Crash Course in Supercomputing

Computing Sciences Summer Student Program Training 2020

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Course Outline

Parallelism & MPI (10 am - noon)

I. Parallelism
II. Supercomputer Architecture
III. Basic MPI

(Interlude 1: Computing Pi in parallel)

IV. MPI Collectives

(Interlude 2: Computing Pi using parallel collectives)

OpenMP & Hybrid Programming (1 - 3 pm)

Course Outline

Parallelism & MPI (10 am - noon)

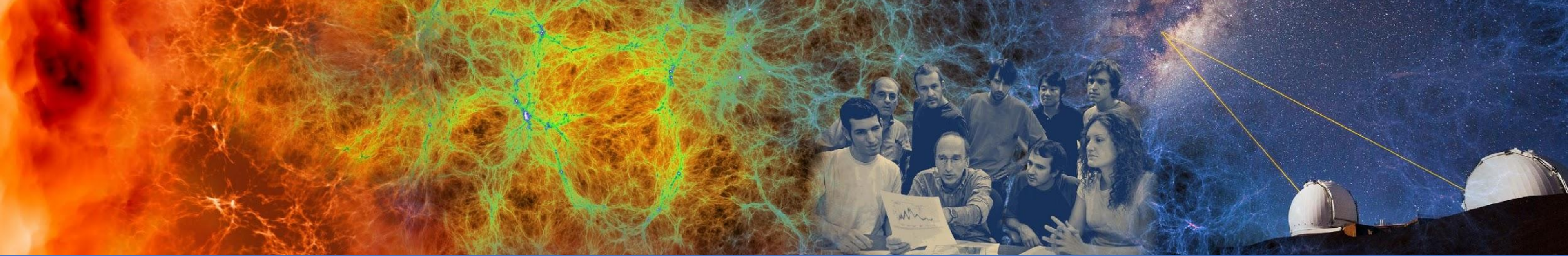
OpenMP & Hybrid Programming (1 - 3 pm)

I. About OpenMP
II. OpenMP Directives
III. Data Scope
IV. Runtime Library Routines & Environment
V. Using OpenMP

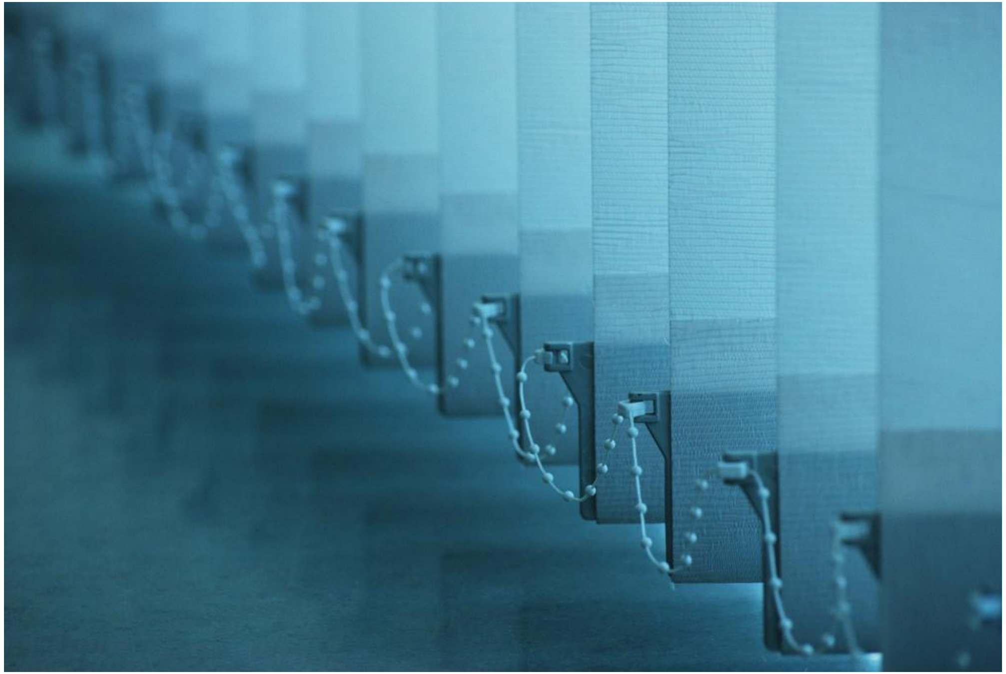
(Interlude 3: Computing Pi with OpenMP)

VI. Hybrid Programming

(Interlude 4: Computing Pi with Hybrid Programming)



Parallelism & MPI



I. PARALLELISM

"Parallel Worlds" by aloshbennett from
http://www.flickr.com/photos/aloshbennett/3209564747/sizes/l/in/photostream/

I. Parallelism

- Concepts of parallelization
- Serial vs. parallel
- Parallelization strategies

Parallelization Concepts

- When performing task, some subtasks depend on one another, while others do not
- Example: Preparing dinner
  - Salad prep independent of lasagna baking
  - Lasagna must be assembled before baking
- Likewise, in solving scientific problems, some tasks independent of one another

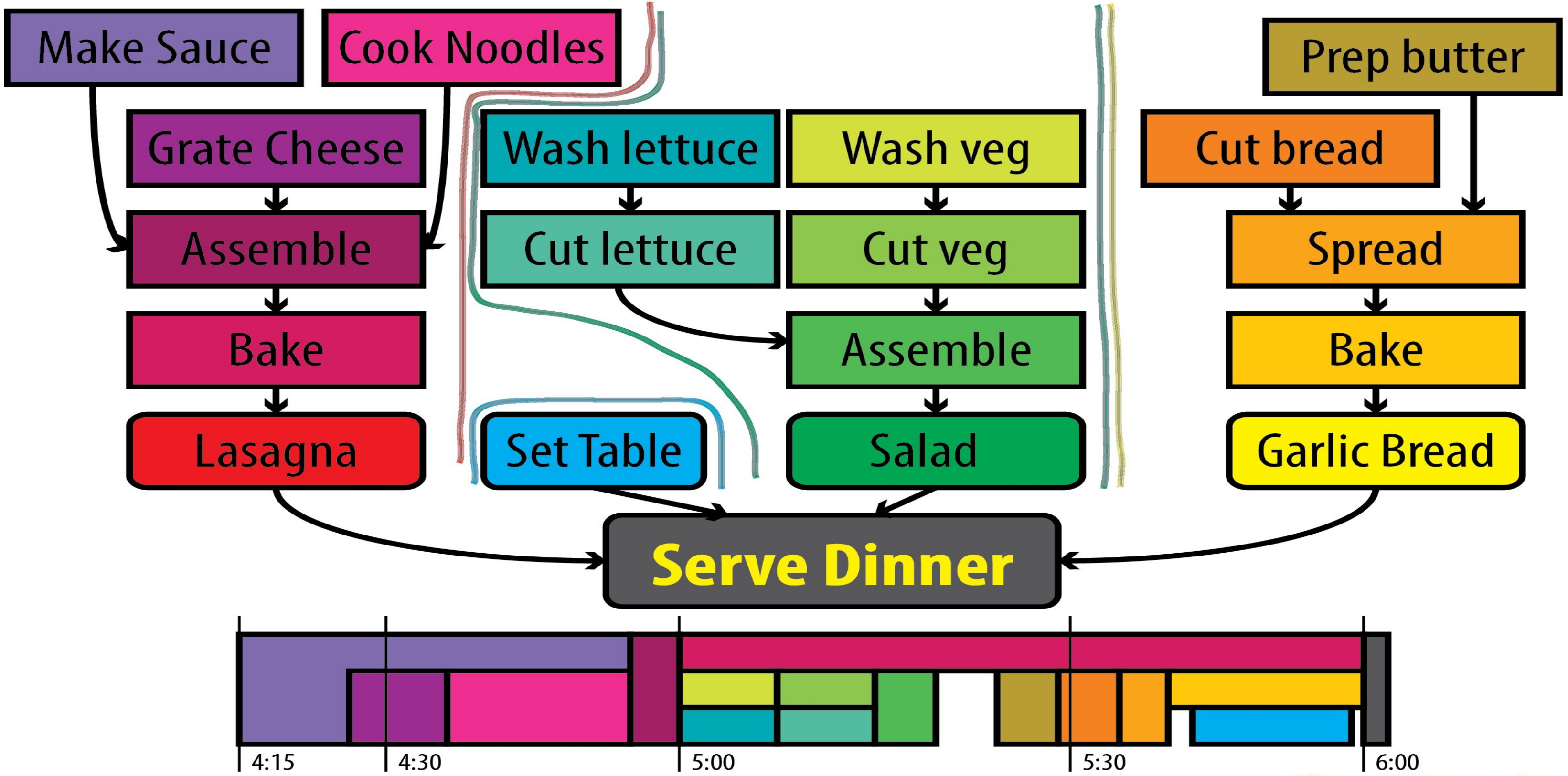
Serial vs. Parallel

- *Serial:* tasks must be performed in sequence
- *Parallel:* tasks can be performed independently in any order

