CME 213, ME 339 Spring 2023
Introduction to parallel computing using MPI, openMP, and CUDA

Eric Darve, ICME, Stanford

"Any fool can write code that a computer can understand. Good programmers write code that humans can understand." (Martin Fowler)

Stanford University

- C++ threads
- How to pass arguments by value and reference
- `join` and `detach`
- `promise` and `future`
- `mutex` and `lock_guard`

OpenMP

C++ std::thread for scientific computing

- C++ thread is a powerful and efficient mechanism to program shared memory computers.
- High performance and flexible.
- But engineering codes demand a higher productivity.
- There are certain patterns of computing in engineering codes that are common and can be leveraged.

OpenMP

Key objectives:

- Simplify multithreaded programming
- Improve performance
- Allow same code to run on both sequential or multicore processors

Common patterns in parallel scientific computing

1. `for` loops are at the core of most computation: perform a repetitive calculation on large arrays. This form of structured parallel computation is ideal for OpenMP.

2. Hand-off a block of code to a separate thread; this is closer to C++ std::thread. OpenMP makes this process more efficient and takes care of many “boilerplate” optimizations.

OpenMP makes scientific multithreaded programming very easy!

- OpenMP simplifies the programming significantly.
- In many cases, adding one line is sufficient to make it run in parallel.
- OpenMP is the standard approach in scientific computing for multicore processors.

Goals of OpenMP

- **Standardization:**
  - Provide a **standard** among a variety of shared memory architectures/platforms
  - Jointly defined and endorsed by a **group of major** computer hardware and software vendors
- **Simple but powerful:**
  - Establish a simple and limited set of **directives** for programming shared memory machines.
  - Significant parallelism can be implemented by using just **3 or 4 directives.**
  - This goal is becoming less true with each new release, unfortunately.

