# Introduction to Parallel Programming and MPI

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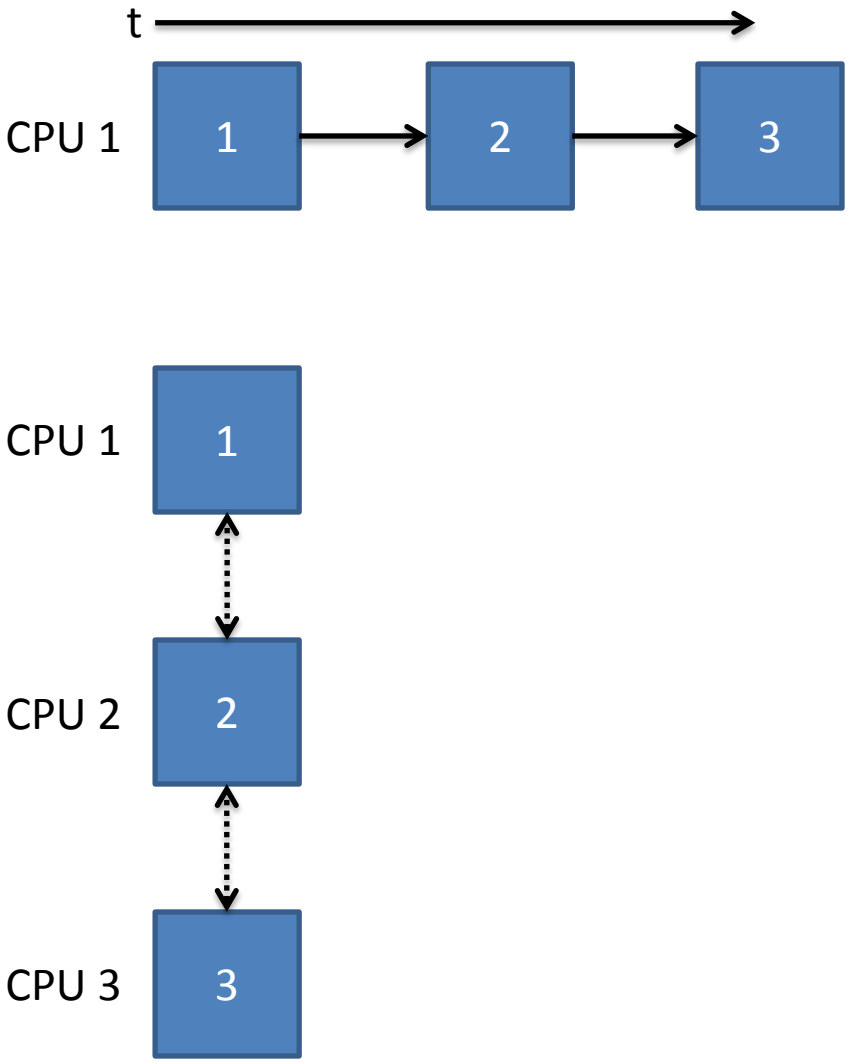
# Outline

