High Performance Parallel Programming (CS61064)

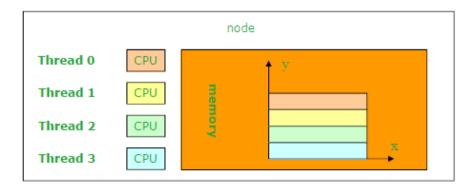
Week – 2 Part 1

Pralay Mitra

Parallel Software Models and Languages

- Programming Models
 - Shared Memory (OpenMP)
 - Message Passing (MPI)
 - Hardware Accelerators (CUDA, OpenCL)
 - Hybrid
- Programming Language:
 - С
 - C++
 - Fortran

Shared Memory



Shared Memory

OpenMP

Main Characteristics

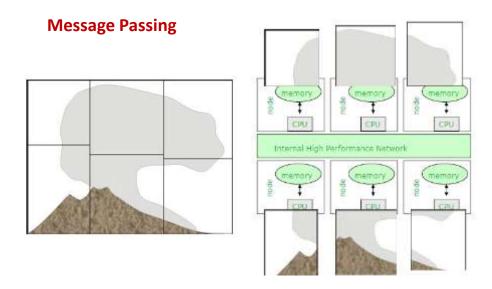
- · Compiler directives
- Medium grain
- Intra node parallelization
- Loop or iteration partition
- Shared memory
- Many HPC App

- Open Issues

- Thread creation overhead
- Memory/core affinity
- Interface with MPI

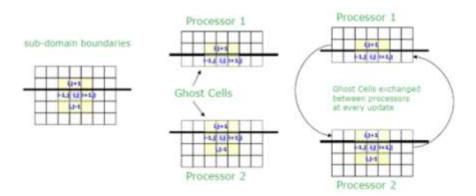
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Private Memory



Private Memory

Message Passing



Private Memory

MPI

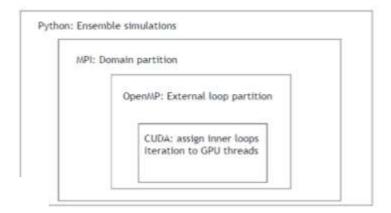
Main Characteristics

- Library
- · Coarse grain
- Inter node parallelization
- · Domain partition
- Distributed memory
- Almost all HPC parallel App

Open Issues

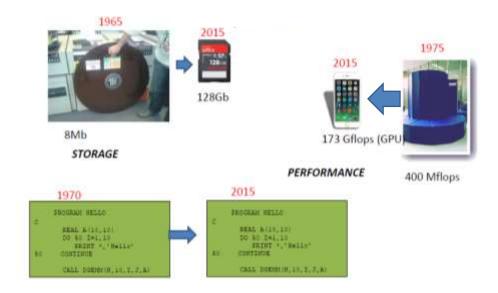
- Latency
- · OS Jitter
- Scalability

Hybrid Parallel Programming



Spring 2021

Advances: Hardware vs Software



Real HPC Crisis: Software

A supercomputer application and software are usually much more long-lived than a hardware

- Hardware life typically four-five years at most.
- Fortran and C are still the main programming models

Programming is stuck

- Arguably hasn't changed so much since the 70's

Software is a major cost component of modern technologies.

 The tradition in HPC system procurement is to assume that the software is free.

It's time for a change

- Complexity is rising dramatically
- Challenges for the applications on Petaflop systems
- Improvement of existing codes will become complex and partly impossible.
- The use of O(100K) cores implies dramatic optimization effort.
- New paradigm as the support of a hundred threads in one node implies new parallelization strategies
- Implementation of new parallel programming methods in existing large applications can be painful

Software Difficulties

- Legacy applications (includes most scientific applications) not designed with good software engineering principles. Difficult to parallelise programs with many global variables, for example.
- Memory/core decreasing.
- I/O heavy impact on performance, esp. for BlueGene where I/O is handled by dedicated nodes.
- Checkpointing and resilience.
- Fault tolerance over potentially many thousands of threads.
 - In MPI, if one task fails all tasks are brought down.

Summary

- HPC is only possible via parallelism and this must increase to maintain performance gains.
- Parallelism can be achieved at many levels but because of limited code scalability with traditional cores increasing role for accelerators (e.g. GPUs, MICs). The Top500 is becoming now becoming dominated by hybrid systems.
- Hardware trends forcing code re-writes with OpenMP, OpenCL, CUDA, OpenACC, etc in order to exploit large numbers of threads.
- Unfortunately, for many applications the parallelism is determined by problem size and not application code.
- Energy efficiency (Flops/Watt) is a crucial issue. Some batch schedulers already report energy consumed and in the near future your job priority may depend on predicted energy consumption.