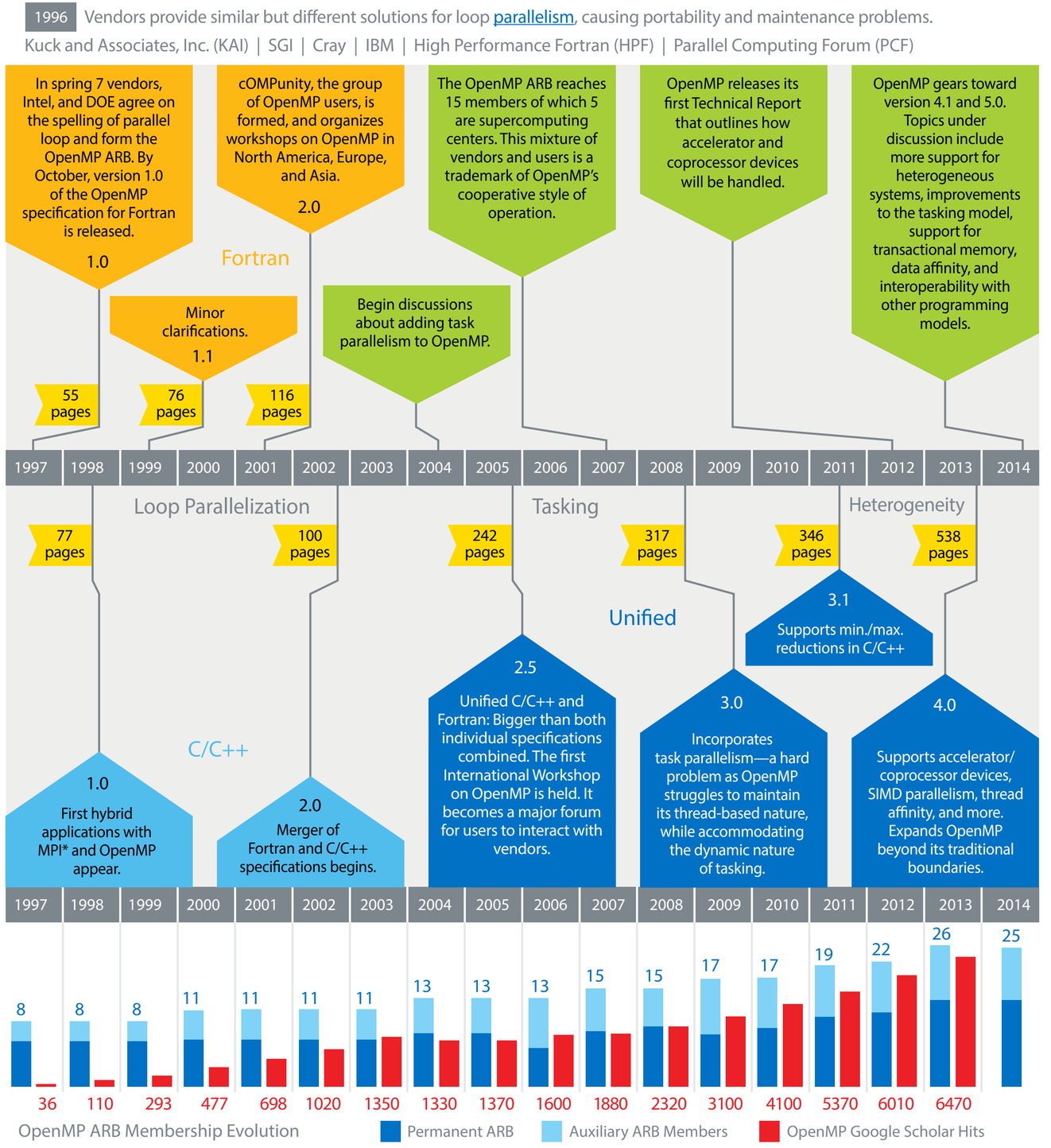
Goals of OpenMP

- **Ease of use:**
  - Provide capability to **incrementally** parallelize a serial program
  - Provide the capability to implement both coarse-grained and fine-grained parallelism
- **Portability:**
  - The API is specified for C/C++ and Fortran
  - Public forum for API and membership
  - **Most major platforms have been implemented including Unix/Linux platforms and Windows**

Reference material

- OpenMP website https://openmp.org
- Wikipedia https://en.wikipedia.org/wiki/OpenMP
- LLNL tutorial https://hpc-tutorials.llnl.gov/openmp
- Intel https://www.intel.com/content/dam/www/public/apac/xa/en/pdfs/ssg/Programming_with_OpenMP-Linux.pdf

History of OpenMP



https://www.openmp.org/uncategorized/openmp-timeline/

OpenMP release history

Month/Year	Version
Oct 1997	Fortran 1.0
Oct 1998	C/C++ 1.0
Nov 1999	Fortran 1.1
Nov 2000	Fortran 2.0
Mar 2002	C/C++ 2.0
May 2005	OpenMP 2.5
May 2008	OpenMP 3.0
Jul 2011	OpenMP 3.1
Jul 2013	OpenMP 4.0
Nov 2018	OpenMP 5.0
Nov 2020	OpenMP 5.1
Nov 2021	**OpenMP 5.2**