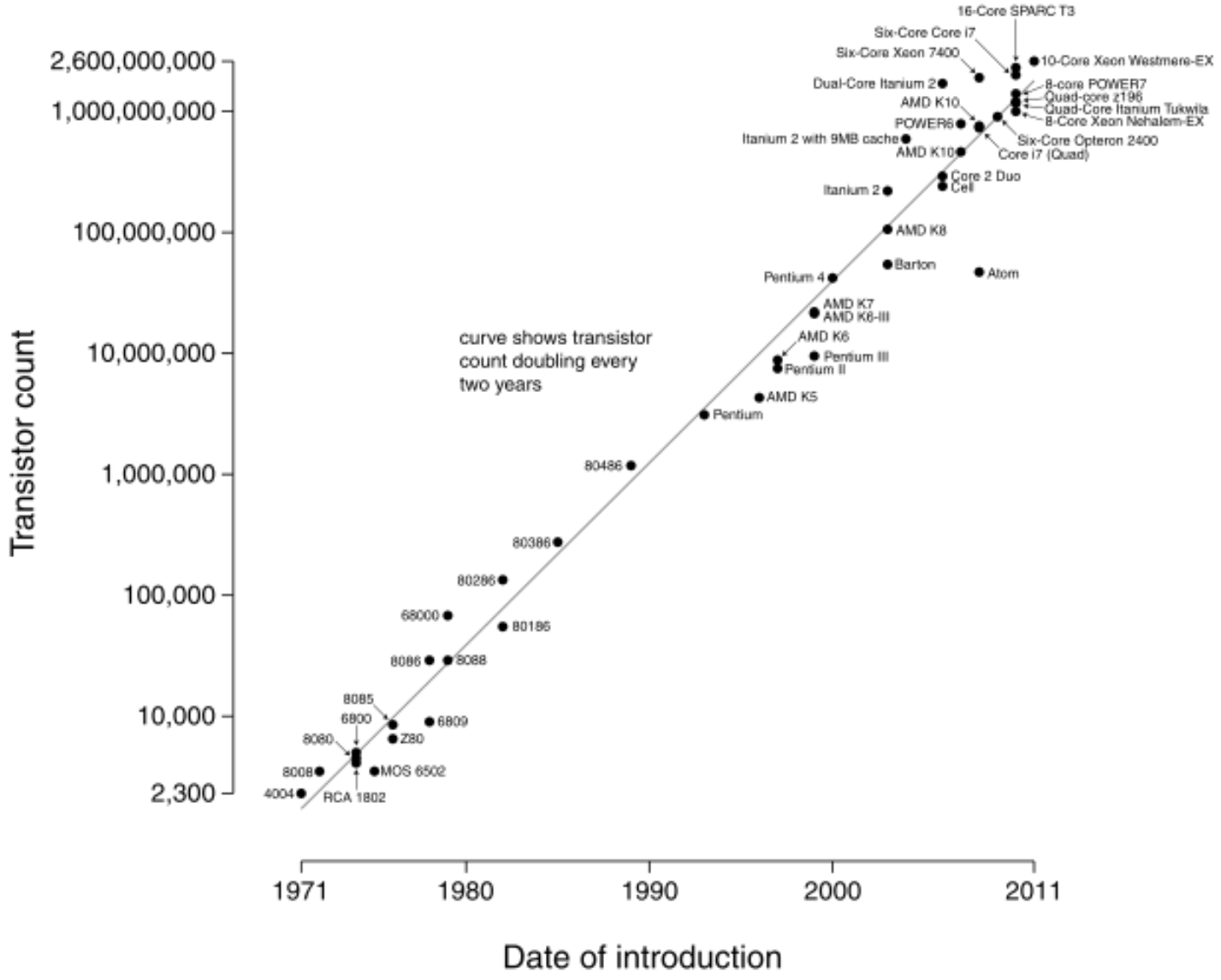
- What is parallel computing?
- Theory
- Message Passing Interface

# Parallel vs. Serial

- Serial: A logically sequential execution of steps. The result of next step depends on the previous step.
- Parallel: Steps can be contemporaneously and are not immediately interdependent or are mutually exclusive.



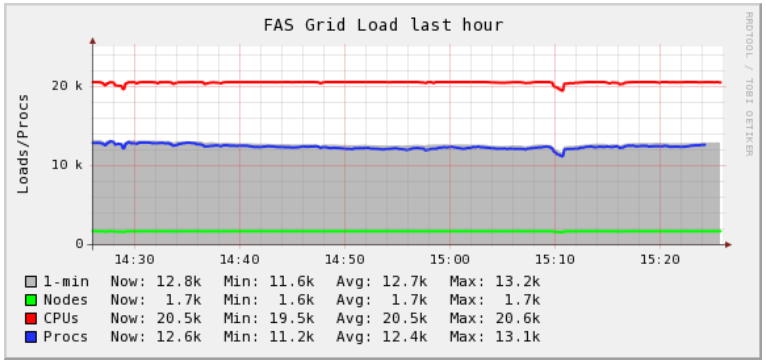
# Microprocessor Transistor Counts 1971-2011 & Moore's Law



