

A short parallel computing class for C/C++

Andrew W. Steiner

UTK/ORNL

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- Logins on bridges2.psc.edu and neutrino.desktop.utk.edu
- Slack channel
- Github repository: <https://github.com/awsteiner/parallel>

Outline

- Makefiles and Environment Variables
- HPC Filesystems
- OpenMP or Shared Memory Parallelism
- Group Exercises

- Terminal is a GUI, plus a "shell"
- Interaction between the user and the operating systems
- I will often assume bash, but the default on MacOS is zsh
- Determine your shell using e.g. ps
- Setting and displaying environment variables depends on which shell you use
- On bash, show your environment variables using env and set using e.g. export VAR=value
- Particularly important environment variables: PATH, LD_LIBRARY_PATH, EDITOR, CC, CXX, OMP_NUM_THREADS, DISPLAY, PS1, USER, SHELL, TERM, LS_COLORS, HOME
- Common pattern: env | grep -i path

- Basic structure

target: dependencies
build rules

- e.g.

code: code.o
\$(CXX) -o code code.o

code.o: code.cpp code.h
\$(CXX) -o code.o -c code.cpp

- Notice how these targets uses environment variables?
- Make creates a "subshell" and executes commands within that subshell (defaults to sh)
- @ prefix doesn't echo commands
- - prefix allows commands to fail
- Variables referred to by \$()
- Need two \$\$'s for one \$
- Makefile is picky about tabs

Makefiles and Environment Variables III

- Two tricks:
 - Variable as the result of a shell command
 - Foreach

- System configurations vary widely: always read the HPC documentation
- Can be significantly different compared to logging into a standard Unix computer
- Login nodes and compute nodes
- Networked file systems: user directories and project directories
- Not all file systems are accessible from both the login and the compute nodes
- Frequently, output files must be stored on a scratch filesystem, and copied to a user (or project) directory later

- Login nodes are shared among many users (and thus slow), so be careful
 - No computation, especially no parallelism
 - No parallel compiling with "make -j"
 - No time-consuming tasks (e.g. no `ls -lR /`)
- File I/O can be the **most time-consuming part of code execution.**
- Often, Globus is preferred over ssh for large file transfers

Modules

- Code often needs to access libraries, but different users need different libraries
- Some of these libraries require different compilers or environment variables
- In most systems, this is handled by the `module` command
- `module load`, `module purge` `module help`
- Unfortunately, many of these modules are poorly documented

- Often it is better to use previously-developed code
- But even then, it is better to understand the concepts behind the code you are using

OpenMP or Shared Memory parallelism

- Memory space shared between "threads"
- OpenMP, POSIX threads, Boost threads, etc.
- Relatively small code changes
- Can lead to very confusing behavior
- Requires compiling with, e.g. `-fopenmp` and `#include <omp.h>`
- Danger zones:
 - Multiple threads writing and reading the same location at the same time
 - Multiple threads waiting for each other to complete ("deadlock")
 - Algorithms which depend sensitively on the order of operations ("race conditions")

OpenMP or Shared Memory parallelism II

- Simple parallel region:

```
#include <omp.h>
#pragma omp parallel
{
    #pragma omp for
    for(size_t i=0;i<100;i++) {
        // ... do something 100 times
    }
}
```

OpenMP or Shared Memory parallelism III

- Determine the number of threads: `omp_get_num_threads()`
- Determine the current thread: `omp_get_thread_num()`
- These latter two functions are only well-defined inside a parallel region
- By default, objects created in the work sharing region are private.
- "Some variables need to be shared, some need to be private, and you the programmer have to specify what you want."

- Accessing shared memory:
 - Reading memory locations at the same time from multiple threads is typically (but not always) safe
 - Writing memory locations at the same time from multiple threads is typically (but not always) unsafe
- A simple paradigm is to perform a difficult parallel calculation and store the results for every OpenMP thread
- and then to perform a simple calculation to sort or process those results afterwards in a non-parallel region

- In C/C++, care must be taken to understand if constructors and destructors are inside or outside parallel regions
- It is dangerous to create an object inside a parallel region, and destroy it outside the parallel region
- Not all objects are "thread-safe"
- Reading is often thread-safe, but writing is rarely thread-safe
- You can use const references to help write thread-safe code
- omp_test*.cpp example

- Special regions inside parallel regions:
 - critical: the enclosed code block will be executed by only one thread at a time, and not simultaneously executed by multiple threads. It is often used to protect shared data from race conditions.
 - atomic: the memory update (write, or read-modify-write) in the next instruction will be performed atomically. It does not make the entire statement atomic; only the memory update is atomic. A compiler might use special hardware instructions for better performance than when using critical.
 - ordered: the structured block is executed in the order in which iterations would be executed in a sequential loop

- Special regions inside parallel regions:
 - barrier: each thread waits until all of the other threads of a team have reached this point. A work-sharing construct has an implicit barrier synchronization at the end.
 - nowait: specifies that threads completing assigned work can proceed without waiting for all threads in the team to finish. In the absence of this clause, threads encounter a barrier synchronization at the end of the work sharing construct.

OpenMP or Shared Memory parallelism VIII

- The for loop cannot exit early, for example:

```
// BAD - cannot parallelize with OpenMP
for (int i=0;i < 100; i++) {
    if (i > 50)
        break;
}
```

OpenMP or Shared Memory parallelism IX

- Values of the loop control expressions must be the same for all iterations of the loop.

For example:

```
// BAD - cannot parallelize with OpenMP
for (int i=0; i < 100; i++) {
    if (i == 50)
        i = 0;
}
```

- Threads that exceed their stack allocation may or may not seg fault. An application may continue to run while data is being corrupted.

Group Exercises

- Create a OpenMP parallel program, including makefile targets, to compute Pascal's triangle (using addition) to a user-specified number of rows, and output the result to a file at the end.
- Ensure that, at some point during the execution, the program prints out the current number of OpenMP threads

References

- Some material taken from: bowdoin.edu/~ltoma
- A good reference is at LLNL