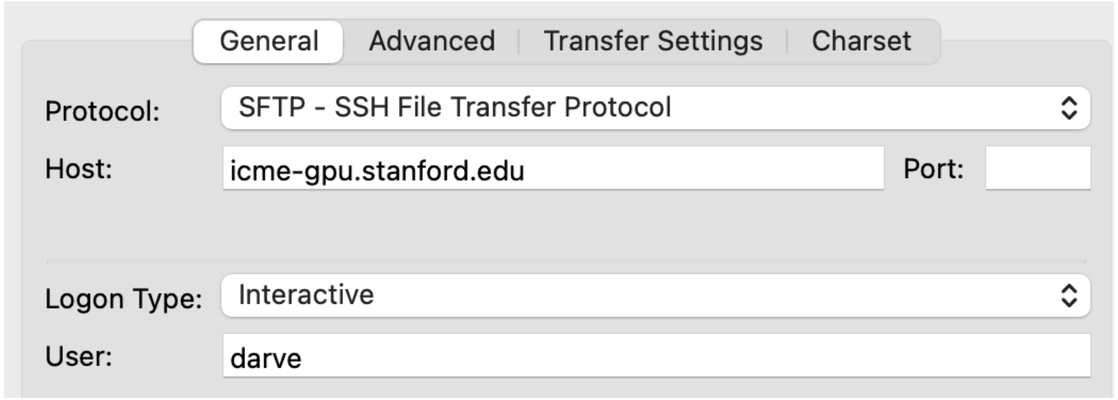
How to use the icme-gpu cluster

Connecting to the cluster

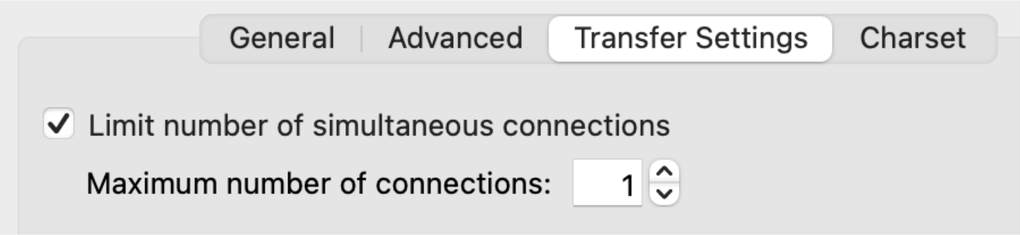
- Use scp or ssh.
- Example:
  - FileZilla
  - VSCode

FileZilla

- Use Site Manager with these options.
- Make sure the Logon type is **interactive**.

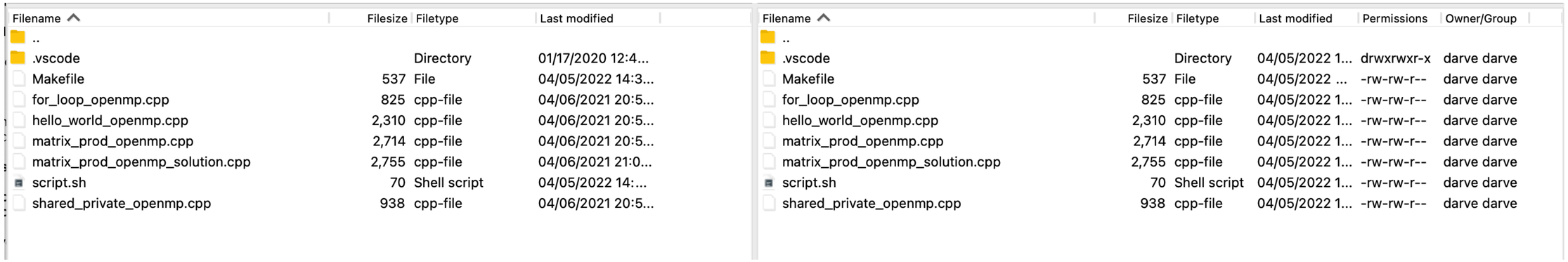


- Select only **one connection** at a time to avoid having to enter your password repeatedly.



- Use graphical interface to transfer files.

FileZilla transfer window



Filename	Filesize	Filetype	Last modified
..			
.vscode		Directory	01/17/2020 12:4...
Makefile	537	File	04/05/2022 14:3...
for_loop_openmp.cpp	825	cpp-file	04/06/2021 20:5...
hello_world_openmp.cpp	2,310	cpp-file	04/06/2021 20:5...
matrix_prod_openmp.cpp	2,714	cpp-file	04/06/2021 20:5...
matrix_prod_openmp_solution.cpp	2,755	cpp-file	04/06/2021 21:0...
script.sh	70	Shell script	04/05/2022 14:...
shared_private_openmp.cpp	938	cpp-file	04/06/2021 20:5...

Filename	Filesize	Filetype	Last modified	Permissions	Owner/Group
..					
.vscode		Directory	04/05/2022 1...	drwxrwxr-x	darve darve
Makefile	537	File	04/05/2022 ...	-rw-rw-r--	darve darve
for_loop_openmp.cpp	825	cpp-file	04/05/2022 1...	-rw-rw-r--	darve darve
hello_world_openmp.cpp	2,310	cpp-file	04/05/2022 1...	-rw-rw-r--	darve darve
matrix_prod_openmp.cpp	2,714	cpp-file	04/05/2022 1...	-rw-rw-r--	darve darve
matrix_prod_openmp_solution.cpp	2,755	cpp-file	04/05/2022 1...	-rw-rw-r--	darve darve
script.sh	70	Shell script	04/05/2022 1...	-rw-rw-r--	darve darve
shared_private_openmp.cpp	938	cpp-file	04/05/2022 1...	-rw-rw-r--	darve darve

Visual Studio Code

Open the Command Palette (F1, ⇧⌘P) and enter:

```
Remote-SSH: Connect to Host
```

