()
```

```
24 {  int i;
25    for (i = 0; i < n*n; i++)
26       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 consist 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):

```
MPI_Comm_size(MPI_COMM_WORLD,&nnodes);
MPI_Comm_rank(MPI_COMM_WORLD,&me);
...
// declare variables to bind to groups
MPI_Group worldgroup, subgroup;
// declare variable to bind to a communicator
MPI_Comm subcomm;
...
int i,startrank,nn2 = nnodes/2;
int *subranks = malloc(nn2*sizeof(int));
if (me < nn2) start = 0;
else start = nn2;
for (i = 0; i < nn2; i++)
   subranks[i] = i + start;
// bind the world to a group variable
MPI_Comm_group(MPI_COMM_WORLD, &worldgroup);
// take worldgroup the nn2 ranks in "subranks" and form group
// "subgroup" from them
MPI_Group_incl(worldgroup, nn2, subranks, subgroup);
// create a communicator for that new group
MPI_Comm_create(MPI_COMM_WORLD, subgroup, subcomm);
// get my rank in this new group
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 **??** and **??**.

8.9 Other MPI Examples in This Book

- The pipelined prime number finder in Chapter 1.
- Bucket sort with sampling, in Section 12.5.

Chapter 9

MapReduce Computation

As the world emerged into an era of Big Data, demand grew for a computing paradigm that (a) is generally applicable and (b) works on *distributed* data.The latter term means that data is physically distributed over many chunks, possibly on different disks and maybe even different geographical locations. Having the data stored in a distributed manner facilitates parallel computation — different chunks can be read simultaneously — and also enables us to work with data sets that are too large to fit into the memory of a single machine. Demand for such computational capability led to the development of various systems using the *MapReduce* paradigm.

MapReduce is really a form of the scatter-gather pattern we've seen frequently in this book, with the added feature of a sorting operation added in the middle. In rough form, it works like this. The input is in a (distributed) file, fed into the following process:

- **Map phase:** There are various parallel processes known as *mappers*, all running the same code. For each line of the input file, the mapper handling that chunk of the file reads the line, processes it in some way, and then emits an output line, consisting of a key-value pair.

- **Shuffle/sort phase:** All the mapper output lines that share the same key are gathered together.

- **Reduce phase:** There are various parallel processes known as *reducers*, all running the same code. Each reducer will work on its own set of keys, i.e. for any given key, all mapper output lines having the same key will go to the same reducer. Moreover, the lines fed into any given reducer will be sorted by key.

9.1 Apache Hadoop

At this writing, the most popular MapReduce software package is Hadoop. It is written in Java, and is most efficiently used in that language (or C++), but it includes a *streaming* feature that enables one to use Hadoop from essentially any language, including R. Hadoop includes is into distributed file system, unsurprisingly called the Hadoop Distributed File System (HDFS). Note that one advantage of HDFS is that it is replicated, thus achieving some degree of fault tolerance.

9.1.1 Hadoop Streaming

As noted, Hadoop is really written for Java or C++ applications. However, Hadoop can work with programs in any language under Hadoop's streaming option, by reading from **stdin** and writing to **stdout**, in text, line-oriented form in both cases.

Input to the mappers is from an HDFS file, and output from the reducers is again to an HDFS file, one chunk per reducer. The file line format is

```
key \t data
```

where \t is the Tab character.

The usage of text format does cause some slowdown in numeric programs, for the conversion of strings to numbers and vice versa, but again, Hadoop is not designed for maximum efficiency.

9.1.2 Example: Word Count

The typical "Hello World," introductory example is word count for a text file. The mapper program breaks a line into words, and emits (key,value) pairs in the form of (word,1). (If a word appears several times in a line, there would be several pairs emitted for that word.) In the Reduce stage, all those 1s for a given word are summed, giving a frequency count for that word. In this way, we get counts for all words.

Here is the mapper code:

```
#! /usr/bin/env Rscript

# wordmapper.R

si <- file("stdin",open="r")
while (length(inln <-
      scan(si,what="",nlines=1,quiet=TRUE,blank.lines.skip=FALSE))) {
   for (w in inln) {
```

```
        cat(w,"\t 1\n")
    }
}
```

And here is the reducer:

```
#! /usr/bin/env Rscript

# wordreducer.R

si <- file("stdin",open="r")
oldword <- ""

while (length(inln <- scan(si,what="",nlines=1,quiet=TRUE))) {
    word <- inln[1]
    if (word != oldword) {
        if (oldword != "")
            cat(oldword,"\t ",count,"\n")
        oldword <- word
        count <- 1
    } else {
        count <- count + as.integer(inln[2])
    }
}
```

The above code is not very refined, for instance treating *The* as different from *the*. The main point, though, is just to illustrate the principles.

9.1.3 Running the Code

I ran the following code from the top level of the Hadoop directory tree, with obvious modifications possible for other run points. First, I needed to place my data file, **rnyt**,[1]

```
$ bin/hadoop fs -put ../rnyt rnyt
$ bin/hadoop jar contrib/streaming/*.jar \
    -input rnyt \
    -output wordcountsnyt \
    -mapper ../wordmapper.R
    -reducer ../wordreducer.R
```

That first command specifies that it will be for the file system (**fs**, and that I am placing a file in that system. My ordinary version of the file was in my home directory.

Hadoop, being Java-based, runs Java archive, **.jar** files. So, the second command above specifies that I want to run in streaming mode. It also states that I wan the output to go to a file **word-**

[1]The file was the contents of the article "Data Analysts Captivated by Rs Power," *New York Times*, January 6, 2009.

countsnyt in my HDFS system. Finally, I specify my mapper and reducer code files. in my HDFS system, after which I ran the program. I allowed Hadoop to use its default values for the number of mappers and reducers, and could have specified them above if desired.

Recall that the final output comes in chunks in the HDFS. Here's how to check (some material not shown), and to view the actual file contents:

```
$ bin/hadoop fs -ls wordcountsnyt

Found 3 items
-rw-r--r--   1 ... /user/matloff/wordcountsnyt/_SUCCESS
drwxr-xr-x   - ... /user/matloff/wordcountsnyt/_logs
-rw-r--r--   1 ... /user/matloff/wordcountsnyt/part-00000
$ bin/hadoop fs -cat wordcountsnyt1/part-00000
1           NA
$2          1
1,600       1
18th        1
1991,       1
1996,       1
2009        1
2009,       1
250,000             1
6,          1
7,          1
A           1
ASHLEE      1
According           1
America,            1
Analysts            2
Anne        1
Another             1
Apache,             1
Are         1
At          1
...
```

So, in HDFS, one distributed file is stored as a directory, with the chunks in **part-00000**, **part-00001** and so on. We only had enough data to fill one chunk here.

9.1.4 Analysis of the Code

The first thing to notice is that these two R files are not executed directly by R, but instead under Rscript. This is standard for running R in *batch*, i.e. noninteractive, mode.

Next, as noted earlier, input to the mappers is from **stdin**, in this case from the redirected file **rnyt** in my HDFS, seen here in the identifier **si** in the mapper. Final output is to **stdout**, redirected

to the specified HDFS file, hence the call to **cat()** in the reducer. The mapper output goes to the shuffle and then to the reducers, again using STDOUT, visible here in the call to **cat()** in the mapper code.

The reader might be wondering here about the line

```
count <- count + as.integer(inln[2])
```

in the reducer. The way things have been described so far, it would seem that the expression **as.integer(inln[2])** — a word count output from a mapper — should always be 1. However, there is more to the story, as Hadoop also allows one to specify *combiner* code, as follows.

Remember, all the communication, e.g. from the mappers to the shuffler, is via our network, with one (key,value) pair per network message. So, we may have an enormous number of short messages, thus incurring the network latency penalty many times, as well as huge network congestion due to, for instance, many mappers trying to use the network at once. The solution is to have each mapper try to coalesce its messages before sending to the shuffler.

The coalescing is done by a *combiner* specified by the user. Often the combiner will be the same as the reducer. So, what occurs is that each mapper will run the reducer on its own mapper output, then send the combiner output to the shuffler, after which it goes to the reducers as usual.

Thus in our word count example here, when a line arrives at a reducer, its count field may already have a value greater than 1. The combiner code, by the way, is specified via the **-combiner** field in the run command, like **-mapper** and **-reducer**.

9.1.5 Role of Disk Files

As ntoed, Hadoop has its own file system, HDFS, which is built on top of the native OS' file system of the machines. It is replicated for the sake of reliability, with each HDFS block existing in at least 3 copies, i.e. on at least 3 separate disks. Very large files are possible, in some cases spanning more than one disk/machine.

Disk files play a major role in Hadoop programs:

- Input is from a file in the HDFS system.
- The output of the mappers goes to temporary files in the native OS' file system.
- Final output is to a file in the HDFS system. As noted earlier, that file may be distributed across several disks/machines.

Note that by having the input and output files in HDFS, we minimize communications costs in

shipping the data between nodes of a cluster. The slogan used is "Moving computation is cheaper than moving data." However, all that disk activity can be quite costly in terms of run time.

9.2 Other MapReduce Systems

As of late 2014, there has been increasing concern regarding Hadoop's performance. One of the problems is that one cannot keep intermediate results in memory between Hadoop runs. This is a serious problem, for instance, with iterative or even multi-pass algorithms.

The Spark package now being developed aims to remedy many of Hadoop's shortcomings. Early reports indicate some drastic speed improvements, while retaining the ability to read HDFS files, and continuing to have fault tolerance features.

9.3 R Interfaces to MapReduce Systems

Given the widespread usage of Hadoop, a number of R interfaces have been developed. The most popular is probably **rmr**, developed by Revolution Analytics, and RHIPE, written by Saptarshi Guha as part of his PhD dissertation. An R interface package, **sparkr**, is available.

9.4 An Alternative: "Snowdoop"

So, what does Hadoop really give us? The two main features are (a) distributed data access and (b) an efficient distributed file sort. Hadoop works well for many applications, but a realization developed that Hadoop can be very slow, and very limited in available data operations.

Both of those shortcomings are addressed to a large extent by the new kid on the block, Spark. Spark is apparently much faster than Hadoop, sometimes dramatically so, due to strong caching ability and a wider variety of available operations. Recently **distributedR** has also been released, again with the goal of using R on voluminous data sets, and there is also the more established **pbdR**.

But even Spark suffers a very practical problem, shared by the others mentioned above. All of these systems are complicated. There is a considerable amount of configuration to do, worsened by dependence on infrastructure software such as Java or MPI, and in some cases by interface software such as rJava. Some of this requires systems knowledge that many R users may lack. And once they do get these systems set up, they may be required to design algorithms with world views quite different from R, even though they are coding in R.

So, do we really need all that complicated machinery? Hadoop and Spark provide efficient distributed sort operations, but if one's application does not depend on sorting, we have a cost-benefit issue here.

Here is an alternative, a general approach rather than a package, which I call "Snowdoop": One simply does one's own chunking of files into distributed mini-files, and then uses Snow or some other general R tool on those files.

9.4.1 Example: Snowdoop Word Count

Let's use as our example word count, the "Hello World" of MapReduce. It determines which words are in a text file, and calculates frequency counts for each distinct word:

```
1  # each node executes this function
2  wordcensus <- function(basename,ndigs) {
3     fname <- filechunkname(basename,ndigs)
4     words <- scan(fname,what="")
5     tapply(words,words,length, simplify=FALSE)
6  }
7
8  # manager
9  fullwordcount <- function(cls,basename,ndigs) {
10    setclsinfo(cls)  # give workers ID numbers, etc.
11    counts <- clusterCall(cls,wordcensus,basename,ndigs)
12    addlistssum <- function(lst1,lst2)
13       addlists(lst1,lst2,sum)
14    Reduce(addlistssum,counts)
15 }
```

The above code makes use of the following routines, which are general and are used in many "Snowdoop" applications. These and other utilities are included in my **partools** package. Here are the call forms:

```
# give each cluster node an ID, etc.
setclsinfo(cls)

# "add" lists lst1, lst2, applying the operation 'add' to elements in
# common, copying non-null others
addlists(lst1,lst2,add)

# form the file name basename.i, where i is the ID of this node unless
# nodenum is specified
filechunkname(basename,ndigs,nodenum=NULL)
```

All pure R! No Java, no configuration. Indeed, it's worthwhile comparing to the word count example in the **sparkr** distribution. There we see calls to **sparkr** functions such as **flatMap()**,

reduceByKey() and **collect()**. But the **reduceByKey()** function is pretty much the same as R's tried and true **tapply()**. The **collect()** function is more or less our Snowdoop library function **addlists()**. So, again, there is no need to resort to Spark, Hadoop, Java and so on; we just use ordinary R.

We are achieving the parallel-read advantage of Hadoop and Spark,[2] *while avoiding the Hadoop/Spark configuration headaches and while staying with the familiar R programming paradigm.* In many cases, this should be a highly beneficial tradeoff for us.

Of course, this approach lacks the fault tolerance feature of Hadhoop and Spark can, which can be quite advantageous. And as of this writing, it is not yet clear how well this scales, e.g. how well the **parallel** package works with very large numbers of nodes. But Snowdoop is an attractive approach for many applications.

9.4.2 Example: Snowdoop k-Means Clustering

The k-means clustering problem is discussed in Section 14.3. Read ahead, and then see how we can implement it here:

```
1  # k-means clustering, using Snowdoop
2
3  # chunked data with name xname, nitrs iterations, nclus clusters;
4  # assumes for simplicity that a cluster will never become empty; ctrs is
5  # the matrix of initial centroids
6
7  # assumes setclsinfo already called
8
9  kmeans <- function(cls,xname,nitrs,ctrs) {
10    # will tell everyone to read their chunks; first, find cluster size
11    # and compute number of digits in file suffixes
12    addlistssum <- function(lst1,lst2) addlists(lst1,lst2,sum)
13    for (i in 1:nitrs) {
14       # for each data point, find the nearest centroid, and tabulate; at
15       # each worker and for each centroid, we compute a vector whose
16       # first component is the count of the number of data points whose
17       # nearest centroid is that centroid, and whose remainining portion
18       # is the sum of all such data points
19       tmp <- clusterCall(cls,findnrst,xname,ctrs)
20       # sum over all workers
21       tmp <- Reduce(addlistssum,tmp)
22       # compute new centroids
23       for (i in 1:nrow(ctrs)) {
24          tmp1 <- tmp[[as.character(i)]]
25          ctrs[i,] <- (1/tmp1[1]) * tmp1[-1]
```

[2]Note that neither Hadoop, Spark nor Snowdoop will achieve full parallel reading if the file chunks are all on the same disk.

```
26          }
27      }
28      ctrs
29  }
30
31  findnrst <- function(xname,ctrs) {
32      require(pdist)
33      x <- get(xname)
34      dsts <- matrix(pdist(x,ctrs)@dist,ncol=nrow(x))
35      # dsts[,i] now has the distances from row i of x to the centroids
36      nrst <- apply(dsts,2,which.min)
37      # nrst[i] tells us the index of the centroid closest to row i of x
38      mysum <- function(idxs,myx)
39          c(length(idxs),colSums(x[idxs,,drop=F]))
40      tmp <- tapply(1:nrow(x),nrst,mysum,x)
41  }
42
43  test <- function(cls) {
44      m <- matrix(c(4,1,4,6,3,2,6,6),ncol=2)
45      formrowchunks(cls,m,"m")
46      initc <- rbind(c(2,2),c(3,5))
47      kmeans(cls,"m",1,initc)
48  }
```

So again, we are using chunked files as in Hadoop, but writing ordinary R code, e.g. **tapply()** and **Reduce()**. But most important, the data at each worker persists across iterations. In Hadoop, it would be reread from disk at each iteration, and in Spark, we'd need to request caching, but here it comes for free, no special effort needed.

Chapter 10

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 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:

$$x_1 \leftarrow x_0 + x_1 \tag{10.4}$$
$$x_2 \leftarrow x_1 + x_2 \tag{10.5}$$
$$x_3 \leftarrow x_2 + x_3 \tag{10.6}$$
$$x_4 \leftarrow x_3 + x_4 \tag{10.7}$$
$$x_5 \leftarrow x_4 + x_5 \tag{10.8}$$
$$x_6 \leftarrow x_5 + x_6 \tag{10.9}$$
$$x_7 \leftarrow x_6 + x_7 \tag{10.10}$$

Step 2:

$$x_2 \leftarrow x_0 + x_2 \tag{10.11}$$
$$x_3 \leftarrow x_1 + x_3 \tag{10.12}$$
$$x_4 \leftarrow x_2 + x_4 \tag{10.13}$$
$$x_5 \leftarrow x_3 + x_5 \tag{10.14}$$
$$x_6 \leftarrow x_4 + x_6 \tag{10.15}$$
$$x_7 \leftarrow x_5 + x_7 \tag{10.16}$$

Step 3:

$$x_4 \leftarrow x_0 + x_4 \tag{10.17}$$
$$x_5 \leftarrow x_1 + x_5 \tag{10.18}$$
$$x_6 \leftarrow x_2 + x_6 \tag{10.19}$$
$$x_7 \leftarrow x_3 + x_7 \tag{10.20}$$

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 these 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.[1] 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 5.11:

```
1  break the array into p blocks
2  parallel for i = 0,...,p-1
3     Ti does serial 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

```
2 25 26 8 50 3 1 11 7 9 29 10
```

and three threads, and our operation is summing. We break the data into three sections,

2 25 26 8	50 3 1 11	7 9 29 10

[1] This is called a **red/black method**, Think of one array as "red" and the other as "black." It arises often in parallel computation.

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 prefix scan operation is common enough for it to be officially incorporated into various widely-used parallel computation platforms, such as:

- 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.
- Intel's Threads Building Blocks (TBB), similar in nature to OpenMP (though more sophisticated), includes a prefix scan operation.
- 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 Summing in OpenMP

Here is 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 }
```

10.5 Example: Run-Length Coding Decompression in OpenMP

Here is an example applying the code in the last section: A method for compressing data, called **run-length coding**, 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.

```
1  void uncomprle(int *x,int nx,int *tmp,int *y,int *ny)
2  {
3     int i,nx2 = nx/2;
4     int z[MAXTHREADS];
5     for (i = 0; i < nx2; i++) tmp[i+1] = x[2*i];
6     parprfsum(tmp+1,nx2+1,z);
7     tmp[0] = 0;
8     #pragma omp parallel
9     {  int j,k;
10       int me=omp_get_thread_num();
11       #pragma omp for
12       for (j = 0; j < nx2; j++) {
13          // where to start the j-th run?
14          int start = tmp[j];
15          // what value is in the run?
16          int val = x[2*j+1];
17          // how long is the run?
18          int nrun = x[2*j];
19          for (k = 0; k < nrun; k++)
20             y[start+k] = val;
21       }
22    }
23    *ny = tmp[nx2];
24 }
```

10.6 Example: Run-Length Coding 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:

```
1  #include <stdio.h>
2  #include <thrust/device_vector.h>
3  #include <thrust/scan.h>
4  #include <thrust/sequence.h>
5  #include <thrust/remove.h>
6
7  struct iseven {
8     bool operator()(const int i)
9     {  return (i % 2) == 0;
10    }
11 };
12
```

```
13 int main()
14 {  int i;
15    int x[12] = {3,2,2,0,1,5,2,0};
16    int nx = 12;
17    thrust::device_vector<int> out(nx);
18    thrust::device_vector<int> seq(nx);
19    thrust::sequence(seq.begin(),seq.end(),0);
20    thrust::device_vector<int> dx(x,x+nx);
21    thrust::device_vector<int>::iterator newend =
22       thrust::copy_if(dx.begin(),dx.end(),seq.begin(),out.begin(),iseven());
23    thrust::inclusive_scan(out.begin(),out.end(),out.begin());
24    // "out" should be 3,3+2 = 5,3+2+2=7,...
25    thrust::copy(out.begin(), newend,
26       std::ostream_iterator<int>(std::cout, " "));
27    std::cout << "\n";
28 }
```

10.7 Example: Moving Average

A *moving average* is defined as follows. With input $x_1, .., x_n$ and window width w, the output is $a_w, ..., a_n$, where

$$a_i = \frac{x_{i-w+1} + ... + x_i}{w} \tag{10.21}$$

The goal is to address the question, "What has the recent trend been?" at time i, $i = w, ..., n$.

10.7.1 Rth Code

Rth is an R interface to Thrust, for certain algorithms, including moving average, via the function **rthma()**. You can download it from `https://github.com/Rth-org/Rth`.

Below is the C++ code, contents of the file **rthma.cpp** in the **Rth** package. Before reading it, note that the **Rth** code here uses **Rcpp**, a very handy interface from R to C++.[2]

```
1 // Rth interface to Thrust moving-average example,
2 // simple_moving_average.cu in
3 // github.com/thrust/thrust/blob/master/examples/
4
5 // C++ code adapted from example in Thrust docs
6
7 #include <thrust/device_vector.h>
```

[2]Later versions of **Rth** do not use **Rcpp**.

