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Parallel Programming
in C with MPI and OpenMP

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Chapter 13

Finite Difference Methods

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Outline

- Ordinary and partial differential equations
- Finite difference methods
- Vibrating string problem
- Steady state heat distribution problem

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Ordinary and Partial Differential Equations

- Ordinary differential equation: equation containing derivatives of a function of one variable
- Partial differential equation: equation containing derivatives of a function of two or more variables

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Examples of Phenomena Modeled by PDEs

- Air flow over an aircraft wing
- Blood circulation in human body
- Water circulation in an ocean
- Bridge deformations as its carries traffic
- Evolution of a thunderstorm
- Oscillations of a skyscraper hit by earthquake
- Strength of a toy

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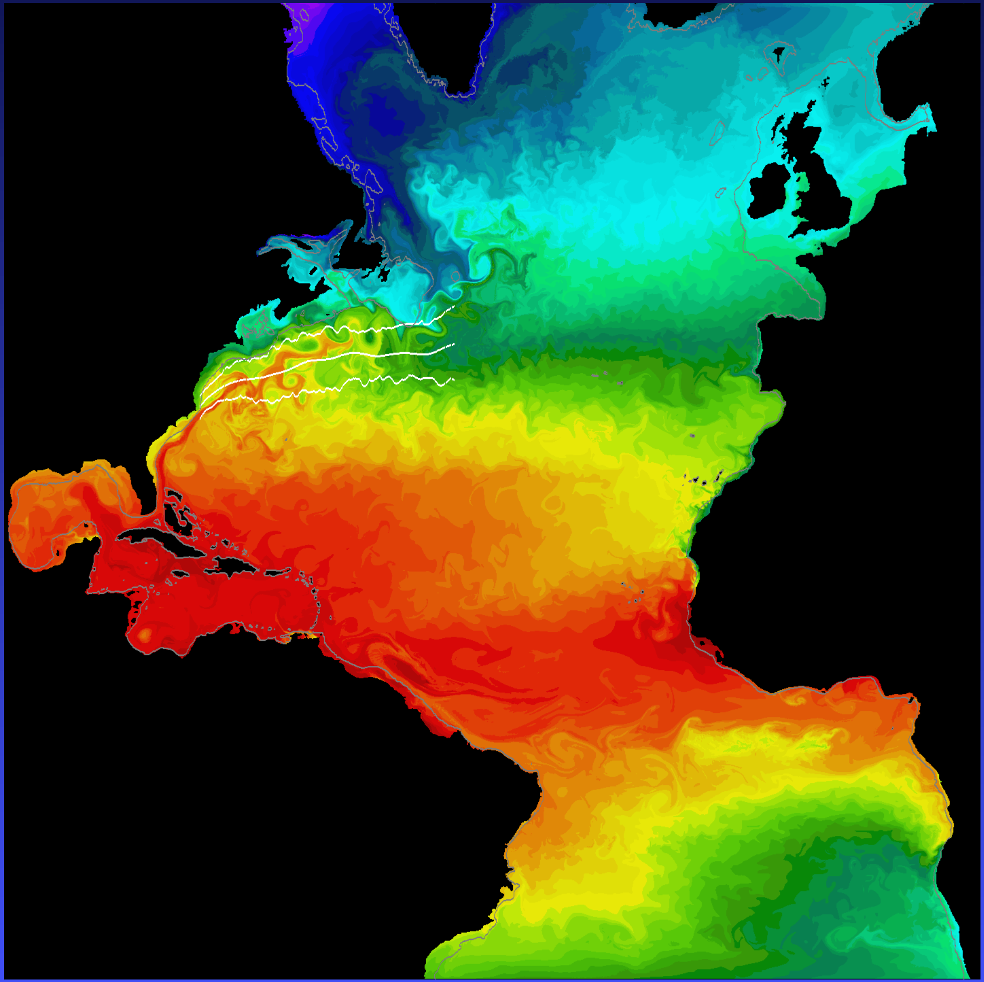
Model of Sea Surface Temperature in Atlantic Ocean



Courtesy MICOM group at the Rosenstiel School of Marine and Atmospheric Science, University of Miami

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Solving PDEs

- Finite element method
- Finite difference method (our focus)
  - Converts PDE into matrix equation
  - Result is usually a sparse matrix
  - Matrix-based algorithms represent matrices explicitly
  - Matrix-free algorithms represent matrix values implicitly (our focus)

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Linear Second-order PDEs

- Linear second-order PDEs are of the form

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + Eu_{x} + Fu_{y} + Gu = H$$

where A - H are functions of x and y only

- Elliptic PDEs: $B^2 - AC < 0$
- Parabolic PDEs: $B^2 - AC = 0$
- Hyperbolic PDEs: $B^2 - AC > 0$

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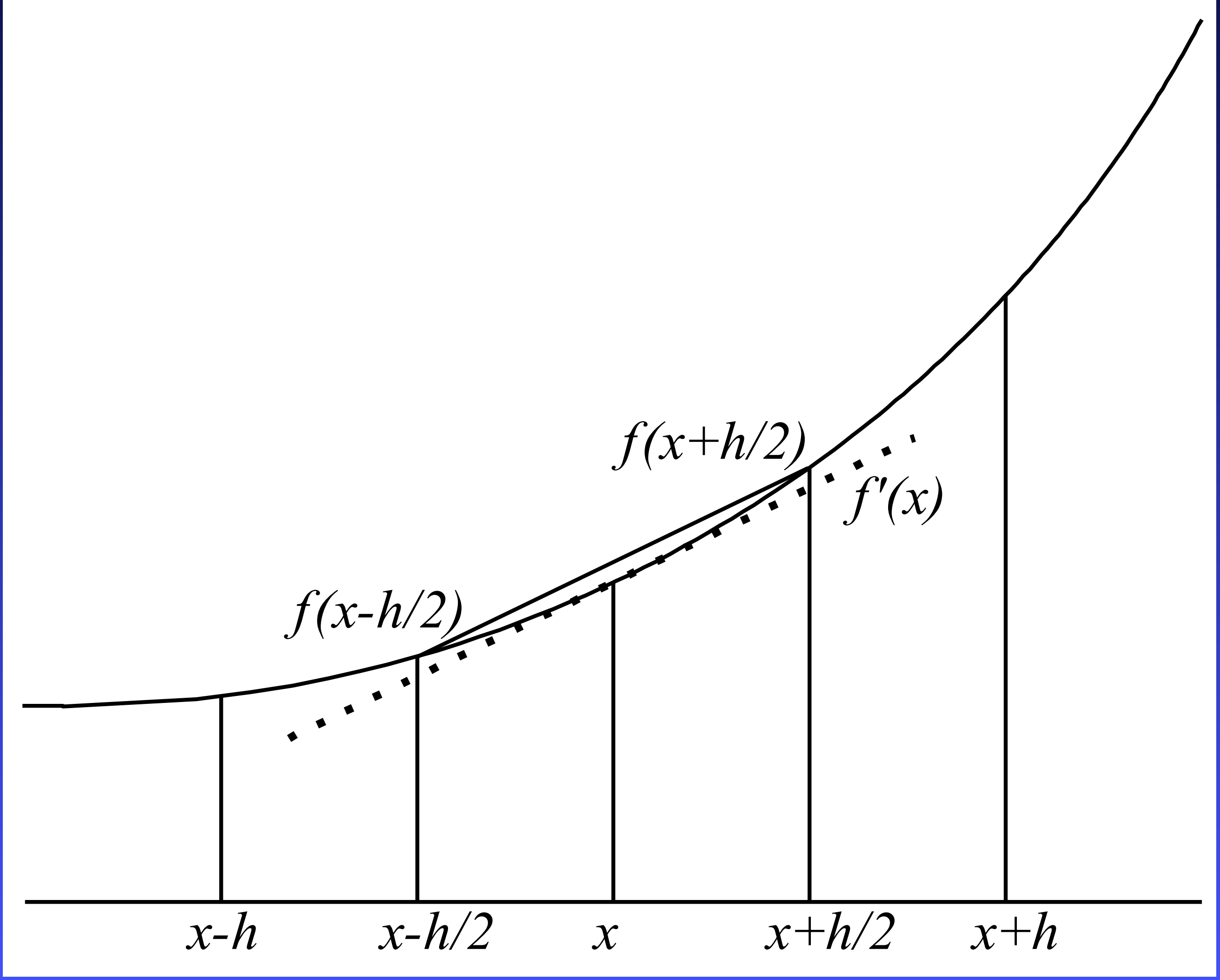
Difference Quotients