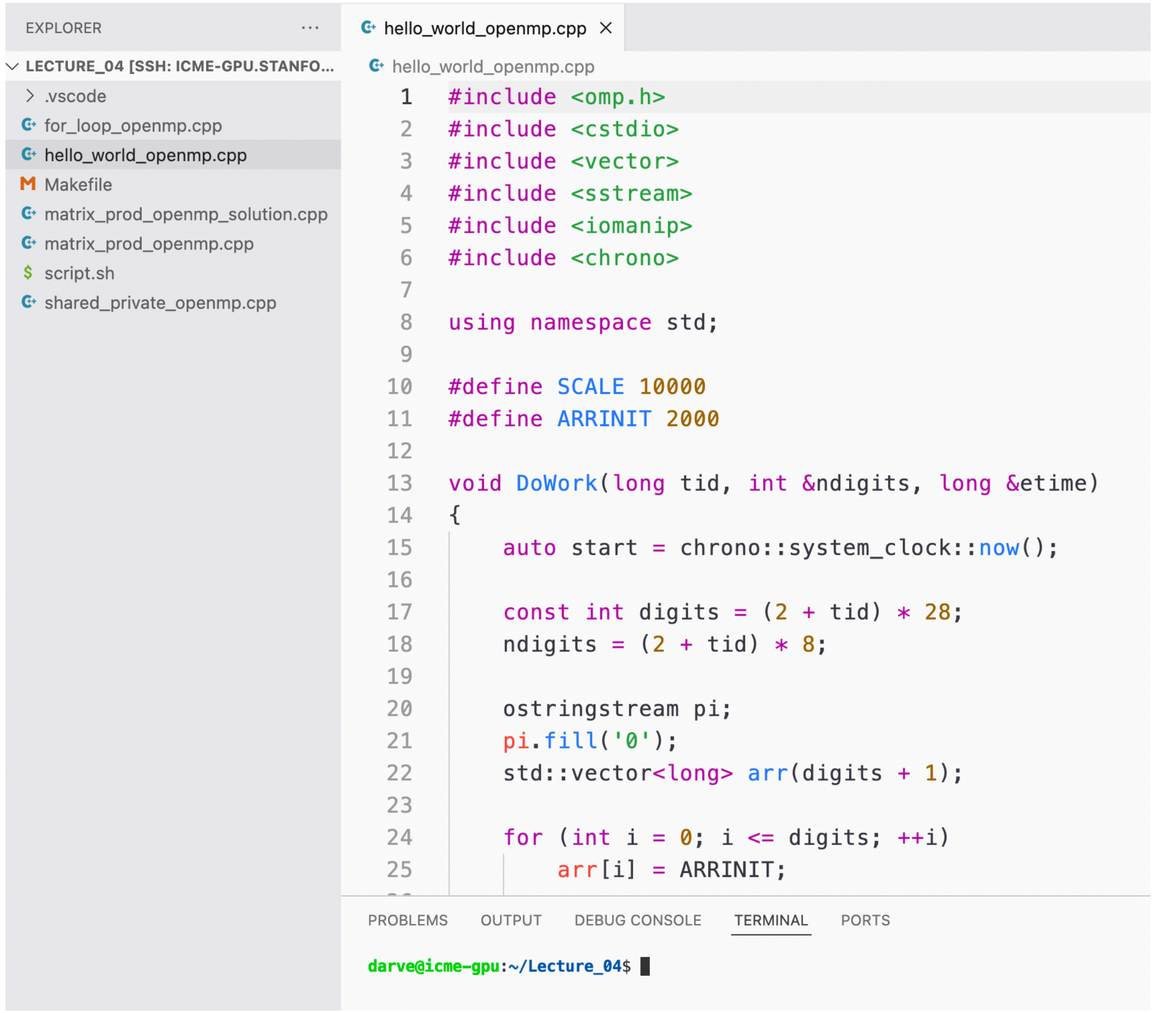
Enter your credentials.

Edit your files as if they were local.

```
$ source /etc/profile
```

may be needed

Visual Studio Code remote interface



Compile

```
darve@icme-gpu1:~/2023/openMP$ make
g++ -std=c++11 -Wall -O2 -fopenmp -o for_loop_openmp for_loop_openmp.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o hello_world_dowork hello_world_dowork.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o hello_world_openmp hello_world_openmp.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o matrix_prod_openmp matrix_prod_openmp.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o matrix_prod_openmp_solution matrix_prod_openmp_solution.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o matrix_prod_simple matrix_prod_simple.cpp
g++ -std=c++11 -Wall -O2 -fopenmp -o shared_private_openmp shared_private_openmp.cpp
darve@icme-gpu1:~/2023/openMP$
```

run code

- The cluster has two types of nodes:
  - **the login node:** where you land when you log in; this node must not be used to run CPU intensive jobs.
  - **the compute nodes:** these are the nodes where you run your code.
- It’s OK to compile on the login node.
- To run a code on the cluster, you need to use a queuing system.

