Supercomputing: Hybrid Parallel Programming Models – OpenMP/MPI

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Today's lecture

On this lecture we will discuss the following topics:

- Brief introduction to Supercomputing
- Supercomputer Architectures
- Quick overview of shared-memory programming
- A brief introduction to distributed memory programming
- Hybrid Parallel Programming
- Summary/Overview

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"Advanced Parallel Scientific Computing"

Explore the use and examples of parallel computing in scientific research applications.

- HPC tools (optimization and performance tools)
- Advanced MPI, MPI-file IO.
- Hybrid MPI-openMP implementations
- CUDA/OpenACC/OpenCL
- Scientific Applications: Smoothed Particle Hydrodynamics, N-body simulations Molecular Dynamics Computational Fluid Dynamics

Prerequisites

- Knowledge of compiled languages, such as C/C++ and/or Fortran, and scientific programming applications.
- Experience editing and compiling code in a Linux environment.
- Previous knowledge/experience of parallel programming, including shared memory (openMP), distribute MPI, and heterogeneous architectures (openACC, GPU, etc...) is desirable.

Supercomputing

Supercomputing

Supercomputing, a.k.a. High Performance Computing, is leveraging larger and/or multiple computers to solve computations in parallel.

What does it involve?

- hardware – pipelining, instruction sets, multi-processors, inter-connects
- algorithms – concurrency, efficiency, communications
- software – parallel approaches, compilers, optimization, libraries

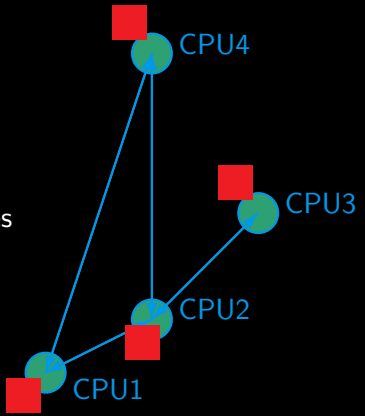
When do I need Supercomputing/HPC?

- My problem takes too long: more/faster computation
- My problem is too big: more memory
- My data is too big: more storage

Supercomputers Architectures

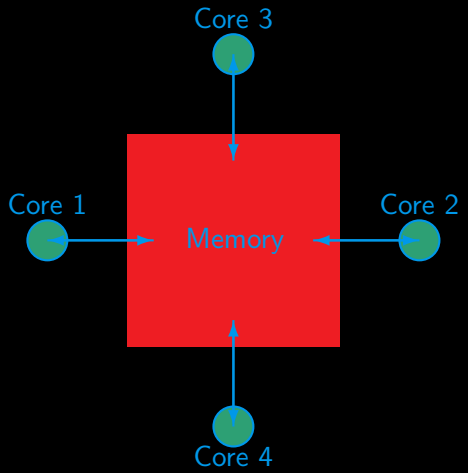
Clusters

- Take existing powerful standalone computers (called a "node"),
- Link them together through a high-speed network (or "interconnect").
- Easy to build and easy to expand.
- Because each node has its own memory that the other nodes cannot see, these are called **distributed memory systems**.
- Nodes communicate and transfer data through messages.
- Programming Model: Message Passing Interface (MPI)



Multi-core Computers

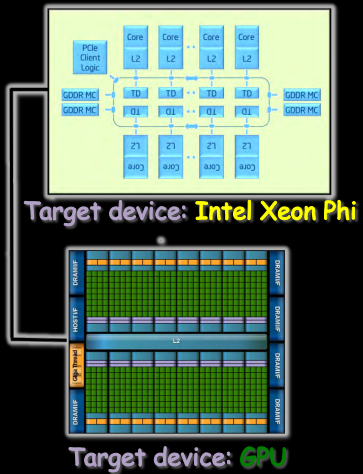
- A collection of processors that can see and use the same memory.
- Limited number of cores, and much more expensive when the number of cores is large.
- Coordination/communication done through memory.
- Also known as **shared-memory systems**.
- Programming model: Threads (e.g. OpenMP)



Your desktop, laptop and cell phone likely use this kind of architecture.