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Formulas for 1st, 2nd Derivatives

$$f'(x) = \frac{f(x+h/2) - f(x-h/2)}{h} + O(h^2)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

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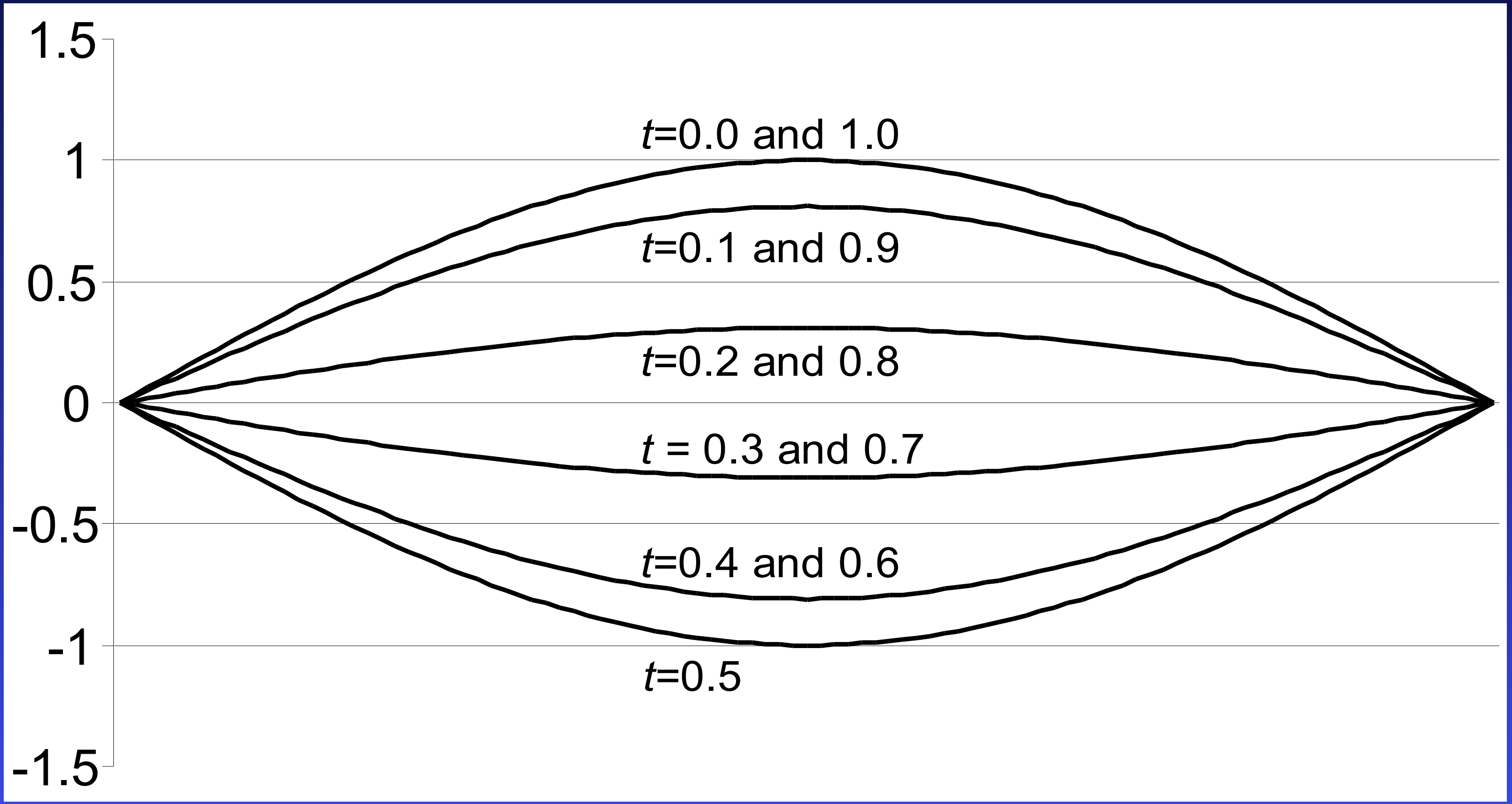
Vibrating String Problem



Vibrating string modeled by a hyperbolic PDE

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Solution Stored in 2-D Matrix

- Each row represents state of string at some point in time
- Each column shows how position of string at a particular point changes with time