# High Performance Computing (HPC)

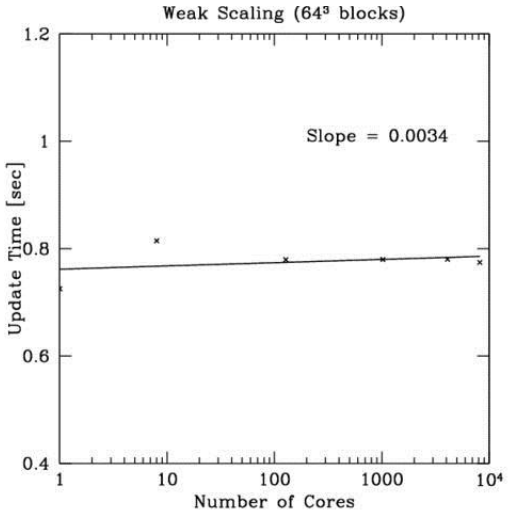
- Goal: Leverage as much computer power as possible with as much efficiency as possible to solve problems that cannot be solve by conventional means

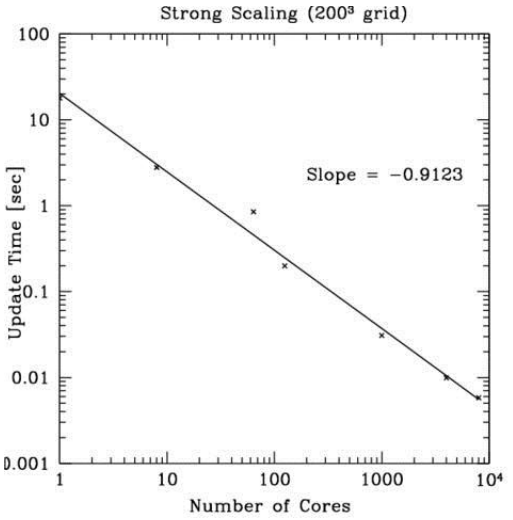
- Sub Types
  - Algorithm and Single Chip Efficiency
  - High Throughput Computing
  - High I/O Computing
  - Tightly Coupled Parallel Computing



# Scaling

- Weak Scaling
  - Keep the size of the problem per core the same, but keep increasing the number of cores.
  - Ideal: Amount of time to solution should not change
- Strong Scaling
  - Keep the total size of the problem the same but keep increasing the number of cores.
  - Ideal: Time to completion should scale linearly with the number of cores
- Reasons for Deviation
  - Communications Latency
  - Blocking Communications
  - Non-overlapped communications and computation.
  - Not enough computational work

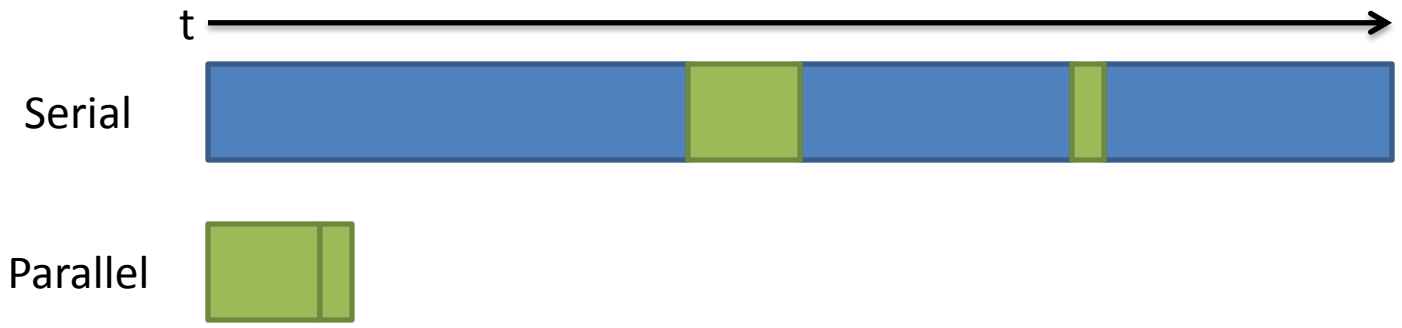


# Amdahl's Law

- The maximum you can speed up any code is limited by the amount that can be effectively parallelized.

