Parallel Programming Workshop

Brought to you by

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Registration

- Please make sure you're signed in.
- Won't need a computer this morning
  - unless you need a calculator to add integers
Important Concepts

- Decomposition
- Scaling
- Speedup

We will jointly “discover” the meaning of these terms through experiment and group exercises – ease into programming only when necessary.
Distributed Memory Programming

- Two main models for doing parallel programming:
- Distributed Memory – workers must talk with one another to get data.
- Shared Memory – Workers view the same memory space.

Each has different issues.
Take on Distributed Memory first.
The Data Set

- Any confusion over the terms “integer” and “real” numbers?
- The data at hand consists of:
  - 50 data cards.
  - 5 integer numbers per card.
  - An integer card identifier.

<table>
<thead>
<tr>
<th>Set: 14</th>
</tr>
</thead>
<tbody>
<tr>
<td>164</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>76</td>
</tr>
<tr>
<td>144</td>
</tr>
<tr>
<td>105</td>
</tr>
</tbody>
</table>
Exercise 1

- Desired analysis: summation over 4 cards
- Divide into groups.
- Each group needs a time keeper.

Pay attention to the process!
Exercise 1 Outcomes

- What was the basic “unit of work” or task?
- What discreet steps were involved?

_Yea verily, computers are lowly beasts and must be instructed tediously._
Exercise 1 Summary

- Process had 3 distinct steps:
  - Hand out cards
  - Sum the numbers
  - Report results
- More formally:
  - Distribute work (tasks).
  - Perform work
  - Gather results
Exercise 2 – Two Workers

- Repeat Ex 1, only with 2 people adding numbers.
- What changes?
Added Workers

- What happened with more workers?
- The process changes a little:
  - Distribute work
    - How to do that? Communicate!
  - Perform work
  - Gather results
    - Gather partial results. Communicate!
  - Compute final result
  - Report result
Exercise 3

- What happens with 3 workers?
- What happens with 4 workers?
- Could we use more than 4 workers?
Exercise 3 Outcomes

- More workers => More communication
- Balanced work assignments?
- Task starvation? (run out of cards)
- How do the input and output compare with Ex 1?

*Everybody's talking at me, I don't hear a word they're saying ...*  

*Fred Neil*
Comment on Scaling

- How does parallel work speed up, i.e. “scale”?

\[ S_p = \frac{T_1}{T_n} \]

\[ S_{\text{serial}} = \frac{T_{\text{serial}}}{T_n} \]

- How efficient is it? Again, two types:

\[ E_p = \frac{T_1}{nT_n} \]

\[ E_{\text{serial}} = \frac{T_{\text{serial}}}{nT_n} \]

Beware of “Lies, damn lies, and statistics . . .”
Hypothetical Speedup Chart

\[ S_4 = 3.2 \quad E_4 = 0.8 \]
Overhead Expense

- 80% efficiency => 20% overhead.
  - If one hour on 5 computers, then 1 computer worth of power is unused!
- Constant trade-off between time-to-answer and expense, even if the usage seems "free".
- Time on most HPC systems is charged in core-hours (or service units), so low efficiency still costs more as service units are used up faster.
Distributing Work (Data)

- Shared data?
  - Each worker has a copy
  - Each worker has an ID
  - Use ID to *compute* what to work on.

- Distributed data?
  - Head worker has all the data.
  - Head worker knows # of workers.
  - Head worker computes decomposition.
  - Head worker *sends pieces* to workers.
Sharing Data

- Parallel file system – all workers see same data files.
- Broadcast – head worker broadcasts all data to all workers.
Considerations

- How much time is required to communicate?
- Does machines have access to shared file systems?
Concept Summary

When you approach problem to programming, ask yourself:

• What algorithm is required?
• How best to decompose the work?
• How is it suppose to scale?
• Minimize comm to get speedup.
• Test to see what has been achieved.
Shared Memory Programming

- Distributed Memory Programming recap:
  - Each worker was isolated.
  - Sent or computed work decomposition info.
  - Sent data or shared via file system.
- What changes with Shared Memory Programming?
  - Workers part of same system (i.e. cores).
  - Each worker can see all data in memory.
  - *Communication* replaced by *coordination* of read/write access.
### Exercise 4

Assume all workers can see all the data - how does summation task change?

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>Sums</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>3</td>
<td>13</td>
<td>78</td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>187</td>
<td>77</td>
<td>216</td>
<td>51</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Exercise 4 Outcomes

• Benefits?
• Difficulties?
Concept Summary

• Shared memory lets all processors see all data, it is just there – no work to distribute it. BUT, need to coordinate changes!

• Shared Memory Model is growing in popularity as more cores per node become available, and new devices such as GPUs become common place – multi-core PCs use shared memory.