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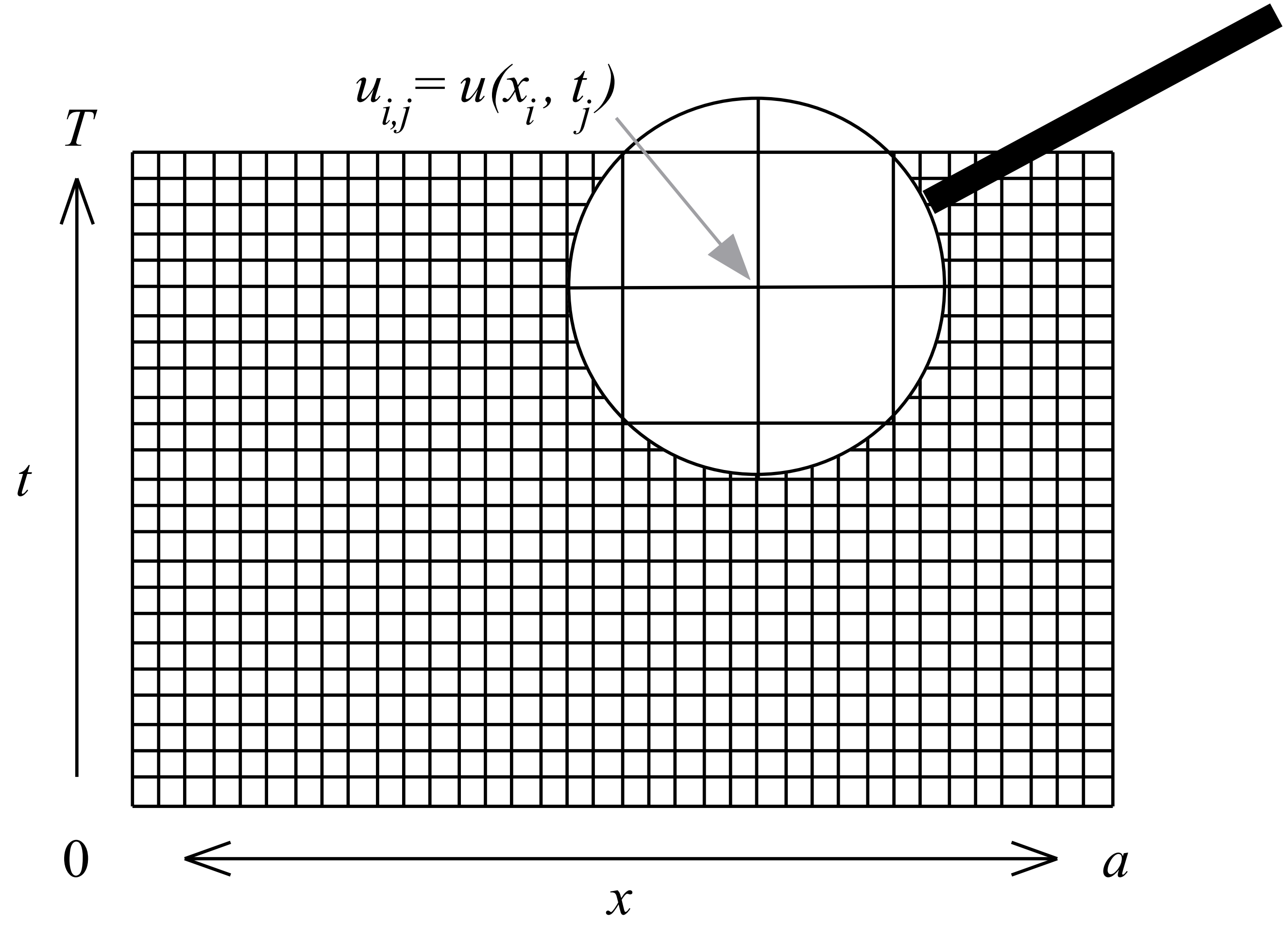
Discrete Space, Time Intervals Lead to 2-D Matrix



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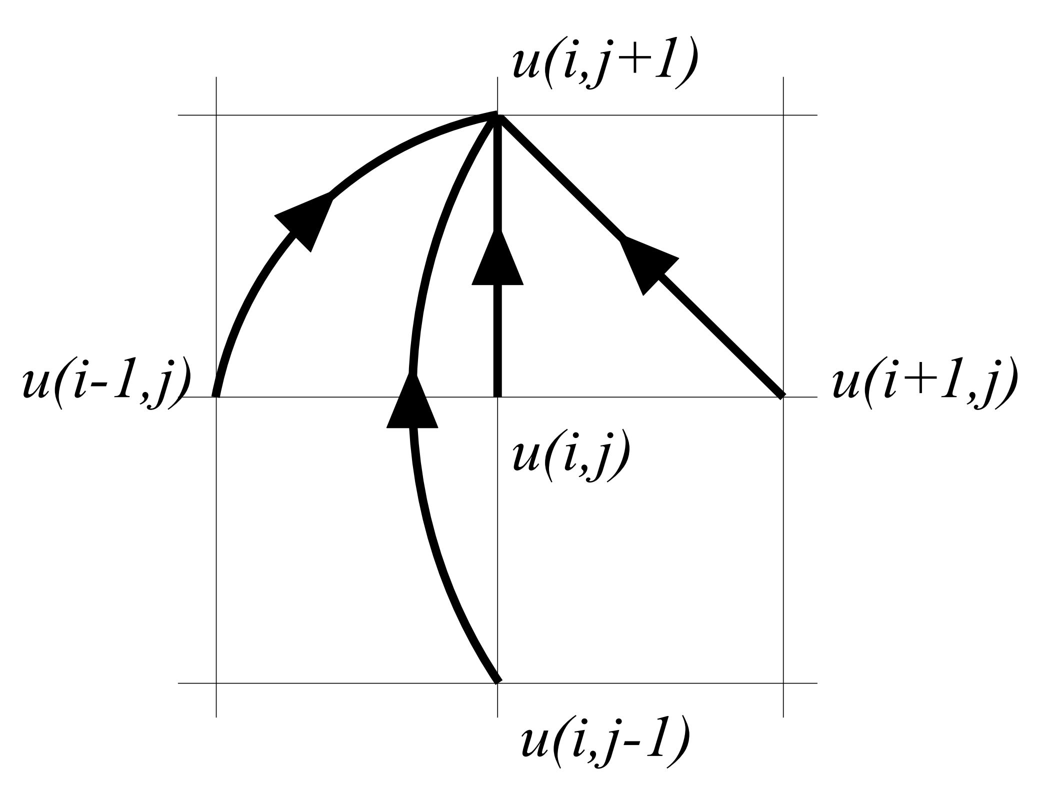
Heart of Sequential Program

```
u[j+1][i] = 2.0*(1.0-L)*u[j][i] +
   L*(u[j][i+1] + u[j][i-1]) - u[j-1][i];
```



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Parallel Program Design

- Associate primitive task with each element of matrix
- Examine communication pattern
- Agglomerate tasks in same column
- Static number of identical tasks
- Regular communication pattern
- Strategy: agglomerate columns, assign one block of columns to each task