- In other words: You are limited by the mandatory serial portions of your code.



# Types of Parallelization

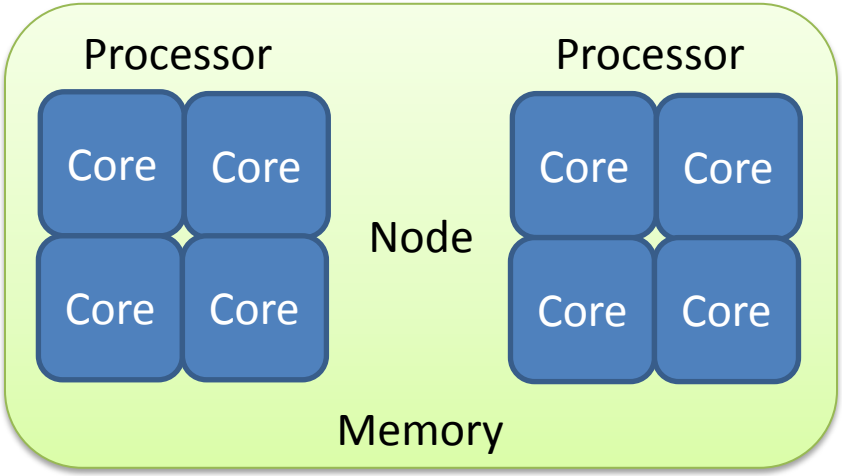
- SIMD
- Thread
- Multinode

# SIMD


- Single Instruction Multiple Data
- Vectorization
  - A(:)=B(:)+C(:)
- Processors natively do this, compilers optimize for it.
  - SSE (Streaming SIMD Extensions): 128 bit register, a=a+b
  - AVX (Advanced Vector Extensions): 128 bit register, a=a+b -> 256 bit register a=b+c
- Note on Optimization Flags:
  - -O0: No optimization
  - -O1: Safe optimization
  - -O2: Mostly Safe optimization
  - -O3: Aggressive optimization
- Always check your answers after your optimize to make sure that you get the same answer back. This is true for any time you recompile or build on a new system. If there are differences make sure they are minor with respect to your expected code outcome.