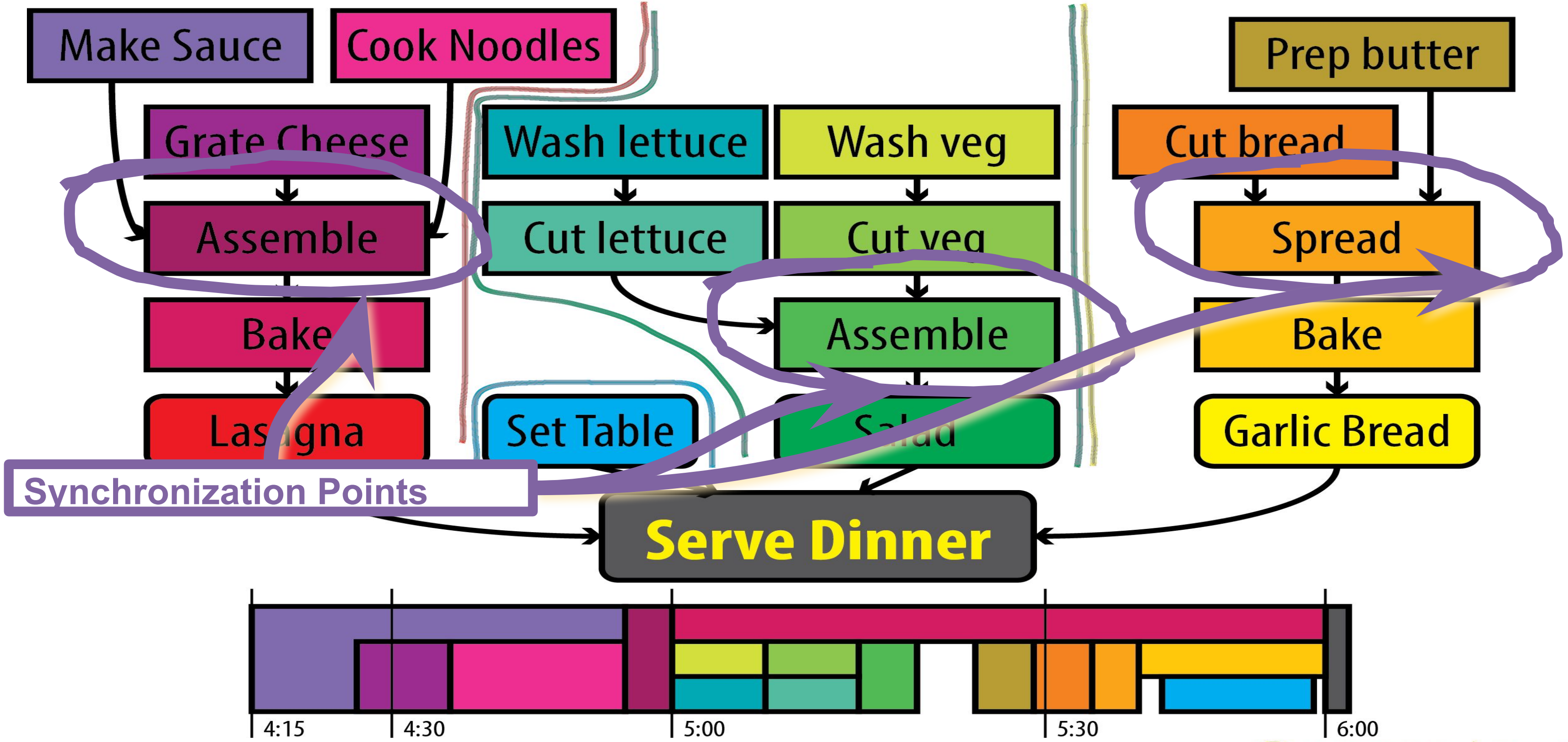
Serial vs. Parallel: Example

- Preparing lasagna dinner
- *Serial tasks:* making sauce, assembling lasagna, baking lasagna; washing lettuce, cutting vegetables, assembling salad
- *Parallel tasks:* making lasagna, making salad, setting table

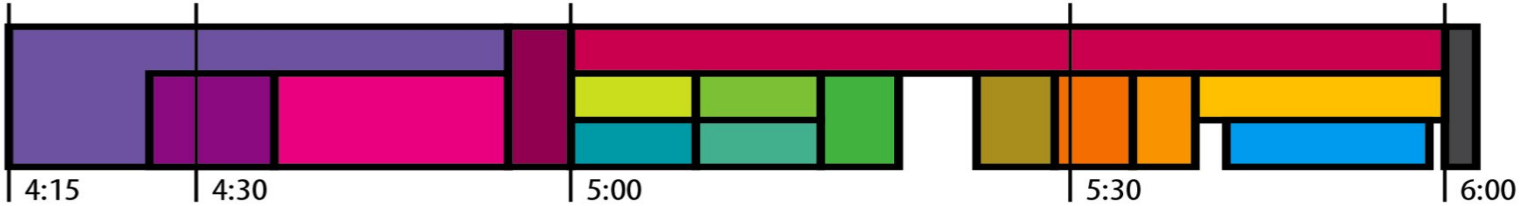
Serial vs. Parallel: Graph



Serial vs. Parallel: Graph



Serial vs. Parallel: Graph

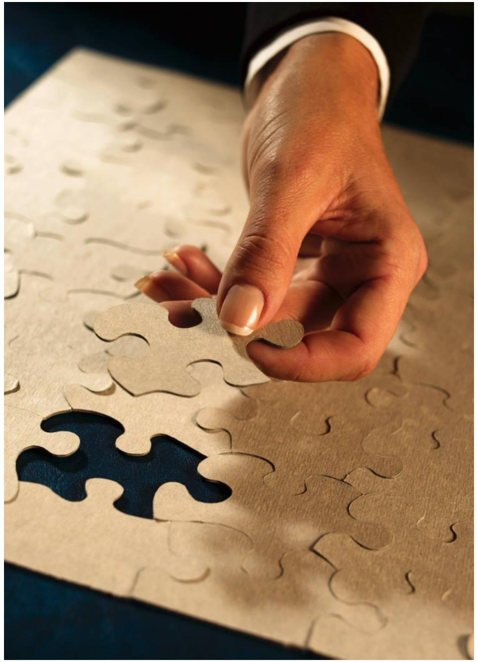


Serial vs. Parallel: Example

- Could have several chefs, each performing one parallel task
- This is concept behind parallel computing

Discussion: Jigsaw Puzzle*

- Suppose we want to do a large, N-piece jigsaw puzzle (e.g., $N = 10{,}000$ pieces)
- Time for one person to complete puzzle: T hours
- How can we decrease walltime to completion?



Discussion: Jigsaw Puzzle

- Impact of having multiple people at the table
  - Walltime to completion
  - Communication
  - Resource contention
- Let number of people = p
  - Think about what happens when $p = 1, 2, 4, \ldots 5000$

Discussion: Jigsaw Puzzle

Alternate setup: p people, each at separate table with N/p pieces each

- What is the impact on
  - Walltime to completion
  - Communication
  - Resource contention?

Discussion: Jigsaw Puzzle

Alternate setup: divide puzzle by features, each person works on one, e.g., mountain, sky, stream, tree, meadow, etc.

- What is the impact on
  - Walltime to completion
  - Communication
  - Resource contention?

Parallel Algorithm Design: PCAM

- *Partition:* Decompose problem into fine-grained tasks to maximize potential parallelism
- *Communication:* Determine communication pattern among tasks
- *Agglomeration:* Combine into coarser-grained tasks, if necessary, to reduce communication requirements or other costs
- *Mapping:* Assign tasks to processors, subject to tradeoff between communication cost and concurrency

(from Heath: *Parallel Numerical Algorithms*)

II. ARCHITECTURE

“Architecture” by marie-II, http://www.flickr.com/photos/grrrl/324473920/sizes/l/in/photostream/

II. Supercomputer Architecture

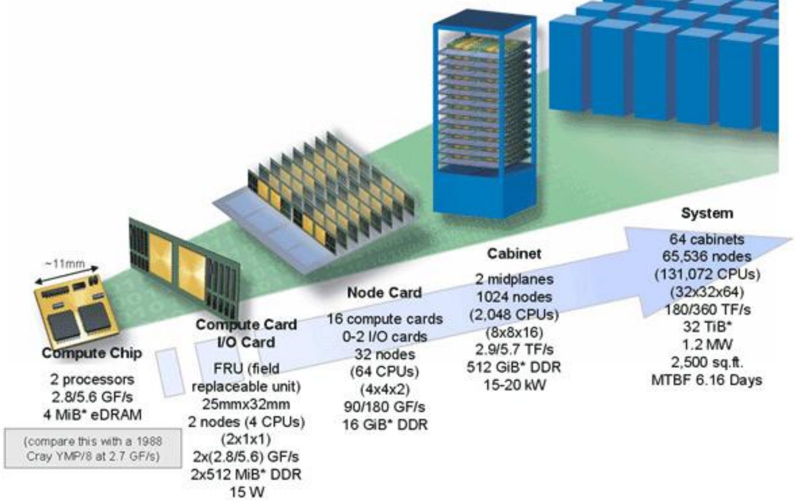
- What is a supercomputer?
- Conceptual overview of architecture

Cray 1 (1976)

IBM Blue Gene (2005)

Cray XT5 (2009)

Architecture of IBM Blue Gene



What Is a Supercomputer?

- “The biggest, fastest computer right this minute.”
  – Henry Neeman
- Generally at least 100 times more powerful than PC
- This field of study known as supercomputing, high-performance computing (HPC), or scientific computing
- Scientists use really big computers to solve really hard problems

SMP Architecture

- Massive memory, shared by multiple processors
- Any processor can work on any task, no matter its location in memory
- Ideal for parallelization of sums, loops, etc.