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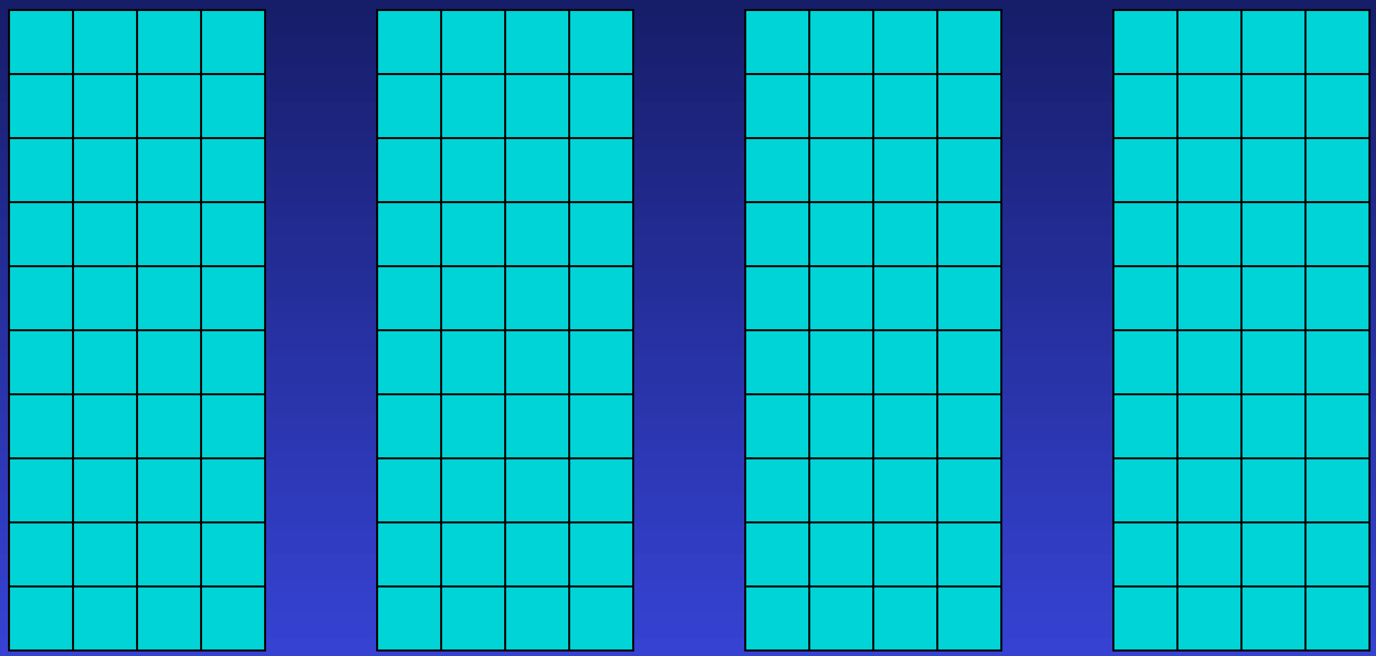
Result of Agglomeration and Mapping



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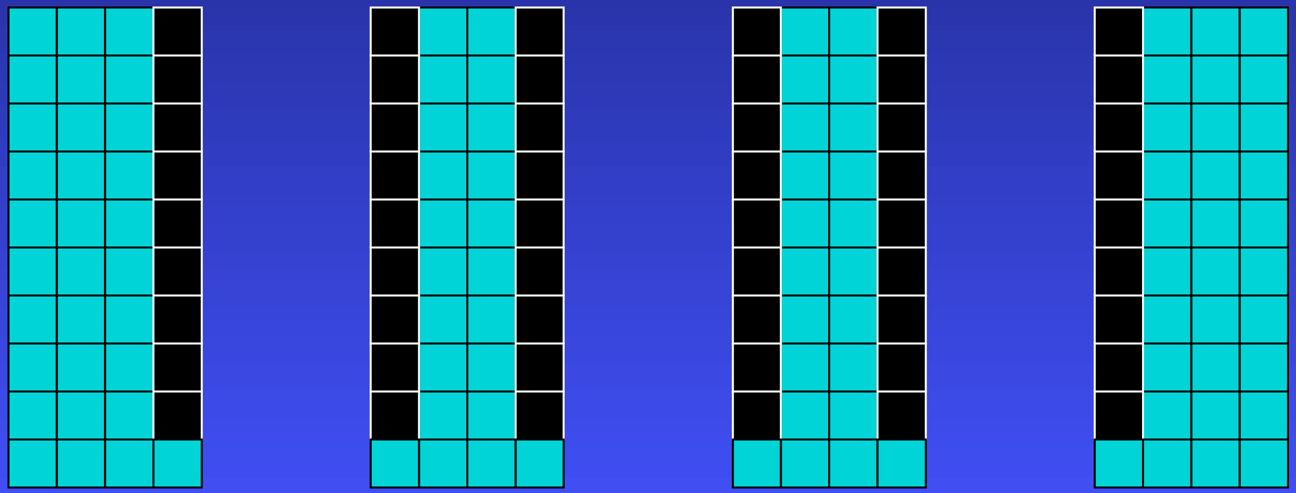
Communication Still Needed

- Initial values (in lowest row) are computed without communication
- Values in black cells cannot be computed without access to values held by other tasks



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Ghost Points

- Ghost points: memory locations used to store redundant copies of data held by neighboring processes
- Allocating ghost points as extra columns simplifies parallel algorithm by allowing same loop to update all cells

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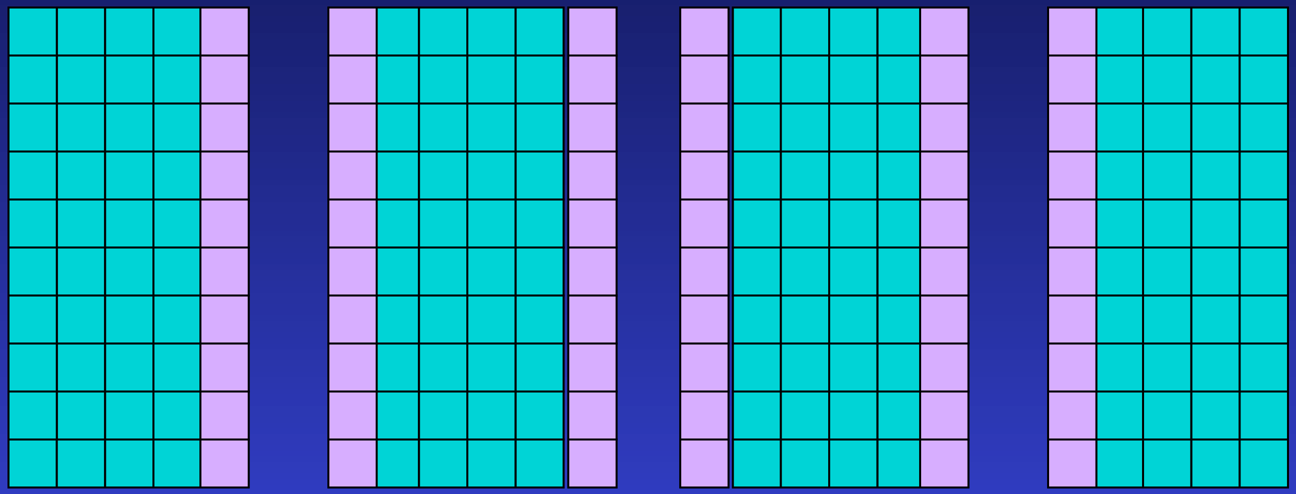
Matrices Augmented with Ghost Points



Lilac cells are the ghost points.