• Hybrid or Heterogeneous models are becoming important as the needed to combine Shared and Distributed models increase.
Parallel Thinking

● What kind of questions do you need to consider when approaching a new program?

   • Algorithm – numerical stability? programmability?
   • Data size – memory needs?
   • Machine architecture – shared/distributed/both?
   • Code lifetime – save FTE's or machine hours?
   • Choice of language?
   • Choice of tools?
Break
The Laplace Heat Equation

- For a “real” problem, consider how to go about solving the Laplace Heat Equation in 2-D. Idea is to determine the temperature at any point on a surface, given the temperature at the boundaries:
Formal Solution

The solution must satisfy:

\[ \nabla^2 \phi = 0 \]

with the application of Dirichlet boundary conditions (constant values around edge of region.)
The Serial Solution

Subdivide the surface into a mesh of points, add boundary points.

Apply the following 5-point stencil iteratively until the temperature stops changing (new temp approximates old temp) to interior only:

\[
T_{i,j}^{n+1} = 0.25 \left( T_{i-1,j}^n + T_{i+1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n \right)
\]
Exercise 5: 1-D Problem

\[
T_i^{n+1} = 0.5 \times (T_{i-1}^n + T_{i+1}^n)
\]

Discuss programming this problem in your group.
Exercise 5: Solution

70 iterations to reach 0.001% convergence bound.

<table>
<thead>
<tr>
<th></th>
<th>0</th>
<th>16.6611</th>
<th>33.3324</th>
<th>49.9988</th>
<th>66.6658</th>
<th>83.3327</th>
<th>100</th>
</tr>
</thead>
</table>
Exercise 6

Now the question is, how would we do this in parallel?

Need one small modification, so try using 2 workers first.
Process Start

Initialize:

```
0 0 0 0 0 0 0 0 100
```

Decompose:

```
Worker 1:
0 0 0 0 0

Worker 2:
0 0 0 0 100
```

“Ghost” or overlapped cells.
Process Iteration

Compute:

Worker 1: 0 0 0 0 0 0
Worker 2: 0 0 0 50 100

Communicate:

Worker 1: 0 0 0 0 0 0
Worker 2: 0 0 0 50 100

Lather, Rinse, Repeat.
What Would 3 Workers Involve?

Communicate:

Workers in the middle have to communicate intermediate results to neighbors on both sides!

Number of workers limited by problem size!
Serial Program

- Grab a copy of the program named: 
  /work/jalupo/laplace_solver_serial.f90
- Open with “less” or “vi” so you can follow along.
- Anyone have trouble reading Fortran?
- Anyone not know how to compile and run a Fortran program?
Main Components

- **program laplace_main** – program main line.
- **subroutine laplace** – the actual solver. It also allocates memory to hold the 2-D mesh based on the requested rows and columns.
- **subroutine initialize** – sets the internal temperatures to 0.
- **subroutine set_bcs** – sets up the boundary conditions.
Compiling Fortran

• Here is a quick summary of how to compile and run this particular program (assumes default environment):
  
  $ ifort -o laplace laplace_solver_serial.f90
  $ ./laplace

• You should see the following line of text on your screen:
  
  Usage: laplace nrows ncols niter iprint relerr

Now try executing the program with some real numbers:

  $ ./laplace 100 200 3000 300 0.001
Results of Run

$ ./laplace 100 200 10000 3000 0.01

Solution has converged.

Iterations: 2241
Max error: 0.01
Total time: 0.079s

What if the problem gets bigger, and error condition was changed to 0.001?
Higher Accuracy Run

$ ./laplace 1000 1000 30000 1000 0.001

Solution has converged.

Iterations: 29812
Max error: 0.001
Total time: 60.546s
Why go to parallel?

What if this was only part of a simulation and the temperatures changed 25,000 times?

Even though 1 solution taking 1 second seems fast, 25,000 solutions would take 7 hours!

Can it be done in parallel to speed up the overall simulation time?

How do we approach the solution in parallel?
Decomposition

Assuming 2 processors, let's divide the surface in half.

What overhead do we have to consider adding to make this give the same answer?
Ghost Cells
Overhead

- Breaking up the problem so multiple processes can work on it introduces *overhead*:
  - Logic must be added so each process knows which part of the mesh it is expected to work on. This directly impacts how the code will start up.
  - Communication must be added so data from adjoining regions can be properly updated.
  - Code must be added so the final results can be communicated. This directly impacts how the code will report results and terminate.
- A serial program is not the same as a parallel program running on 1 processor!
Compute/Communication Bound

- Clearly, if you increase the number of processes working on this problem, the amount of communication required increases.
- With a few processes, this problem exhibits the property of being compute bound.
- When the number of processes approach the number of mesh points, it becomes communication bound.
- All parallel programs exhibit one form or the other depending on the problem specifics.
LUNCH