Cluster Architecture

- CPUs on racks, do computations (fast)
- Communicate through networked connections (slow)
- Want to write programs that divide computations evenly but minimize communication

State-of-the-Art Architectures

- Today, hybrid architectures pervasive
  - Multiple {8, 12, 16, 24, 32, 68}-core nodes, connected to other nodes by (slow) interconnect
  - Cores in node share memory (like small SMP machines)
  - Machine appears to follow cluster architecture (with multi-core nodes rather than single processors)
  - To take advantage of all parallelism, use MPI (cluster) and OpenMP (SMP) hybrid programming

State-of-the-Art Architectures

- Hybrid CPU/GPGPU architectures broadly accepted
    - Nodes consist of one (or more) multicore CPU + one (or more) GPU
    - Heavy computations offloaded to GPGPUs
    - Separate memory for CPU and GPU
    - Complicated programming paradigm, outside the scope of today's training

III. BASIC MPI

"MPI Adventure" by Stefan Jürgensen, from
http://www.flickr.com/photos/94039982@N00/6177616380/sizes/l/in/photostream/

III. Basic MPI

- Introduction to MPI
- Parallel programming concepts
- The Six Necessary MPI Commands
- Example program

Introduction to MPI

- Stands for **M**essage **P**assing **I**nterface
- Industry standard for parallel programming (200+ page document)
- MPI implemented by many vendors; open source implementations available too
  - Cray, IBM, HPE vendor implementations
  - MPICH, LAM-MPI, OpenMPI (open source)
- MPI function library is used in writing C, C++, or Fortran programs in HPC

Introduction to MPI

- MPI-1 vs. MPI-2: MPI-2 has additional advanced functionality and C++ bindings, but everything learned in this section applies to both standards
- MPI-3: Major revisions (e.g., nonblocking collectives, extensions to one-sided operations), released September 2012, 800+ pages
  - MPI-3.1 released June 2015
  - MPI-3 additions to standard will not be covered today
- MPI-4: Standard currently in development

Parallelization Concepts

- Two primary programming paradigms:
  - **SPMD** (single program, multiple data)
  - **MPMD** (multiple programs, multiple data)
- MPI can be used for either paradigm

SPMD vs. MPMD

- SPMD: Write single program that will perform same operation on multiple sets of data
    - Multiple chefs baking many lasagnas
    - Rendering different frames of movie
- MPMD: Write different programs to perform different operations on multiple sets of data
    - Multiple chefs preparing four-course dinner
    - Rendering different parts of movie frame
- Can also write hybrid program in which some processes perform same task

The Six Necessary MPI Commands

```
int MPI_Init(int *argc, char **argv)
int MPI_Finalize(void)
int MPI_Comm_size(MPI_Comm comm, int *size)
int MPI_Comm_rank(MPI_Comm comm, int *rank)
int MPI_Send(void *buf, int count, MPI_Datatype
   datatype, int dest, int tag, MPI_Comm comm)
int MPI_Recv(void *buf, int count, MPI_Datatype
   datatype, int source, int tag, MPI_Comm comm,
   MPI_Status *status)
```

Initiation and Termination

- `MPI_Init(int *argc, char **argv)` initiates MPI
    - Place in body of code after variable declarations and before any MPI commands
- `MPI_Finalize(void)` shuts down MPI
    - Place near end of code, after last MPI command

Environmental Inquiry

- `MPI_Comm_size(MPI_Comm comm, int *size)`
  - Find out number of processes
  - Allows flexibility in number of processes used in program
- `MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Find out identifier of current process
  - `0 ≤ rank ≤ size-1`

Message Passing: Send

- **`MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`**
  - Send message of length **`count`** items and datatype **`datatype`** contained in **`buf`** with tag **`tag`** to process number **`dest`** in communicator **`comm`**
  - E.g., **`MPI_Send(&x, 1, MPI_DOUBLE, manager, me, MPI_COMM_WORLD)`**

Message Passing: Receive

- **`MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`**
- Receive message of length **`count`** items and datatype **`datatype`** with tag **`tag`** in buffer **`buf`** from process number **`source`** in communicator **`comm`**, and record status **`status`**
- E.g. **`MPI_Recv(&x, 1, MPI_DOUBLE, source, source, MPI_COMM_WORLD, &status)`**

Message Passing

- WARNING! Both standard send and receive functions are blocking
- **`MPI_Recv`** returns only after receive buffer contains requested message
- **`MPI_Send`** may or may not block until message received (usually blocks)
- Must watch out for deadlock

Deadlocking Example (Always)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
    MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    printf("Sent %d to proc %d, received %d from proc %d\n", me, sendto, q,
sendto);
    MPI_Finalize();
    return 0;
}
```

Deadlocking Example (Sometimes)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
    printf("Sent %d to proc %d, received %d from proc %d\n", me, sendto, q,
sendto);
    MPI_Finalize();
    return 0;
}
```

Deadlocking Example (Safe)

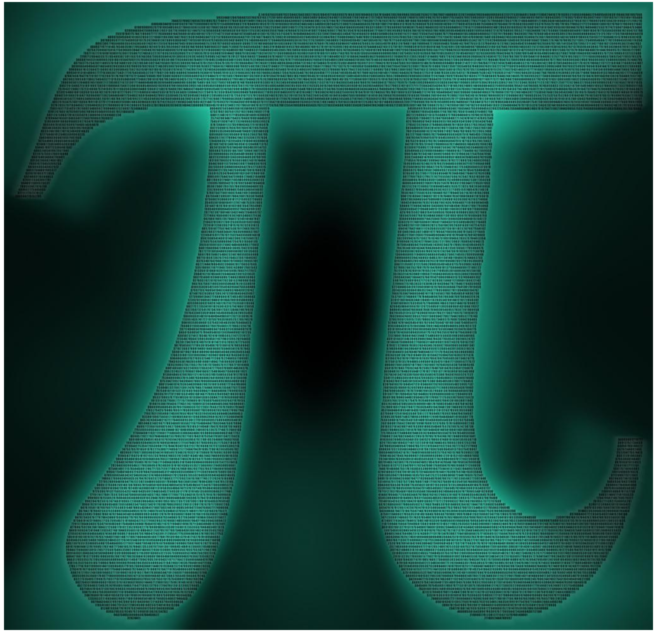
```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    if (me%2 == 0) {
        MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
        MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
     } else {
        MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
        MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    }
    printf("Sent %d to proc %d, received %d from proc %d\n", me, sendto, q, sendto);
    MPI_Finalize();
    return 0;
}
```

Explanation: Always Deadlocking Example

- Logically incorrect
- Deadlock caused by blocking **`MPI_Recv`**s
- All processes wait for corresponding **`MPI_Send`**s to begin, which never happens

Explanation: Sometimes Deadlocking Example

- Logically correct
- Deadlock could be caused by **`MPI_Send`**s competing for buffer space
- Unsafe because depends on system resources
- Solutions:
  - Reorder sends and receives, like safe example, having evens send first and odds send second
  - Use non-blocking sends and receives or other advanced functions from MPI library (see MPI standard for details)



INTERLUDE 1: COMPUTING PI IN PARALLEL

"Pi of Pi" by spellbee2, from
http://www.flickr.com/photos/49825386@N08/7253578340/sizes/l/in/photostream/

Interlude 1: Computing π in Parallel

- Project Description
- Serial Code
- Parallelization Strategies
- Your Assignment

Project Description

- We want to compute π
- One method: method of darts*
- Ratio of area of square to area of inscribed circle proportional to π

“Picycle” by Tang Yau Hoong, from http://www.flickr.com/photos/tangyauhoong/5609933651/sizes/o/in/photostream/

* This is a TERRIBLE way to compute pi! Don’t do this in real life!!!! (See Appendix 1 for better ways)

Method of Darts

- Imagine dartboard with circle of radius R inscribed in square
- Area of circle $= \pi R^2$
- Area of square $= (2R)^2 = 4R^2$
- $\dfrac{\text{Area of circle}}{\text{Area of square}} = \dfrac{\pi R^2}{4R^2} = \dfrac{\pi}{4}$

"Dartboard" by AndyRobertsPhotos, from http://www.flickr.com/photos/aroberts/2907670014/sizes/o/in/photostream/

Method of Darts

- Ratio of areas proportional to π
- How to find areas?
  - Suppose we threw darts (completely randomly) at dartboard
  - Count # darts landing in circle & total # darts landing in square
  - Ratio of these numbers gives approximation to ratio of areas
  - Quality of approximation increases with # darts thrown

Method of Darts

$$\pi = 4 \times \frac{\text{\# darts inside circle}}{\text{\# darts thrown}}$$

Method of Darts cake in celebration of Pi Day 2009, Rebecca Hartman-Baker

Method of Darts

- Okay, Rebecca, but how in the world do we simulate this experiment on a computer?
- Decide on length R
- Generate pairs of random numbers (x, y) s.t.

$$-R \leq (x, y) \leq R$$

- If (x, y) within circle (i.e., if $(x^2+y^2) \leq R^2$) add one to tally for inside circle
- Lastly, find ratio

Serial Code (darts.c)

```
#include "lcgenerator.h"
static long num_trials = 1000000;

int main() {
  long i;
  long Ncirc = 0;
  double pi, x, y;
  double r = 1.0; // radius of circle
  double r2 = r*r;

  for (i = 0; i < num_trials; i++) {
    x = r*lcgrandom();
    y = r*lcgrandom();
    if ((x*x + y*y) <= r2)
      Ncirc++;
  }

  pi = 4.0 * ((double)Ncirc)/((double)num_trials);
  printf("\n For %ld trials, pi = %f\n", num_trials, pi);

  return 0;
}
```

Serial Code (lcgenerator.h)

```
// Random number generator -- and not a very good one, either!

static long MULTIPLIER = 1366;
static long ADDEND = 150889;
static long PMOD = 714025;
long random_last = 0;

// This is not a thread-safe random number generator

double lcgrandom() {
  long random_next;
  random_next = (MULTIPLIER * random_last + ADDEND)%PMOD;
  random_last = random_next;

  return ((double)random_next/(double)PMOD);
}
```

Serial Code (darts.f) (1)

```
! First, the pseudorandom number generator

  real function lcgrandom()
    integer*8, parameter :: MULTIPLIER = 1366
    integer*8, parameter :: ADDEND = 150889
    integer*8, parameter :: PMOD = 714025
    integer*8, save :: random_last = 0

    integer*8 :: random_next = 0
    random_next = mod((MULTIPLIER * random_last + ADDEND), PMOD)
    random_last = random_next
    lcgrandom = (1.0*random_next)/PMOD
    return
  end
```

