Parallel Job Workflows using OpenMP and MPI

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Harvard - FAS Research Computing

Objectives

- To advise you on the best practices for running parallel workflows on the FASRC cluster
- To provide the basic knowledge required for (implementing and) running your parallel OpenMP and MPI applications efficiently on the FASRC cluster

Overview

- Best Practices
- Brief Introduction to Parallel Computing
- Embarrassingly Parallel Jobs / Workflows
- OpenMP Jobs / Workflows
- MPI Jobs / Workflows
- Hybrid (MPI+OpenMP) Jobs / Workflows

Best Practices (1)

- Do small scale testing prior to large scale runs
- Ensure your jobs will run at least 10 minutes
- Make sure your jobs are well constrained
- Make sure your data is on a filesystem that can handle the I/O load
- Be aware of potential bottlenecks in your workflow
- Be cognizant of your fairshare https://docs.rc.fas.harvard.edu/kb/fairshare/

Best Practices (2)

- Ensure your code is operating as expected
- Understand the scaling of your code
- Have your primary code in a `git` repo
- Keep backups of critical data
- Have checkpoints
- Optimize your code and workflow

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What is High Performance Computing (HPC) ?

Summit: ORNL

Sierra: LLNL

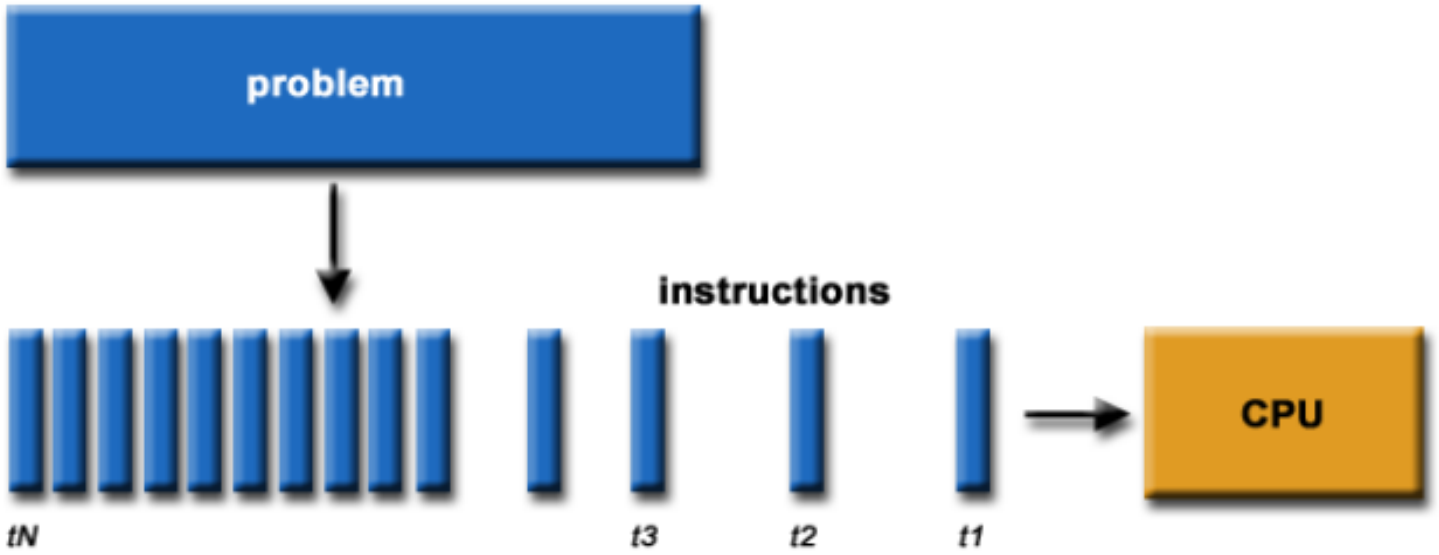
Cannon: Harvard

Using the world's fastest and largest computers to solve large and complex problems.

Serial Computation

Traditionally software has been written for serial computations:

