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.

Set: 14				
164	5	76	144	105

Exercise 1

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

Pay attention to the process.

Ex 1 Outcomes

- **What was the basic "unit of work" or task?**
- **What discreet steps were involved?**

Adding Workers

- **What happens if we add more "workers"?**
- **Do the steps involved change?**

Ex 2 – Two Workers

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

Exercise 3

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

Ex. 3 Outcomes

- More workers => More communication
- Balanced work assignments?
- Task starvation?
- How do the input and output compare with Ex 1?

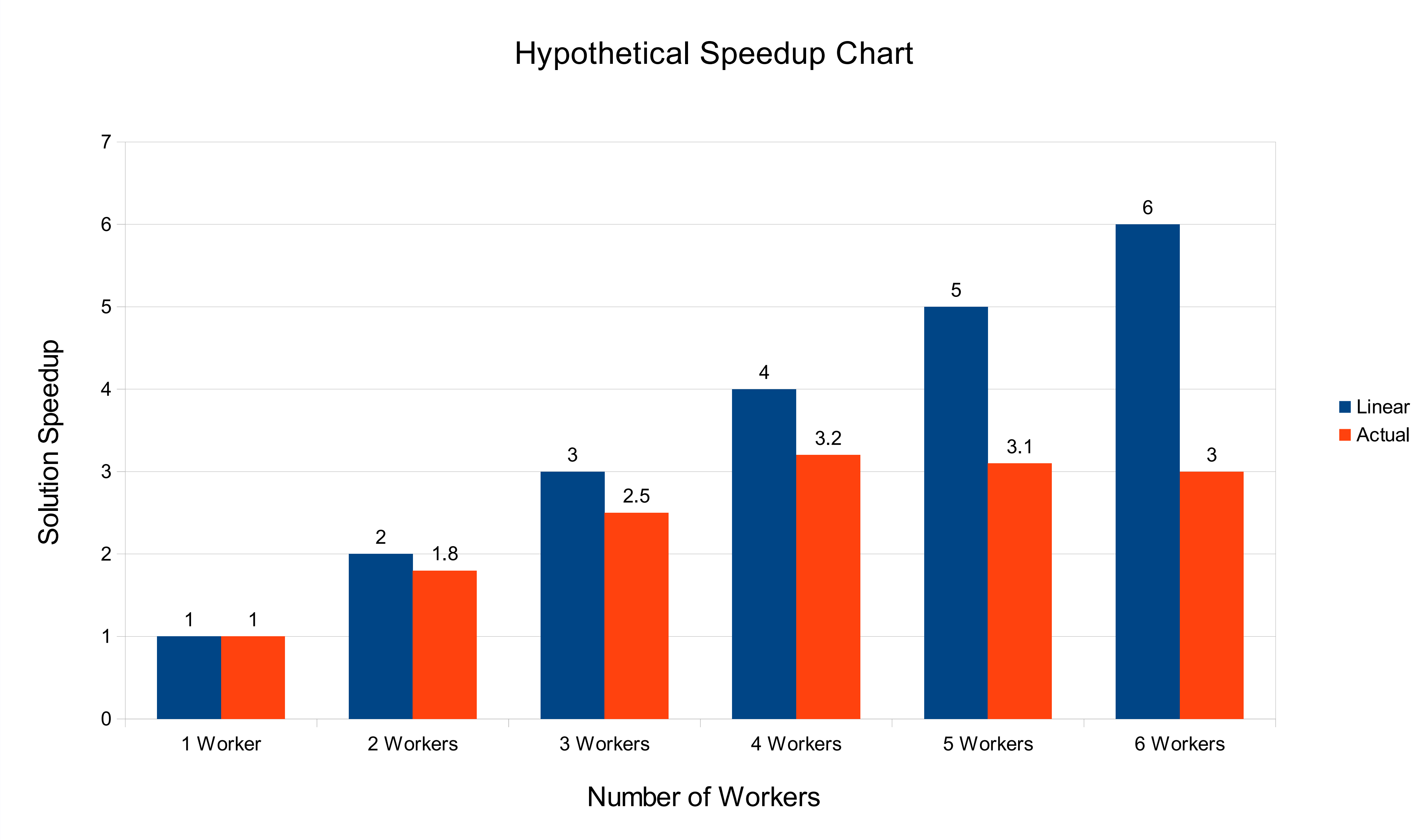
Comment on Scaling

- How does this type of work scale?
- How does it speed up (two types)?

$$S_p = \frac{T_1}{T_n} \qquad S_{serial} = \frac{T_{serial}}{T_n}$$

- How efficient is it (two types)?

$$E_p = \frac{T_1}{n\,T_n} \qquad E_{serial} = \frac{T_{serial}}{n\,T_n}$$


Hypothetical Speedup Chart
Solution Speedup
0
1
2
3
4
5
6
7
1 Worker
2 Workers
3 Workers
4 Workers
5 Workers
6 Workers
Number of Workers
Linear
Actual
1
1
2
1.8
3
2.5
4
3.2
5
3.1
6
3

$S_4 = 3.2$ $E_4 = 0.8$

Distributing 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.**

Trade-offs

- How much time is required to communicate?
- Does program have to work on machines with and without shared file systems?