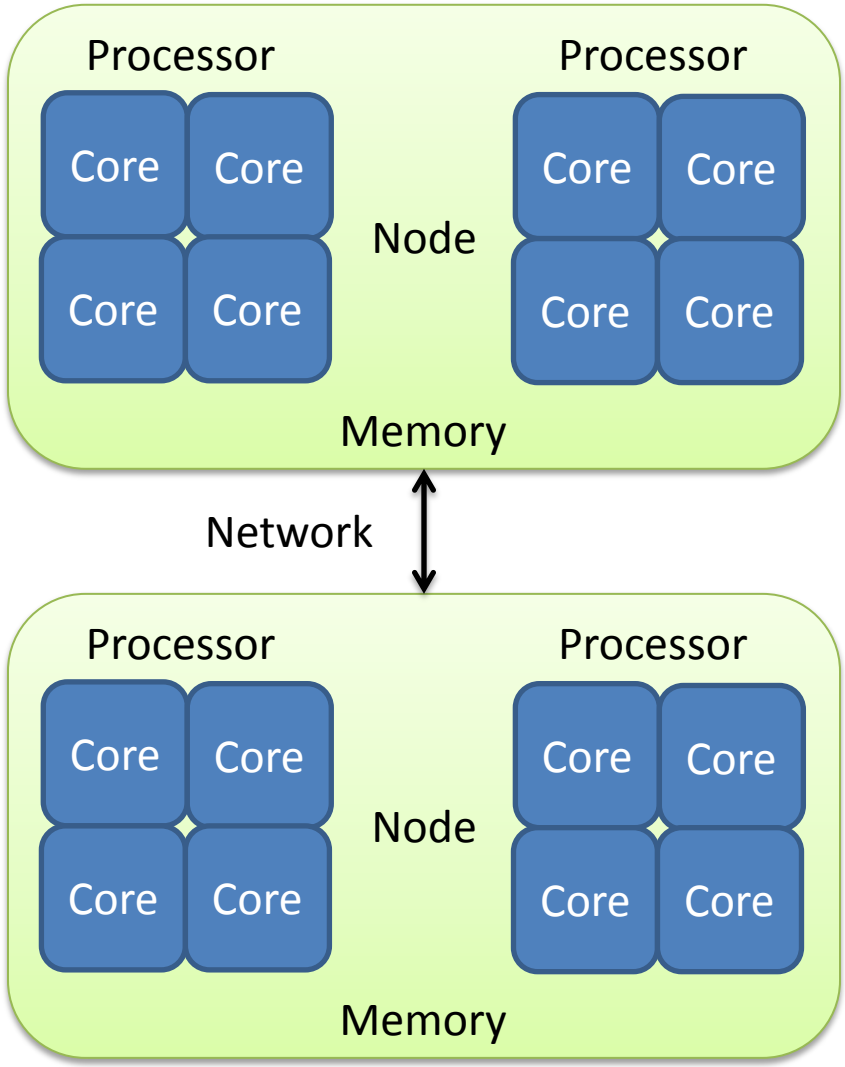
# Thread

- Single Node, program is broken up into threads
- Libraries: OpenMP, pThreads, Cilk
- SMP: Symmetric multiprocessing
- Threads have access to the same memory pool and thus do not have to communicate



# Multinode

- Program is broken up into ranks, each rank runs a part of the code
- Ranks run on multiple nodes
- Ranks do not share memory so they must communicate with each to share information
- Libraries: MPI



# Is my code parallelizable?

- Does it have large loops that repeat the same commands?
- Does your code do multiple tasks that are not dependent one another? If so is the dependency weak?
- Can any dependencies or information sharing be overlapped with computation? If not is the amount communications small?
- Do multiple tasks depend on the same data?
- Does the order of operations matter? If so how strict does it have to be?

# Examples

- Computational Fluid Dynamics
- N-Body and NAMD
- Radiative Transfer and Image Processing
- Markov Chain Monte Carlo
- Embarrassingly Parallel Work

# General Guidelines for Parallelization

- Is it even worth parallelizing my code?
  - Does your code take an intractably long amount of time to complete?
  - Do you run single large models 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: May be easier/faster to do, but may not give good performance or scaling
  - Start from Scratch: Takes longer but will give better performance, accuracy, and gives opportunity to turn a black box code into a code you understand
- Test, test, test, etc.
- Use Nonblocking Communications as often as possible
- Overlap Communications with Computation
- Limit synchronization barriers

# General Guidelines for Parallelization

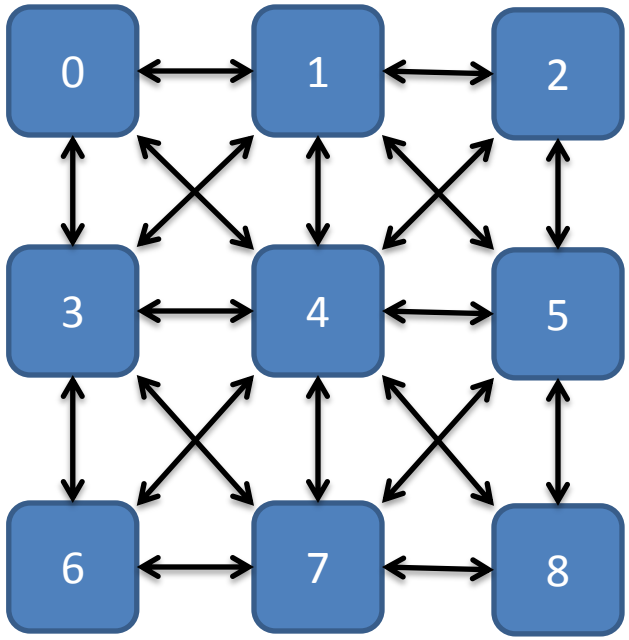
- Limit Collective Communications
- Make messages small
  - Only send essential information
- Make sure messages are well packaged
  - Do one large send with data in a buffer rather than multiple sends
- Use MPI_Iprobe to grease the wheels of nonblocking communications
- Always post nonblocking receives before sends
- Watch out for communications deadlocks
- Be careful of your memory overhead
- Be careful of I/O
  - Avoid having all the cores write to disk at once
  - Alternately don't have all I/O go through one rank.