Accelerators

- Systems with accelerators are machines which contain an "off-host" accelerator, such as a GPU or Xeon Phi.
- These accelerator devices are very fast and good at massively parallel processing (having 500-2000+ cores).
- Complicated to program.
- Programming model: CUDA, OpenACC, and OpenCL.
- Needs to be combine with at least some 'host' code: **heterogeous computing**.



OpenMP for shared-memory Parallel Programming

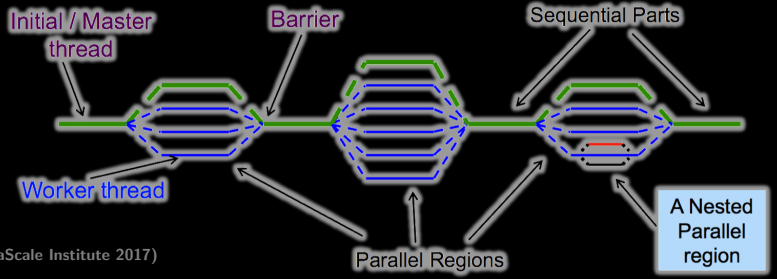
OpenMP

- For shared memory systems.
- Add parallelism to functioning serial code.
- Compiler, run-time environment does a lot of work for us (divides up work)
- But we have to tell it how to use variables, where to run in parallel, . . .
- Works by adding compiler directives to code.
- Industry standard specifying directives (pragmas) to create parallel Fortran, C and C++ programs
- Directives are instructions to a compiler
- API also has library routines and environment variables
- `http://www.openmp.org`

OpenMP Execution Model

- Execution starts with single thread (the initial / master thread)
- Master thread spawns multiple worker threads as needed, together they form a team

  team = master + workers
- Parallel region is a block of code executed by all threads in a team simultaneously

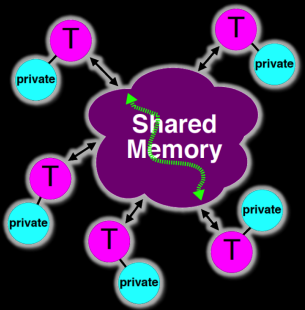


(Credit PetaScale Institute 2017)

- Number of threads in a team may be dynamically adjusted

OpenMP Memory Model

All threads access the same, globally shared memory



(Credit PetaScale Institute 2017)

Data can be shared or private

- **Shared** – only one instance of data
  - Threads can access data simultaneously
  - Changes are visible to all threads
    Not necessarily immediately
- **Private** - Each thread has copy of data
  - No other thread can access it
  - Changes only visible to the thread owning the data

OpenMP has **relaxed-consistency** shared memory model

- Threads may have a temporary view of shared memory that is not consistent with that of other threads
- These temporary views are made consistent at certain places in code

MPI for distributed-memory Parallel Programming

Improving scalability

Issues with shared memory programming

- Parallel tasks are run by threads.
- All threads live on the same node and share the memory.
- Limited to the resources of a single node.
- Creation and deletion of threads can cause overhead.
- Can lead to bugs like race conditions.

Distributed memory programming approach

- Parallel tasks are processes.
- Each process has only its own, private memory.
- Processes need not be on the same node.
- You can scale up the size of your system to as many resources as you have.
- Harder to create race condition bugs, but now you get new bugs like dead-lock.
- Must explicitly code in the communication between processes: Message Passing Interface