The batch queue

- To run a code on the cluster, you need to use the queue.
- This will reserve a compute node and will run your program on that node.
- To do this, you need to write a SHELL script.
- This script will be run on the compute node by SLURM.
- SLURM: a cluster management and job scheduling system.

Example of batch script

- script.sh

```
1   #!/bin/bash
2   #SBATCH -p CME
3
4   ./hello_world_openmp
```

Fancier version

```
#!/bin/bash
#SBATCH --partition=CME
#SBATCH --cpus-per-task=16
#SBATCH --time=00:00:10
#SBATCH --nodes=1
#SBATCH --job-name=slurm
#SBATCH --output=slurm-%j.out
#SBATCH --error=slurm-%j.err

echo "Starting at `date`"
echo "Current working directory is $SLURM_SUBMIT_DIR."
echo "The master node of this job is: $SLURMD_NODENAME."
echo "Running on hosts: $SLURM_JOB_NODELIST"
echo "Using $SLURM_CPUS_PER_TASK CPUs per task."
echo "Number of CPUs on node: $SLURM_CPUS_ON_NODE."
echo

./hello_world_openmp

echo
echo "Environment variables"
export
```

Run your script

```
$ sbatch script.sh
```

- This puts your job in the queue.
- When a resource is available (a compute node), SLURM will run your script on the node.
- The output goes to:

```
slurm_[JOBID].out
```

Example of output

```
Starting at Mon Apr 17 05:44:43 PM UTC 2023
Current working directory is /home/darve/2023/openMP.
The master node of this job is: icmet01.
Running on hosts: icmet01
Using 8 CPUs per task.
Number of CPUs on node: 8.

Let's compute pi =      3.14159265358979323846264338327950288419716939937510582097494459230781640628620899862803482534211706 79
Hello World from thread = 4
Hello World from thread = 2
Hello World from thread = 6
[info] Number of threads = 8
Hello World from thread = 0
Hello World from thread = 3
Hello World from thread = 5
Hello World from thread = 1
Hello World from thread = 7
Thread  0 approximated Pi as     3141592653589793
Thread  2 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592
Thread  6 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592
Thread  4 approximated Pi as     3141592653589793238462643383279502884197169939937
Thread  3 approximated Pi as     3141592653589793238462643383279502884197
Thread  7 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592307816406
Thread  1 approximated Pi as     3141592653589793238462643
Thread  5 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592307816406286208
Thread 0 computed 16 digits of pi in   143 musecs (   8.938 musec per digit)
Thread 1 computed 24 digits of pi in   375 musecs (  15.625 musec per digit)
Thread 2 computed 32 digits of pi in   270 musecs (   8.438 musec per digit)
Thread 3 computed 40 digits of pi in   363 musecs (   9.075 musec per digit)
Thread 4 computed 48 digits of pi in   323 musecs (   6.729 musec per digit)
Thread 5 computed 56 digits of pi in   387 musecs (   6.911 musec per digit)
Thread 6 computed 64 digits of pi in   313 musecs (   4.891 musec per digit)
Thread 7 computed 72 digits of pi in   358 musecs (   4.972 musec per digit)
```

sbatch vs srun

- The `srun` command is designed for interactive use, with someone monitoring the output.
- The output of the application is seen as output of the `srun` command, typically at the user's terminal.
- The `sbatch` command is designed to submit a script for later execution and its output is written to a file.
- Command options used in the job allocation are almost identical.

srun example

```
darve@icme-gpu1:~/2023/openMP$ srun --cpus-per-task=2 -p CME ./hello_world_openmp
Hello World from thread = 0
Number of threads = 2
Hello World from thread = 1
darve@icme-gpu1:~/2023/openMP$ srun --cpus-per-task=4 -p CME ./hello_world_openmp
Hello World from thread = 2
Hello World from thread = 3
Hello World from thread = 1
Hello World from thread = 0
Number of threads = 4
darve@icme-gpu1:~/2023/openMP$ sbatch ./script.sh
Submitted batch job 7269
darve@icme-gpu1:~/2023/openMP$
```

Other SLURM commands

- **sbatch/srun**: run a script on a compute node
- **squeue**: list the jobs currently in the queue
- **sinfo**: view information about Slurm nodes and partitions
- **scancel**: used to cancel a pending or running job or job step