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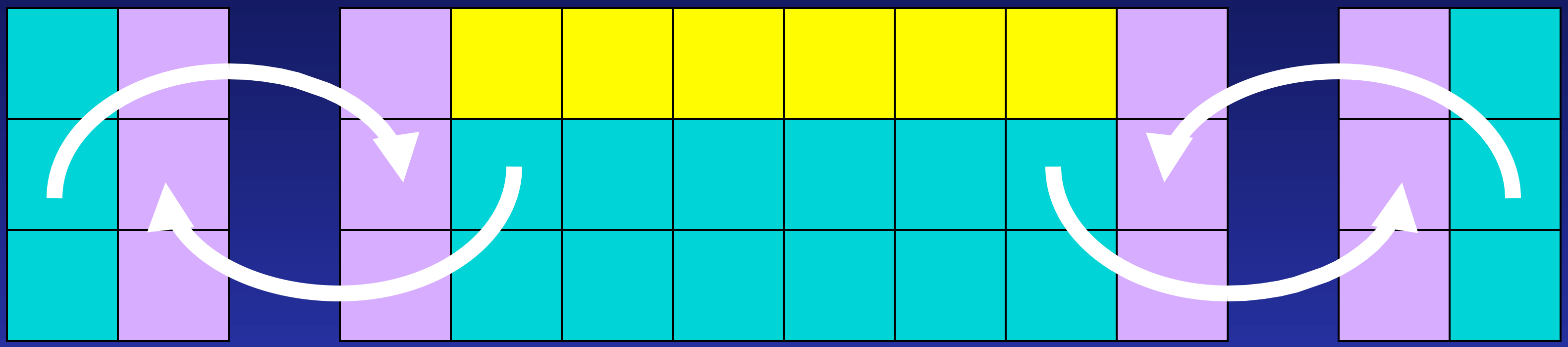
Communication in an Iteration



This iteration the process is responsible for computing the values of the yellow cells.

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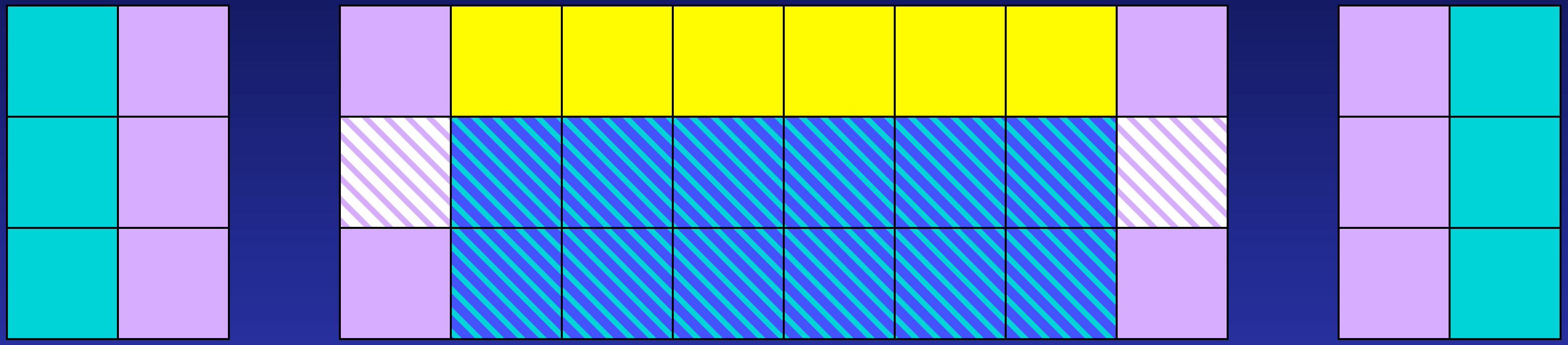
Computation in an Iteration



This iteration the process is responsible for computing the values of the yellow cells. The striped cells are the ones accessed as the yellow cell values are computed.

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Complexity Analysis

- Computation time per element is constant, so sequential time complexity per iteration is $\Theta(n)$
- Elements divided evenly among processes, so parallel computational complexity per iteration is $\Theta(n / p)$
- During each iteration a process with an interior block sends two messages and receives two messages, so communication complexity per iteration is $\Theta(1)$

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Isoefficiency Analysis

- Sequential time complexity: $\Theta(n)$
- Parallel overhead: $\Theta(p)$
- Isoefficiency relation:

  $n \geq Cp$
- To maintain the same level of efficiency, n must increase at the same rate as p
- If $M(n) = n^2$, algorithm has poor scalability
- If matrix of 3 rows rather than m rows is used, $M(n) = n$ and system is perfectly scalable

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Replicating Computations

- If only one value transmitted, communication time dominated by message latency
- We can reduce number of communications by replicating computations
- If we send two values instead of one, we can advance simulation two time steps before another communication

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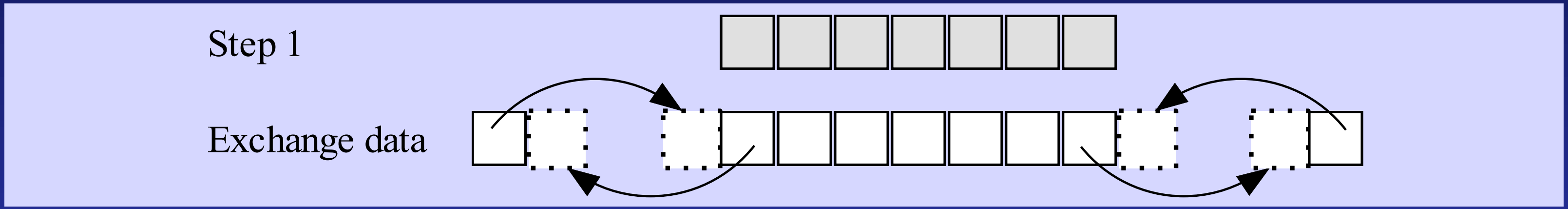
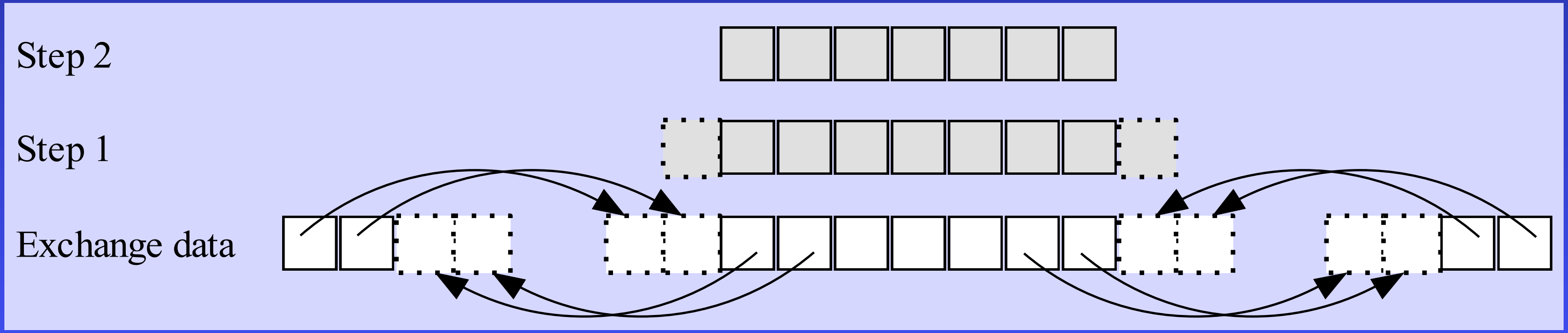
Replicating Computations