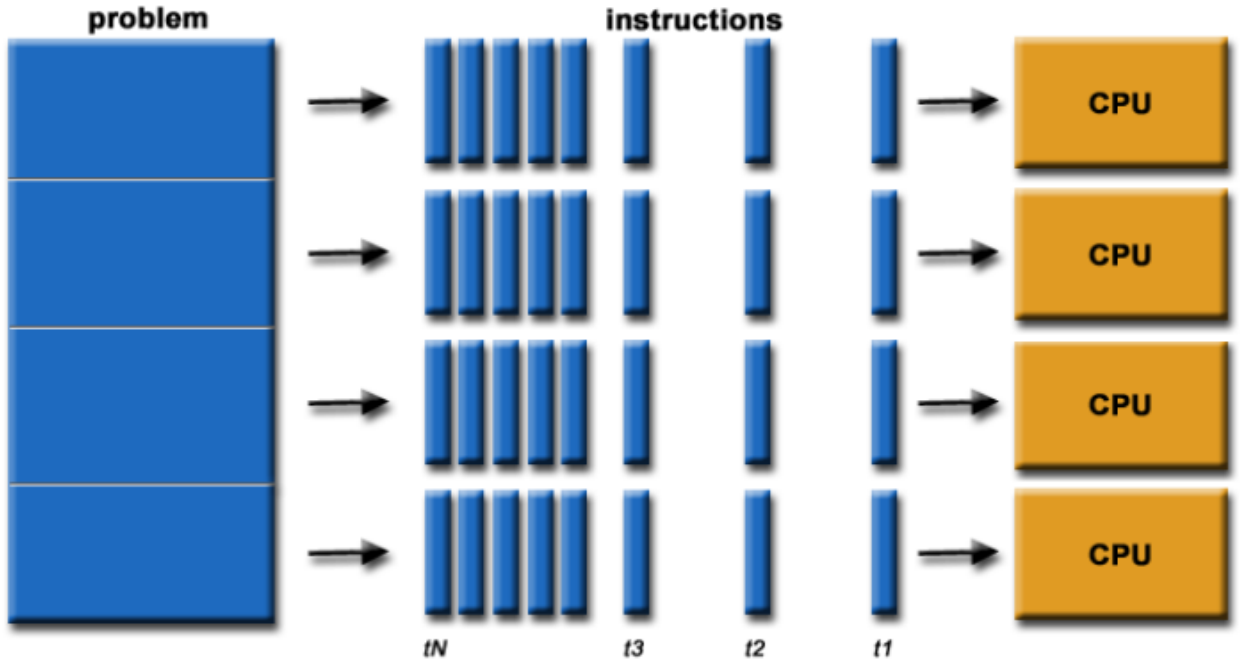
- To be run on a single computer having a single Central Processing Unit (CPU)
- A problem is broken into a discrete set of instructions
- Instructions are executed one after another
- Only one instruction can be executed at any moment in time



Parallel Computation

In the simplest sense, parallel computing is the simultaneous use of multiple compute resources to solve a computational problem:

- To be run using multiple CPUs
- A problem is broken into discrete parts that can be solved concurrently
- Each part is further broken down to a series of instructions
- Instructions from each part execute simultaneously on different CPUs



Why use HPC ?

Major Reasons:

Save time and/or money: In theory, throwing more resources at a task will shorten its time to completion, with potential cost savings. Parallel clusters can be built from cheap, commodity components.

Solve larger / more complex problems: Many problems are so large and/or complex that it is impractical or impossible to solve them on a single computer, especially given limited computer memory.

Provide concurrency: A single compute resource can only do one thing at a time. Multiple computing resources can be doing many things simultaneously.

Use of non-local resources: Using compute resources on a wide area network, or even the Internet when local compute resources are scarce.

Applications of HPC (not a complete list)

- Atmosphere, Earth, Environment, Space Weather
- Physics / Astrophysics – applied, nuclear, particle, condensed matter, high pressure, fusion, photonics
- Bioscience, Biotechnology, Genetics
- Chemistry, Molecular Sciences
- Geology, Seismology
- Mechanical and Aerospace Engineering
- Electrical Engineering, Circuit Design, Microelectronics
- Computer Science, Mathematics