Serial Code (darts.f) (2)

```
! Now, we compute pi
  program darts
    implicit none
    integer*8 :: num_trials = 1000000, i = 0, Ncirc = 0
    real :: pi = 0.0, x = 0.0, y = 0.0, r = 1.0
    real :: r2 = 0.0
    real :: lcgrandom
    r2 = r*r

   do i = 1, num_trials
      x = r*lcgrandom()
      y = r*lcgrandom()
      if ((x*x + y*y) .le. r2) then
        Ncirc = Ncirc+1
      end if
    end do
    pi = 4.0*((1.0*Ncirc)/(1.0*num_trials))
    print*, ' For ', num_trials, ' trials, pi = ', pi

  end
```

Parallelization Strategies

- What tasks independent of each other?
- What tasks must be performed sequentially?
- Using PCAM parallel algorithm design strategy

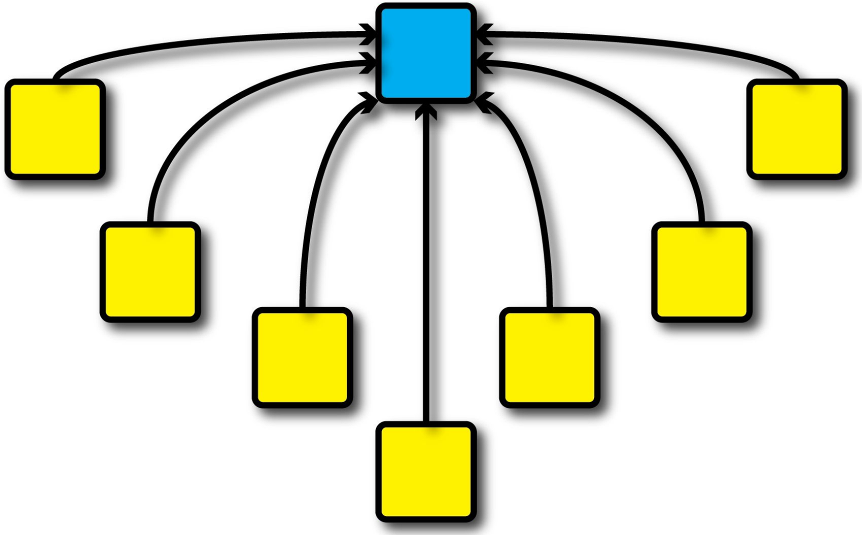
Partition

- *"Decompose problem into fine-grained tasks to maximize potential parallelism"*
- Finest grained task: throw of one dart
- Each throw independent of all others
- If we had huge computer, could assign one throw to each processor

Communication

"Determine communication pattern among tasks"

- Each processor throws dart(s) then sends results back to manager process



Agglomeration

"Combine into coarser-grained tasks, if necessary, to reduce communication requirements or other costs"

- To get good value of π, must use millions of darts
- We don't have millions of processors available
- Furthermore, communication between manager and millions of worker processors would be very expensive
- Solution: divide up number of dart throws evenly between processors, so each processor does a share of work

Mapping

"Assign tasks to processors, subject to tradeoff between communication cost and concurrency"

- Assign role of "manager" to processor 0
- Processor 0 will receive tallies from all the other processors, and will compute final value of π
- Every processor, including manager, will perform equal share of dart throws

Your Assignment

- Clone the whole assignment (including answers!) to Cori from the repository with: **`git clone https://github.com/hartmanbaker/Developing-with-MPI-and-OpenMP.git`**
- Copy **`darts.c/lcgenerator.h`** or **`darts.f`** (your choice) from **`Developing-with-MPI-and-OpenMP/darts-suite/{c,fortran}`**
- Parallelize the code using the 6 basic MPI commands
- Rename your new MPI code **`darts-mpi.c`** or **`darts-mpi.f`**

IV. MPI COLLECTIVES

“The First Tractor” by Vladimir Krikhatsky (socialist realist, 1877-1942). Source: http://en.wikipedia.org/wiki/File:Wladimir_Gawriilowitsch_Krikhatzkij_-_The_First_Tractor.jpg

MPI Collectives

- Communication involving group of processes
- Collective operations
  - Broadcast
  - Gather
  - Scatter
  - Reduce
  - All-
  - Barrier

Broadcast

- Perhaps one message needs to be sent from manager to all worker processes
- Could send individual messages
- Instead, use broadcast – more efficient, faster
- `int MPI_Bcast(void* buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm)`

Gather

- All processes need to send same (similar) message to manager
- Could implement with each process calling **`MPI_Send(…)`** and manager looping through **`MPI_Recv(…)`**
- Instead, use gather operation – more efficient, faster
- Messages concatenated in rank order
- **`int MPI_Gather(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`**
- Note: **`recvcount`** = # items received from each process, not total

Gather

- Maybe some processes need to send longer messages than others
- Allow varying data count from each process with **`MPI_Gatherv(…)`**
- **`int MPI_Gatherv(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int *recvcounts, int *displs, MPI_Datatype recvtype, int root, MPI_Comm comm)`**
- **`recvcounts`** is array; entry **`i`** in **`displs`** array specifies displacement relative to **`recvbuf[0]`** at which to place data from corresponding process number

Scatter

- Inverse of gather: split message into **`NP`** equal pieces, with **`i`**th segment sent to **`i`**th process in group
- **`int MPI_Scatter(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`**
- Send messages of varying sizes across processes in group: **`MPI_Scatterv(…)`**
- **`int MPI_Scatterv(void* sendbuf, int *sendcounts, int *displs, MPI_datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`**

Reduce

- Perhaps we need to do sum of many subsums owned by all processors
- Perhaps we need to find maximum value of variable across all processors
- Perform global reduce operation across all group members
- `int MPI_Reduce(void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)`

Reduce: Predefined Operations

MPI_Op	Meaning	Allowed Types
MPI_MAX	Maximum	Integer, floating point
MPI_MIN	Minimum	Integer, floating point
MPI_SUM	Sum	Integer, floating point, complex
MPI_PROD	Product	Integer, floating point, complex
MPI_LAND	Logical and	Integer, logical
MPI_BAND	Bitwise and	Integer, logical
MPI_LOR	Logical or	Integer, logical
MPI_BOR	Bitwise or	Integer, logical
MPI_LXOR	Logical xor	Integer, logical
MPI_BXOR	Bitwise xor	Integer, logical
MPI_MAXLOC	Maximum value & location	*
MPI_MINLOC	Minimum value & location	*

Reduce: Operations

- `MPI_MAXLOC` and `MPI_MINLOC`
  - Returns {max, min} and rank of first process with that value
  - Use with special MPI pair datatype arguments:
    - `MPI_FLOAT_INT` (`float` and `int`)
    - `MPI_DOUBLE_INT` (`double` and `int`)
    - `MPI_LONG_INT` (`long` and `int`)
    - `MPI_2INT` (pair of `int`)
  - See MPI standard for more details
- User-defined operations
  - Use `MPI_Op_create(...)` to create new operations
  - See MPI standard for more details

All- Operations

- Sometimes, may want to have result of gather, scatter, or reduce on all processes
- Gather operations
  - `int MPI_Allgather(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)`
  - `int MPI_Allgatherv(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int *recvcounts, int *displs, MPI_Datatype recvtype, MPI_Comm comm)`

All-to-All Scatter/Gather

- Extension of Allgather in which each process sends distinct data to each receiver
- Block **`j`** from process **`i`** is received by process **`j`** into **`i`**th block of **`recvbuf`**
- **`int MPI_Alltoall(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)`**
- Corresponding **`MPI_Alltoallv`** function also available

All-Reduce

- Same as **`MPI_Reduce`** except result appears on all processes
- **`int MPI_Allreduce(void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)`**

Barrier

- In algorithm, may need to synchronize processes
- Barrier blocks until all group members have called it
- **`int MPI_Barrier(MPI_Comm comm)`**

Bibliography/Resources: MPI/MPI Collectives

- Snir, Marc, Steve W. Otto, Steven Huss-Lederman, David W. Walker, and Jack Dongarra. (1996) *MPI: The Complete Reference.* Cambridge, MA: MIT Press. (also available at http://www.netlib.org/utk/papers/mpi-book/mpi-book.html)
- MPICH Documentation http://www.mpich.org/documentation/guides/

Bibliography/Resources: MPI/MPI Collectives

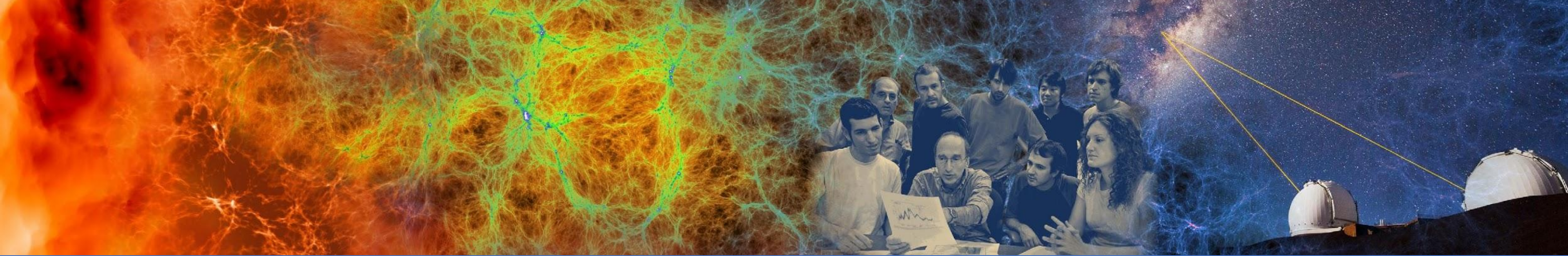
- Message Passing Interface (MPI) Tutorial https://computing.llnl.gov/tutorials/mpi/
- MPI Standard at MPI Forum
  - MPI 1.1: http://www.mpi-forum.org/docs/mpi-11-html/mpi-report.html
  - MPI-2.2: http://www.mpi-forum.org/docs/mpi22-report/mpi22-report.htm
  - MPI 3.1: https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf

INTERLUDE 2: COMPUTING PI WITH MPI COLLECTIVES

“Pi-Shaped Power Lines at Fermilab” by Michael Kappel from
http://www.flickr.com/photos/m-i-k-e/4781834200/sizes/l/in/photostream/

Interlude 2: Computing π with MPI Collectives

- In previous Interlude, you used the 6 basic MPI routines to develop a parallel program using the Method of Darts to compute π
- The communications in previous program could be made more efficient by using collectives
- Your assignment: update your MPI code to use collective communications
- Rename it `darts-collective.c` or `darts-collective.f`



OpenMP & Hybrid Programming

Outline

I. About OpenMP
II. OpenMP Directives
III. Data Scope
IV. Runtime Library Routines and Environment Variables
V. Using OpenMP
VI. Hybrid Programming

I. ABOUT OPENMP

About OpenMP

- Industry-standard shared memory programming model
- Developed in 1997
- OpenMP Architecture Review Board (ARB) determines additions and updates to standard
- Current standard: 5.0 (November 2018)

Advantages to OpenMP

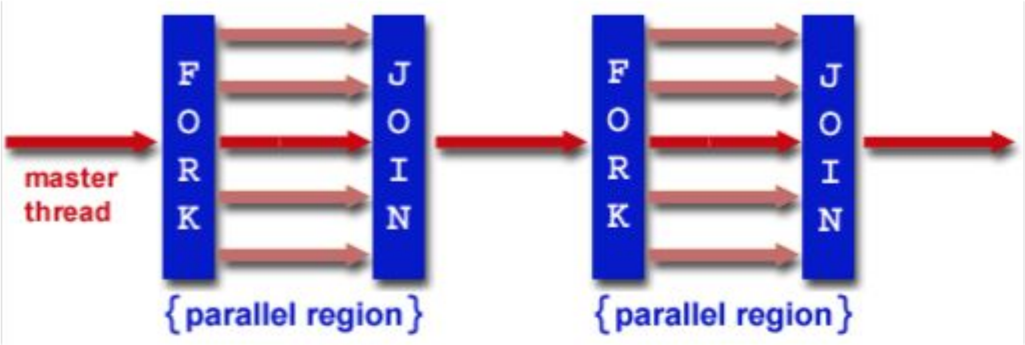
- Parallelize small parts of application, one at a time (beginning with most time-critical parts)
- Can express simple or complex algorithms
- Code size grows only modestly
- Expression of parallelism flows clearly, so code is easy to read
- Single source code for OpenMP and non-OpenMP – non-OpenMP compilers simply ignore OMP directives

OpenMP Programming Model

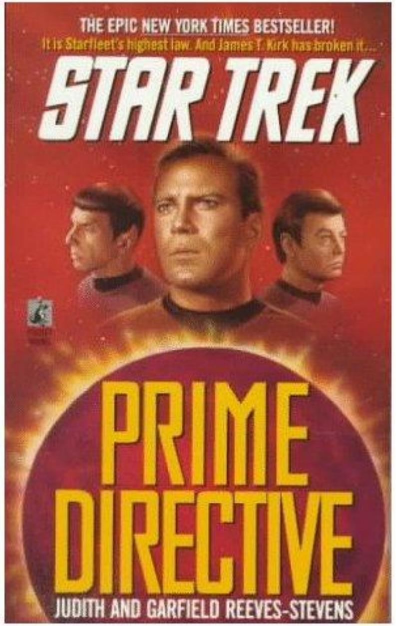
- Application Programmer Interface (API) is combination of
  - Directives
  - Runtime library routines
  - Environment variables
- API falls into three categories
  - Expression of parallelism (flow control)
  - Data sharing among threads (communication)
  - Synchronization (coordination or interaction)

Parallelism

- Shared memory, thread-based parallelism
- Explicit parallelism (parallel regions)
- Fork/join model



Source: https://computing.llnl.gov/tutorials/openMP/



II. OPENMP DIRECTIVES

Star Trek: Prime Directive by Judith and Garfield Reeves-Stevens, ISBN 0671744666

II. OpenMP Directives

- Syntax overview
- Parallel
- Loop
- Sections
- Synchronization
- Reduction

Syntax Overview: C/C++

- Basic format
  - **#pragma omp** ***directive-name*** *[clause]* ***newline***
- All directives followed by newline
- Uses pragma construct (pragma = Greek for “thing done”)
- Case sensitive
- Directives follow standard rules for C/C++ compiler directives
- Use curly braces (not on pragma line) to denote scope of directive
- Long directive lines can be continued by escaping newline character with \

Syntax Overview: Fortran

- Basic format:
  - ***sentinel directive-name*** *[clause]*
- Three accepted sentinels: **`!$omp`** **`*$omp`** **`c$omp`**
- Some directives paired with end clause
- Fixed-form code:
  - Any of three sentinels beginning at column 1
  - Initial directive line has space/zero in column 6
  - Continuation directive line has non-space/zero in column 6
  - Standard rules for fixed-form line length, spaces, etc. apply
- Free-form code:
  - **`!$omp`** only accepted sentinel
  - Sentinel can be in any column, but must be preceded by only white space and followed by a space
  - Line to be continued must end in **`&`** and following line begins with sentinel
  - Standard rules for free-form line length, spaces, etc. apply

OpenMP Directives: Parallel

- A block of code executed by multiple threads
- Syntax:

```
#pragma omp parallel private(list) shared(list)
{
   /* parallel section */
}

!$omp parallel private(list) &
!$omp shared(list)
! Parallel section
!$omp end parallel
```

Simple Example (C/C++)

```
#include <stdio.h>
#include <omp.h>
int main (int argc, char *argv[]) {
    int tid;
    printf("Hello world from threads:\n");
    #pragma omp parallel private(tid)
    {
        tid = omp_get_thread_num();
        printf("<%d>\n", tid);
    }
    printf("I am sequential now\n");
    return 0;
}
```

Simple Example (Fortran)

```
program hello
integer tid, omp_get_thread_num
write(*,*) 'Hello world from threads:'
!$omp parallel private(tid)
tid = omp_get_thread_num()
write(*,*) '<', tid, '>'
!$omp end parallel
write(*,*) 'I am sequential now'
end
```

Simple Example: Output

Output 1

```
Hello world from threads:
<0>
<1>
<2>
<3>
<4>
I am sequential now
```

Output 2

```
Hello world from threads:
<1>
<2>
<4>
<3>
I am sequential now
```

<u>Order of execution is scheduled by OS!!!</u>

OpenMP Directives: Loop

- Iterations of the loop following the directive are executed in parallel
- Syntax (C):

```
#pragma omp for schedule(type [,chunk]) private(list)\
shared(list) nowait
 {
    /* for loop */
 }
```

OpenMP Directives: Loop

- Syntax (Fortran):

```
!$omp do schedule (type [,chunk]) &
!omp private(list) shared(list)
C do loop goes here
!$omp end do nowait
```

- *type* = {static, dynamic, guided, runtime}
- If `nowait` specified, threads do not synchronize at end of loop

OpenMP Directives: Loop Scheduling

- Default scheduling determined by implementation
- Static
  - ID of thread performing particular iteration is function of iteration number and number of threads
  - Statically assigned at beginning of loop
  - Load imbalance may be issue if iterations have different amounts of work
  - Low overhead
- Dynamic
  - Assignment of threads determined at runtime (round robin)
  - Each thread gets more work after completing current work
  - Load balance is possible
  - Introduces extra overhead

OpenMP Directives: Loop Scheduling

Type	Chunks ?	Chunk Size	# Chunks	Overhead	Description
`static`	N	N/P	P	Lowest	Simple Static
`static`	Y	C	N/C	Low	Interleaved
`dynamic`	N	N/P	P	Medium	Simple dynamic
`dynamic`	Y	C	N/C	High	Dynamic
`guided`	N/A	$\leq N/P$	$\leq N/C$	Highest	Dynamic optimized
`runtime`	Varies	Varies	Varies	Varies	Set by environment variable

Note: N = size of loop, P = number of threads, C = chunk size

Which Loops are Parallelizable?