# General Guidelines for Parallelization

- Do as much as is possible asynchronously
- See if some one has parallelized a code similar to yours and look at what they did
- Beware of portions of the code that depend on order of operations
- Avoid gratuitous IF statements
- Do not use GOTO unless absolutely necessary
- KISS: Keep it simple stupid.
- Print statements are your friend for debugging
- So is replicating the problem on a small number of ranks
- Think at scale

# Message Passing Interface

- MPI standard: Set by MPI Forum
- Current full standard is MPI-2
  - MPI-3 is in the works which includes nonblocking collectives
- MPI allows the user to control passing data between processes through well defined subroutines
- API: C, C++, Fortran
- Libraries: C#, Java, Python, R
- MPI is “agnostic” about network architecture, all it cares is that the location that is being run on can be addressed by whatever transport method you are using



# MPI Nomenclature

- Rank: The ID of a process, starts counting from 0
- Handle: The unique ID for the communication that is being done
- Buffer: An array or string, either controlled by the user or MPI, which is being transported
- Core: An individual compute element
- Node: A collection of compute elements that share the same network address, share memory, and are typically on the same main board
- Hostfile: The list of hosts you will be running on
- MPI Fabric: The communications network MPI constructs either by itself or using a daemon
- Blocking: Means the communications subroutine waits for the completion of the routine before moving on.
- Collective: All ranks talk to everyone else to solve some problem.