Without replication:



With replication:



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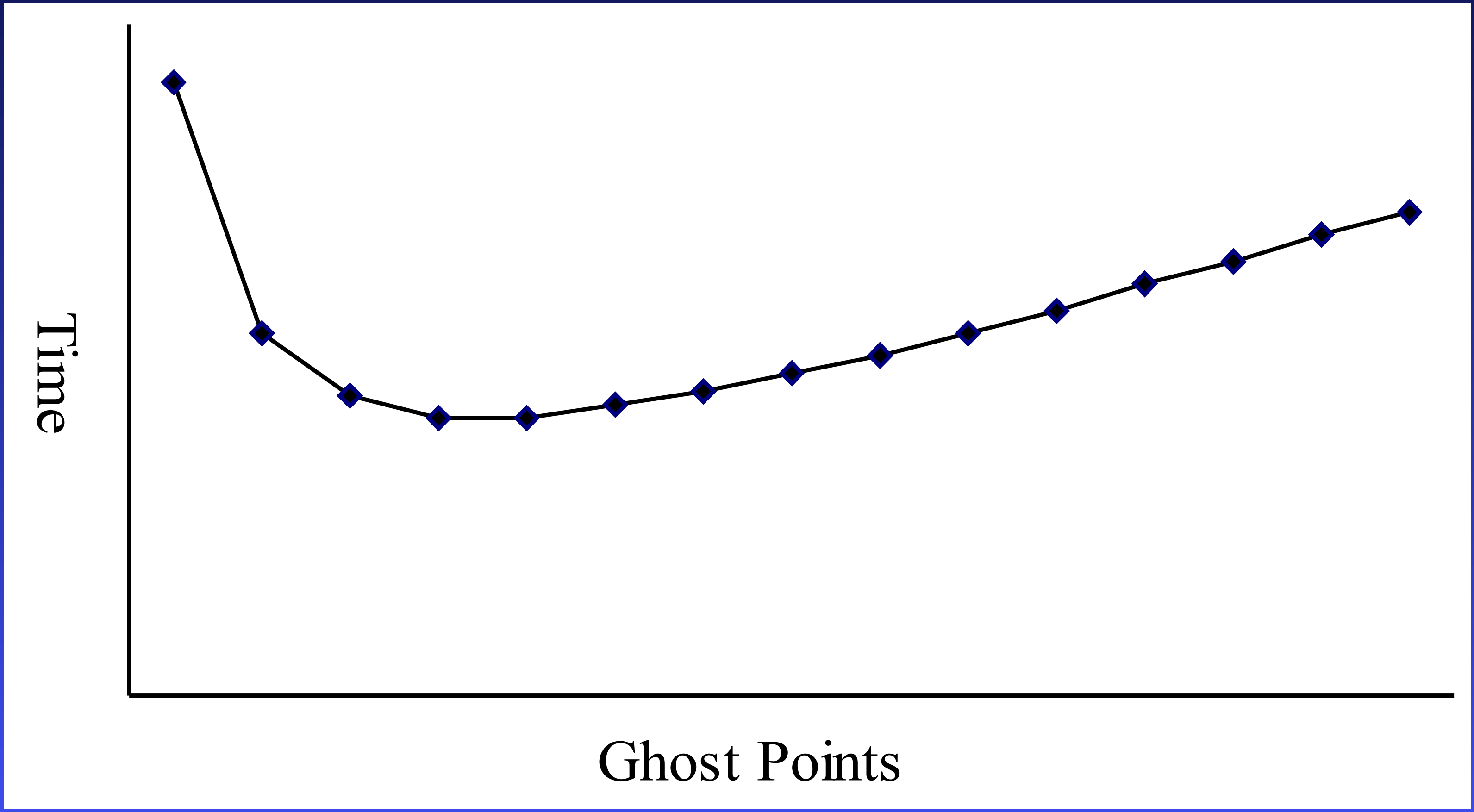
Communication Time vs. Number of Ghost Points



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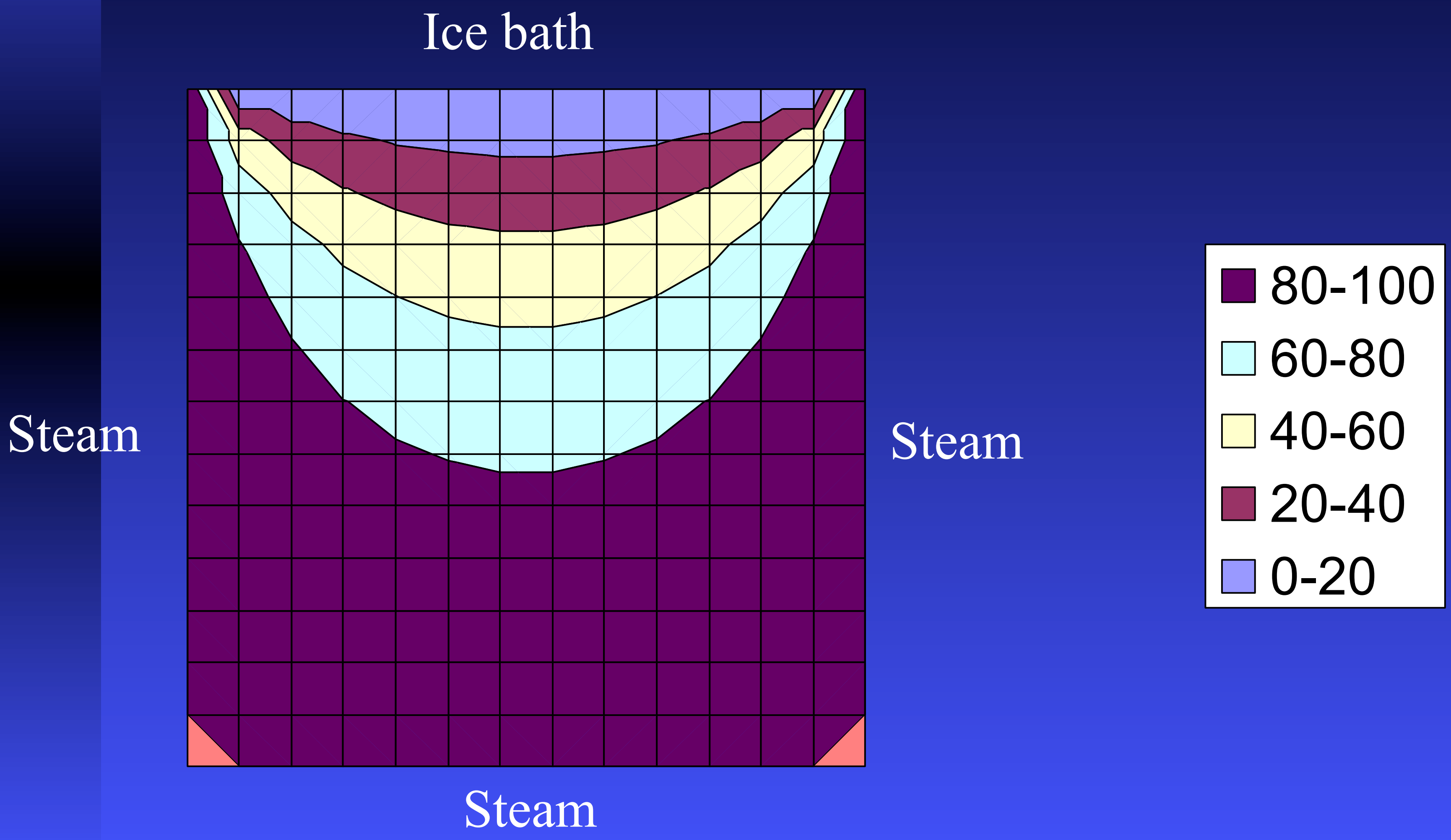
Steady State Heat Distribution Problem