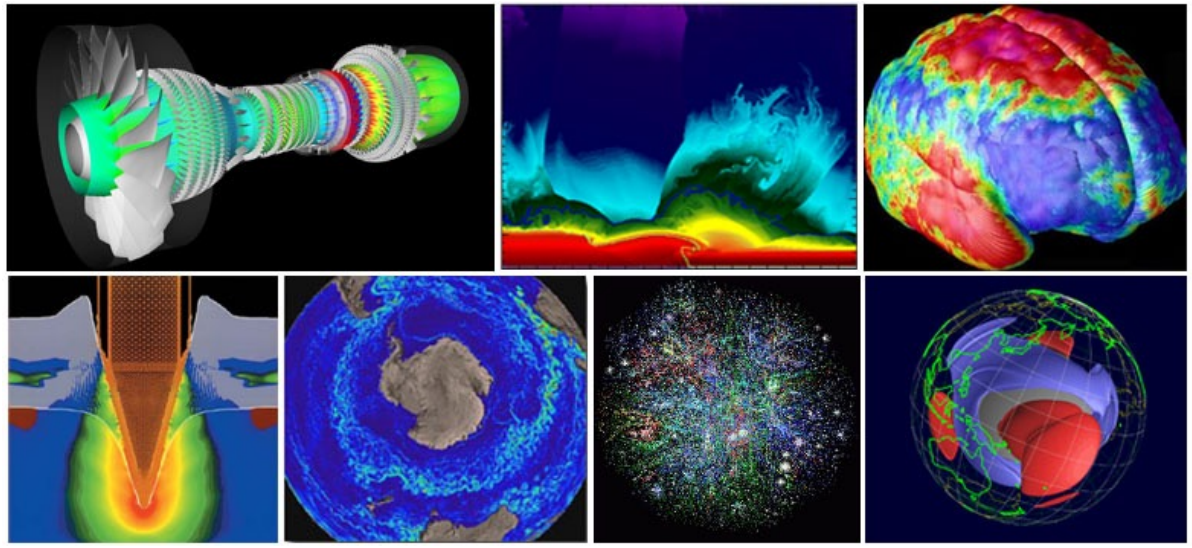


Image credit: LLNL

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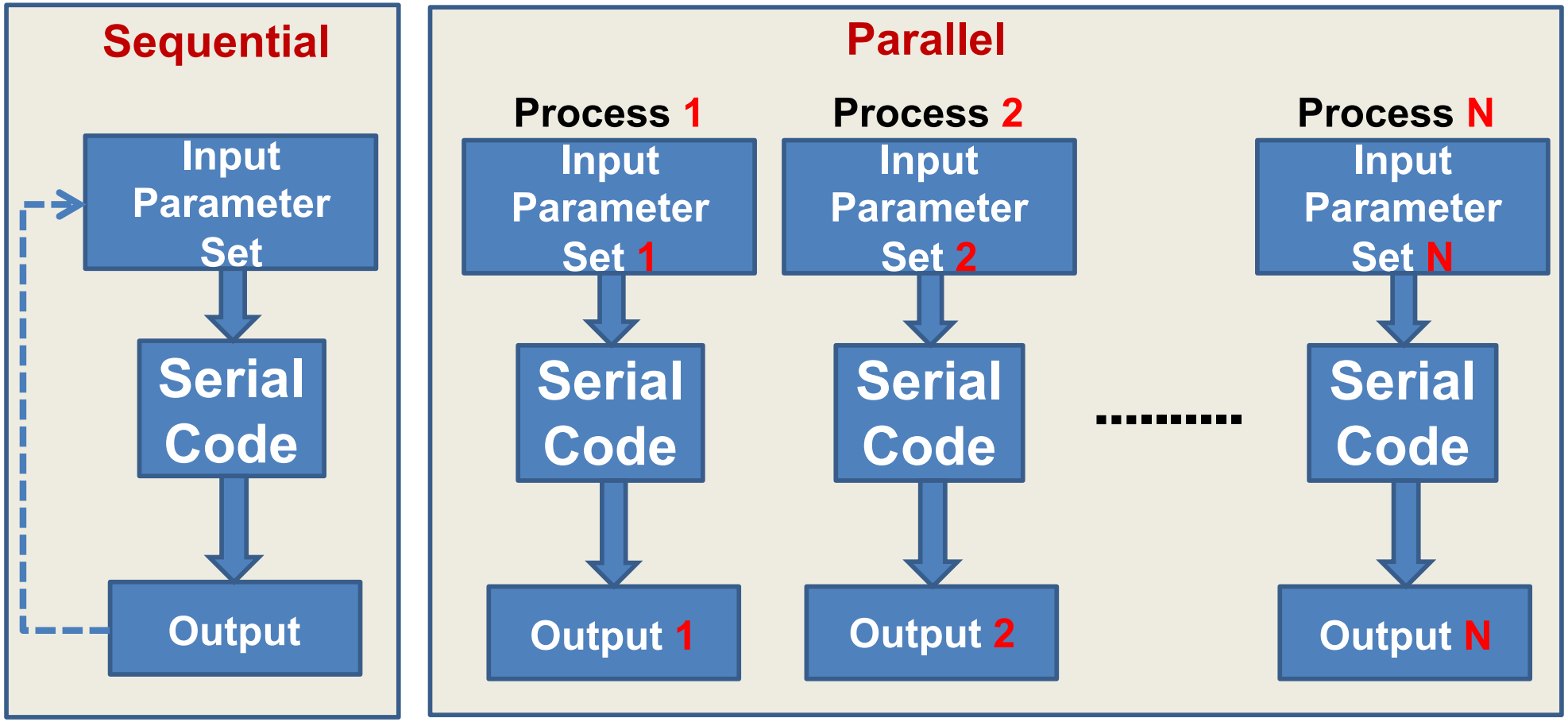
Embarrassingly Parallel



Embarrassingly Parallel

- Running many serial jobs in parallel
  - Parameter Sweeps
    https://www.rc.fas.harvard.edu/wp-content/uploads/2015/04/Parameter-Sweep.pdf
  - Data Transfers
  - Data Analysis Pipelines
- When possible, use `serial_requeue` partition
- Potential Problems/Bottlenecks
  - Filesystem I/O
  - Re-queue
  - SLURM Thrashing
    - Short runs
    - Lots of scheduler queries

Submitting Large Number of Serial Jobs

- Job Launcher Scripts
  - Use scripting language (e.g., `Bash`, `Python`, `Perl`, `R`) to construct and submit jobs
- SLURM Job Arrays
  - Works best for individual tasks that take 10+ minutes
- Single job: *for loop* in job-script
  - Works best for lots really short tasks (seconds)

Genuine Warning: Resist the urge to use R / bash to create 1000s of files and submit each as a separate job

Reference:

https://docs.rc.fas.harvard.edu/kb/submitting-large-numbers-of-jobs/

Job Launcher Scripts

- Use scripting language (e.g., `Bash`, `Python`, `R`, `Perl`) to construct and submit jobs

- Advantages
  - Full Flexibility and Control

- Disadvantage
  - Can get rather complex depending on workflow

- Examples:
  - https://github.com/fasrc/slurm_migration_scripts

SLURM Job Arrays

- Use **SLURM job arrays** to process data

- Advantages
  - Easy to use
  - Quick
  - Easy on the scheduler

- Disadvantages
  - Problems must fit into the Job Array style

- Examples:
  - https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/EP/Example1

SLURM Job Arrays

- #SBATCH --array=*indexes*

1-10	1,2,3,4,5,6,7,8,9,10
2-20:2	2,4,6,8,10,12,14,16,18,20
1,3,5,7,11,21	1,3,5,7,11,21
2-20%2	2,4 then 6,8 then 10,12 …

- SLURM job script variables
  - %A = JobId and %a = IndexID

    Ex: `$SBATCH -o stdout-%A_%a.o`
  - $SLURM_ARRAY_TASK_ID

    Ex: `R CMD input.R input.$SLURM_ARRAY_TASK_ID.out`

SLURM Job Arrays Example

```
#!/bin/bash
#SBATCH -J array_test
#SBATCH -p shared
#SBATCH -c 1
#SBATCH -t 00:10:00
#SBATCH --mem=4G
#SBATCH -o %A-%a.o
#SBATCH -e %A-%a.e
#SBATCH --array=100,200,300
```

