Advanced Crash Course in Supercomputing: Programming Project

OLCF
Oak Ridge Leadership Computing Facility

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Programming Project

I. Project Description
II. Programming Concepts
III. Parallelization Strategies
IV. Implementation Details

I. PROJECT DESCRIPTION

Source: http://www.ehow.com/how_2141082_best-berry-pie-ever.html

I. 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

***Disclaimer: this is a <u>TERRIBLE</u> way to compute π. Don't even think about doing it this way except for the purposes of this project!**

Method of Darts

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

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Method of Darts

- So, ratio of areas proportional to π
- How to find areas?
  - Suppose we threw darts (completely randomly) at dartboard
  - Could count number of darts landing in circle and total number of darts landing in square
  - Ratio of these numbers gives approximation to ratio of areas
  - Quality of approximation increases with number of darts
- $\pi = 4 \times \dfrac{\text{\# darts inside circle}}{\text{\# darts thrown}}$

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Method of Darts

- Okay, Rebecca, but how in the world do we simulate this experiment on 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

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II. PROGRAMMING CONCEPTS

Nissan Pivo Concept Car. Source: http://www.gizmag.com/go/4683/picture/15670/

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II. Programming Concepts

- Pseudorandom numbers
- Typecast and coercion
- Datatypes

Pseudorandom Numbers

- In C language, function `int rand(void)` generates "pseudo-random integer in range 0 to `RAND_MAX`"
- `RAND_MAX`: C-language constant denoting maximum random number generated; actual value varies with implementation
- Divide "random" number by maximum random number to get a number between 0 and 1*
- Numbers generated by `rand()` not really random; same sequence every time
- Change seed for random number generator with `void srand(unsigned int seed)`

***Disclaimer: this is a TERRIBLE way to compute a pseudorandom number. Don't even think about doing it this way except for the purposes of this project!**

Type Cast and Coercion

- `int a = rand(); double b = a/RAND_MAX;`
  - b equals 0
- `int a = rand(); double b = ((double) a)/((double) RAND_MAX);`
  - b equals correct value
- Type conversion rules:
  - `int/int` → `int`
  - `int/double` → `double`
  - `double/int` → `double`
  - `double/double` → `double`

Datatypes

- For large number of darts, need larger datatype than `int` or risk overflow
- On some computers (varies by platform):

Data Type	Range
`int`	-32,768 → +32,767
`long int`	-2,147,483,648 → +2,147,483,647
`unsigned long int`	0 → +4,294,967,295

III. PARALLELIZATION STRATEGIES

III. Parallelization Strategies

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

Partition

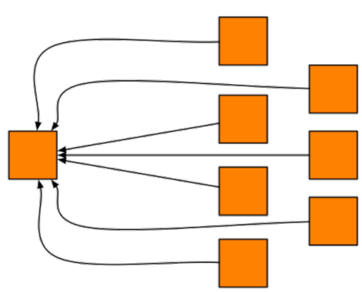
"Decompose problem into fine-grained tasks to maximize potential parallelism"

- 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

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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

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IV. IMPLEMENTATION DETAILS

Detail from Vincent van Gogh's Sunflowers. Source:
http://painting.about.com/od/famouspainters/ig/Van-Gogh-and-Expressionism/Sunflower-Detail.htm

IV. Implementation Details

1. Implement using six basic MPI functions
2. Add OpenMP capabilities
3. Implement using collective operations

Step 1

- Create function `pi_basic(...)` that uses only six basic functions covered in part 1
  - `pi_basic(...)` should call function `throw_darts(...)` to perform the actual throwing of darts
- Test your implementation and make sure it works

Step 2

- Use OpenMP to parallelize `throw_darts(...)` over a node
- Parallelization will occur in loop
- Make sure code works properly

Step 3

- Create function `pi_advanced(…)` that uses MPI collective operations
- This should require trivial change from `pi_basic(…)`

Skeleton Code

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char
  **argv) {
/* declarations here */
  MPI_Init(&argc,
  &argv);
  double start =
  MPI_Wtime();
   pi_simple(…);
   double finish =
  MPI_Wtime();
   printf("Processor %d
  took %f s for
  pi_simple", me,
  finish-start);
```

```
  double start =
  MPI_Wtime();
   pi_advanced(…);
   double finish =
  MPI_Wtime();
   printf("Processor %d
  took %f s for
  pi_advanced", me,
  finish-start);
  MPI_Finalize();
 return 0;
}
```

Doing this Project on Smoky

- Bring up shell on Mac or Linux or PuTTY shell on Windows
- Log into jaguar with your username (temporary guest accounts or your regular account)
  - `ssh -Y hqi@smoky.ccs.ornl.gov`
  - Enter your PIN number and then 6-digit SECURID number
- Create directory for program and write program
- Compile using `mpicc` (e.g. `mpicc -o pi.o pi.c`)
  - For OpenMP, use `-mp=nonuma` flag, i.e., `mpicc -mp=nonuma pi.c`
- No link to MPI or OpenMP libraries necessary – Smoky takes care of that
- Write batch script and submit using `qsub scriptname`

Bibliography/Resources

- Heath, Michael T. (2006) *Notes for CS554: Parallel Numerical Algorithms,* http://www.cse.illinois.edu/courses/cs554/notes/index.html
- Kernighan, Brian W. and Dennis M. Ritchie. *The C Programming Language, 2nd ed.* Upper Saddle River, NJ: Prentice-Hall, 1988.
- C: The float and double Data Types and the sizeof Operator http://www.iota-six.co.uk/c/b3_float_double_and_sizeof.asp
- C Data types http://www.phim.unibe.ch/comp_doc/c_manual/C/CONCEPT/data_types.html
- OLCF Webpages http://olcf.ornl.gov/

Appendix: Better Ways to Compute π

- Look it up on the internet, e.g. http://oldweb.cecm.sfu.ca/projects/ISC/data/ pi.html
- Compute using the 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: Better Ways to Generate Pseudorandom Numbers

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