MPI is a Library for Message-Passing

- An open standard library interface for message passing, ratified by the MPI Forum
- Not built in to compiler.
- Function calls that can be made from any compiler, many languages.
- "Just" link to it.
- Multiple implementations: OpenMPI, MPICH, ...
- Wrappers: `mpicc`, `mpif90`, `mpicxx`.

```
#include <iostream>
#include <string>
#include <mpi.h>
using namespace std;

int main(int argc, char **argv) {

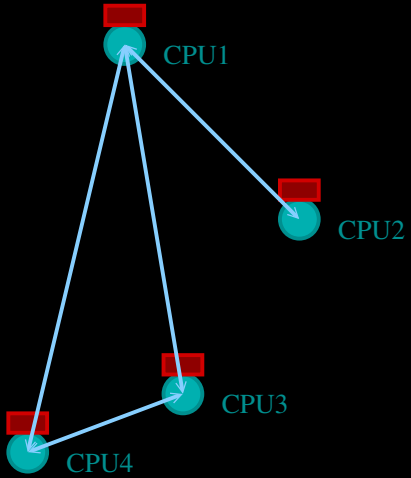
    int rank, size;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    cout << "Hello from task " +
  to_string(rank) + " of " +
  to_string(size) + "World \n";

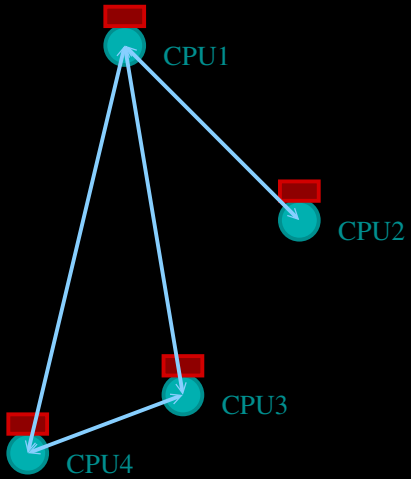
    MPI_Finalize();
}
```

MPI is a Library for Message Passing



- Communication/coordination between tasks done by sending and receiving messages.
- Each message involves a function call from each of the programs.

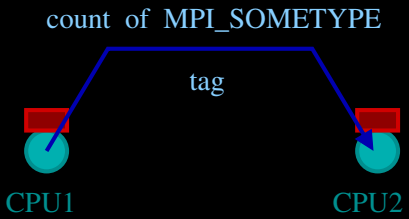
MPI is a Library for Message Passing



Three basic sets of functionality:

- Pairwise communications via messages;
- Collective operations via messages;
- Efficient routines for getting data from memory into messages and vice versa.

Messages



- Messages have a **sender** and a **receiver**.
- When you are sending a message, you don't need to specify the sender (it is the current processor).
- A sent message has to be actively received by the receiving process

Size of MPI Library

- Many, many functions (>200).
- Not nearly so many concepts.
- We'll get started with just 10-12, use more as needed.

```
MPI_Init()
MPI_Comm_size()
MPI_Comm_rank()
MPI_Ssend()
MPI_Recv()
MPI_Sendrecv()
MPI_Finalize()

// Special destinations
MPI_PROC_NULL()
MPI_ANY_SOURCE()
```

Example: Hello World

Compile with MPI

MPI provides compiler wrappers

- mpicc
- mpicxx
- mpif90

that set all the -I, -L, -l, etc. options properly for the base compiler.

```
#include <iostream>
#include <string>
#include <mpi.h>
using namespace std;

int main(int argc, char **argv) {

    int rank, size;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

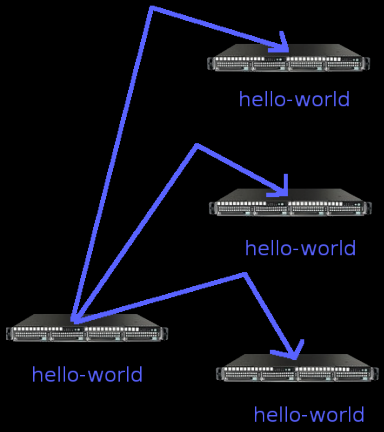
    cout << "Hello from task " +
  to_string(rank) + " of " +
  to_string(size) + "World \n";

    MPI_Finalize();
}
```

```
#Compilation:
mpicxx -O2 --std=c++14 -o mpi-hello-world mpi-hello-world.cc

# Execution:
mpirun -np 16  ./mpi-hello-world
```

What `mpirun` Does



- Launches *n* processes, assigns each an MPI **rank** and starts the program.
- Usually, the processes run the same executable, therefore **each process runs the exact same code**.
- For multinode runs, has a list of nodes, and logs in (effectively) to each node, where it launches the program.
- `mpirun` can run **any** program, eg.

```
mpirun -np 8 hostname
mpirun -np 4 ls
```