# Available MPI Compilers on Odyssey

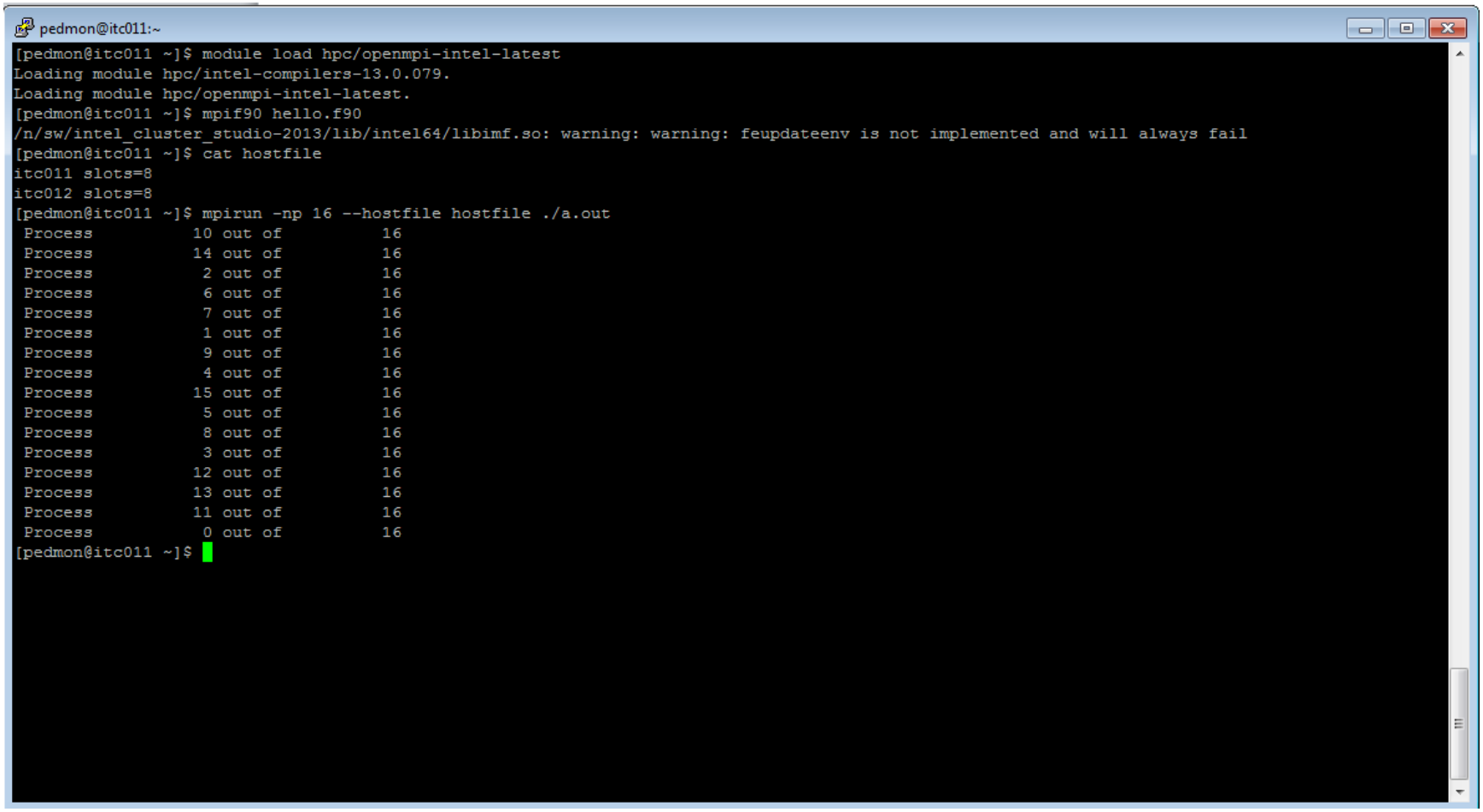
- OpenMPI
  - Open Source project
  - No daemon required
  - Supports MPI-2
  - Even releases are stable, odd releases are development
- MVAPICH2
  - Ohio State University project
  - Old versions require daemon, Latest version does not require daemon
  - MPI-2.2 support as well as some support for MPI-3
- Intel MPI
  - Version of MVAPICH2 optimized by Intel
  - Requires daemon
- All compile for C, C++ and Fortran

# MPI Hello World (Fortran/C)

```
PROGRAM hello

    !### Need to include this to be able to hook into the MPI API ###
    INCLUDE 'mpif.h'

    INTEGER*4 :: numprocs, rank, ierr

    !### Initializes MPI ###
    CALL MPI_INIT(ierr)

    !### Figures out the number of processors I am asking for ###
    CALL MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

    !### Figures out which rank we are ###
    CALL MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierr)

    write(*,*) 'Process', rank, 'out of', numprocs

    !### Need this to shutdown MPI ###
    CALL MPI_FINALIZE(ierr)

END PROGRAM hello
```

```
#include <stdio.h>
/* Need to include this to be able to hook into the MPI API */
#include <mpi.h>

int main(int argc, char *argv[]) {
    int numprocs, rank;

    /* Initializes MPI */
    MPI_Init(&argc, &argv);

    /* Figures out the number of processors I am asking for */
    MPI_Comm_size(MPI_COMM_WORLD, &numprocs);

    /* Figures out which rank we are */
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    printf("Process %d out of %d\n", rank, numprocs);

    /* Need this to shutdown MPI */
    MPI_Finalize();
}
```

# Compiling and Running OpenMPI



# Compiling and Running in other versions of MPI

- MVAPICH2: Same as OpenMPI but hostfile is different
  - OpenMPI: hostname slots=8
  - MVAPICH: hostname:8
- Intel MPI: Same as MVAPICH2 but you first need to start the daemon using the following line
  - mpdboot –f hostfile –n 2
  - mpirun –np 16 ./a.out
  - Where n in this is the number of nodes

# Stay tuned

- Next presentation by Plamen will cover more complex topics such as:
  - MPI Collectives
  - Point to Point Communications
  - Asynchronous Communications
  - MPI and non-C and non-Fortran codes
  - I/O in Parallel Environments