Crash Course in Supercomputing

Rebecca Hartman-Baker, PhD
User Engagement Group Lead
Charles Lively III, PhD
Science Engagement Engineer

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Course Outline

Parallelism & MPI (01:00 - 3:00 pm)

I. Parallelism
II. Supercomputer Architecture
III. Basic MPI
   (Interlude 1: Computing Pi in parallel)
I. MPI Collectives
   (Interlude 2: Computing Pi using parallel collectives)

OpenMP & Hybrid Programming (3:30 - 5 pm)
Course Outline

Parallelism & MPI (01:00 – 3:00 pm)

OpenMP & Hybrid Programming (3:30 - 5 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
What is Parallelism?

● Generally Speaking:
  ○ Parallelism lets us work smarter, not harder, by simultaneously tackling multiple tasks.
  ○ How?
    ■ the concept of dividing a task or problem into smaller subtasks that can be executed simultaneously.
  ○ Benefit?
    ■ Work can get done more efficiently, thus quicker!
Parallelization Concepts

This concept applies to both everyday activities like preparing dinner:

- Imagine preparing a lasagna dinner with multiple tasks involved.
- Some tasks, such as making the sauce, assembling the lasagna, and baking it, can be performed independently and concurrently.
- These tasks do not depend on each other's completion, allowing for parallel execution.
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 the sauce
- Assembling the lasagna
- Baking the lasagna
- Washing lettuce
- Cutting vegetables
- Assembling the salad

**PARALLEL TASKS**
- Making the lasagna
- Making the salad
- Setting the table
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

II. Supercomputer Architecture

- What is a supercomputer?
- Conceptual overview of architecture

- Cray 1 (1976)
- IBM Blue Gene (2005)
- Cray XT5 (2009)
- HPE-Cray Shasta Architecture (2021)
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 utilize supercomputers to solve complex problems.
  - Really hard problems need really LARGE (super)computers
SMP Architecture

- **SMP stands for Symmetric Multiprocessing architecture**
  - commonly used in supercomputers, servers, and high-performance computing environments.
  - all processors have equal access to memory and input/output devices.
    - 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.
- **SMP systems and architectures allow for better load balancing and resource utilization across multiple processors.**
Cluster Architecture

- CPUs on racks, do computations (fast)
- Communicate through networked connections (slow)
- Want to write programs that divide computations evenly but minimize communication
SMP Architecture vs Cluster Architecture
State-of-the-Art Architectures

● Today, hybrid architectures very common
  ○ Multiple \{16, 24, 32, 64, 68, 128\}-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 also very common
  - 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
    - Often use CUDA to directly program GPU offload portions of code
    - Alternatives: standards-based directives, OpenACC or OpenMP offloading; programming environments such as Kokkos or Raja
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 **Message Passing Interface**
- 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 released June, 2021
  - MPI-4 additions to standard will also not be covered today
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
  - $0 \leq \text{rank} \leq \text{size}-1$
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
Message Passing Interface

Message passing interface (MPI)

MPI_COMM_WORLD

Process ID (rank):
0
1
2
3
4
5

CLUSTER

node 1
CPU 0
CPU 1

node 2
CPU 0

node 3
CPU 0
CPU 1

node 4
CPU 0
Deadlocking Example (Always)

```c
#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;
}
```
```
#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;
}
```
#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_Recvs`
- All processes wait for corresponding `MPI_Sends` to begin, which never happens
Explanation: Sometimes Deadlocking Example

- Logically correct
- Deadlock could be caused by `MPI_Sends` 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 $\pi$ in Parallel

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

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

* 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 \( = (2R)^2 = 4R^2 \)
- Area of circle \( \frac{\pi R^2}{4R^2} = \frac{\pi}{4} \)

Method of Darts

- Ratio of areas proportional to $\pi$
- 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 and Charles, 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)

```c
#include "lcregister.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 (lcggenerator.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);
}
First, the pseudorandom number generator

```fortran
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
```
! 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
“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 $\pi$, 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 Perlmutter from the repository with: `git clone https://github.com/NERSC/crash-course-supercomputing.git`

● Copy `darts.c/lcgenerator.h` or `darts.f` (your choice) from `crash-course-supercomputing/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

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