MPI - Hello World (cont)

```
$ mpirun -np 4 ./mpi-hello-world
 Hello from task 2 of 4 World
 Hello from task 1 of 4 World
 Hello from task 0 of 4 World
 Hello from task 3 of 4 World

$ mpirun --tag-output -np 4 ./mpi-hello-world
 [1,2]<stdout>:Hello from task 2 of 4 World
 [1,3]<stdout>:Hello from task 3 of 4 World
 [1,0]<stdout>:Hello from task 0 of 4 World
 [1,1]<stdout>:Hello from task 1 of 4 World
```

The `--tag-output` flag is specific for the OpenMPI implementation of MPI.

MPI Basics

Basic MPI Components

- `#include <mpi.h>`
  MPI library definitions
- `MPI_Init(&argc,&argv)`
  MPI Intialization, must come first
- `MPI_Finalize()`
  Finalizes MPI, must come last

Communicator Components

- A communicator is a handle to a group of processes that can communicate.
- `MPI_Comm_rank(MPI_COMM_WORLD,&rank)`
- `MPI_Comm_size(MPI_COMM_WORLD,&rank)`

```
#include <iostream>
#include <string>
#include <mpi.h>
using namespace std;

int main(int argc, char **argv) {

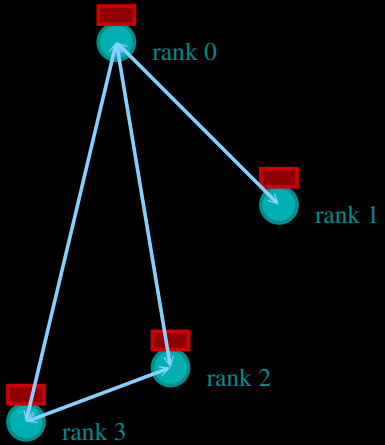
    int rank, size;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    cout << "Hello from task " +
  to_string(rank) + " of " +
  to_string(size) + "World \n";

    MPI_Finalize();
}
```

Communicators



- MPI groups processes into communicators.
- Each communicator has some size – number of tasks.
- Every task has a rank 0..size-1
- Every task in your program belongs to `MPI_COMM_WORLD`.

`MPI_COMM_WORLD`:

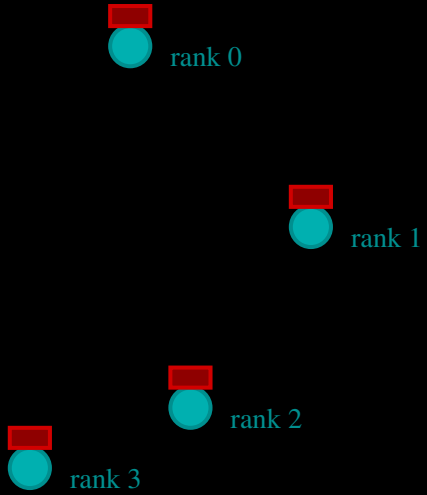
size = 4, ranks = 0..3

- `MPI_COMM_WORLD`: Global Communicator
- `MPI_Comm_rank(MPI_COMM_WORLD,&rank)` Get current tasks rank
- `MPI_Comm_size(MPI_COMM_WORLD,&size)` Get communicator size

MPI = Rank and Size

Rank and Size are much more important in MPI than in OpenMP

- In OpenMP, the compiler assigns jobs to each thread; you do not need to know which one is which (usually).
- In MPI, all proceses run the same code.
- In MPI, processes determine amongst themselves which piece of puzzle to work on, based on their **rank**, then communicate with appropriate others.



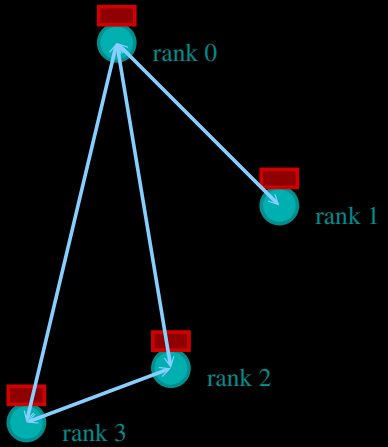
MPI = Communication

Explicit Communication between Tasks

- In OpenMP, threads can communicate using the memory.
- In MPI, a process which needs data of another process needs to communicate with that process by passing messages.