Your first openMP program

Your first openMP program

```
Check your system support: locate omp.h /usr/lib/gcc/x86_64-redhat-linux/4.8.2/include/omp.h
```

Compilation: g++ -fopenmp first_openMP.c

Conditional Compilation:

Execution: ./a.out

Flags:

```
GNU: -fopenmp for Linux, Solaris, AIX, MacOSX, Windows. IBM: -qsmp=omp for Windows, AIX and Linux. Sun: -xopenmp for Solaris and Linux. Intel: -openmp on Linux or Mac, or -Qopenmp on Windows PGI: -mp
```

Your first openMP program

\$./a.out

Hello world!

Setting Environmental Variable

Know your shell

\$ echo \$SHELL

\$ /bin/bash

\$ export OMP_NUM_THREADS=16

Your first openMP program

Setting Environmental Variable and Executing

```
//Know your shell
$ echo $SHELL
$ /bin/bash
//Setting environmental variables
$ export OMP_NUM_THREADS=8
//Compilation
$ g++ -fopenmp first_openMP.c
//Execution
$ ./a.out
Hello world!
```

Directives

- · Syntactically directives are just comments
 - #pragma omp directive-name [clause[[,] clause]...] new-line
- Examples
 - #pragma omp parallel
- · Clause is one of the followings
 - if(scalar-expression)
 - private(variable-list)
 - firstprivate(variable-list)
 - default(shared | none)
 - shared(variable-list)
 - copyin(variable-list)
 - reduction(operator: variable-list)
 - num_threads(integer-expression)
- Multiple directive names are not allowed
 - #pragma omp parallel barrier

parallel construct

#pragma omp parallel

- Forms a team of N threads before starting executing parallel region
- N is set by OMP_NUM_THREADS environment or using function omp_set_num_threads()
- Semantics is (almost) same as serial program

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Comments on parallel construct

- At most one **if** clause can appear on the directive (serial/parallel)
- It is unspecified whether any side effects inside the if expression or num_threads expression occur.
- Only a single num_threads clause can appear on the directive. The num_threads expression is evaluated outside the context of the parallel region, and must evaluate to a positive integer value.
- The order of evaluation of the **if** and **num_threads** clauses is unspecified.
- A nested parallel region is executed by a team composed of one thread.
 The default behavior may be changed by using either the runtime library function omp_set_nested.
- If the num_threads clause is present then it supersedes the number of threads requested by the omp_set_num_threads library function or the OMP_NUM_THREADS environment variable only for the parallel region it is applied to. Subsequent parallel regions are not affected by it.

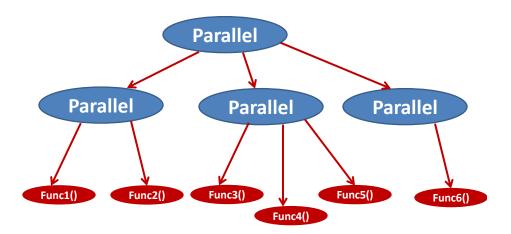
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Week – 2 Part 2

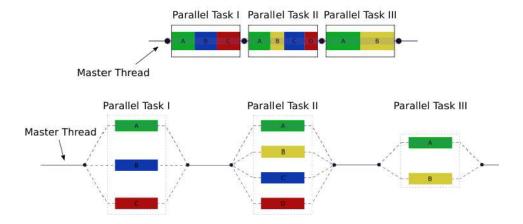
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OpenMP

Overview



Overview



Amdahl's law

 If a proportion (in time) P of a code can get S speed up then total speedup will be (less than)

$$S_{latency}(S) = \frac{1}{(1-P) + \frac{P}{S}}$$

• Improving **P** is more important than improving **S** that is often more difficult too.

Parallelization

- A serial code has three parts (A, B, C).
 - A takes 5secs (wish to make it 2 times faster)
 - B takes 1secs (wish to make it 7 times faster)
 - C takes 2secs (wish to make it 3 times faster)
 - You are allowed to parallelize only one part.

How many computing resources are required to achieve maximum speed up (which one will you choose)? What is the percentage of improvement?

Take home message

 Do you need infinite number of computing and storage power?

Possibly NO!!

Run time library functions

#include <omp.h>

- omp get num threads()
- omp_get_thread_num()
- omp_set_num_threads()
- omp_get_wtime()
- omp_get_max_threads()
- omp_get_num_procs()
- omp_in_parallel()
- omp_set_dynamic()
- omp_get_dynamic()
- omp_set_nested()
- omp_get_nested()

returns number of threads
returns the thread ID of the current thread
sets number of threads
returns the wall clock time in sec

```
# include <stdio.h>
# include <omp.h>
int main (int argc, char *argv[]) {
double wtime;
printf ("Number of processors available = %d\n", omp_get_num_procs ());
                                   %d\n", omp_get_max_threads ( ) );
printf ( "Number of threads =
wtime = omp_get_wtime ();  
printf ( "OUTSIDE the parallel region.\n" );
id = omp_get_thread_num (); <
printf ("HELLO from process %d\n Going INSIDE the parallel region:\n ", id );
# pragma omp parallel \
private (id) {
 id = omp_get_thread_num ();
 printf (" Hello from process %d\n", id );
wtime = omp_get_wtime () - wtime; <
printf ("Back OUTSIDE the parallel region.\nNormal end of execution.\nElapsed wall clock time = %f\n", wtime );
return 0;
```