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Solving the Problem

- Underlying PDE is the Poisson equation

$$u_{xx} + u_{yy} = f(x, y)$$

- This is an example of an elliptical PDE
- Will create a 2-D grid
- Each grid point represents value of state solution at particular (x, y) location in plate

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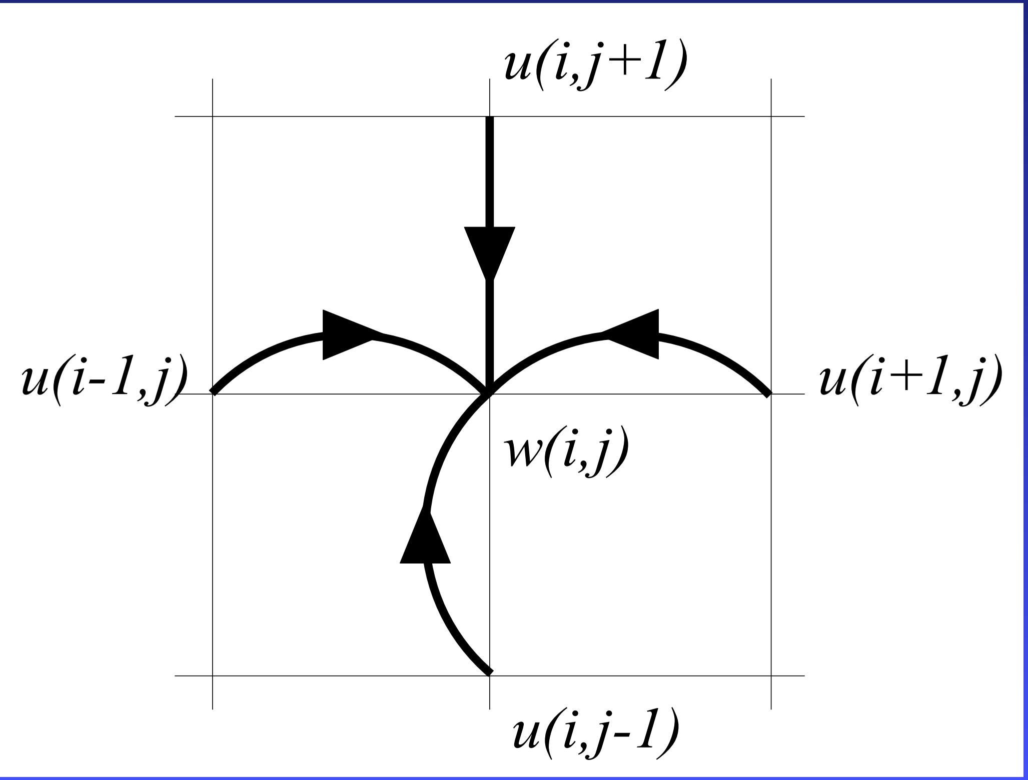
Heart of Sequential Program

```
w[i][j] = (u[i-1][j] + u[i+1][j] +
           u[i][j-1] + u[i][j+1]) / 4.0;
```



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Parallel Algorithm 1

- Associate primitive task with each matrix element
- Agglomerate tasks in contiguous rows (rowwise block striped decomposition)
- Add rows of ghost points above and below rectangular region controlled by process

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Ghost Points

- Ghost points: memory locations used to store redundant copies of data held by neighboring processes
- Allocating ghost points as extra rows simplifies parallel algorithm by allowing same loop to update all cells

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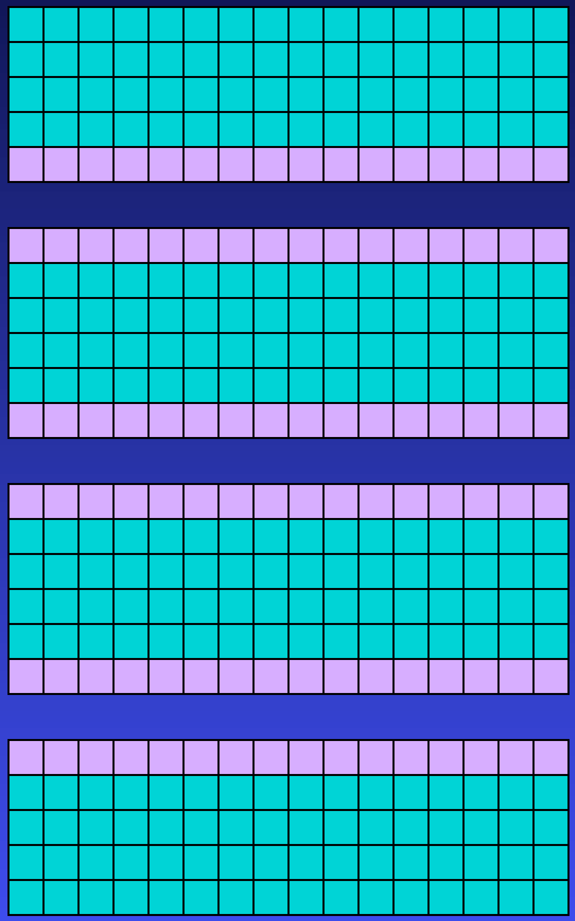
Example Decomposition