```
 8 #include <thrust/scan.h>
 9 #include <thrust/transform.h>
10 #include <thrust/functional.h>
11 #include <thrust/sequence.h>
12 #include <Rcpp.h>  // Rcpp includes
13 #include "backend.h"  // from Rth
14
15 // update function, to calculate current moving average value from the
16 // previous one
17 struct minus_and_divide :
18    public thrust::binary_function<double,double,double>
19 {
20     double w;
21     minus_and_divide(double w) : w(w) {}
22     __host__ __device__
23     double operator()(const double& a, const double& b) const
24     { return (a - b) / w; }
25 };
26
27 // computes moving averages from x of window width w; SEXP ("S
28 // expression") is the name of the struct type used by R for internal
29 // storage of objects
30 RcppExport SEXP rthma(SEXP x, SEXP w, SEXP nthreads)
31 {
32    Rcpp::NumericVector xa(x);  // convert to C++ array
33    int wa = INTEGER(w)[0];  // convert this SEXP to int
34
35    #if RTH_OMP
36    omp_set_num_threads(INT(nthreads));
37    #elif RTH_TBB
38    tbb::task_scheduler_init init(INT(nthreads));
39    #endif
40
41    // set up device vector and copy xa to it
42    thrust::device_vector<double> dx(xa.begin(), xa.end());
43
44    int xas = xa.size();
45    if (xas < wa)
46        return 0;
47
48    // allocate device storage for cumulative sums, and compute them
49    thrust::device_vector<double> csums(xa.size() + 1);
50    thrust::exclusive_scan(dx.begin(), dx.end(), csums.begin());
51    // need one more sum at (actually past) the end
52    csums[xas] = xa[xas-1] + csums[xas-1];
53
54    // compute moving averages from cumulative sums
55    Rcpp::NumericVector xb(xas - wa + 1);
56    thrust::transform(csums.begin() + wa, csums.end(),
57       csums.begin(), xb.begin(), minus_and_divide(double(wa)));
```

```
58
59      return xb;
60  }
```

10.7.2 Algorithm

Again with the x_i as inputs, it first computes the cumulative sums c_i, using the Thrust function **exclusive_scan()**:

```
thrust::exclusive_scan(dx.begin(), dx.end(), csums.begin());
```

Here **dx** contains a copy of the x_i on the device (GPU or OpenMP/TBB), and **csums** will contain our cumulative sums c_i.

Since the numerator of (10.21) is

$$x_{i-w+1} + ... + x_i = c_i - c_{i-w} \tag{10.22}$$

We then need only compute these differences $c_i - c_{i-w}$and divide by w.

To do all this, we use Thrust's **transform()** function:

```
thrust::transform(csums.begin() + wa, csums.end(), csums.begin(),
   xb.begin(), minus_and_divide(double(wa)));
```

As the name implies, **transform()** takes one or more inputs, applies a user-specified transformation, and writes to an output vector. You can see that the first two arguments are first the c_i, shifted left by w, and then the c_i themselves. The functor computes the values in (10.22) and divides by w:

```
struct minus_and_divide :
   public thrust::binary_function<double,double,double>
{
    double w;
    minus_and_divide(double w) : w(w) {}
    __host__ __device__
    double operator()(const double& a, const double& b) const
    { return (a - b) / w; }
};
```

10.7.3 Use of Lambda Functions

If you have a compiler that allows C++11 *lambda functions*, these can make life much simpler for you if you use Thrust, TBB or anything that uses functors. Let's see how this would work with

our C++ function **rthma()** above (scroll down to "changed code").

```
1  #include <thrust/device_vector.h>
2  #include <thrust/scan.h>
3  #include <thrust/transform.h>
4  #include <thrust/functional.h>
5  #include <thrust/sequence.h>
6  #include <Rcpp.h>
7  #include "backend.h"  // from Rth
8
9  // struct minus_and_divide now deleted
10
11 RcppExport SEXP rthma(SEXP x, SEXP w, SEXP nthreads)
12 {
13    Rcpp::NumericVector xa(x);
14    int wa = INTEGER(w)[0];
15    #if RTH_OMP
16    omp_set_num_threads(INT(nthreads));
17    #elif RTH_TBB
18    tbb::task_scheduler_init init(INT(nthreads));
19    #endif
20    thrust::device_vector<double> dx(xa.begin(), xa.end());
21    int xas = xa.size();
22    if (xas < wa) return 0;
23    thrust::device_vector<double> csums(xa.size() + 1);
24    thrust::exclusive_scan(dx.begin(), dx.end(), csums.begin());
25    csums[xas] = xa[xas-1] + csums[xas-1];
26    Rcpp::NumericVector xb(xas - wa + 1);
27
28    // changed code
29    thrust::transform(csums.begin() + wa, csums.end(),
30       csums.begin(), xb.begin(),
31       // lambda function
32       [=] (double& a, double& b) {  return( (a-b)/wa);  });
33
34    return xb;
35 }
```

Just what is going on in the line

```
[=] (double& a, double& b) {  return( (a-b)/wa);  });
```

We are creating a function object here, as we did in the earlier version with an **operator()** notation within a **struct**. But here we are doing so right on the spot, in one of the arguments to **thrust::transform()**. It's similar to the concept of *anonymous* functions in R. Here are the details:

- The brackets in [=] tells the compiler that a function object is about to begin. (The = sign will be explained shortly.)

- The variable **wa** that was local to the function **rthma()** is considered "global" to our lambda function, thus accessible to it *without passing* **wa** *as an argument to that function).* (This too is similar to the R case.) We say that **wa** is *captured* by that function.

  The = indicates that we wish to use **wa** *by value*, i.e. just for its value alone, rather than it being a pointer that we wish to reference. If it had been the latter (with the capability of changing the pointed-to location), we'd use & instead of =.

- Here **a** and **b** are ordinary arguments.

All this is so much clearer and cleaner than using a functor!

By the way, in using **g++** for the compilation, I did need to add the **-std=c++11** compiler flag to use lambda functions.

Chapter 11

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

$$A = \begin{pmatrix} 1 & 5 & 12 \\ 0 & 3 & 6 \\ 4 & 8 & 2 \end{pmatrix} \tag{11.1}$$

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

$$B_{10} = \begin{pmatrix} 1 & 1 \end{pmatrix}. \tag{11.11}$$

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.

11.3.1.1 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.

11.3.1.2 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

11.3.2.1 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.

11.3.2.2 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

$$C_{00} = A_{00}B_{00} + A_{01}B_{10} + A_{02}B_{20} \tag{11.18}$$

$$= \begin{pmatrix} 1 & 2 \\ 7 & 8 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 5 & 6 \end{pmatrix} + ... \tag{11.19}$$

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:

```
int c = (dc_wB * BLOCK_SIZE * by) + (BLOCK_SIZE*bx);
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 1.6.3.1 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 (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.

(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

So, matrix powers can help use determine graph connectivity. Another application of matrix powers is Fibonacci numbers.

The basic problem is well known: Find the Fibonacci numbers f_n, where

$$f_0 = f_1 = 1 \tag{11.27}$$

and

$$f_n = f_{n-1} + f_{n-2},\ n > 1 \tag{11.28}$$

The point is that (11.28) can be couched in matrix terms as

$$\begin{pmatrix} f_{n+1} \\ f_n \end{pmatrix} = A \begin{pmatrix} f_n \\ f_{n-1} \end{pmatrix} \tag{11.29}$$

where

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{11.30}$$

Given the initial conditions (11.27) and (11.29), we have

$$\begin{pmatrix} f_{n+1} \\ f_n \end{pmatrix} = A^{n-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{11.31}$$

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 also a power series method.

Recall that for numbers x that are smaller than 1 in absolute value,

$$\frac{1}{1-x} = 1 + x + x^2 + ... \tag{11.32}$$

In algebraic terms, this would be that for an n x n matrix C,

$$(I - C)^{-1} = I + C + C^2 + ... \tag{11.33}$$

This can be shown to converge if

$$\sum_{i,j} c_{ij}^2 | < 1 \tag{11.34}$$

To invert our matrix A, then, we can set C = I - A, giving us

$$A^{-1} = (I - C)^{-1} = I + C + C^2 + ... = I + (I - A) + (I - A)^2 + ... \tag{11.35}$$

To meet the convergence condition, we could set $\tilde{A} = dA$, where d is small enough so that (11.34) 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.

Serial matrix multiplication has time complexity $O(n^3)$, and so does matrix inversion. So the above trick does not save time in the serial case, but since matrix multiplication is much more effectively parallelized than is matrix inversion, it may pay off.

11.4.4 Parallel Computation

So, how can we speed up the computation of matrix powers? Of course, our primary tools are the parallel methods for matrix multiplication seen earlier.

For the case in which we want only one power, 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.

11.5 Solving Systems of Linear Equations

Suppose we have a system of equations

$$a_{i0}x_0 + ... + a_{i,n-1}x_{n-1} = b_i, i = 0, 1, ..., n-1, \tag{11.36}$$

where the x_i are the unknowns to be solved for.