  `MPI_Ssend(...)`

  `MPI_Recv(...)`



MPI: Send & Receive

`MPI_Ssend(sendptr, count, MPI_TYPE, destination,tag, Communicator);`

`MPI_Recv(recvptr, count, MPI_TYPE, source, tag, Communicator, MPI_status)`

- `sendptr/recvptr`: pointer to message
- `count`: number of elements in message
- `MPI_TYPE`: one of MPI_DOUBLE, MPI_FLOAT, MPI_INT, MPI_CHAR, etc.
- `destination/source`: rank of sender/reciever
- `tag`: unique id for message pair
- `Communicator`: MPI_COMM_WORLD or user created
- `status`: receiver status (error, source, tag)

```
int main(int argc, char **argv) {
  int rank, size;
  int tag = 1;
  double msgsent, msgrcvd;
  MPI_Status rstatus;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &size);

  msgsent = 111.;
  msgrcvd = -999.;

  if (rank == 0) {
    MPI_Ssend(&msgsent, 1, MPI_DOUBLE, 1,
        tag, MPI_COMM_WORLD);
    cout << "Sent " + to_string(msgsent) +
        " from " + to_string(rank) + "\n";
  }

  if (rank == 1) {
    MPI_Recv(&msgrcvd, 1, MPI_DOUBLE, 0,
        tag, MPI_COMM_WORLD, &rstatus);
    cout << "Received " + to_string(
        msgrcvd) + " on " + to_string(rank)
        + "\n";
  }

  MPI_Finalize();
}
```

MPI: Send & Receive

```
int main(int argc, char **argv) {
  int rank, size, left, right, tag = 1;
  double msgsent, msgrcvd;
  MPI_Status rstatus;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &size);

  left = rank - 1;
  if (left < 0) left = MPI_PROC_NULL;

  right = rank + 1;
  if (right >= size) right = MPI_PROC_NULL;

  msgsent = rank*rank;
  msgrcvd = -999.;
  MPI_Ssend(&msgsent, 1, MPI_DOUBLE, right, tag, MPI_COMM_WORLD);
  MPI_Recv(&msgrcvd, 1, MPI_DOUBLE, left, tag, MPI_COMM_WORLD, &rstatus);

  cout << to_string(rank) + ": Sent " + to_string(msgsent)
    + " and got " + to_string(msgrcvd) + "\n";

  MPI_Finalize();
}
```

Hybrid Parallel Programming

Shared and Distributed Memory Systems

- Modern clusters have a hybrid architecture.
- Mulitcore machines linked together with an (specialized) interconnect.
- Machines with GPU or other coprocessors: GPU is multi-core, but the amount of shared memory is limited.

Hybrid Parallel Programming

On Modern HPC systems, we need a solution to enable parallelism across nodes

- MPI was developed primarily for inter-address space (inter means between or among)
- OpenMP was developed for shared memory or intra-node, and now supports accelerators as well (intra means within)
- Several solutions $\boldsymbol{MPI + X}$
  - MPI + OpenMP
  - MPI + MPI
  - MPI + other languages
  - Non-MPI solutions such as HPX, ParallelX, ...
- *Hybrid Programming* is when we use a solution with different programming models for inter vs intra-node parallelism

MPI vs OpenMP

We have OpenMP for shared memory programming.

We have MPI to program distributed memory machines.

model	memory	latency	mem.overhead	scalable	incremental
OpenMP	shared mem	low	low	limited	yes
MPI	distributed	high(er)	higher	yes	no

- Could we have the best of both worlds?

MPI vs OpenMP

We have OpenMP for shared memory programming.

We have MPI to program distributed memory machines.

model	memory	latency	mem.overhead	scalable	incremental
OpenMP	shared mem	low	low	limited	yes
MPI	distributed	high(er)	higher	yes	no

- Could we have the best of both worlds?
  - NUMA/memory herarchy/cache-lines/...
  - processor affinity
  - memory affinity (NUMA...)