```c
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(...)`

```c
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
- \( \text{int } MPI\text{-Scatter}(\text{void* } \text{sendbuf}, \text{int } \text{sendcount}, \text{MPI\_Datatype } \text{sendtype}, \text{void* } \text{recvbuf}, \text{int } \text{recvcount}, \text{MPI\_Datatype } \text{recvtype}, \text{int } \text{root}, \text{MPI\_Comm } \text{comm}) \)
- Send messages of varying sizes across processes in group: \( \text{MPI\_Scatterv}(...) \)
- \( \text{int } MPI\text{-Scatterv}(\text{void* } \text{sendbuf}, \text{int } *\text{sendcounts}, \text{int } *\text{displs}, \text{MPI\_datatype } \text{sendtype}, \text{void* } \text{recvbuf}, \text{int } \text{recvcount}, \text{MPI\_Datatype } \text{recvtype}, \text{int } \text{root}, \text{MPI\_Comm } \text{comm}) \)
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

<table>
<thead>
<tr>
<th><strong>MPI_Op</strong></th>
<th><strong>Meaning</strong></th>
<th><strong>Allowed Types</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_MAX</td>
<td>Maximum</td>
<td>Integer, floating point</td>
</tr>
<tr>
<td>MPI_MIN</td>
<td>Minimum</td>
<td>Integer, floating point</td>
</tr>
<tr>
<td>MPI_SUM</td>
<td>Sum</td>
<td>Integer, floating point, complex</td>
</tr>
<tr>
<td>MPI_PROD</td>
<td>Product</td>
<td>Integer, floating point, complex</td>
</tr>
<tr>
<td>MPI_LAND</td>
<td>Logical and</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_BAND</td>
<td>Bitwise and</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_LOR</td>
<td>Logical or</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_BOR</td>
<td>Bitwise or</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_LXOR</td>
<td>Logical xor</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_BXOR</td>
<td>Bitwise xor</td>
<td>Integer, logical</td>
</tr>
<tr>
<td>MPI_MAXLOC</td>
<td>Maximum value &amp; location</td>
<td>*</td>
</tr>
<tr>
<td>MPI_MINLOC</td>
<td>Minimum value &amp; location</td>
<td>*</td>
</tr>
</tbody>
</table>
Reduce: Operations

- **MPI_MAXLOC** and **MPI_MINLOC**
  - Returns \(\{\text{max, min}\}\) 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 $\text{recvbuf}$
- `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

- MPICH Documentation http://www.mpich.org/documentation/guides/
Bibliography/Resources: MPI/MPI Collectives

● Message Passing Interface (MPI) Tutorial [https://hpc-tutorials.llnl.gov/mpi/](https://hpc-tutorials.llnl.gov/mpi/)

● MPI Standard at MPI Forum: [https://www.mpi-forum.org/docs/](https://www.mpi-forum.org/docs/)
  ○ MPI 3.1: [https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf](https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf)
  ○ MPI 4.0: [https://www.mpi-forum.org/docs/mpi-4.0/mpi40-report.pdf](https://www.mpi-forum.org/docs/mpi-4.0/mpi40-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 $\pi$ 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 $\pi$.
- 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: 5.2 (November 2021)
- Standard includes GPU offloading (since 4.5), not discussed today
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://hpc-tutorials.llnl.gov/openmp/](https://hpc-tutorials.llnl.gov/openmp/)
II. OPENMP DIRECTIVES

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:** `!$omp` `*omp` `&omp`
- **Some directives paired with end clause**
- **Fixed-form code:**
  - Any of three sentinels beginning at column 1
  - Initial directive line has space/zero in column 6
  - Continuation directive line has non-space/zero in column 6
  - Standard rules for fixed-form line length, spaces, etc. apply
- **Free-form code:**
  - `$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:

```c
#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++)

```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;
}
```
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>
<3>
<4>
<0>
I am sequential now

Order of execution is scheduled by OS!!!
OpenMP Directives: Loop

- Iterations of the loop following the directive are executed in parallel
- Syntax (C):
  
  ```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
  - Best for known, predictable amount of work per iteration
  - Low overhead
- Dynamic
  - Assignment of threads determined at runtime (round robin)
  - Each thread gets more work after completing current work
  - Load balance is possible for variable work per iteration
  - Introduces extra overhead
## OpenMP Directives: Loop Scheduling

<table>
<thead>
<tr>
<th>Type</th>
<th>Chunks</th>
<th>Chunk Size</th>
<th># Chunks</th>
<th>Overhead</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>static</td>
<td>N</td>
<td>$N/P$</td>
<td>$P$</td>
<td>Lowest</td>
<td>Simple Static</td>
</tr>
<tr>
<td>static</td>
<td>Y</td>
<td>$C$</td>
<td>$N/C$</td>
<td>Low</td>
<td>Interleaved</td>
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<tr>
<td>dynamic</td>
<td>N</td>
<td>$N/P$</td>
<td>$P$</td>
<td>Medium</td>
<td>Simple dynamic</td>
</tr>
<tr>
<td>dynamic</td>
<td>Y</td>
<td>$C$</td>
<td>$N/C$</td>
<td>High</td>
<td>Dynamic</td>
</tr>
<tr>
<td>guided</td>
<td>N/A</td>
<td>$\leq N/P$</td>
<td>$\leq N/C$</td>
<td>Highest</td>
<td>Dynamic optimized</td>
</tr>
<tr>
<td>runtime</td>
<td>Varies</td>
<td>Varies</td>
<td>Varies</td>
<td>Varies</td>
<td>Set by environment variable</td>
</tr>
</tbody>
</table>

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): \( x = \mathbf{A\backslash b} \) */

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?