As you know, this system can be represented compactly as

$$Ax = b, \tag{11.37}$$

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

Below is CUDA code for the reduced row echelon form version. As with much of the CUDA code in this book, we have sacrificed speed for clarity, in this case using only one block.

```
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 (11.36) as

$$x_i = \frac{1}{a_{ii}}[b_i - (a_{i0}x_0 + ... + a_{i,i-1}x_{i-1} + a_{i,i+1}x_{i+1} + ... + a_{i,n-1}x_{n-1})], i = 0, 1, ..., n-1. \quad (11.38)$$

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 kth iteration, we find our (k+1)st guess by plugging in our kth guess into the right-hand side of (11.38). 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 (11.38) can be expressed as

$$x^{(k+1)} = D^{-1}(b - Ox^{(k)}) \tag{11.39}$$

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 ithiteration. 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:

```
1  #include <omp.h>
2
3  // partitions s..e into nc chunks, placing the ith in first and last (i
4  // = 0,...,nc-1)
5  void chunker(int s, int e, int nc, int i, int *first, int *last)
6  {  int chunksize = (e-s+1) / nc;
7     *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

$$x^{(k)} = \frac{A^k x}{\parallel A^k x \parallel} \tag{11.40}$$

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

$$B = A - \lambda_1 v_1 v_1' \tag{11.41}$$

where we've now scaled v_1 to have length 1.

Then

$$
\begin{aligned}
Bv_1 &= Av_1 - \lambda_1 v1(v_1' v_1) && (11.42)\\
&= \lambda_1 v_1 - \lambda_1 v1(1) && (11.43)\\
&= 0 && (11.44)
\end{aligned}
$$

and for $i > 0$,

$$
\begin{aligned}
Bv_i &= Av_i - \lambda_1 v1(v_1' v_i) && (11.45)\\
&= \lambda_i v_i - \lambda_1 v1(0) && (11.46)\\
&= \lambda_i v_i && (11.47)
\end{aligned}
$$

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 (11.40). 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

[1] The term *singular value* is a synonym for *eigenvalue*.

either on the diagonal or on subdiagonals just below or above the diagonal, and all other elements are guaranteed to be 0, such as

$$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 1 & 1 & 8 & 0 & 0 \\ 0 & 1 & 5 & 8 & 0 \\ 0 & 0 & 0 & 8 & 8 \\ 0 & 0 & 0 & 3 & 5 \end{pmatrix} \tag{11.48}$$

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 (11.48) (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 PLAPACK.

For multicore machines, OpenBLAS provides a very fast implementation of basic matrix operations, using OpenMP. Note that R users can replace the built-in BLAS by OpenBLAS, thus automatically getting big speedups for large matrices.

Chapter 12

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 sorted 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:

```
for i = d downto 1
   for each i-cube:
      root of the i-cube broadcasts its median to all in the i-cube,
         to serve as pivot
      consider the two (i-1)-subcubes of this i-cube
```

[1] See Chapter 7 for definitions of hypercube terms.

```
each pair of partners in the (i-1)-subcubes exchanges data:
   low-numbered PE gives its partner its data larger than pivot
   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.

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:

```
do
   if my left-child datum < my right-child datum
      pass my left-child datum to my parent
   else
      pass my right-child datum to my parent
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:

```
send all my data to partner
receive all my partner's data
if I have a lower id than my partner
   I keep the lower half of the pooled data
else
   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:

```
1  // x is bitonic of length n, n a power of 2
2  void sortbitonic(int *x, int n)
3  {  do the pairwise compare-exchange operations
4     if (n > 2) {
5        sortbitonic(x,n/2);
6        sortbitonic(x+n/2,n/2);
7     }
8  }
```

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**:

```
1  void bubblesort(int *x, int n)
2  {  for i = n-1 downto 1
3        for j = 0 to i
4           compare-exchange(x,i,j,n)
5  }
```

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:

```
1  // the argument "me" is this thread's ID
2  void oddevensort(int *x, int n, int me)
3  {  for i = 1 to n
4        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. Below is the pseudocode for the case of n, the array length, being a perfect square (row numbers start at 1).

```
1  for i = 1 to ceiling(log2(n)) + 1
2      if i is odd
3         sort each even row in descending order
4         sort each odd row in ascending order
5      else
6         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 1.6.1.1. Here is similar MPI code below (various improvements could be made, e.g. with broadcast):

```
1  // bucket sort, bin boundaries known in advance
2
3  // node 0 is manager, all else worker nodes; node 0 sends full data, bin
4  // boundaries to all worker nodes; i-th worker node extracts data for
5  // bin i-1, sorts it, sends sorted chunk back to node 0; node 0 places
6  // sorted results back in original array
7
8  // not claimed efficient; e.g. could be better to have manager place
9  // items into bins
10
11 #include <mpi.h>
12
13 #define MAX_N 100000  // max size of original data array
14 #define MAX_NPROCS 100  // max number of MPI processes
15 #define DATA_MSG 0  // manager sending original data
16 #define BDRIES_MSG 0  // manager sending bin boundaries
17 #define CHUNKS_MSG 2  // workers sending their sorted chunks
18
19 int nnodes,  //
20     n,  // size of full array
21     me,  // my node number
22     fulldata[MAX_N],
23     tmp[MAX_N],
24     nbdries,  // number of bin boundaries
25     counts[MAX_NPROCS];
26 float bdries[MAX_NPROCS-2];  // bin boundaries
27
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 $\mathbf{x}$, which for convenience we assume contains no tied values. Then the pseudocode for this algorithm, placing the results in $\mathbf{y}$, is

```
for all i in 0...n-1:
   count = 0
   elt = x[i]
   for all j in 0...n-1:
      if x[j] < elt then count++
   y[count] = elt
```

The outer (or inner) loop is easily parallelized.

Chapter 13

Parallel Computation for Audio and Image Processing

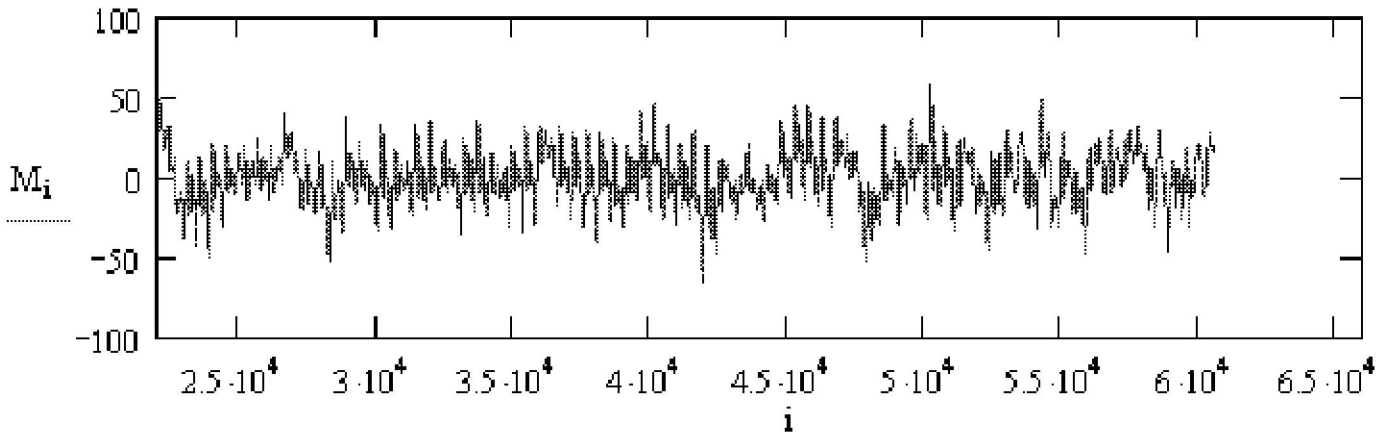
Mathematical computations involving images can become quite intensive, and thus parallel methods are of great interest. Here we will be primarily interested in methods involving **Fourier** analysis.

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]

[1]Reproduced here by permission of Prof. Peter Hamburger, Indiana-Purdue University, Fort Wayne. See http://www.ipfw.edu/math/Workshop/PBC.html



Recall that we say a function of time g(t) is **periodic** ("repeating," in our casual wording above) 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 nf_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.

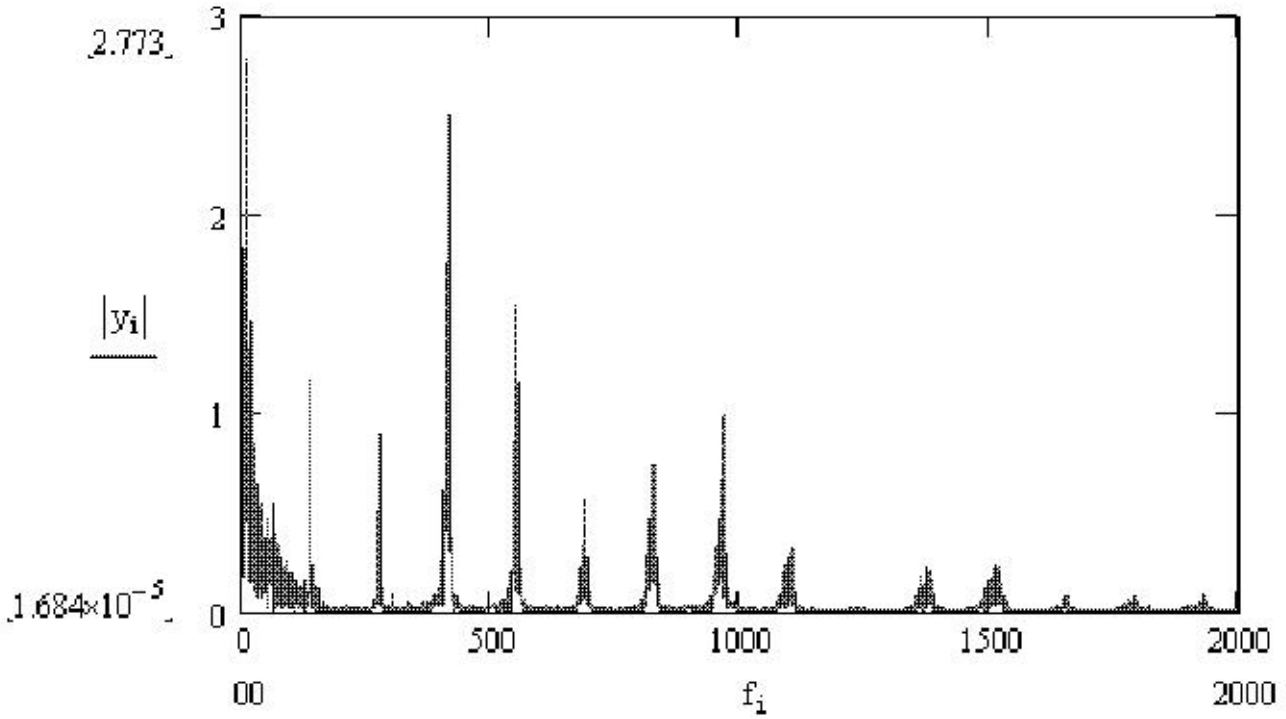
Since g(t) is a graph of loudness against time, this representation of the sound is called the **time domain**. When we find the Fourier series of the sound, the set of weights a_n and b_n is said to be a

[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.