MPI and OpenMP

Hybrid programming model of using MPI and OpenMP

- MPI across nodes
- OpenMP within nodes
- Minimizes communication
- Scalable
- Not much more complicated than pure MPI
- MPI+X / X=openMP

MPI and OpenMP

Hybrid programming model of using MPI and OpenMP

- MPI across nodes
- OpenMP within nodes
- Minimizes communication
- Scalable
- Not much more complicated than pure MPI
- MPI+X / X=openMP

Many Computations are amenable to a Hybrid (often MPI + OpenMP) approach

- Domains (often resulting from the decomposition of PDE's) are spread across the large system and only need to communicate "ghost zone" information as time advances
- MPI is used to communicate these ghost zone values in the form of messages passed among the nodes
- In various hybrid approaches, different programming models can be used for the shared memory region. OpenMP is one choice.

Hybrid Programming

Pros

- No decomposition on node
- Lower latency, less communication
- Less duplication of data (and perhaps computation)
- OpenMP has load balance capabilities

Cons

- One more layer to maintain
- OpenMP has more hidden side effects
- May have to worry about NUMA

MPI + OpenMP has been targeted for optimized use on many systems

- For example, systems with many threads to keep busy
- MPI + OpenMP is one obvious programming model
  - may not fit into node using pure MPI across all HW cores and threads because of the memory overhead for each MPI task.
  - Conceptually nice: OpenMP within node, MPI between
  - Provides a way to increase fine-scale parallel granularity
  - Some problems have natural two-level parallelism;

Hybrid Programming

Example

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

int main(int argc, char ** argv) {

  int size,rank;

  MPI_Init(&argc,&argv);
  MPI_Comm_get_rank(MPI_COMM_WORLD,&rank);
  MPI_Comm_get_size(MPI_COMM_WORLD,&size);

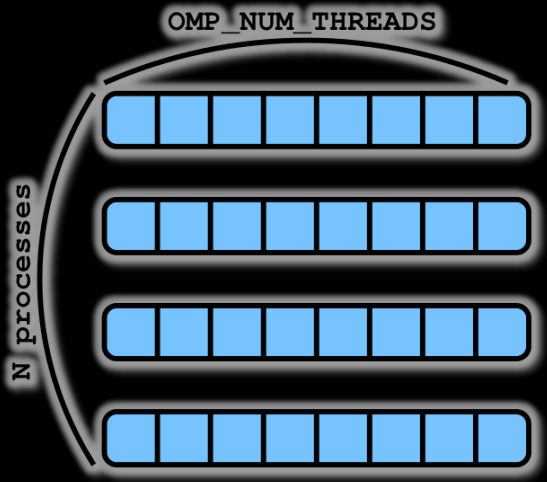
  #pragma omp parallel for
  for (int i=0;i<4;i++)
    std::cout << "Hello world from thread "
      << omp_get_thread_num() << std::endl;

  MPI_Finalize();
}
```

PseudoCode (Fortran-ish...)

```
Program hybrid
 call MPI_INIT (ierr)
 call MPI_COMM_RANK (...)
 call MPI_COMM_SIZE (...)
  ... some computation and MPI communication
 call OMP_SET_NUM_THREADS(4)
!$OMP PARALLEL DO PRIVATE(i)
!$OMP&                  SHARED(n)
  do i=1,n
     ... computation
  enddo
 !$OMP END PARALLEL DO
  ... some computation and MPI communication
call MPI_FINALIZE (ierr)
end
```

Hybrid Programming



- Memory shared among threads of same process
- Memory not shared among threads of different processes

Hybrid Programming – Technicalities

- Note: OpenMP inside MPI
- Often, one starts with an MPI code and adds in OpenMP.
- Compilation:

```
mpicxx -fopenmp [filename] -o [executable]
```

- Execution:

```
export OMP_NUM_THREADS=M
mpirun -np N --bynode [executable]
```

- This starts `N` processes
- Between `MPI_Init` and `MPI_Finalize`, each process spawns `OMP_NUM_THREADS` threads in `#pragma omp parallel` blocks.

Hybrid MPI+OpenMP Scalability Performance

- MPI/OpenMP Code can sometimes be slower
- All threads are idle except one while MPI communication
  - Need overlap comp and comm for better performance.
  - Critical Section for shared variables.
- Thread creation overhead
- Cache coherence, false sharing.
- Data placement, NUMA effects.
- Natural one level parallelism problems.
- Check performance of pure OpenMP in a node to pure MPI in a node

If a Routine Does Not Scale Well

- Examine code for serial/critical sections, eliminate if possible.
- Reduce number of OpenMP parallel regions to reduce overhead costs.
- Perhaps loop collapse, loop fusion or loop permutation is required to give all threads enough work, and to optimize thread cache locality.
- Pay attention to load imbalance. If needed, try dynamic scheduling or implement own load balance scheme.
- Experiment with different combinations of MPI tasks and number of threads per task. Less MPI tasks may not saturate inter-node bandwidth.
- Test different process and thread affinity options.
- Leave some cores idle on purpose, for memory capacity or bandwidth capacity.

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- Test different process and thread affinity options.
- Leave some cores idle on purpose, for memory capacity or bandwidth capacity.

*** Vary MPI ranks and OpenMP threads to find optimal configuration**

$\rightsquigarrow$ **find the sweet spot for hybrid MPI/OpenMP**

Summary

Summary

- Supercomputing/HPC
- Shared memory programming: openMP (pragmas, directives to the compiler)
- Distributed memory programming: MPI (library)
- Hybrid parallel programming: MPI+$\boldsymbol{X}$, $\boldsymbol{X}$=openMP (openACC, CUDA, ...)

Appendix

MPI Example

Let's consider a diffusion equation with an explicit **finite-difference**, **time-marching** method.

We'll imagine that the problem is too large to fit in the memory of one node, so we need to do **domain decomposition**, and use **MPI**.

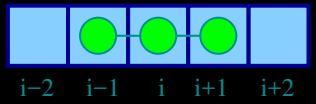
Discretizing Derivatives

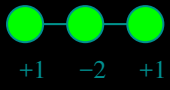
- Partial Differential Equations like the diffusion equation

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2}$$

  are usually numerically solved by finite differencing the discretized values.
- Implicitly or explicitly involves interpolating data and taking the derivative of the interpolant.
- Larger 'stencils' $\rightarrow$ More accuracy.

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$





Diffusion equation in higher dimensions

Spatial grid separation: Δx. Time step Δt.

Grid indices: i, j. Time step index: (n)

1D

$$\left.\frac{\partial T}{\partial t}\right|_i \approx \frac{T_i^{(n)} - T_i^{(n-1)}}{\Delta t}$$

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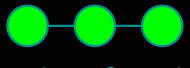
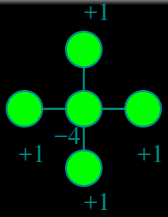


2D



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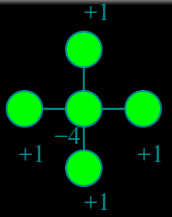

$$\left.\frac{\partial T}{\partial t}\right|_{i,j} \approx \frac{T_{i,j}^{(n)} - T_{i,j}^{(n-1)}}{\Delta t}$$

$$\left.\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)\right|_{i,j} \approx \frac{T_{i-1,j}^{(n)} + T_{i,j-1}^{(n)} - 4T_{i,j}^{(n)} + T_{i+1,j}^{(n)} + T_{i,j+1}^{(n)}}{\Delta x^2}$$

Stencils and Boundaries

- How do you deal with boundaries?
- The stencil juts out, you need info on cells beyond those you're updating.
- Common solution:
  Guard cells:
  - Pad domain with these guard celss so that stencil works even for the first point in domain.
  - Fill guard cells with values such that the required boundary conditions are met.

1D

- Number of guard cells $n_g = 1$
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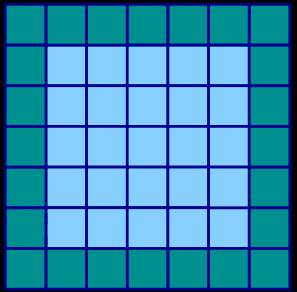
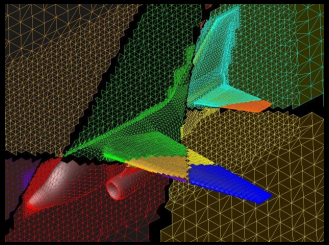
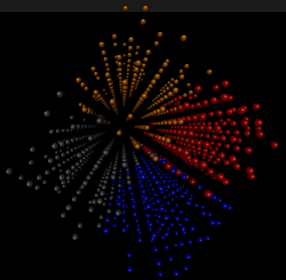
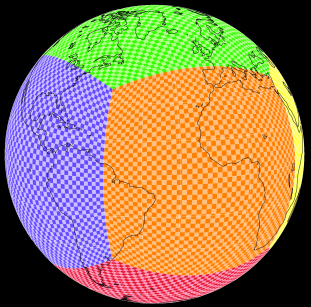


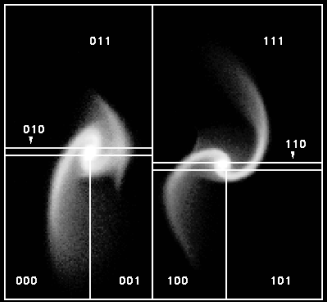
Domain decomposition

- A very common approach to parallelizing on distributed memory computers.
- Subdivide the domain into contiguous subdomains.
- Give each subdomain to a different MPI process.
- No process contains the full data!
- Maintains locality.
- Need mostly local data, ie., only data at the boundary of each subdomain will need to be sent between processes.



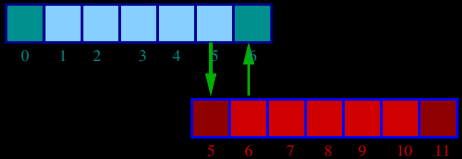






Guard cell exchange

- In the domain decomposition, the stencils will jut out into a neighbouring subdomain.
- Much like the boundary condition.
- One uses guard cells for domain decomposition too.
- If we managed to fill the guard cell with values from neighbouring domains, we can treat each coupled subdomain as an isolated domain with changing boundary conditions.



- Could use even/odd trick, or sendrecv.

1D diffusion with MPI

Before MPI