Parallelizable

- Number of iterations known upon entry, and does not change
- Each iteration independent of all others
- No data dependence

Not Parallelizable

- Conditional loops (many while loops)
- Iterator loops (e.g., iterating over `std:: list<…>` in C++)
- Iterations dependent upon each other
- Data dependence

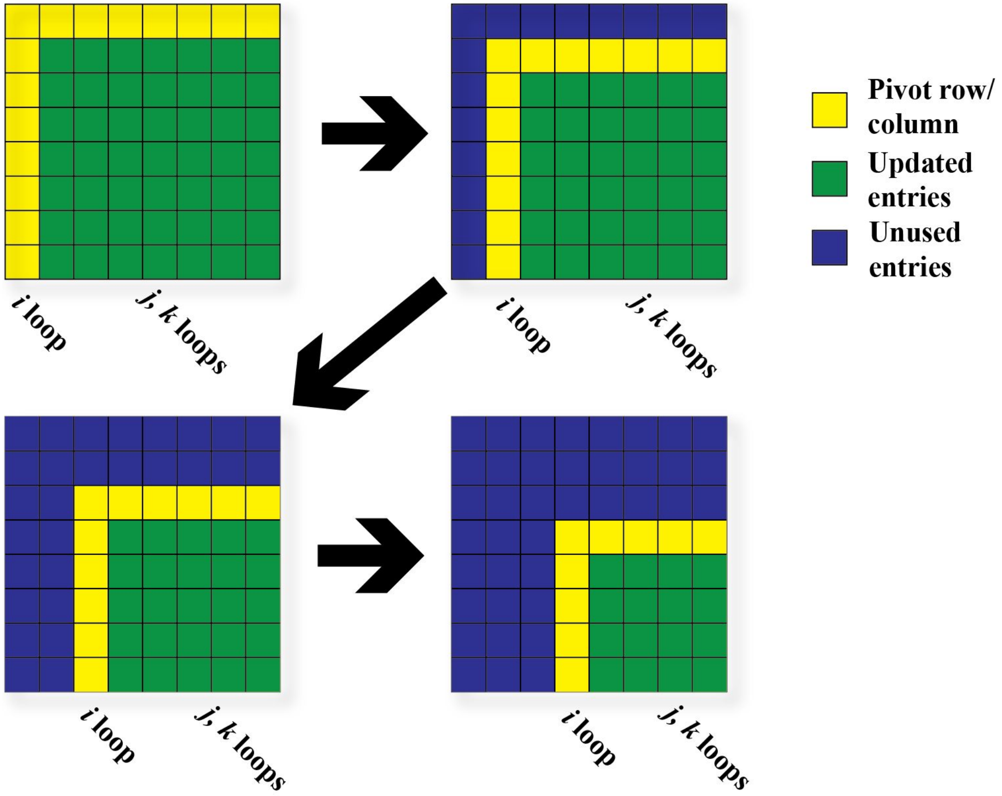
Trick: If a loop can be run backwards and get the same results, then it is almost always parallelizable!

Example: Parallelizable?

```
/* Gaussian Elimination (no pivoting):   x = A\b   */

for (int i = 0; i < N-1; i++) {
  for (int j = i; j < N; j++) {
    double ratio = A[j][i]/A[i][i];
    for (int k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

Example: Parallelizable?



Example: Parallelizable?

- Outermost Loop (`i`):
  - `N-1` iterations
  - Iterations depend upon each other (values computed at step `i-1` used in step `i`)
- Inner loop (`j`):
  - `N-i` iterations (constant for given `i`)
  - Iterations can be performed in any order
- Innermost loop (`k`):
  - `N-i` iterations (constant for given `i`)
  - Iterations can be performed in any order

Example: Parallelizable?

```
/* Gaussian Elimination (no pivoting):   x = A\b   */

for (int i = 0; i < N-1; i++) {
#pragma omp parallel for
  for (int j = i; j < N; j++) {
    double ratio = A[j][i]/A[i][i];
    for (int k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

Note: can combine **`parallel`** and **`for`** into single **`pragma`**

OpenMP Directives: Sections

- Non-iterative work-sharing construct
- Divide enclosed sections of code among threads
- Section directives nested within sections directive
- Syntax: C/C++ Fortran

```
#pragma omp sections
{
  #pragma omp section
  /* first section */
  #pragma omp section
  /* next section */
}
```

```
!$omp sections

!$omp section
c First section
!$omp section
c Second section
!$omp end sections
```

Example: Sections

```
#include <omp.h>
#define N     1000
int main () {
  int i;
  double a[N], b[N];
  double c[N], d[N];
  /* Some initializations */
  for (i=0; i < N; i++) {
    a[i] = i * 1.5;
    b[i] = i + 22.35;
  }
```

```
#pragma omp parallel shared(a,b,c,d)
private(i)
  {
    #pragma omp sections nowait
    {
      #pragma omp section
        for (i=0; i < N; i++)
          c[i] = a[i] + b[i];
      #pragma omp section
        for (i=0; i < N; i++)
          d[i] = a[i] * b[i];
     }  /* end of sections */
   }  /* end of parallel section */
return 0;
}
```

OpenMP Directives: Synchronization

- Sometimes, need to make sure threads execute regions of code in proper order
  - Maybe one part depends on another part being completed
  - Maybe only one thread need execute a section of code
- Synchronization directives
  - Critical
  - Barrier
  - Single

OpenMP Directives: Synchronization

- Critical
  - Specifies section of code that must be executed by only one thread at a time
  - Syntax: C/C++

```
#pragma omp critical (name)
```

  - Fortran

```
!$omp critical (name)
!$omp end critical
```

  - Names are global identifiers – critical regions with same name are treated as same region

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OpenMP Directives: Synchronization

- Single
  - Enclosed code is to be executed by only one thread
  - Useful for thread-unsafe sections of code (e.g., I/O)
  - Syntax: C/C++ Fortran

```
#pragma omp single
```

```
!$omp single
!$omp end single
```

OpenMP Directives: Synchronization

- Barrier
  - Synchronizes all threads: thread reaches barrier and waits until all other threads have reached barrier, then resumes executing code following barrier
  - Syntax: C/C++ Fortran

    `#pragma omp barrier` **`!$OMP barrier`**
  - Sequence of work-sharing and barrier regions encountered must be the same for every thread

OpenMP Directives: Reduction

- Reduces list of variables into one, using operator (e.g., max, sum, product, etc.)
- Syntax

```
#pragma omp reduction(op : list)
!$omp reduction(op : list)
```

  - where list is list of variables and op is one of following:
    - C/C++: `+, -, *, &, ^, |, &&, ||, max, min`
    - Fortran: `+, -, *, .and., .or., .eqv., .neqv., max, min, iand, ior, ieor`

III. VARIABLE SCOPE

"M119A2 Scope" by Georgia National Guard, source:
http://www.flickr.com/photos/ganatlguard/5934238668/sizes/l/in/photostream/

III. Variable Scope

- About variable scope
- Scoping clauses
- Common mistakes

About Variable Scope

- Variables can be shared or private within a parallel region
- Shared: one copy, shared between all threads
  - Single common memory location, accessible by all threads
- Private: each thread makes its own copy
  - Private variables exist only in parallel region

About Variable Scope

- By default, all variables shared *except*
  - Index values of parallel region loop – **private by default**
  - Local variables and value parameters within subroutines called within parallel region – **private**
  - Variables declared within lexical extent of parallel region – **private**
- Variable scope is the most common source of errors in OpenMP codes
  - Correctly determining variable scope is key to correctness and performance of your code

Variable Scoping Clauses: Shared

- Shared variables: **`shared (list)`**
  - By default, all variables shared unless otherwise specified
  - All threads access this variable in same location in memory
  - Race conditions can occur if access is not carefully controlled

Variable Scoping Clauses: Private

- Private: `private (list)`
  - Variable exists only within parallel region
  - Value undefined at start and after end of parallel region
- Private starting with defined values: `firstprivate (list)`
  - Private variables initialized to be the value held immediately before entry into parallel region
- Private ending with defined value: `lastprivate(list)`
  - At end of loop, set variable to value set by final iteration of loop

Common Mistakes

- A variable that should be private is public
  - Something unexpectedly gets overwritten
  - Solution: explicitly declare all variable scope
- Nondeterministic execution
  - Different results from different executions
- Race condition
  - Sometimes you get the wrong answer
  - Solutions:
    - Look for overwriting of shared variable
    - Use a tool such as Cray Reveal or Parallelware Analyzer to rescope your loop

Find the Mistake(s)!

```
/* Gaussian Elimination (no pivoting):   x = A\b   */
int i, j, k;
double ratio;
for (i = 0; i < N-1; i++) {
#pragma omp parallel for
  for (j = i; j < N; j++) {
    ratio = A[j][i]/A[i][i];
    for (k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

`j`, **`k`**, & **`ratio`** are shared variables by default. Depending on compiler, **`j`** & **`k`** may be optimized out & therefore not impact correctness, but **`ratio`** will always lead to errors! Depending how loop is scheduled, you will see different answers.

Fix the Mistake(s)!

```
/* Gaussian Elimination (no pivoting):   x = A\b   */
int i, j, k;
double ratio;
for (i = 0; i < N-1; i++) {
#pragma omp parallel for private (j, k, ratio) \
shared (A, b, N) default none
  for (j = i; j < N; j++) {
    ratio = A[j][i]/A[i][i];
    for (k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

By setting **`default none`**, compiler will catch any variables not explicitly scoped

IV. RUNTIME LIBRARY ROUTINES & ENVIRONMENT VARIABLES

Panorama with snow-capped Mt. McKinley in Denali National Park, Alaska, USA, May 2011, by Rebecca Hartman-Baker.