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:



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]

[3]There is basically no physical interpretation of complex numbers. Instead, they are just mathematical abstrac-

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.

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

tions. 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.

[4] See Section 13.10 for the reasons behind this.

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:

$$c_k = \frac{1}{n} \sum_{j=0}^{n-1} x_j e^{-2\pi ijk/n} = \frac{1}{n} \sum_{j=0}^{n-1} x_j q^{jk} \tag{13.13}$$

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 n^{th} 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

$$C = \frac{1}{n} AX, \tag{13.16}$$

[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.

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:

```
makeamat <- function(n,u)  {
   m <- matrix(nrow=n,ncol=n)
   for (i in 1:n) {
      for (j in i:n) {
         if (i == j) {
            m[i,i] <- u^((i-1)^2)
         }
         else {
            m[i,j] <- u^((i-1)*(j-1))
            m[j,i] <- m[i,j]
         }
      }
   }
   m
}
```

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).

13.2.2.1 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

$$C = \frac{1}{n} AX \tag{13.25}$$

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:

$$c_{rs} = \frac{1}{n} \sum_{j=0}^{n-1} \left(\frac{1}{m} \sum_{k=0}^{m-1} x_{jk} e^{-2\pi i (\frac{ks}{m})} \right) e^{-2\pi i (\frac{jr}{n})} \tag{13.26}$$

$$= \frac{1}{n} \sum_{j=0}^{n-1} y_{js} e^{-2\pi i (\frac{jr}{n})} \tag{13.27}$$

Note that y_{js}, i.e. the expression between the large parentheses, is the s^{th} component of the DFT of the j^{th} 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.

[6] In fact, one can obtain the new matrix easily from the old, as explained in Section 13.9.

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 **??**. 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).

```
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  }
```

[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.

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"),

$$[u,w] = \frac{1}{n}\sum_{j=0}^{n-1} u_j \bar{w}_j. \tag{13.29}$$

[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.

Define

$$v_h = (1, q^{-h}, q^{-2h}, ..., q^{-(n-1)h}), h = 0, 1, ..., n-1. \tag{13.30}$$

Then it turns out that the v_h form an orthonormal basis for V.[11] 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.

[11] 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}.

[12] And in fact will probably be deliberately filtered out.

The radio and TV frequency ranges are large also, which is why, for example, we can have many 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.

Chapter 14

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]

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 i^{th} 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.

[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.

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 = φ
    for each I in F_{i-1}
        for each K in F_1
            Q = I ∪ K
            if support(Q) exceeds support threshold
              add Q to F_i
    if F_i is empty break
return ∪_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 ^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

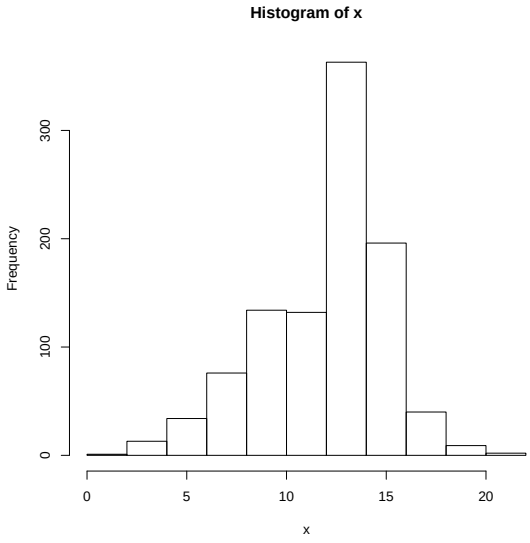
[3]Some statistical programs will choose default values, based on theory.

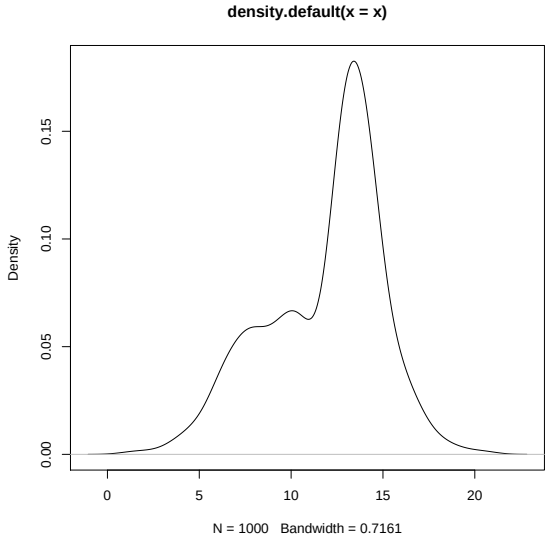
weight in our estimation of f(25.8). Well, it won't have much weight at all, because the quantity

$$u = \frac{25.8 - 88}{6} \tag{14.4}$$

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:





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.

[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

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:

```
for i = 1,...,numintenslevels:
   count = 0
   for row = 1,...,numrows:
      for col = 1,...,numcols:
         if image[row][col] == i: count++
   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.

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 i^{th} 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 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.

The subhistograms will be stored together in a two-dimensional array, the j^{th} 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.

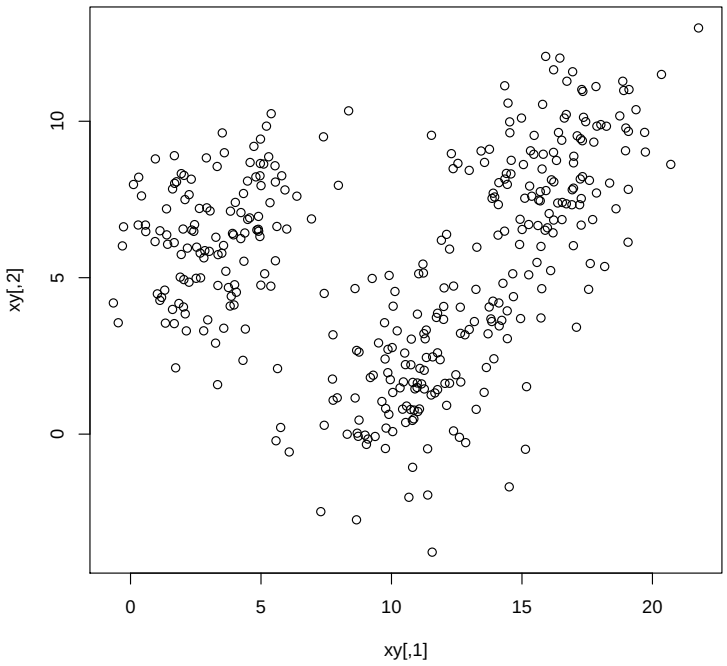
In the end, the many subhistograms within a block must be merged, and those merged counts must in turn be merged across all blocks. The former operation is done again by careful ordering to avoid any bank conflicts, and then the latter is done **atomicAdd()**.

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:
```

```
   for j = 1,...,n:
      find the closest center[i] to (x[j],y[j])
      cl[j] = the i you got in the previous line
   for i = 1,...,k:
      group[i] = all (x[j],y[j]) such that cl[j] = i
      center[i] = average of all (x,y) in group[i]
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

$$\sqrt{(b_1 - a_1)^2 + ... + (b_p - a_p)^2} \tag{14.6}$$

  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:

```
# 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) {
```

```
19      ngrps <- nrow(currctrs)
20      spacedim <- ncol(currctrs)  # what dimension space are we in?
21      # set up the return matrix
22      sumcounts <- matrix(rep(0,ngrps*(spacedim+1)),nrow=ngrps)
23      for (i in 1:nrow(mchunk)) {
24          dsts <- dst(mchunk[i,],t(currctrs))
25          j <- which.min(dsts)
26          sumcounts[j,] <- sumcounts[j,] + c(mchunk[i,],1)
27      }
28      sumcounts
29  }
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.

Appendix A

Miscellaneous Systems Issues

The material in this appendix pops up often throughout the book, so it's worth the time spent. For further details, see my computer systems book, `http://heather.cs.ucdavis.edu/~matloff/50/PLN/CompSystsBook.pdf`.

A.1 Timesharing

A.1.1 Many Processes, Taking Turns

Suppose you and someone else are both using the computer **pc12** in our lab, one of you at the console and the other logged in remotely. Suppose further that the other person's program will run for five hours! You don't want to wait five hours for the other person's program to end. So, the OS arranges things so that the two programs will take turns running, neither of them running to completion all at once. It won't be visible to you, but that is what happens.

Timesharing involves having several programs running in what appears to be a simultaneous manner. (These programs could be from different users or the same user; in our case with threaded code, several processes actually come from a single invocation of a program.) If the system has only one CPU, which we'll assume temporarily, this simultaneity is of course only an illusion, since only one program can run at any given time, but it is a worthwhile illusion, as we will see.

First of all, how is this illusion attained? The answer is that we have the programs all take turns running, with each turn—called a **quantum** or **timeslice**—being of very short duration, for example 50 milliseconds. (We'll continue to assume 50 ms quanta below.)