This is per array task resource needs

```
# Load software environment
module load R/4.3.1-fasrc01

input=serial_sum.R

# Execute code
srun -n 1 -c 1 R CMD BATCH $input $input.$SLURM_ARRAY_TASK_ID.out
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/EP/Example1

Using SLURM Array Index in R

```
tid <- as.integer(Sys.getenv('SLURM_ARRAY_TASK_ID'))
res <- serial_sum(x=tid)
print(res)
```

Single Job: *for loop* in in job-script

```
#!/bin/bash
#SBATCH -J test_job
#SBATCH -p shared
#SBATCH -c 1
#SBATCH -t 00:10:00
#SBATCH --mem=4G
#SBATCH -o test_job.out
#SBATCH -e test_job.err
```

```
# Load software environment
module load R/4.1.0-fasrc01

input=serial_sum.R

# Execute code
for i in 100 200 300; do
   export inp=$i
   srun -n 1 -c 1 R CMD BATCH $input $input.${inp}.out
done
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/EP/Example2

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What is OpenMP ?

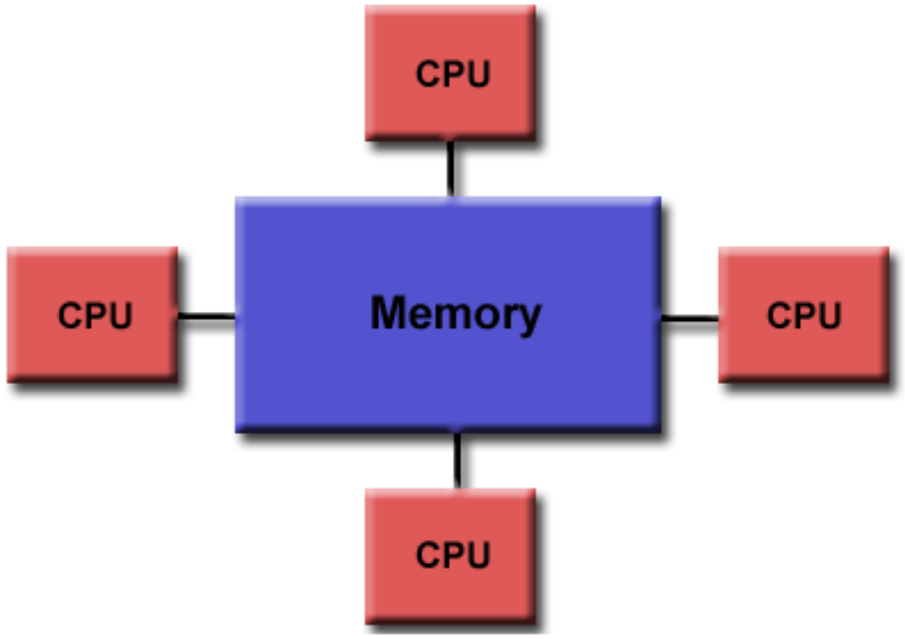
- **OpenMP** = **Open M**ulti-**P**rocessing

- An Application Program Interface (API) that may be used to explicitly direct **multi-threaded**, **shared memory** parallelism

- Comprised of three primary API components:
  - Compiler Directives
  - Runtime Library Routines
  - Environment Variables

OpenMP Programming Model

- Shared Memory
- Single Node
- One thread per core
- Explicit Parallelism
- Not designed to handle parallel I/O



Threading Languages Interfaces

Pthreads

OpenMP

OpenCL/CUDA

OpenACC

Python

R

Perl

MATLAB (PCT)

Others

Compiling OpenMP Programs

Compiler/Platform	Compiler	Flag
Intel	icx (C) icpx (C++) ifx (Fortran)	-qopenmp
GNU	gcc g++ g77 gfortran	-fopenmp

Intel:

```
module load  intel/23.2.0-fasrc01
icx -o omp_test.x omp_test.c -qopenmp
```

GNU:

```
module load gcc/13.2.0-fasrc01
gcc -o omp_test.x omp_test.c -fopenmp
```

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/OpenMP

Running OpenMP Programs (1)

Interactive / test jobs:

(1) Start an interactive bash shell

```
> salloc -p test -c 4 --mem=4G -t 0-06:00
```

(2) Load required modules, e.g.,

```
> module load gcc/10.2.0-fasrc01
```

(3) Compile (or use a Makefile)

```
> gcc -o omp_hello.x omp_hello.c -fopenmp
```

(4) Set number of OpenMP threads

```
> export OMP_NUM_THREADS=4
```

(5) Run the executable

```
> ./omp_hello.x
```

```
[pkrastev@holy7c19314 Example1]$ ./omp_hello.x
Hello World from thread = 1
Hello World from thread = 3
Hello World from thread = 2
Hello World from thread = 0
Number of threads = 4
```

Running OpenMP Programs (2)

Batch Jobs:

(1) Prepare a batch-job submission script

```
#!/bin/bash
#SBATCH -J omp_job              # Job name
#SBATCH -o slurm.out            # STD output
#SBATCH -e slurm.err            # STD error
#SBATCH -p shared               # Queue / Partition
#SBATCH -t 0-00:30              # Time (D-HH:MM)
#SBATCH --mem=4000              # Reserved memory (default in MB)
#SBATCH -c 8                    # Number of threads
#SBATCH -N 1                    # Number of nodes
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
module load gcc/13.2.0-fasrc01 # Load required modules
srun -c $SLURM_CPUS_PER_TASK ./omp_test.x
```

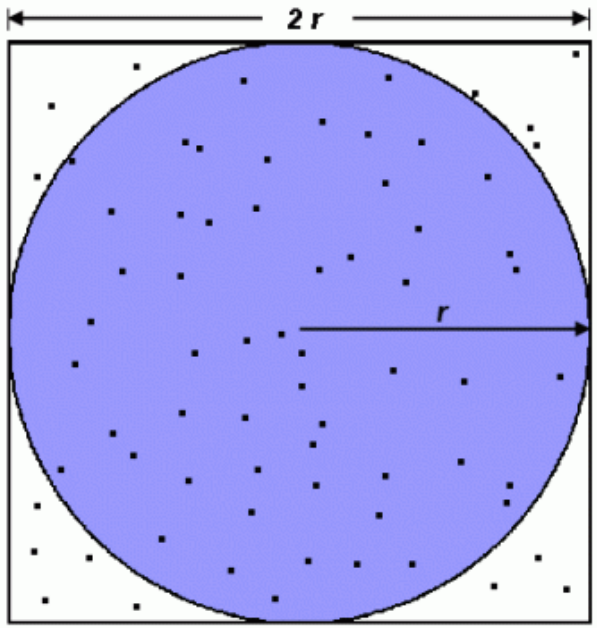
(2) Submit the job to the queue

```
> sbatch omp_test.run
```

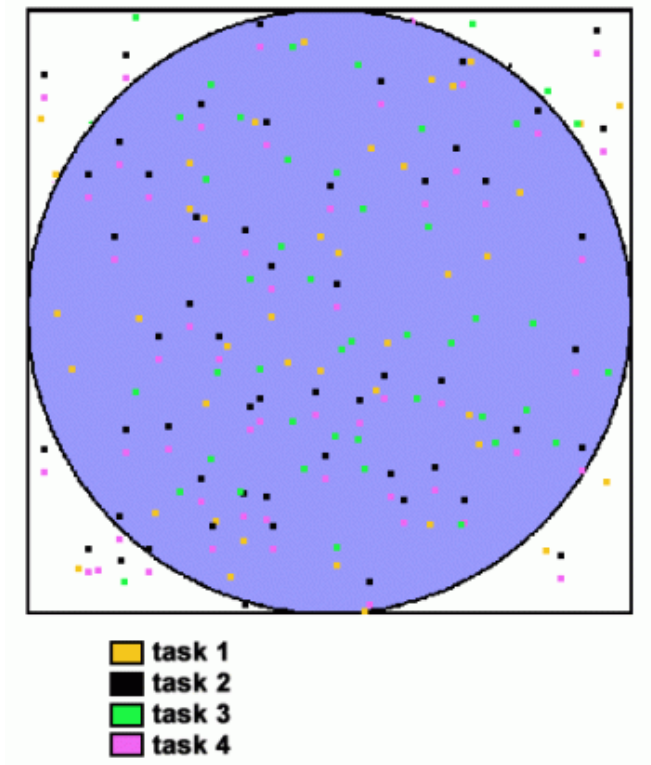
Example: Scaling - Compute PI in Parallel

Monte-Carlo approximation of PI

Calculating PI in serial



Calculating PI in parallel



Images credit: LLNL

https://hpc.llnl.gov/documentation/tutorials/introduction-parallel-computing-tutorial##ExamplesPI

Example: Scaling - Compute PI in Parallel

(1) Setup - get a copy of the code and compile it, e.g.,

```
> mkdir ~/OpenMP
> cd OpenMP
> git clone https://github.com/fasrc/User_Codes.git
```

(2) Review the source code and compile the program

```
> cd User_Codes/Parallel_Computing/OpenMP/Example3
> module load intel/23.2.0-fasrc01
> make
```

(3) Run the program

```
> sbatch sbatch.run
```

(4) Explore the output (the "`omp_dot.dat`" file), e.g.,

```
> cat omp_pi.dat
Number of threads:  8
Exact value of PI: 3.14159
Estimate of PI:    3.14158
Time:    0.32 sec.
```

(5) Run the program with different thread number – 1, 2, 4, 8 – and record the run times for each case. This will be needed to compute the speedup and efficiency (*NOTE: Currently set up to run directly with 1, 2, 4, 8 threads and generate speedup figure*)

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/Example3

Example: Scaling - Compute PI in Parallel

How much faster will the program run?