Example -2

Initialization:

export OMP_NUM_THREADS=16

Compilation:

g++ -fopenmp example.c

Execution:

./a.out

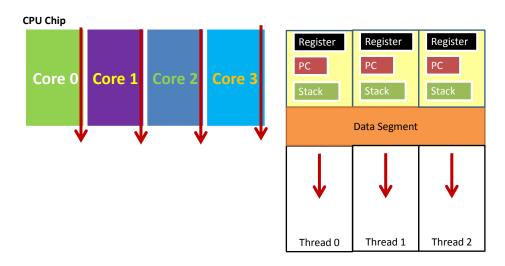
HELLO from process 0 Going INSIDE the parallel region: Hello from process 4 Hello from process 0 Hello from process 2 Hello from process 14 Hello from process 12 Hello from process 13 Hello from process 3 Hello from process 7 Hello from process 1 Hello from process 8 Hello from process 9 Hello from process 10 Hello from process 11 Hello from process 5

Hello from process 6
Hello from process 15
Back OUTSIDE the parallel region.
Normal end of execution.
Elapsed wall clock time = 0.001034

Number of processors available = 8

Number of threads = OUTSIDE the parallel region.

Multi-core CPU



Example -4

```
#include <stdio.h>
#include <unistd.h>
#include <omp.h>
int main()
{
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        sleep(1);
        a[temp][j]=temp+100*(j-1);
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    printf("\n");
    return 0;
}
```

```
$ ./a.out
1
    101
           201
                 301
                       401
                             501
                                   601
2
                 302
                                   602
    102
           202
                       402
                             502
3
           203
                 303
                                   603
    103
                       403
                             503
4
    104
           204
                 304
                       404
                             504
                                   604
5
    105
           205
                 305
                       405
                             505
                                   605
6
    106
           206
                 306
                       406
                             506
                                   606
7
     107
           207
                 307
                                   607
                       407
                             507
```

```
#include <stdio.h>
#include <unistd.h>
#include <omp.h>
int main()
{
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    #pragma omp parallel
    {
            for(i=0;i<=n*m-1;i++) {
                temp=i/m+1;
                j=i%m+1;
                sleep(1);
                a[temp][j]=temp+100*(j-1);
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    printf("\n");
    return 0;
```

```
$ ./a.out
1
          201
                     401
                                601
     0
                0
                           0
0
     102
           0
                302
                      0
                           502
                                 0
3
          203
                                603
     0
                0
                     403
                           0
0
     104
           0
                304
                      0
                           504
                                 0
5
     0
          205
                0
                     405
                           0
                                605
0
     106
           0
                0
                     0
                          506
                                606
7
          207
                0
                     407
                           0
                                607
```

Example -4

```
#include <stdio.h>
#include <unistd.h>
#include <omp.h>
int main()
    int i,j,n,m,temp,a[100][100];
    n=m=7;
    #pragma omp parallel private (temp, j)
            for(i=0;i<=n*m-1;i++) {
                temp=i/m+1;
               j=i%m+1;
                sleep(1);
                a[temp][j]=temp+100*(j-1);
           }
    for(i=0;i<=n*m-1;i++) {
        temp=i/m+1;
        j=i%m+1;
        if(i%m==0) printf("\n");
        printf("%d\t",a[temp][j]);
    printf("\n");
    return 0;
```

```
$ ./a.out
1
    101
         201
              301
                   401
                         501
                              601
2
    102
         202
              302 402
                         502
                              602
3
              303
    103
         203
                   403
                         503
                              603
4
   104
         204
              304
                   404
                         504
                              604
5
   105
         205
              305 405
                         505
                              605
6
    106
         206
              306
                   406
                         506
                              606
    107
         207
              307
                   407
                         507
                              607
```

Work-sharing Constructs

for Construct

- #pragma omp for [clause[[,] clause] ...] new-line for-loop

Clause

- private(variable-list)
- firstprivate(variable-list)
- lastprivate(variable-list)
- reduction(operator: variable-list)
- ordered
- schedule(kind[, chunk_size])
- nowait

Work-sharing Constructs

- for (init-expr; var logical-op b; incr-expr)
 - init-expr/incr-expr: same as C
 - var: A signed integer variable. If this variable would otherwise be shared, it is implicitly made private for the duration of the for. This variable must not be modified within the body of the for statement. Unless the variable is specified lastprivate, its value after the loop is indeterminate.
 - logical-op: >, <, >=, <=
 - *Ib, b,* and *incr:* Loop invariant integer expressions. There is no synchronization during the evaluation of these expressions. Thus, any evaluated side effects produce indeterminate results.

Loop Construct

Work out - 1

- Write a serial program to output the prime numbers occurring between 1 and 131072.
 Report the time required to compute the ith prime (where i will be taking as input).
- Convert it to a OpenMP code. Report the percentage of improvement over serial program using 4 and 16 cores.