SLURM documentation

- https://slurm.schedmd.com/overview.html
- https://slurm.schedmd.com/tutorials.html

Let’s compile our first OpenMP code

- Header file:

```
#include <omp.h>
```

Compiler flag

Compiler / Platform	Compiler	Flag
Intel Linux Opteron/Xeon	icc icpc ifort	-openmp
PGI Linux Opteron/Xeon	pgcc pgCC pgf77 pgf90	-mp
GNU Linux Opteron/Xeon IBM Blue Gene	gcc g++ g77 gfortran	**-fopenmp**

OpenMP version supported by the compiler

```
darve@icme-gpu:~$ echo | cpp -fopenmp -dM | grep OPENMP
#define _OPENMP 201511
darve@icme-gpu:~$
```

Mapping table

Year	OpenMP version
200505	2.5
200805	3.0
201107	3.1
201307	4.0
201511	**4.5**
201811	5.0

Structure of an OpenMP program

- OpenMP breaks the code into sequential and parallel regions.
- **Sequential region:** only a single thread executes that block of code.
- **Parallel regions:**
  - OpenMP creates a pool of threads available to do work.
  - This is more efficient than creating threads. The pool of threads is reused throughout the program and efficiently managed by openMP.
  - All threads in the pool run the parallel region.

Hello World example

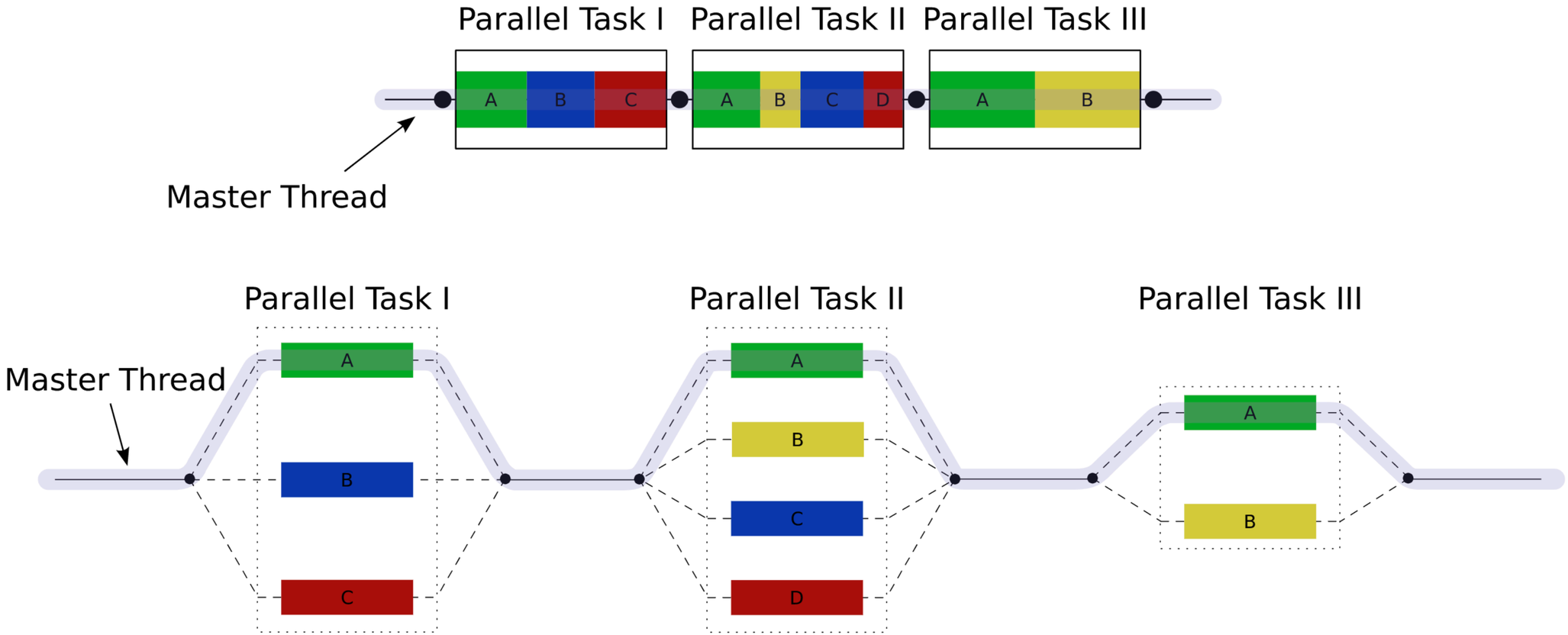
File `hello_world_openmp.cpp`

```
darve@icme-gpu1:~/2023/openMP$ srun --cpus-per-task=8 -p CME ./hello_world_openmp
Hello World from thread = 0
Number of threads = 8
Hello World from thread = 2
Hello World from thread = 5
Hello World from thread = 4
Hello World from thread = 7
Hello World from thread = 3
Hello World from thread = 6
Hello World from thread = 1
darve@icme-gpu1:~/2023/openMP$
```