Say we have four programs, **u**, **v**, **x** and **y**, running currently. What will happen is that first **u** runs for 50 milliseconds, then **u** is suspended and **v** runs for 50 milliseconds, then **v** is suspended

and **x** runs for 50 milliseconds, and so on. After **y** gets its turn, then **u** gets a second turn, etc. Since the turn-switching, formally known as **context-switching**,[1] is happening so fast (every 50 milliseconds), it appears to us humans that each program is running continuously (though at one-fourth speed), rather than on and off, on and off, etc.[2]

But how can the OS enforce these quanta? For example, how can the OS force the program **u** above to stop after 50 milliseconds? The answer is, "It can't! The OS is dead while **u** is running." Instead, the turns are implemented via a timing device, which emits a hardware interrupt at the proper time. For example, we could set the timer to emit an interrupt every 50 milliseconds. When the timer goes off, it sends a pulse of current (the interrupt) to the CPU, which is wired up to suspend its current process and jump to the driver of the interrupting device (here, the timer). Since the driver is in the OS, the OS is now running!

We will make such an assumption here. However, what is more common is to have the timer interrupt more frequently than the desired quantum size. On a PC, the 8253 timer interrupts 100 times per second. Every sixth interrupt, the OS will perform a context switch. That results in a quantum size of 60 milliseconds. But this can be changed, simply by changing the count of interrupts needed to trigger a context switch.

The timer device driver saves all **u**'s current register values, including its Program Counter value (the address of the current instruciton) and the value in its EFLAGS register (flags that record, for instance, whether the last instruction produced a 0 result). Later, when **u**'s next turn comes, those values will be restored, and **u** including its PC value and the value in its EFLAGS register. Later, when **u**'s next turn comes, those values will be restored, and **u** will resume execution as if nothing ever happened. For now, though, the OS routine will restore **v**'s's previously-saved register values, making sure to restore the PC value last of all. That last action forces a jump from the OS to **v**, right at the spot in **v** where **v** was suspended at the end of its last quantum. (Again, the CPU just "minds its own business," and does not "know" that one program, the OS, has handed over control to another, **v**; the CPU just keeps performing its fetch/execute cycle, fetching whatever the PC points to, oblivious to which process is running.)

A process' turn can end early, if the current process voluntarily gives us control of the CPU. Say the process reaches a point at which it is supposed to read from the keyboard, with the source code calling, say, **scanf()** or **cin**. The process will make a systems call to do this (the compiler placed that there), which means the OS will now be running! The OS will mark this process as being in Sleep state, meaning that it's waiting for some action. Later, when the user for that process hits a key, it will cause an interrupt, and since the OS contains the keyboard device driver, this means the OS will then start running. The OS will change the process' entry in the process table from Sleep to Run—meaning only that it is ready to be given a turn. Eventually, after some other process'

[1] We are switching from the "context" of one program to another.

[2] Think of a light bulb turning on and off extremely rapidly, with half the time on and half off. If it is blinking rapidly enough, you won't see it go on and off. You'll simply see it as shining steadily at half brightness.

turn ends, the OS will give this process its next turn.

On a multicore machine, several processes can be physically running at the same time, but the operation is the same as above. On a Linux system, to see all the currently running threads, type

```
ps -eLf
```

A.2 Memory Hierarchies

A.2.1 Cache Memory

Memory (RAM) is usually not on the processor chip, which makes it "far away." Signals must go through thicker wires than the tiny ones inside the chip, which slows things down. And of course the signal does have to travel further. All this still occurs quite quickly by human standards, but not relative to the blinding speeds of modern CPUs.

Accordingly, a section of the CPU chip is reserved for a **cache**, which at any given time contains a copy of part of memory. If the requested item (say **x** above) is found in the cache, the CPU is in luck, and access is quick; this is called a **cache hit**. If the CPU is not lucky (a **cache miss**), it must bring in the requested item from memory.

Caches organize memory by chunks called **blocks**. When a cache miss occurs, the entire block containing the requested item is brought into the cache. Typically a block currently in the cache must be **evicted** to make room for the new one.

A.2.2 Virtual Memory

Most modern processor chips have virtual memory (VM) capability, and most general-purpose OSs make use of it.

A.2.2.1 Make Sure You Understand the Goals

VM has the following basic goals:

- **Overcome limitations on memory size:**

  We want to be able to run a program, or collectively several programs, whose memory needs are larger than the amount of physical memory available.

- **Relieve the compiler and linker of having to deal with real addresses**

We want to facilitate **relocation** of programs, meaning that the compiler and linker do not have to worry about where in memory a program will be loaded when it is run. They can, say, arrange for every program to be loaded into memory starting at address 20200, without fear of conflict, as the actualy address will be different.

- **Enable security:**

  We want to ensure that one program will not accidentally (or intentionally) harm another program's operation by writing to the latter's area of memory, read or write to another program's I/O streams, etc.

A.2.2.2 How It Works

Suppose a variable **x** has the virtual address 1288, i.e. **&x = 1288** in a C/C++ program. But, when the OS loads the program into memory for execution, it rearranges everything, and the actual physical address of **x** may be, say, 5088.

The high-order bits of an address are considered to be the **page number** of that address, with the lower bits being the **offset** within the page. For any given item such as **x**, the offset is the same in both its virtual and physical addresses, but the page number differs.

To illustrate this simply, suppose that our machine uses base-10 numbering instead of base-2, and that page size is 100 bytes. Then **x** above would be in offset 88 of virtual page 12. Its physical page would be 50, with the same offset. In other words, **x** is stored 88 bytes past the beginning of page 50 in memory.

The correspondences between virtual and physical page numbers is given in the **page table**, which is simply an array in the OS. The OS will set up this array at the time it loads the program into memory, so that the virtual-to-physical address translations can be done.

Those translations are done by the hardware. When the CPU executes a machine instruction that specifies access to 1288, the CPU will do a lookup on the **page table**, in the entry for virtual page 12, and find that the actual page is 50. The CPU will then know that the true location is 5088, and it would place 5088 in the address lines in the system bus to then access 5088.

On the other hand, **x** may not currently be **resident** in memory at all, in which case the page table will mark it as such. If the CPU finds that page 12 is nonresident, we say a **page fault** occurs, and this will cause an internal interrupt, which in turn will cause a jump to the operating system (OS). The OS will then read the page containing **x** in from disk, place it somewhere in memory, and then update the page table to show that virtual page 12 is now in some physical page in memory. The OS will then execute an interrupt return instruction, and the CPU will restart the instruction which triggered the page fault.

A.2.3 Performance Issues

Upon a cache miss, the hardware will need to read an entire block from memory, and if an eviction is involved, an entire block will be written as well, assuming a **write-back** policy. (See the reference at the beginning of this appendix.) All this is obviously slow.

The cache[3] is quite small relative to memory, so you might guess that cache misses are very frequent. Actually, though, they aren't, due to something called **locality of reference**. This term refers to the fact that most programs tend to either access the same memory item repeatedly within short time periods (**temporal** locality), and/or access items within the same block often during short periods (**spatial** locality). Hit rates are typically well above 90%. Part of this depends on having a good **block replacement policy**, which decides which block to evict (hopefully one that won't be needed again soon!).

A page fault is pretty catastrophic in performance terms. Remember, the disk speed is on a mechanical scale, not an electronic one, so it will take quite a while for the OS to service a page fault, much worse than for a cache miss. So the page replacement policy is even more important as well.

On Unix-family machines, the **time** command not only tells how long your program ran, but also how many page faults it caused. Note that since the OS runs every time a page fault occurs, it can keep track of the number of faults. This is very different from a cache miss, which although seems similar to a page fault in many ways, the key point is that a cache miss is handled solely in hardware, so no program can count the number of misses.[4]

Note that in a VM system each memory access becomes two memory accesses—the page table read and the memory access itself. This would kill performance, so there is a special cache just for the page table, called the Translation Lookaside Buffer.

A.3 Array Issues

A.3.1 Storage

It is important to understand how compilers store arrays in memory, an overview of which will now be presented.

Consider the array declaration

```
int y[100];
```

[3] Or caches, plural, as there are often multiple levels of caches in today's machines.

[4] Note by the way that cache misses, though harmful to program speed, aren't as catastrophic as page faults, as the disk is not involved.

The compiler will store this in 100 consecutive words of memory. You may recall that in C/C++, an expression consisting of an array name, no subscript, is a pointer to the array. Well, more specifically, it is the address of the first element of the array.

An array element, say `y[8]` actually means the same as the C/C++ pointer expression `y+8`, which in turn means "the word 8 **int**s past the beginning of **y**."

Two-dimensional arrays, say

```
int z[3][10];
```

exist only in our imagination. They are actually treated as one-dimensional arrays, in the above case consisting of $3 \times 10 = 30$ elements. C/C++ arranges this in **row-major** order, meaning that all of row 0 comes first, then all of row 1 and so on. So for instance `z[2][5]` is stored in element $10 + 10 + 5$ of **z**, and we could for example set that element to 8 with the code

```
z[25] = 8;
```

or

```
*(z+25) = 8;
```

Note that if we have a c-column two-dimensional array, element (i,j) is stored in the word $i \times c + j$ of the array. You'll see this fact used a lot in this book, and in general in code written in the parallel processing community.

A.3.2 Subarrays

The considerations in the last section can be used to access subarrays. For example, here is code to find the sum of a **float** array of length k:

```
1  float sum(float x,int k)
2  {  float s = 0.0; int i;
3     for (i = 0; i < k; i++) s += x[i];
4     return s;
5  }
```

Quite ordinary, but suppose we wish to find the sum in row 2 of the two-dimensional array **z** above. We could do this as `sum(z+20,10)`.

A.3.3 Memory Allocation

Very often one needs to set up an array whose size is not known at compile time. You are probably accustomed to doing this via **malloc()** or **new**. However, in large parallel programs, this approach may be quite slow.

With an array with size known at compile time, and which is declared local to some function, it will be allocated on the stack and you might run out of stack space. The easiest solution is probably to make the array global, of fixed size.

To accommodate larger arrays under **gcc** on a 64-bit system, use the **-mcmodel=medium** command line option.