```
a = 0.25*dt/pow(dx,2);
guardleft = 0;
guardright = n+1;

for (int t=0;t<maxt;t++) {
  T[guardleft] = 0.0;
  T[guardright] = 0.0;

  for (int i=1; i<=n; i++)
    newT[i] = T[i] + a*(T[i+1]+T[i
        -1]-2*T[i]);

  for (int i=1; i<=n; i++)
    T[i] = newT[i];
}
```

Note:

- the for-loop over `i` could also easily be parallelized with OpenMP ($\Rightarrow$ hybrid MPI-OpenMP code).

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}
```

Note:

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After MPI

```
MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);

left = rank-1; if(left<0)left=MPI_PROC_NULL;
right = rank+1; if(right>=size)right=
    MPI_PROC_NULL; localn = n/size;

a = 0.25*dt/pow(dx,2); guardleft = 0;
guardright = localn+1;
for (int t=0;t<maxt;t++) {
  MPI_Sendrecv(&T[1], 1, MPI_DOUBLE, left, 11,
       &T[guardright], 1, MPI_DOUBLE,right,11,
       MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  MPI_Sendrecv(&T[nlocal], 1, MPI_DOUBLE,
      right,11, &T[guardleft], 1, MPI_DOUBLE,
      left, 11, MPI_COMM_WORLD,
      MPI_STATUS_IGNORE);
  if (rank==0) T[guardleft] = 0.0;
  if (rank==size-1) T[guardright] = 0.0;
  for (int i=1; i<=localn; i++)
    newT[i] = T[i] + a*(T[i+1]+T[i-1]-2*T[i]);
  for (int i=1; i<=n; i++)
    T[i] = newT[i];
}
MPI_Finalize();
```