Concept Summary

When you approach programming a problem, ask yourself:

- What algorithm?
- How do I decompose the work?
- How is it suppose to scale?
- Minimize comm to get speedup.

Shared Memory Programming

- Distributed Memory Programming:
  - Each worker was isolated.
  - Sent or computed work decomposition info.
  - Sent data or shared via file system.
- Shared Memory Programming:
  - Workers part of same system (i.e. cores).
  - Workers can see same data in memory.
  - Problem will be coordinating access.

Exercise 4

Example of *sharing memory:* all workers can see all the data.

	A	B	C	D	E	Sums
1	6	3	13	78	35	
2	49	60	138	34	79	
3	59	108	108	188	110	
4	137	50	4	167	189	
5	83	136	215	26	140	
6	0	187	77	216	51	

Total

Ex 4 Outcomes

- **Benefits?**
- **Difficulties?**

Concept Summary

- Shared memory lets all processors see all data, it is just there – no work to distribute it.
- 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 are 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 problems?**

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

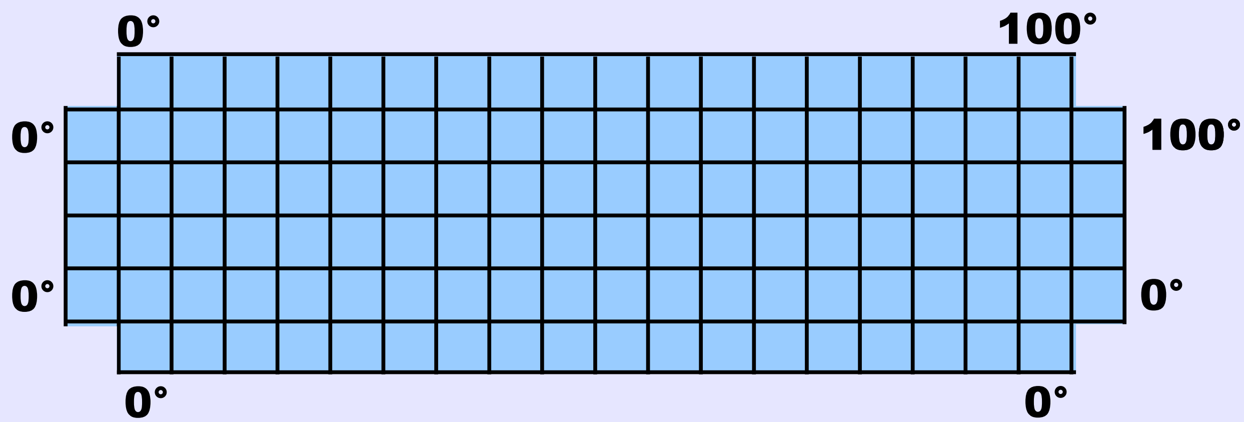
The solution must satisfy:

$$\nabla^2 \phi = 0$$

with the application of Dirichlet boundary conditions (constant values around edge of region.

The Serial Solution

Subdivide the surface into a mesh of points.



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

$$T_{i,j}^{n+1} = 0.25 * \left(T_{i-1,j}^{n} + T_{i+1,j}^{n} + T_{i,j-1}^{n} + T_{i,j+1}^{n} \right)$$

Ex 5: 1-D Problem

0	?	?	?	?	?	100

$$T_i^{n+1} = 0.5 * \left(T_{i-1}^n + T_{i+1}^n \right)$$

Think about working this problem in your group.

Step 1: Array 1 → Array 2

Array 1	0	0	0	0	0	0	100
Array 2	0	0	0	0	0	50	100

Step 2: Array 2 → Array 1

Array 1	0	0	0	0	25	50	100
Array 2	0	0	0	0	0	50	100

Step 3: Array 1 → Array 2

Array 1	0	0	0	0	25	50	100
Array 2	0	0	0	12.5	25	50	100

Ex 5: Solution

70 iterations to reach 0.001% convergence bound.

0	16.6661	33.3324	49.9988	66.6658	83.3327	100

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 0.001

 Solution has converged.
Iterations:             8437
Max error:             0.001
Total time:            0.461
```

What if the error condition was changed to 0.0001?

Higher Accuracy Run