Speedup:

$$S(n) = \frac{T(1)}{T(n)}$$

Time to complete the job on **one** thread

Time to complete the job on **n** threads

Efficiency:

$$E(n) = \frac{S(n)}{n}$$

Tells you how efficiently you parallelize your code

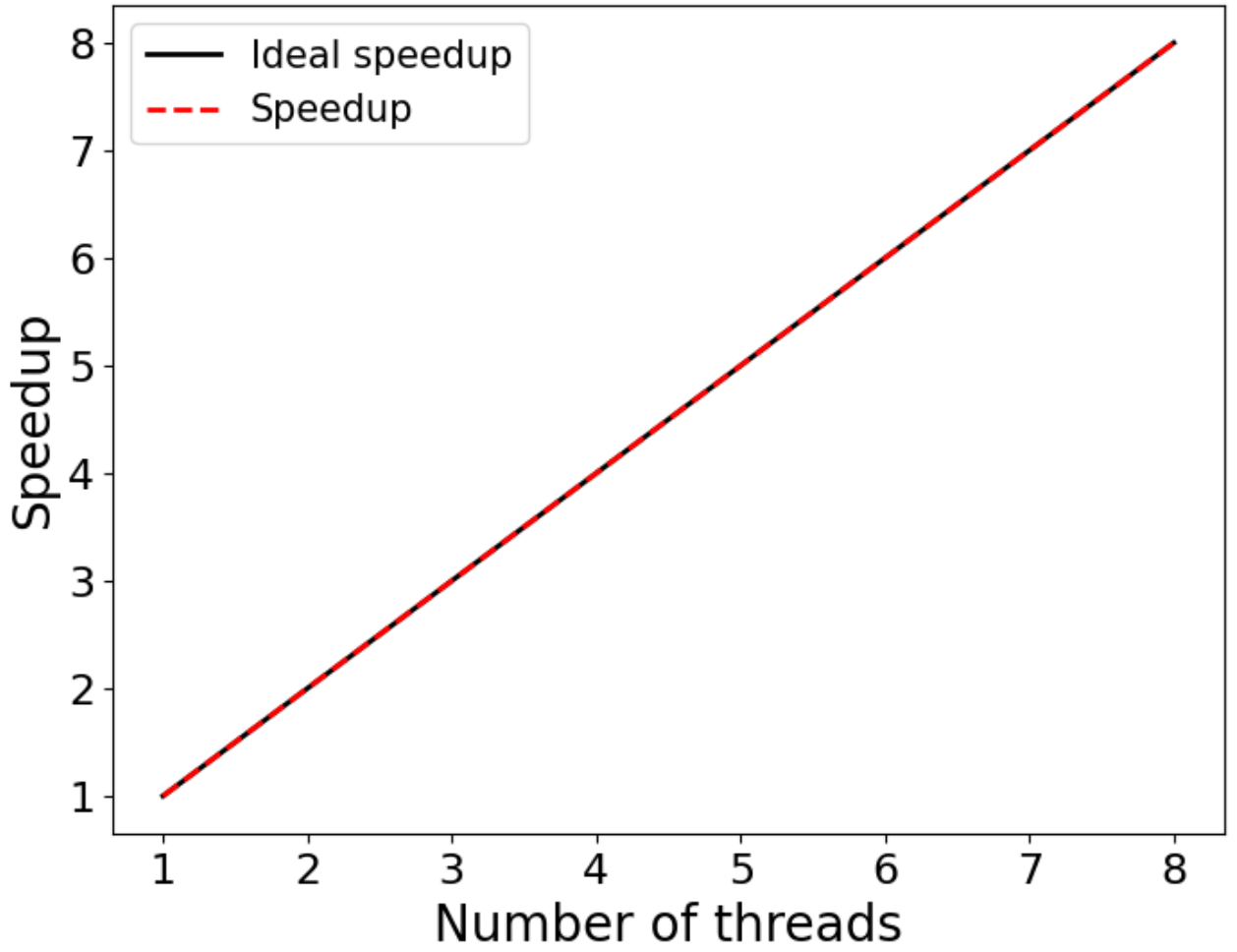
Example: Scaling - Compute PI in Parallel

You may use the `speedup.py` Python code to generate to calculate the speedup and efficiency. It generates the below table plus a speedup figure.

Nthreads	Walltime	Speedup	Efficiency (%)
1	2.56	1.00	100.00
2	1.28	2.00	100.00
4	0.64	4.00	100.00
8	0.32	8.00	100.00

https://github.com/fasrc/User_Codes/tree/master/Parallel_Computing/Example3

Example: Scaling - Compute PI in Parallel



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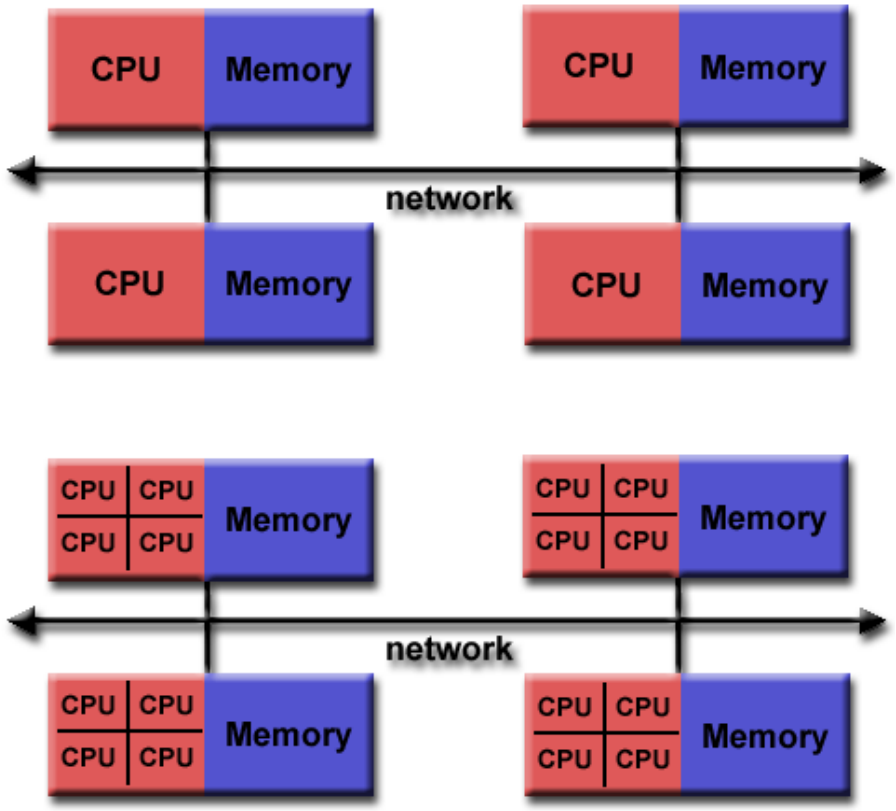
What is MPI?