Appendix B

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.

B.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

$$\| X \| = \sqrt{\sum_{i=1}^{n} x_i^2} \tag{B.1}$$

B.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.

$$\begin{pmatrix} 1 & 5 \\ 0 & 3 \\ 4 & 8 \end{pmatrix} + \begin{pmatrix} 6 & 2 \\ 0 & 1 \\ 4 & 0 \end{pmatrix} = \begin{pmatrix} 7 & 7 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \tag{B.2}$$

- Multiplication of a matrix by a **scalar**, i.e., a number, is also defined elementwise, e.g.

$$0.4 \begin{pmatrix} 7 & 7 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} = \begin{pmatrix} 2.8 & 2.8 \\ 0 & 1.6 \\ 3.2 & 3.2 \end{pmatrix} \tag{B.3}$$

- The **inner product** or **dot product** of equal-length vectors X and Y is defined to be

$$\sum_{k=1}^{n} x_k y_k \tag{B.4}$$

- 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

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{B.5}$$

  For instance,

$$\begin{pmatrix} 7 & 6 \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \begin{pmatrix} 1 & 6 \\ 2 & 4 \end{pmatrix} = \begin{pmatrix} 19 & 66 \\ 8 & 16 \\ 24 & 80 \end{pmatrix} \tag{B.6}$$

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:

$$\begin{pmatrix} \mathbf{7} & \mathbf{6} \\ 0 & 4 \\ 8 & 8 \end{pmatrix} \begin{pmatrix} \mathbf{1} & 6 \\ \mathbf{2} & 4 \end{pmatrix} = \begin{pmatrix} \mathbf{1}9 & 66 \\ 8 & 16 \\ 24 & 80 \end{pmatrix} \tag{B.7}$$

- Matrix multiplication is associative and distributive, but in general not commutative:

$$A(BC) = (AB)C \tag{B.8}$$

$$A(B + C) = AB + AC \tag{B.9}$$

$$AB \neq BA \tag{B.10}$$

B.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.

$$\begin{pmatrix} 7 & 70 \\ 8 & 16 \\ 8 & 80 \end{pmatrix}' = \begin{pmatrix} 7 & 8 & 8 \\ 70 & 16 & 80 \end{pmatrix} \tag{B.11}$$

- If $A + B$ is defined, then

$$(A + B)' = A' + B' \tag{B.12}$$

- If A and B are conformable, then

$$(AB)' = B'A' \tag{B.13}$$

B.3 Linear Independence

Equal-length vectors X_1,...,X_k are said to be **linearly independent** if it is impossible for

$$a_1X_1 + ... + a_kX_k = 0 \tag{B.14}$$

unless all the a_i are 0.

B.4 Determinants

Let A be an $n \times n$ 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 jth column. Then the determinant can be computed recursively across the kth row of A as

$$det(A) = \sum_{m=1}^{n} (-1)^{k+m} det(A_{-(k,m)}) \tag{B.15}$$

where

$$det \begin{pmatrix} s & t \\ u & v \end{pmatrix} = sv - tu \tag{B.16}$$

Generally, determinants are mainly of theoretical importance, but they often can clarify one's understanding of concepts.

B.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

$$(AB)^{-1} = B^{-1}A^{-1} \tag{B.17}$$

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 obtained 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 invertible, A^{-1} is easily found:

$$A^{-1} = (QR)^{-1} = R^{-1}Q' \tag{B.18}$$

Again, though, in some cases A is part of a more complex system, and the inverse is not explicitly computed.

B.6 Eigenvalues and Eigenvectors

Let A be a square matrix.[1]

- A scalar λ and a nonzero vector X that satisfy

$$AX = \lambda X \tag{B.19}$$

  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

$$U'AU = D \tag{B.20}$$

  for a diagonal matrix D. The elements of D are the eigenvalues of A, and the columns of U are the eigenvectors of A.

[1] For nonsquare matrices, the discussion here would generalize to the topic of **singular value decomposition**.

A different sufficient condition for B.20 is that the eigenvalues of A are distinct. In this case, U will not necessarily be orthogonal.

By the way, this latter sufficient condition shows that "most" square matrices are diagonalizable, if we treat their entries as continous random variables. Under such a circumstance, the probability of having repeated eigenvalues would be 0.

B.7 Rank of a Matrix

Definition: The rank of a matrix A is the maximal number of linearly independent columns in A.

Let's denote the rank of A by rk(A). Rank has the following properties:

- rk(A') = rk(A)
- Thus the rank of A is also the maximal number of linearly independent rows in A.
- Let A be $r \times s$. Then

$$\text{rk}(A) \leq \min(r, s) \tag{B.21}$$

- rk($A'A$) = rk(A)

B.8 Matrix Algebra in R

The R programming language has extensive facilities for matrix algebra, introduced here. Note by the way that R uses column-major order.

A linear algebra vector can be formed as an R vector, or as a one-row or one-column matrix.

```
> # constructing matrices
> a <- rbind(1:3,10:12)
> a
     [,1] [,2] [,3]
[1,]    1    2    3
[2,]   10   11   12
> b <- matrix(1:9,ncol=3)
> b
     [,1] [,2] [,3]
[1,]    1    4    7
[2,]    2    5    8
[3,]    3    6    9
# multiplication, etc.
```

```
> c <- a %*% b; c + matrix(c(1,-1,0,0,3,8),nrow=2)
     [,1] [,2] [,3]
[1,]   15   32   53
[2,]   67  167  274
> c %*% c(1,5,6)  # note 2 different c's
     [,1]
[1,]  474
# be careful! -- if you extract a submatrix that ends up
# consisting of a single row, the result will be a vector
# rather than a matrix, unless one specifies drop = FALSE:
> x <- rbind(3:5,c(6,2,9),c(5,12,13))
> class(x[1,])
[1] "numeric"
> x[1,]
[1] 3 4 5
> class(x[1,,drop=FALSE])
[1] "matrix"
> x[1,,drop=FALSE]
     [,1] [,2] [,3]
[1,]    3    4    5
> # transpose, inverse
> t(a)  # transpose
     [,1] [,2]
[1,]    1   10
[2,]    2   11
[3,]    3   12
> u <- matrix(runif(9),nrow=3)
> u
          [,1]      [,2]      [,3]
[1,] 0.08446154 0.86335270 0.6962092
[2,] 0.31174324 0.35352138 0.7310355
[3,] 0.56182226 0.02375487 0.2950227
> uinv <- solve(u)
> uinv
          [,1]      [,2]      [,3]
[1,]  0.5818482 -1.594123  2.576995
[2,]  2.1333965 -2.451237  1.039415
[3,] -1.2798127  3.233115 -1.601586
> u %*% uinv  # note roundoff error
             [,1]          [,2]          [,3]
[1,] 1.000000e+00 -1.680513e-16 -2.283330e-16
[2,] 6.651580e-17  1.000000e+00  4.412703e-17
[3,] 2.287667e-17 -3.539920e-17  1.000000e+00
> # eigenvalues and eigenvectors
> eigen(u)
$values
[1]  1.2456220+0.0000000i -0.2563082+0.2329172i
-0.2563082-0.2329172i

$vectors
```

```
                [,1]                          [,2]                          [,3]
[1,] -0.6901599+0i  -0.6537478+0.0000000i
-0.6537478+0.0000000i
[2,] -0.5874584+0i  -0.1989163-0.3827132i
-0.1989163+0.3827132i
[3,] -0.4225778+0i   0.5666579+0.2558820i
0.5666579-0.2558820i
> # diagonal matrices (off-diagonals 0)
> diag(3)
     [,1] [,2] [,3]
[1,]    1    0    0
[2,]    0    1    0
[3,]    0    0    1
> diag((c(5,12,13)))
     [,1] [,2] [,3]
[1,]    5    0    0
[2,]    0   12    0
[3,]    0    0   13
```

We can obtain matrix inverse using **solve()**, e.g.

```
> m <- rbind(1:2,3:4)
> m
     [,1] [,2]
[1,]    1    2
[2,]    3    4
> minv <- solve(m)
> minv
     [,1] [,2]
[1,] -2.0  1.0
[2,]  1.5 -0.5
> m %*% minv  # should get I back
     [,1]          [,2]
[1,]    1 1.110223e-16
[2,]    0 1.000000e+00
```

Note the roundoff error, even with this small matrix. We can try the QR method, provided to us in R via **qr()**. In fact, if we just want the inverse, **qr.solve()** will compute (B.18) for us.

We can in principle obtain rank from, for example, the **rank** component from the output of **qr()**. Note however that although rank is clearly defined in theory, the presence of roundoff error in computation make may rank difficult to determine reliably.

Appendix C

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//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.).

C.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, logical
logical values	true, false	TRUE, FALSE (abbreviated T, F)
mechanism for combining modules	include, link	library()
run method	batch	interactive, batch
comment symbol	//	#

C.2 Starting R

To invoke R, just type "R" into a terminal window, e.g. **xterm** in Linux or Macs, **CMD** in Windows.

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.[1]

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!" For batch work, use **Rscript**, which is in the R package.

C.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. This is actually preferred style in the R community.

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.[2]

```
1 > source("odd.R")  # load code from the given file
2 > ls()  # what objects do we have?
```

[1] I personally use **vim**, as I want to have the same text editor no matter what kind of work I am doing. But I have my own macros to help with R work.