OpenMP Runtime Library Routines

- `void omp_set_num_threads(int num_threads)`
  - Sets number of threads used in next parallel region
  - Must be called from serial portion of code
- `int omp_get_num_threads()`
  - Returns number of threads currently in team executing parallel region from which it is called
- `int omp_get_thread_num()`
  - Returns rank of thread
  - `0 ≤ omp_get_thread_num() < omp_get_num_threads()`

OpenMP Environment Variables

- Set environment variables to control execution of parallel code
- **`OMP_SCHEDULE`**
  - Determines how iterations of loops are scheduled
  - E.g., **`export OMP_SCHEDULE="dynamic, 4"`**
- **`OMP_NUM_THREADS`**
  - Sets maximum number of threads
  - E.g., **`export OMP_NUM_THREADS=4`**

V. USING OPENMP

Conditional Compilation

- Can write single source code for use with or without OpenMP
  - Pragmas are ignored if OpenMP disabled
- What about OpenMP runtime library routines?
  - **`_OPENMP`** macro is defined if OpenMP available: can use this to conditionally include **`omp.h`** header file, else redefine runtime library routines

Conditional Compilation

```
#ifdef _OPENMP
  #include <omp.h>
#else
  #define omp_get_thread_num() 0
#endif
…
int me = omp_get_thread_num();
…
```

Enabling OpenMP

- Most standard compilers support OpenMP directives
- Enable using compiler flags

Compiler	Intel	GNU	PGI	Cray
Flag	`-qopenmp`	`-fopenmp`	`-mp`	`-h omp`

Running Programs with OpenMP Directives

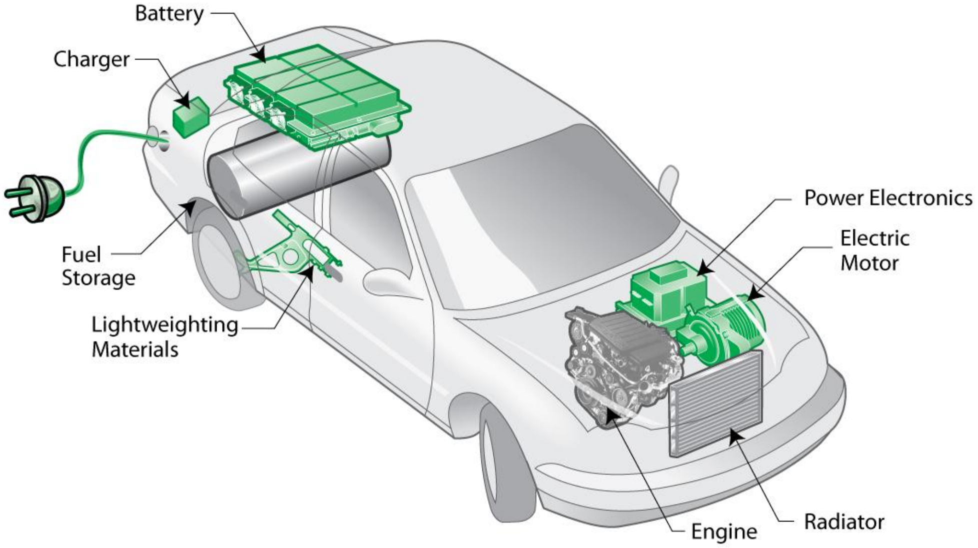
- Set OpenMP environment variables in batch scripts (e.g., include definition of **OMP_NUM_THREADS** in script)
- Example: to run a code with 8 MPI processes and 4 threads/MPI process on Cori:
  - `export OMP_NUM_THREADS=4`
  - `export OMP_PLACES=threads`
  - `export OMP_PROC_BIND=spread`
  - `srun -n 8 -c 8 --cpu_bind=cores ./myprog`
- Use the NERSC jobscript generator for best results: https://my.nersc.gov/script_generator.php

INTERLUDE 3: COMPUTING PI WITH OPENMP

“Happy Pi Day (to the 69th digit)!” by Mykl Roventine from http://www.flickr.com/photos/myklroventine/3355106480/sizes/l/in/photostream/

Interlude 3: Computing π with OpenMP

- Think about the original darts program you downloaded (**`darts.c/lcgenerator.h`** or **`darts.f`**)
- How could we exploit shared-memory parallelism to compute π with the method of darts?
- What possible pitfalls could we encounter?
- Your assignment: parallelize the original darts program using OpenMP
- Rename it **`darts-omp.c`** or **`darts-omp.f`**



VI. HYBRID PROGRAMMING

VI. Hybrid Programming

- Motivation
- Considerations
- MPI threading support
- Designing hybrid algorithms
- Examples

Motivation

- Multicore architectures are here to stay
  - Macro scale: distributed memory architecture, suitable for MPI
  - Micro scale: each node contains multiple cores and shared memory, suitable for OpenMP
- Obvious solution: use MPI between nodes, and OpenMP within nodes
- Hybrid programming model

Considerations

- Sounds great, Rebecca, but is hybrid programming always better?
  - No, not always
  - Especially if poorly programmed ☺
  - Depends also on suitability of architecture
- Think of accelerator model
  - in omp parallel region, use power of multicores; in serial region, use only 1 processor
  - If your code can exploit threaded parallelism “a lot”, then try hybrid programming

Considerations

- Hybrid parallel programming model
  - Are communication and computation discrete phases of algorithm?
  - Can/do communication and computation overlap?
- Communication between threads
  - Communicate only outside of parallel regions
  - Assign a manager thread responsible for inter-process communication
  - Let some threads perform inter-process communication
  - Let all threads communicate with other processes

MPI Threading Support

- MPI-2 standard defines four threading support levels
  - (0) MPI_THREAD_SINGLE   only one thread allowed
  - (1) MPI_THREAD_FUNNELED   master thread is only thread permitted to make MPI calls
  - (2) MPI_THREAD_SERIALIZED   all threads can make MPI calls, but only one at a time
  - (3) MPI_THREAD_MULTIPLE   no restrictions
  - (0.5) MPI calls not permitted inside parallel regions (returns MPI_THREAD_SINGLE) – this is MPI-1

What Threading Model Does My Machine Support?

```
#include <mpi.h>
#include <stdio.h>

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

MPI_Init_thread(&argc, &argv, MPI_THREAD_MULTIPLE, &provided);

printf("Supports level %d of %d %d %d %d\n", provided,
  MPI_THREAD_SINGLE, MPI_THREAD_FUNNELED,
  MPI_THREAD_SERIALIZED, MPI_THREAD_MULTIPLE);

MPI_Finalize();
return 0;
}
```

What Threading Model Does My Machine Support?

```
rjhb@cori03:~/test> cc -o threadmodel threadmodel.c
rjhb@cori03:~/test> salloc -C haswell -q interactive
salloc: Granted job allocation 22559071
salloc: Waiting for resource configuration
salloc: Nodes nid00189 are ready for job
rjhb@nid00189:~/test> srun -n 1 ./threadmodel

Supports level 2 of 0 1 2 3
```

MPI_Init_thread

- **`MPI_Init_thread(int required, int *supported)`**
  - Use this instead of **`MPI_Init(…)`**
  - **`required`**: the level of thread support you want
  - **`supported`**: the level of thread support provided by implementation (ideally = **`required`**, but if not available, returns lowest level > **`required`**; failing that, largest level < **`required`**)
  - Using **`MPI_Init(…)`** is equivalent to **`required = MPI_THREAD_SINGLE`**
- **`MPI_Finalize()`** should be called by same thread that called **`MPI_Init_thread(…)`**

Other Useful MPI Functions

- **`MPI_Is_thread_main(int *flag)`**
  - Thread calls this to determine whether it is main thread
- **`MPI_Query_thread(int *provided)`**
  - Thread calls to query level of thread support

Supported Threading Models: Single

- Use single pragma

```
#pragma omp parallel
{
  #pragma omp barrier
  #pragma omp single
  {
    MPI_Xyz(...);
  }
  #pragma omp barrier
}
```

Supported Threading Models: Funneled

- Cray & Intel MPI implementations support funneling
- Use master pragma

```
#pragma omp parallel
{
  #pragma omp barrier
  #pragma omp master
  {
    MPI_Xyz(…);
  }
  #pragma omp barrier
}
```

Supported Threading Models: Serialized

- Cray & Intel MPI implementations support serialized
- Use single pragma

```
#pragma omp parallel
{
  #pragma omp barrier
  #pragma omp single
  {
    MPI_Xyz(…);
  }
  //Don't need omp barrier
}
```

Supported Threading Models: Multiple

- Intel MPI implementation supports multiple!
  - (Cray MPI can turn on multiple support with env variables, but performance is sub-optimal)
- No need for pragmas to protect MPI calls
- Constraints:
  - Ordering of MPI calls maintained within each thread but not across MPI process -- user is responsible for preventing race conditions
  - Blocking MPI calls block only the calling thread
- Multiple is rarely required; most algorithms can be written without it

Which Threading Model Should I Use?

Depends on the application!

Model	Advantages	Disadvantages
Single	Portable: every MPI implementation supports this	Limited flexibility
Funneled	Simpler to program	Manager thread could get overloaded
Serial	Freedom to communicate	Risk of too much cross-communication
Multiple	Completely thread safe	Limited availability; sub-optimal performance

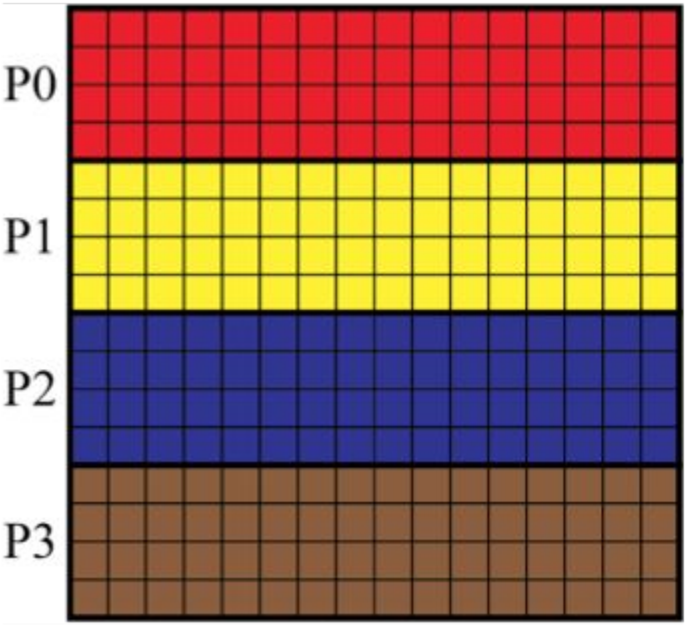
Designing Hybrid Algorithms

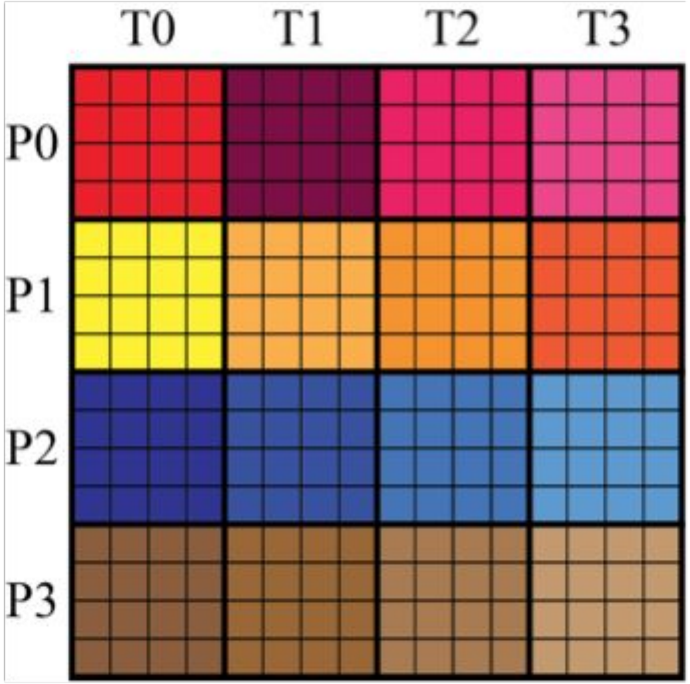
- Just because you *can* communicate thread-to-thread, doesn't mean you *should*
- Tradeoff between lumping messages together and sending individual messages
  - Lumping messages together: one big message, one overhead
  - Sending individual messages: less wait time (?)
- Programmability: performance will be great, when you finally get it working!