- M P I = Massage Passing Interface
- MPI is a specification for the developers and users of message passing libraries. By itself, it is NOT a library
- MPI primarily addresses the message-passing parallel programming model: data is moved from the address space of one process to that of another process through cooperative operations on each process
- Most recent version is MPI-3
- Actual MPI library implementations differ in which version and features of the MPI standard they support

MPI Programming Model

- Originally MPI was designed for distributed memory architectures
- As architectures evolved, MPI implementations adapted their libraries to handle shared, distributed, and hybrid architectures
- Today, MPI runs on virtually any hardware platform
  - Shared Memory
  - Distributed Memory
  - Hybrid
- Programing model remains clearly distributed memory model, regardless of the underlying physical architecture of the machine
- Explicit parallelism – programmer is responsible for correct implementation of MPI



Reasons for using MPI

- **Standardization** - MPI is the only message passing specification which can be considered a standard. It is supported on virtually all HPC platforms
- **Portability** - There is little or no need to modify your source code when you port your application to a different platform that supports (and is compliant with) the MPI standard
- **Performance Opportunities** - Vendor implementations should be able to exploit native hardware features to optimize performance. Any implementation is free to develop optimized algorithms
- **Functionality** - There are over 430 routines defined in MPI-3, which includes the majority of those in MPI-2 and MPI-1
- **Availability** - A variety of implementations are available, both vendor and public domain

MPI Language Interfaces

- C/C++
- Fortran
- Java
- Python (mpi4py, pyMPI, pypar, MYMPI)
- R (Rmpi)
- Perl (Parallel::MPI)
- MATLAB (Matlab Parallel Server / DCS)
- Others

Compiling MPI Programs

MPI Implementation	Compiler	Flag
OpenMPI Mpich	mpicc mpicxx mpif90 mpif77 mpifort	None
Intel MPI	mpiicx mpiicpx mpiifx	None

Intel + OpenMPI / Mpich:

```
module load  intel/23.2.0-fasrc01
module load  openmpi/4.1.5-fasrc03
mpicxx -o mpitest.x mpitest.cpp
```

GNU + OpenMPI / Mpich:

```
module load gcc/10.2.0-fasrc01
module load openmpi/4.1.1-fasrc01
mpicxx -o mpi_test.x mpi_test.cpp
```

Intel + Intel-MPI:

```
module load  intel/23.2.0-fasrc01
module load intelmpi/2021.10.0-fasrc01
mpiicpx -o mpi_test.x mpi_test.cpp
```

Running MPI Programs (1)

Interactive test jobs:

(1) Start an interactive bash shell

```
> salloc -p test -n 4 --mem=4G -t 0-06:00
```

(2) Load required modules, e.g.,

```
> module load gcc/13.2.0-fasrc01 openmpi/4.1.5-fasrc03
```

(3) Compile your code (or use a Makefile)

```
> mpicxx -o mpitest.x mpitest.cpp
```

(4) Run the code

```
> mpirun -np 4 ./mpitest.x
Rank 0 out of 4
Rank 1 out of 4
Rank 2 out of 4
Rank 3 out of 4
End of program.
```

Running MPI Programs (2)

Batch jobs:

(1) Compile your code, e.g.,

```
> module load gcc/13.2.0-fasrc01 openmpi/4.1.5-fasrc03
> mpicxx -o mpitest.x mpitest.cpp
```

(2) Prepare a batch-job submission script

```
#!/bin/bash
#SBATCH -J mpi_job                                  # Job name
#SBATCH -o slurm.out                                # STD output
#SBATCH -e slurm.err                                # STD error
#SBATCH -p shared                                   # Queue / partition
#SBATCH -t 0-00:30                                  # Time (D-HH:MM)
#SBATCH --mem-per-cpu=4000                          # Memory per MPI task
#SBATCH -n 8                                        # Number of MPI tasks
module load gcc/13.2.0-fasrc01 openmpi/4.1.5-fasrc03 # Load required modules
srun -n $SLURM_NTASKS --mpi=pmix ./hello_mpi.x
```

(3) Submit the job to the queue

```
> sbatch mpi_test.run
```

Running MPI Programs (3)

Intel & Intel-MPI

```
#!/bin/bash
#SBATCH -J mpitest              # job name
#SBATCH -o mpitest.out          # standard output file
#SBATCH -e mpitest.err          # standard error file
#SBATCH -p test                 # partition
#SBATCH -n 8                    # ntasks
#SBATCH -t 00:30:00             # time in HH:MM:SS
#SBATCH --mem-per-cpu=4000      # memory in megabytes


# --- Load the required software modules., e.g., ---
module load intel/23.2.0-fasrc01 intelmpi/2021.10.0-fasrc01


# --- Run the executable ---
# --- With Intel-MPI, you need to ensure it uses pmi2 instead of pmix ---
srun -n $SLURM_NTASKS --mpi=pmi2 ./mpitest.x
```