```
$ ./laplace 100 200 25000 1000 0.0001

 Solution has converged.
Iterations:          15909
Max error:           0.000
Total time:          0.887
```

Why go to parallel?

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

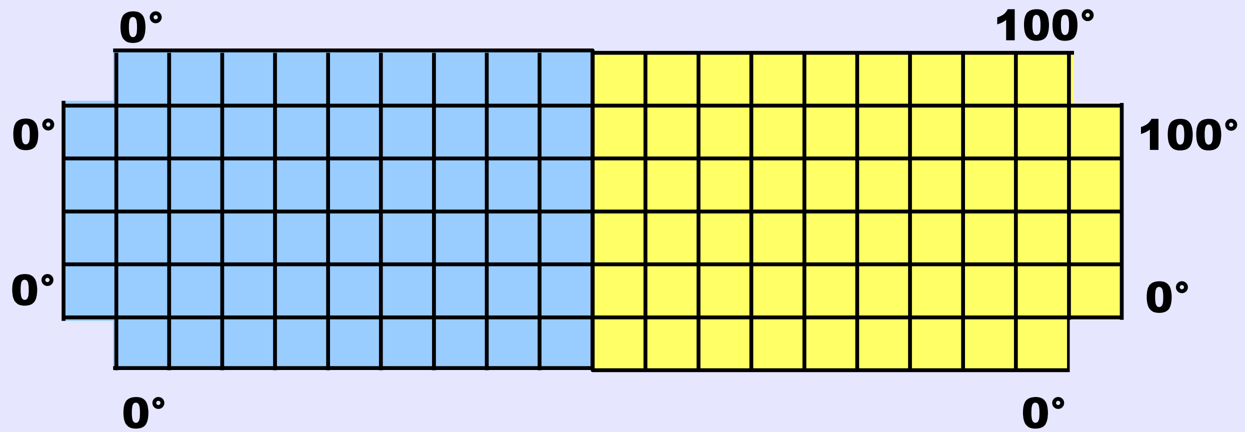
Even though 1 solution taking 1 second seems fast, 25,000 solutions would take 7 hours!

Can it be done in parallel to speed up the over all 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?

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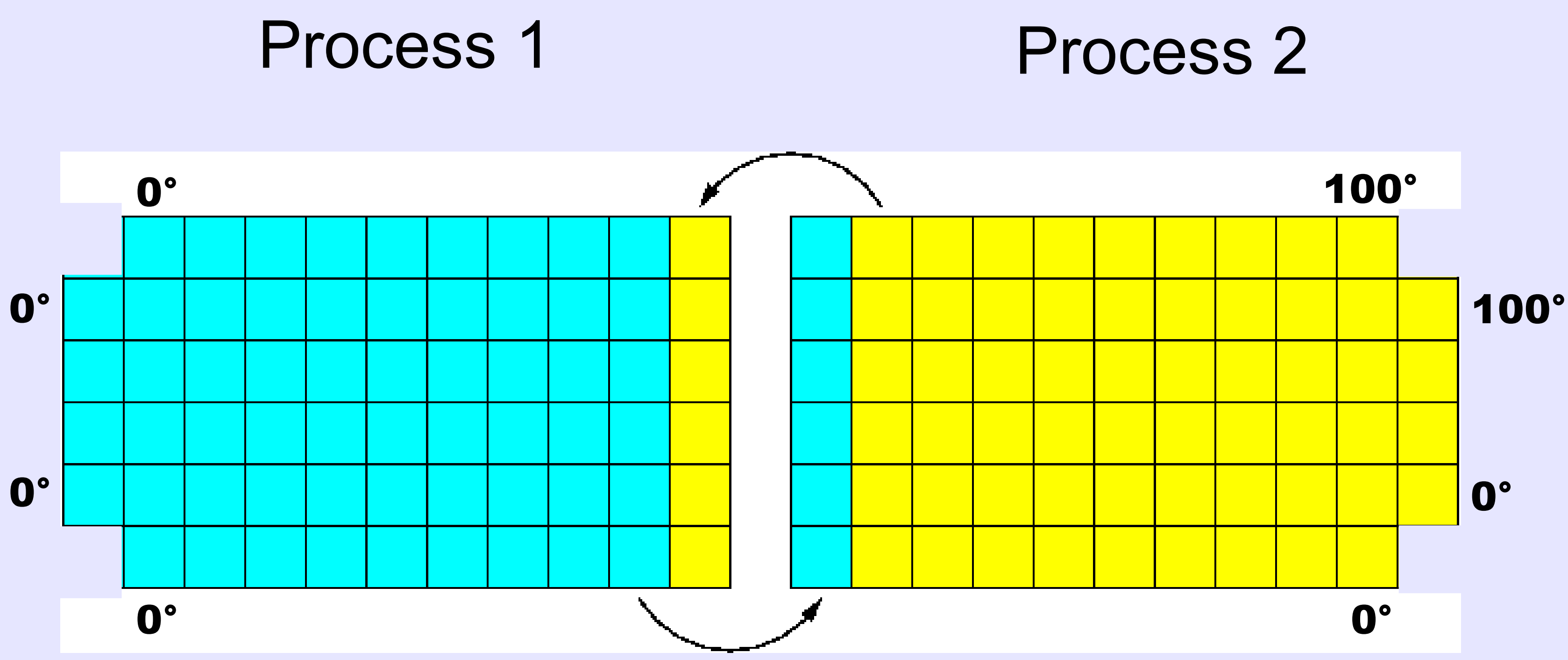
Ghost Cells



Extreme Science and Engineering Discovery Environment

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.

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