16 × 16 grid

divided among 4 processors

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Complexity Analysis

- Sequential time complexity: $\Theta(n^2)$ each iteration
- Parallel computational complexity: $\Theta(n^2 / p)$ each iteration
- Parallel communication complexity: $\Theta(n)$ each iteration (two sends and two receives of n elements)

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Isoefficiency Analysis

- Sequential time complexity: $\Theta(n^2)$
- Parallel overhead: $\Theta(pn)$
- Isoefficiency relation:
  $n^2 \geq Cnp \Rightarrow n \geq Cp$

$$M(Cp)/p = C^2p^2/p = C^2p$$

- This implementation has poor scalability

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Parallel Algorithm 2

- Associate primitive task with each matrix element
- Agglomerate tasks into blocks that are as square as possible (checkerboard block decomposition)
- Add ghost points to all four sides of rectangular region controlled by process

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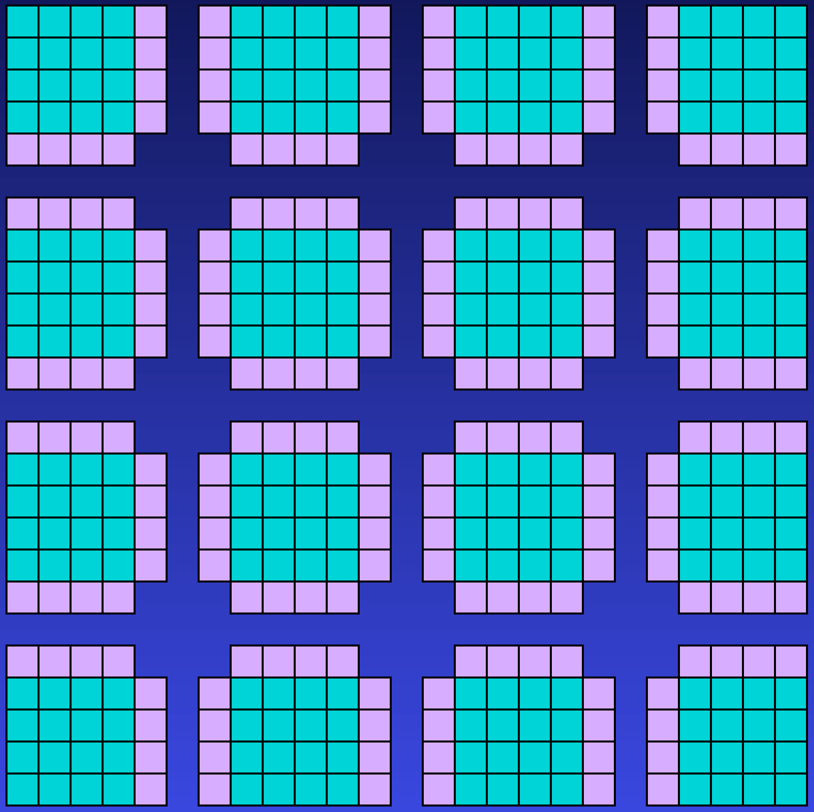
Example Decomposition



16 × 16 grid divided among 16 processors

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Implementation Details

- Using ghost points around 2-D blocks requires extra copying steps
- Ghost points for left and right sides are not in contiguous memory locations
- An auxiliary buffer must be used when receiving these ghost point values
- Similarly, buffer must be used when sending column of values to a neighboring process

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Complexity Analysis

- Sequential time complexity: $\Theta(n^2)$ each iteration
- Parallel computational complexity: $\Theta(n^2 / p)$ each iteration
- Parallel communication complexity: $\Theta(n / \sqrt{p})$ each iteration (four sends and four receives of $n / \sqrt{p}$ elements each)

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Isoefficiency Analysis

- Sequential time complexity: $\Theta(n^2)$
- Parallel overhead: $\Theta(n \sqrt{p})$
- Isoefficiency relation:
  $n^2 \geq Cn \sqrt{p} \Rightarrow n \geq C \sqrt{p}$

$$M(C\sqrt{p})/p = C^2 p/p = C^2$$

- This system is perfectly scalable

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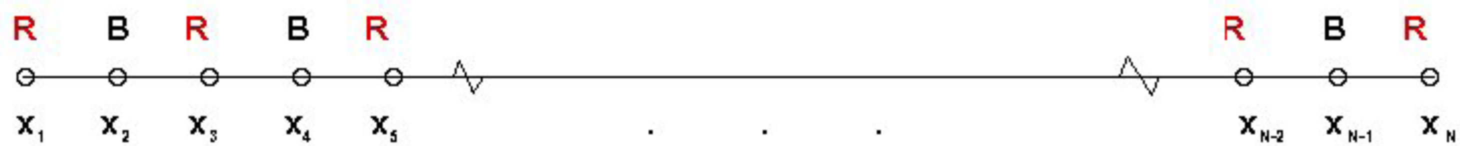
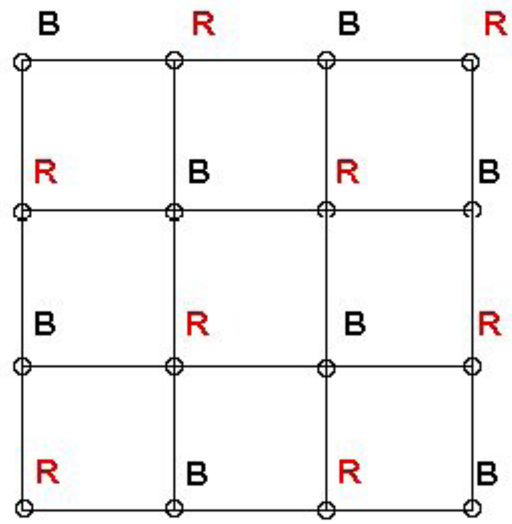
Gauss-Seidel: Red-black ordering





Red-Black grid orderings for 1-D (top) and 2-D (right). Odd and even numbered grid points can simply be assigned to Red and Black colors respectively.

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"Red-black" GS iteration

1. Exchange black edge values with neighboring processes
2. Perform GS updates on all red points
3. Exchange red edge values with neighboring processes
4. Perform GS updates on all black points

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Summary (1/4)

- PDEs used to model behavior of a wide variety of physical systems
- Realistic problems yield PDEs too difficult to solve analytically, so scientists solve them numerically
- Two most common numerical techniques for solving PDEs
  - finite element method
  - finite difference method

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Summary (2/4)

- Finite different methods
  - Matrix-based methods store matrix explicitly
  - Matrix-free implementations store matrix implicitly
- We have designed and analyzed parallel algorithms based on matrix-free implementations

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Summary (3/4)

- Linear second-order PDEs
  - Elliptic (e.g., heat equation)
  - Hyperbolic
  - Parabolic (e.g., wave equation)
- Hyperbolic PDEs typically solved by methods not as amenable to parallelization

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Summary (4/4)

- Ghost points store copies of values held by other processes
- Explored increasing number of ghost points and replicating computation in order to reduce number of message exchanges
- Optimal number of ghost points depends on characteristics of parallel system