Running MPI Programs (4)

- Sometimes programs can be picky about having MPI available on all the nodes it runs on, so it is good to have MPI module loads in your `.bashrc` file

- Some codes are topology sensitive thus the following slurm options can be helpful
  - `--contiguous` `# Contiguous set of nodes`
  - `--ntasks-per-node` `# Number of tasks per node`
  - `--hint` `# Bind tasks according to hints`
  - `--distribution, -m` `# Specify distribution method for tasks`

- For hybrid mode jobs you would set both `-c` and `-n`

https://slurm.schedmd.com/sbatch.html
https://slurm.schedmd.com/mc_support.html
https://www.rc.fas.harvard.edu/resources/documentation/software-development-on-odyssey/hybrid-mpiopenmp-codes-on-odyssey

MPI Examples

1. MPI Hello World program
2. Parallel FOR loops in MPI – dot product
3. Scaling – speedup and efficiency
4. Parallel Matrix-Matrix multiplication
5. Parallel Lanczos algorithm

https://github.com/fasrc/User_Codes/tree/master/Courses/CS205/MPI_2021

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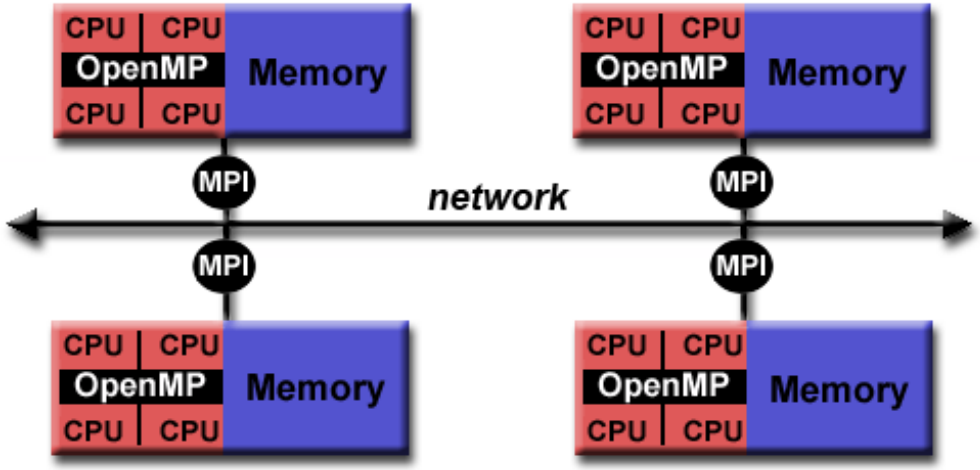
Hybrid (MPI+OpenMP) Parallel Programming

- **OpenMP** is used for computationally intensive work on **each node**
- **MPI** is used for communication and data sharing **between nodes**
- This allows parallelism to be implemented to the full scale of a cluster



https://docs.rc.fas.harvard.edu/kb/hybrid-mpiopenmp-codes-on-odyssey/

Running Hybrid Applications

Example 1: 2 MPI tasks with 4 OpenMP threads per MPI task, using 8 cores in total

```
#!/bin/bash
#SBATCH -J hybrid_test
#SBATCH -o hybrid_test.out
#SBATCH -e hybrid_test.err
#SBATCH -p shared
#SBATCH -n 2
#SBATCH -c 4
#SBATCH -t 180
#SBATCH --mem-per-cpu=4G

export OMP_NUM_THREADS=4
srun -n 2 -c 4 --mpi=pmix ./hybrid_test.x
```

Example 2: 4 Nodes with 1 MPI task per node and 32 OpenMP threads per MPI task, using 128 cores in total (across 4 nodes)

```
#!/bin/bash
#SBATCH -J hybrid_test
#SBATCH -o hybrid_test.out
#SBATCH -e hybrid_test.err
#SBATCH -p shared
#SBATCH -n 4
#SBATCH -c 32
#SBATCH --ntasks-per-node=1
#SBATCH -t 180
#SBATCH --mem-per-cpu=128G

export OMP_NUM_THREADS=32
srun -n 4 -c 32 --mpi=pmix ./hybrid_test.x
```

Summary and hints for efficient parallelization

- Is it even worth parallelizing my code?
  - Does your code take an intractably long amount of time to complete?
  - Do you run a single large model or do statistics on multiple small runs?
  - Would the amount of time it take to parallelize your code be worth the gain in speed?
- Parallelizing established code vs. starting from scratch
  - Established code: Maybe easier / faster to parallelize, but my not give good performance or scaling
  - Start from scratch: Takes longer, but will give better performance, accuracy, and gives the opportunity to turn a “black box” into a code you understand

Summary and hints for efficient parallelization

- Increase the fraction of your program that can be parallelized. Identify the most time-consuming parts of your program and parallelize them. This could require modifying your intrinsic algorithm and code's organization
- Balance parallel workload
- Minimize time spent in communication
- Use simple arrays instead of user defined derived types
- Partition data. Distribute arrays and matrices – allocate specific memory for each MPI process
- For I/O intensive applications implement parallel I/O in conjunction with a high-performance parallel filesystem, e.g., Lustre

Thank you! Questions? Comments?

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