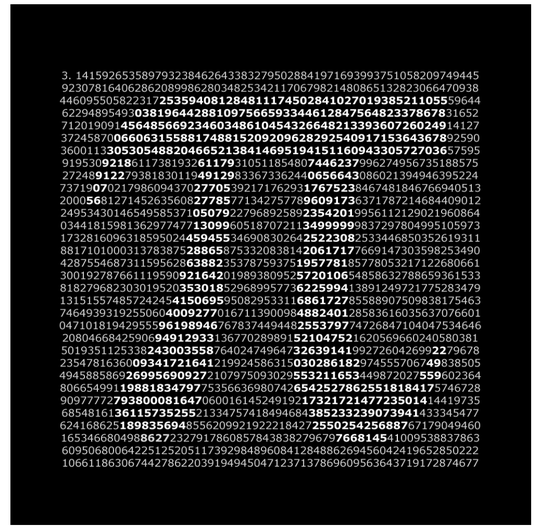
Directives

- `#pragma omp parallel`
- Creates a parallel region with the default number of threads.
- All threads execute the following block of code.

fork-join model



Example: computing π using openMP



- Formula used to compute π:

$$\frac{\pi}{2} = 1 + \frac{1}{3}\left(1 + \frac{2}{5}\left(1 + \frac{3}{7}\left(1 + \frac{4}{9}\left(1 + \cdots\right)\right)\right)\right)$$

- Each thread will compute a varying number of digits in π.
- File `hello_world_dowork.cpp`

Output

```
darve@icme-gpu1:~/2023/openMP$ srun --cpus-per-task=8 -p CME ./hello_world_dowork
Let's compute pi =              3.14159265358979323846264338327950288419716939937510582097494459230781640628620899862803482534211706 79
Hello World from thread = 4
Hello World from thread = 1
Hello World from thread = 2
[info] Number of threads = 8
Hello World from thread = 0
Hello World from thread = 7
Hello World from thread = 6
Hello World from thread = 3
Hello World from thread = 5
Thread  0 approximated Pi as     3141592653589793
Thread  4 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592307816406286208998628034825342117067
Thread  7 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592307816406
Thread  2 approximated Pi as     3141592653589793238462643383279
Thread  1 approximated Pi as     3141592653589793238462
Thread  3 approximated Pi as     3141592653589793238462643383279502884197
Thread  5 approximated Pi as     3141592653589793238462643383279502884197169399375105820
Thread  6 approximated Pi as     3141592653589793238462643383279502884197169399375105820974944592
Thread 0 computed 16 digits of pi in   122 musecs (   7.625 musec per digit)
Thread 1 computed 24 digits of pi in   343 musecs (  14.292 musec per digit)
Thread 2 computed 32 digits of pi in   303 musecs (   9.469 musec per digit)
Thread 3 computed 40 digits of pi in   312 musecs (   7.800 musec per digit)
Thread 4 computed 48 digits of pi in   228 musecs (   4.750 musec per digit)
Thread 5 computed 56 digits of pi in   321 musecs (   5.732 musec per digit)
Thread 6 computed 64 digits of pi in   366 musecs (   5.719 musec per digit)
Thread 7 computed 72 digits of pi in   225 musecs (   3.125 musec per digit)
darve@icme-gpu1:~/2023/openMP$
```

Using Google Colab

File
`openMP.ipynb`

OpenMP

Hello World in OpenMP

File: `hello_world_openmp.cpp`

```
[ ]  1 !name=hello_world_openmp; g++ -I. -o $name $name.cpp gtest_main.a -fopenmp && ./$name
```

```
Running main() from googletest-1.13.0/googletest/src/gtest_main.cc
[==========] Running 1 test from 1 test suite.
[----------] Global test environment set-up.
[----------] 1 test from openmp
[ RUN      ] openmp.hello_world
Hello World from thread = 0
Number of threads = 2
Hello World from thread = 1
[       OK ] openmp.hello_world (0 ms)
[----------] 1 test from openmp (0 ms total)

[----------] Global test environment tear-down
[==========] 1 test from 1 test suite ran. (0 ms total)
[  PASSED  ] 1 test.
```

for loops

- So far we have not done much with OpenMP.
- The syntax was simpler than std::thread but the coding is still cumbersome.
- In most cases, scientific codes can be parallelized by partitioning for loops across multiple threads.