Example: Mesh Partitioning

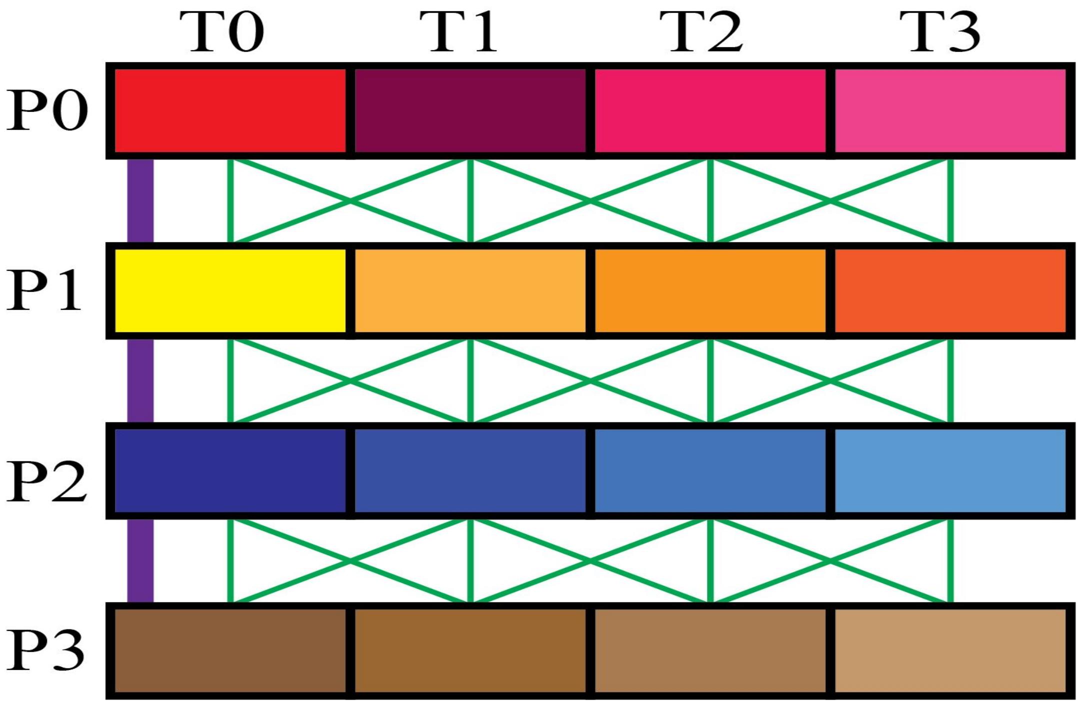
- Regular mesh of finite elements
- When we partition mesh, need to communicate information about (domain) adjacent cells to (computationally) remote neighbors

Example: Mesh Partitioning





Example: Mesh Partitioning



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- OpenMP Standard: https://www.openmp.org/specifications/
  - 5.0 Specification: https://www.openmp.org/spec-html/5.0/openmp.html
  - 5.0 code examples: https://www.openmp.org/wp-content/uploads/openmp-examples-5.0.0.pdf

Bibliography/Resources: Hybrid Programming

- Cuma, Martin (2015) *Hybrid MPI/OpenMP Programming*, https://www.chpc.utah.edu/presentations/images-and-pdfs/MPI-OMP15.pdf
- INTERTWinE (2017) *Best Practice Guide to Hybrid MPI + OpenMP Programming*, http://www.intertwine-project.eu/sites/default/files/images/INTERTWinE_Best_Practice_Guide_MPI%2BOpenMP_1.1.pdf
- Rabenseifner, Rolf, Georg Hager, Gabriele Jost (2013) SC13 Hybrid MPI and OpenMP Parallel Programming Tutorial, https://openmp.org/wp-content/uploads/HybridPP_Slides.pdf

APPENDIX 1: COMPUTING PI

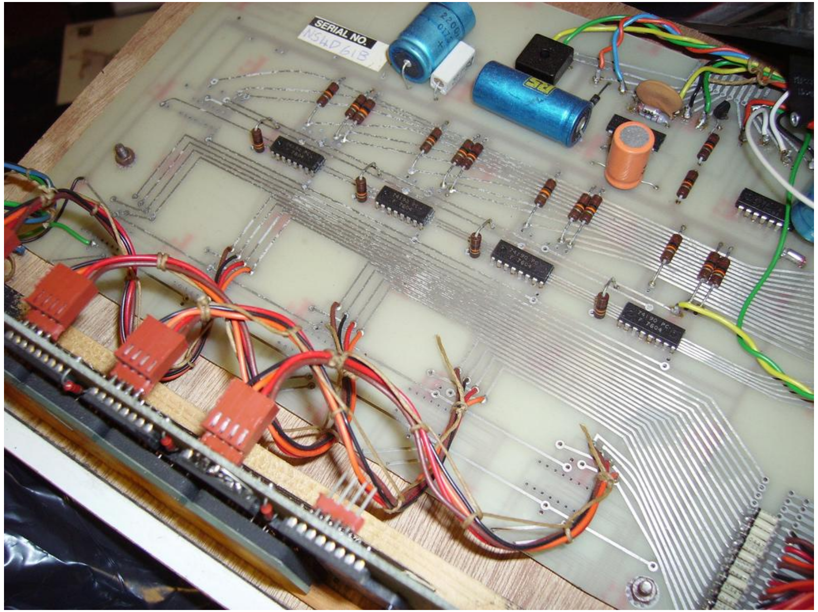
“Pi” by Gregory Bastien, from
http://www.flickr.com/photos/gregory_bastien/2741729411/sizes/z/in/photostream/

Computing π

- Method of Darts is a TERRIBLE way to compute π
  - Accuracy proportional to square root of number of darts
  - For one decimal point increase in accuracy, need 100 times more darts!
- Instead,
  - Look it up on the internet, e.g., http://www.geom.uiuc.edu/~huberty/math5337/groupe/digits.html
  - Compute using BBP (Bailey-Borwein-Plouffe) formula:

$$\pi = \sum_{n=0}^{\infty}\left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6}\right)\left(\frac{1}{16}\right)^n$$

  - For less accurate computations, try your programming language's constant, or quadrature or power series expansions



APPENDIX 2: ABOUT RANDOM NUMBER GENERATION

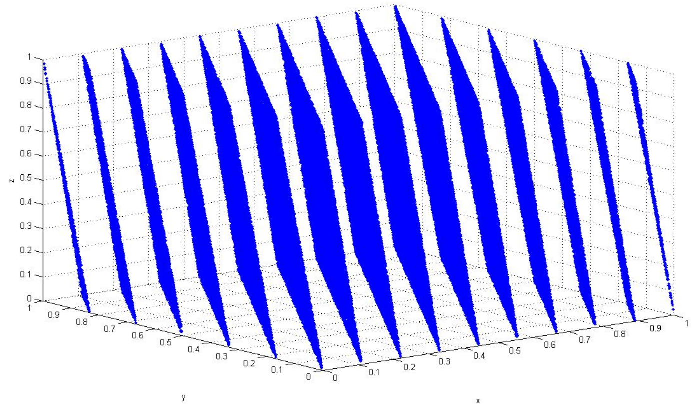
“Random Number Generator insides” by mercuryvapour, from
http://www.flickr.com/photos/mercuryvapour/2743393057/sizes/l/in/photostream/

About Random Number Generation

- No such thing as random number generation – proper term is pseudorandom number generator (PRNG)
- Generate long sequence of numbers that seems “random”
- Properties of good PRNG:
    - Very long period
    - Uniformly distributed
    - Reproducible
    - Quick and easy to compute

Pseudorandom Number Generator

- Generator from `lcgenerator.h` is a Linear Congruential Generator (LCG)
  - Short period (= `PMOD`, 714025)
  - Not uniformly distributed – known to have correlations
  - Reproducible
  - Quick and easy to compute
  - Poor quality (don't do this at home)



Correlation of RANDU LCG (source: http://upload.wikimedia.org/wikipedia/commons/3/38/Randu.png)

Good PRNGs

- For serial codes
  - Mersenne twister
  - GSL (GNU Scientific Library), many generators available (including Mersenne twister) http://www.gnu.org/software/gsl/
  - Also available in Intel MKL
- For parallel codes
  - SPRNG, regarded as leading parallel pseudorandom number generator http://sprng.cs.fsu.edu/