```c
/* 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: 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
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++
    ```c
    #pragma omp single
    ```
  - Fortran
    ```fortran
    !$omp single
    ```

  ```c
  !$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++
    ```
    #pragma omp barrier
    ```
  - Fortran
    ```
    !$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 Codee to rescope your loop
Find the Mistake(s)!

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

```c
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]);
      }
    }
}
```

\( k \) & \( \text{ratio} \) are shared variables by default. Depending on compiler, \( k \) may be optimized out & therefore not impact correctness, but \( \text{ratio} \) will always lead to errors! Depending how loop is scheduled, you will see different answers.
Fix the Mistake(s)!

/* Gaussian Elimination (no pivoting): \( \mathbf{x} = \mathbf{A} \mathbf{b} \) */

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

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 \leq \text{omp}_\text{get}_\text{thread}_\text{num}() < \text{omp}_\text{get}_\text{num}_\text{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

```c
#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

<table>
<thead>
<tr>
<th>Compiler</th>
<th>Intel</th>
<th>GNU</th>
<th>PGI/Nvidia</th>
<th>Cray</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flag</td>
<td>-qopenmp</td>
<td>-fopenmp</td>
<td>-mp</td>
<td>-h omp</td>
</tr>
</tbody>
</table>
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](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 $\pi$ 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 $\pi$ 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?

```c
#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_SERIALIZE, MPI_THREAD_MULTIPLE);
    MPI_Finalize();
    return 0;
}
```
What Threading Model Does My Machine Support?

```
rjhb@perlmutter> cc -o threadmodel threadmodel.c
rjhb@perlmutter> salloc -C cpu -q interactive
salloc: Granted job allocation 10504403
salloc: Waiting for resource configuration
salloc: Nodes nid005664 are ready for job
rjhb@nid005664:~/test> srun -n 1 ./threadmodel

Supports level 3 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

```c
#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

```c
#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

```c
#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!

<table>
<thead>
<tr>
<th>Model</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single</td>
<td>Portable: every MPI implementation supports this</td>
<td>Limited flexibility</td>
</tr>
<tr>
<td>Funneled</td>
<td>Simpler to program</td>
<td>Manager thread could get overloaded</td>
</tr>
<tr>
<td>Serial</td>
<td>Freedom to communicate</td>
<td>Risk of too much cross-communication</td>
</tr>
<tr>
<td>Multiple</td>
<td>Completely thread safe</td>
<td>Limited availability; sub-optimal performance</td>
</tr>
</tbody>
</table>
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
INTERLUDE 4: COMPUTING PI WITH HYBRID PROGRAMMING

“pi” by Travis Morgan from http://www.flickr.com/photos/morgantj/5575500301/sizes/l/in/photostream/
Interlude 4: Computing $\pi$ with Hybrid Programming

● Putting it all together:
  ○ How can we combine inter-node and intra-node parallelism to create a hybrid program that computes $\pi$ using the method of darts?
  ○ What potential pitfalls do you see?
● Your assignment: create a code, `darts-hybrid.c` or `darts-hybrid.f`, developed from `darts-collective.c`/`darts-collective.f` and `darts-omp.c`/`darts-omp.f`, that uses OpenMP to exploit parallelism within the node, and MPI for parallelism between nodes
Bibliography/Resources: OpenMP

- LLNL OpenMP Tutorial, https://computing.llnl.gov/tutorials/openMP/
Bibliography/Resources: OpenMP

- OpenMP.org: https://www.openmp.org/
- OpenMP Standard: https://www.openmp.org/specifications/
Bibliography/Resources: Hybrid Programming

APPENDIX 1: COMPUTING PI

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

- Method of Darts is a TERRIBLE way to compute $\pi$
  - 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](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](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/](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/](http://sprng.cs.fsu.edu/)