[2] 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
```

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**.

C.4 Vectorization

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
```

C.5 Second Sample Programming Session

A matrix is a special case of a vector, with added class attributes, the numbers of rows and columns.

```
> # "rowbind() function combines rows of matrices; there's a cbind() too
> m1 <- rbind(1:2,c(5,8))
> m1
     [,1] [,2]
[1,]    1    2
[2,]    5    8
> rbind(m1,c(6,-1))
     [,1] [,2]
[1,]    1    2
[2,]    5    8
[3,]    6   -1

> # form matrix from 1,2,3,4,5,6, in 2 rows; R uses column-major storage
> m2 <- matrix(1:6,nrow=2)
> m2
     [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6
> ncol(m2)
[1] 3
> nrow(m2)
[1] 2
> m2[2,3]  # extract element in row 2, col 3
[1] 6
# get submatrix of m2, cols 2 and 3, any row
> m3 <- m2[,2:3]
> m3
     [,1] [,2]
[1,]    3    5
[2,]    4    6

> m1 * m3  # elementwise multiplication
     [,1] [,2]
[1,]    3   10
[2,]   20   48
> 2.5 * m3  # scalar multiplication (but see below)
     [,1] [,2]
[1,]  7.5 12.5
[2,] 10.0 15.0
> m1 %*% m3  # linear algebra matrix multiplication
     [,1] [,2]
[1,]   11   17
[2,]   47   73

> # matrices are special cases of vectors, so can treat them as vectors
> 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
```

C.6 Recycling

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

$$\begin{pmatrix} 2.5 & 2.5 \\ 2.5 & 2.5 \end{pmatrix} \tag{C.1}$$

in order to conform with **m3** for (elementwise) multiplication.

C.7 More on Vectorization

The **ifelse()** function is another example of vectorization. Its call has the form

```
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,

```
> ifelse(m2 %%3 == 1,0,m2) # (see below)
```

the expression `m2 %%3 == 1` evaluated to the boolean matrix

$$\begin{pmatrix} T & F & F \\ F & T & F \end{pmatrix} \tag{C.2}$$

(TRUE and FALSE may be abbreviated to T and F.)

The 0 was recycled to the matrix

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{C.3}$$

while **vectorexpression3**, **m2**, evaluated to itself.

C.8 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]
[1,]  6.0 -1.0
[2,] -2.5  0.5
```

C.9 Default Argument Values

Consider the **sort()** function, which is built-in to R, though the following points hold for any function, including ones you write yourself.

The online help for this function, invoked by

```
> ?sort
```

shows that the call form (the simplest version) is

```
sort(x, decreasing = FALSE, ...)
```

Here is an example:

```
> x <- c(12,5,13)
> sort(x)
[1]  5 12 13
> sort(x,decreasing=FALSE)
[1] 13 12  5
```

So, the default is to sort in ascending order, i.e. the argument **decreasing** has TRUE as its default value. If we want the default, we need not specify this argument. If we want a descending-order sort, we must say so.

C.10 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.

C.10.1 The Basics

Here is example usage:

```
> g <- list(x = 4:6, s = "abc")
> g
$x
[1] 4 5 6

$s
[1] "abc"

> g$x  # can reference by component name
[1] 4 5 6
```

```
> g$s
[1] "abc"
> g[[1]]  # can reference by index, but note double brackets
[1] 4 5 6
> g[[2]]
[1] "abc"
> for (i in 1:length(g)) print(g[[i]])
[1] 4 5 6
[1] "abc"

# now have ftn oddcount() return odd count AND the odd numbers themselves,
# using the R list type
> source("odd.R")
> oddcount
function(x)  {
   x1 <- x[x %% 2 == 1]
   return(list(odds=x1, numodds=length(x1)))
}
> # R's list type can contain any type; components delineated by $
> oddcount(y)
$odds
[1]  5 13

$numodds
[1] 2

> ocy <- oddcount(y)  # save the output in ocy, which will be a list
> ocy
$odds
[1]  5 13

$numodds
[1] 2

> ocy$odds
[1]  5 13
> ocy[[1]]  # can get list elements using [[ ]] instead of $
[1]  5 13
> ocy[[2]]
[1] 2
```

C.10.2 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
```

C.10.3 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*:

```
> print.employee <- function(wrkr) {
+     cat(wrkr$name,"\n")
+     cat("salary",wrkr$salary,"\n")
+     cat("union member",wrkr$union,"\n")
+ }
> print(j)
Joe
salary 55000
union member TRUE
> j
Joe
salary 55000
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:

```
> rm(print.employee)  # remove the function, to see what happens with print
> j
$name
[1] "Joe"

$salary
[1] 55000

$union
[1] TRUE

attr(,"class")
[1] "employee"
```

C.11 Some Workhorse Functions

```
> m <- matrix(sample(1:5,12,replace=TRUE),ncol=2)
> m
[,1] [,2]
[1,]    2    1
[2,]    2    5
[3,]    5    4
[4,]    5    1
[5,]    2    1
[6,]    1    3
# call sum() on each row
> apply(m,1,sum)
[1] 3 7 9 6 3 4
# call sum() on each column
> apply(m,2,sum)
[1] 17 15
> f <- function(x) sum(x[x >= 4])
# call f() on each row
> apply(m,1,f)
[1] 0 5 9 5 0 0
> l <- list(x = 5, y = 12, z = 13)
# apply the given funciton to each element of l, producing a new list
> lapply(l,function(a) a+1)
$x
[1] 6

$y
```

```
[1] 13

$z
[1] 14
# group the first column of m by the second
> sout <- split(m[,1],m[,2])
> sout
$`1`
[1] 2 5 2
$`3`
[1] 1
$`4`
[1] 5
                                                                    $`5`
[1] 2
# find the size of each group, by applying the length() function
> lapply(sout,length)
$`1`
[1] 3
                                                                    $`3`
[1] 1
$`4`
[1] 1

$`5`
[1] 1
# like lapply(), but sapply() attempts to make vector output
> sapply(sout,length)
1 3 4 5
3 1 1 1
```

C.12 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:

```
> z <- list(a = runif(50), b = list(u=sample(1:100,25), v="blue sky"))
> z
$a
 [1] 0.301676229 0.679918518 0.208713522 0.510032893 0.405027042
0.412388038
 [7] 0.900498062 0.119936222 0.154996457 0.251126218 0.928304164
0.979945937
[13] 0.902377363 0.941813898 0.027964137 0.992137908 0.207571134
0.049504986
[19] 0.092011899 0.564024424 0.247162004 0.730086786 0.530251779
0.562163986
[25] 0.360718988 0.392522242 0.830468427 0.883086752 0.009853107
0.148819125
[31] 0.381143870 0.027740959 0.173798926 0.338813042 0.371025885
0.417984331
[37] 0.777219084 0.588650413 0.916212011 0.181104510 0.377617399
0.856198893
[43] 0.629269146 0.921698394 0.878412398 0.771662408 0.595483477
0.940457376
[49] 0.228829858 0.700500359

$b
$b$u
 [1] 33 67 32 76 29  3 42 54 97 41 57 87 36 92 81 31 78 12 85 73 26 44
86 40 43

$b$v
[1] "blue sky"
> names(z)
[1] "a" "b"
> str(z)
List of 2
 $ a: num [1:50] 0.302 0.68 0.209 0.51 0.405 ...
 $ b:List of 2
  ..$ u: int [1:25] 33 67 32 76 29 3 42 54 97 41 ...
  ..$ v: chr "blue sky"
> names(z$b)
[1] "u" "v"
> summary(z)
  Length Class  Mode
a 50     -none- numeric
b  2     -none- list
```

C.13 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]  # wind 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,]
  Ozone Solar.R Wind Temp Month Day  Celsius
```

```
1    41     190  7.4   67     5   1 19.44444
2    36     118  8.0   72     5   2 22.22222
3    12     149 12.6   74     5   3 23.33333
> aqjune <- airquality[airquality$Month == 6,]  # filter op
> nrow(aqjune)
[1] 30
> mean(aqjune$Temp)
[1] 79.1
> write.table(aqjune,"AQJune")  # write data frame to file
> aqj <- read.table("AQJune",header=T)  # read it in
```

C.14 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 beginners 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:

```
pr2file
function (filename)
{
    origdev <- dev.cur()
    parts <- strsplit(filename, ".", fixed = TRUE)
    nparts <- length(parts[[1]])
    suff <- parts[[1]][nparts]
    if (suff == "pdf") {
        pdf(filename)
    }
    else if (suff == "png") {
        png(filename)
    }
    else jpeg(filename)
    devnum <- dev.cur()
    dev.set(origdev)
    dev.copy(which = devnum)
    dev.set(devnum)
    dev.off()
    dev.set(origdev)
}
```

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.

C.15 Packages

The analog of a library in C/C++ in R is called a **package** (and often loosely referred to as a **library**). Some are already included in base R, while others can be downloaded, or written by yourself.

```
> library(parallel) # load the package named 'parallel'
> ls(package:parallel) # let's see what functions it gave us
 [1] "clusterApply"          "clusterApplyLB"       "clusterCall"
 [4] "clusterEvalQ"          "clusterExport"        "clusterMap"
 [7] "clusterSetRNGStream"   "clusterSplit"         "detectCores"
[10] "makeCluster"           "makeForkCluster"      "makePSOCKcluster"
[13] "mc.reset.stream"       "mcaffinity"           "mccollect"
[16] "mclapply"              "mcMap"                "mcmapply"
[19] "mcparallel"            "nextRNGStream"        "nextRNGSubStream"
[22] "parApply"              "parCapply"            "parLapply"
[25] "parLapplyLB"           "parRapply"            "parSapply"
[28] "parSapplyLB"           "pvec"                 "setDefaultCluster"
[31] "splitIndices"          "stopCluster"
> ?pvec # let's see how one of them works
```

The CRAN repository of contributed R code has thousands of R packages available. It also includes a number of "tables of contents" for specific areas, say time series, in the form of CRAN Task Views. See the R home page, or simply Google "CRAN Task View."

```
> install.packages("cts","~/myr") # download into desired directory
--- Please select a CRAN mirror for use in this session ---
...
downloaded 533 Kb


The downloaded binary packages are in
        /var/folders/jk/dh9zkds97sj23kjcfkr5v6q00000gn/T//RtmplkKzOU/downloaded_packages
> ?library
> library(cts,lib.loc="~/myr")

Attaching package:    cts
...
```

C.16 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`.

C.17 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

```
> ?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

```
> example(wireframe())
```

will show examples—R code and resulting pictures—of **wireframe()**, one of R's 3-dimensional graphics functions.

C.18 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.
- For Emacs users, there is **ess-tracebug**.
- 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*.

C.19 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.

C.20 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, as well as Hadley Wickham's *Advanced R*, Chapman and Hall, 2014.

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, and even Andrie de Vries' *R for Dummies*, 2012.