Manual partitioning

- Following our previous examples, we can manually partition the for loop across threads.
- The code runs correctly and will use all the threads.
- See `matrix_prod_simple.cpp`

```
#pragma omp parallel
  {
    const long tid = omp_get_thread_num();
    const int n_threads = omp_get_num_threads();
    for (int i = tid; i < size; i += n_threads)
```

Output

```
darve@icme-gpu1:~/2023/openMP$ srun -c 2 -p CME ./matrix_prod_simple
Running main() from /home/darve/googletest-1.13.0/googletest/src/gtest_main.cc
[==========] Running 1 test from 1 test suite.
[----------] Global test environment set-up.
[----------] 1 test from matrix_prod
[ RUN      ] matrix_prod.simple
Size of matrix = 512
Number of threads to create = 2
[       OK ] matrix_prod.simple (221 ms)
[----------] 1 test from matrix_prod (221 ms total)

[----------] Global test environment tear-down
[==========] 1 test from 1 test suite ran. (221 ms total)
[  PASSED  ] 1 test.
darve@icme-gpu1:~/2023/openMP$
```

OpenMP directives

- But openMP provides a much more concise and simple mechanism to do this.
- This is a very common operation in scientific computing.
- OpenMP has many mechanisms to optimize this type of parallelism.

pragma omp for

- `#pragma omp parallel` creates a parallel region
- Adding `for` at the end results in a parallel execution of the for loop that follows.
- See `matrix_prod_openmp.cpp`

```
#pragma omp parallel for
  for (int i = 0; i < size; ++i)
    for (int j = 0; j < size; ++j) {
      float c_ij = 0;
      for (int k = 0; k < size; ++k) {
        c_ij += MatA(i, k) * MatB(k, j);
      }
      mat_c[i * size + j] = c_ij;
    }
```

Syntax options

```
#pragma omp parallel
#pragma omp for
    for (int i = 0; i < size; ++i)
```

```
#pragma omp parallel for
    for (int i = 0; i < size; ++i)
```

Performance and scalability

```
darve@icme-gpu1:~/2023/openMP$ srun -c 16 -p CME ./matrix_prod_openmp
Running main() from /home/darve/googletest-1.13.0/googletest/src/gtest_main.cc
[==========] Running 2 tests from 1 test suite.
[----------] Global test environment set-up.
[----------] 2 tests from matrix_prod
[ RUN      ] matrix_prod.parallel_for
Size of matrix = 512
Number of threads to create = 2
[       OK ] matrix_prod.parallel_for (183 ms)
[ RUN      ] matrix_prod.nthreads
Number of threads:  1; elapsed time [millisec]:  117
Number of threads:  2; elapsed time [millisec]:   59
Number of threads:  4; elapsed time [millisec]:   37
[       OK ] matrix_prod.nthreads (213 ms)
[----------] 2 tests from matrix_prod (397 ms total)

[----------] Global test environment tear-down
[==========] 2 tests from 1 test suite ran. (397 ms total)
[  PASSED  ] 2 tests.
darve@icme-gpu1:~/2023/openMP$
```

Loop scheduling

- Loop scheduling is important for performance.
- Some fine-tuning is often required.
- A parallel for loop often has a barrier at the end.
- At the barrier, the other members of the team must wait for the last thread to arrive.
- To minimize this wait time, shared work should be distributed so that all threads arrive at the barrier at about the same time.
- The schedule clause allows optimizing this execution.

General syntax

```
#pragma omp for schedule(kind,chunk_size)
```

`kind = static, dynamic, guided`

`chunk_size` the exact meaning varies depending on `kind` but generally this is the number of iterations in a given chunk assigned to a thread.

`static`

- This is the simplest.
- chunk size is fixed (and equal `chunk_size`).
- The chunk assignment is done using a round-robin assignment.
- Pro: low-overhead
- Con: will not work well if the runtime of each iteration varies significantly.