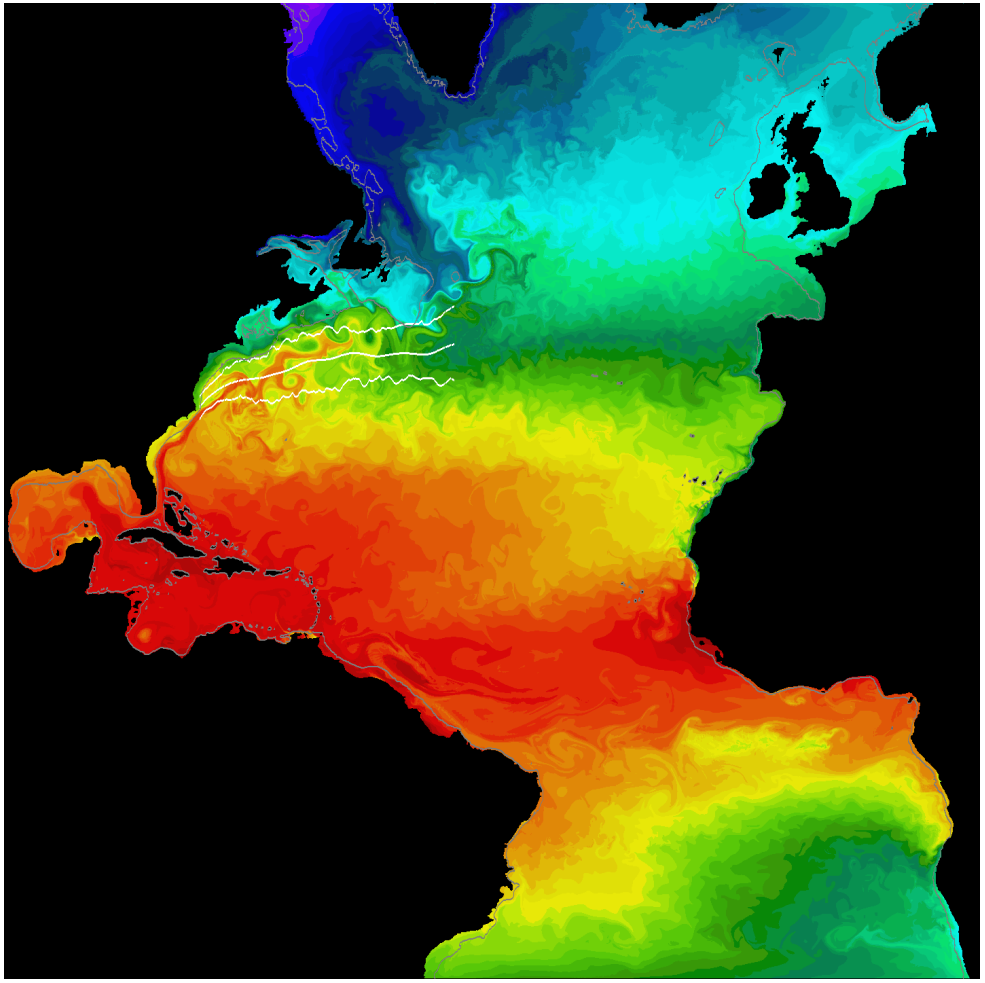
CS6068-Fall 2020: Numerical Methods

- Solving ordinary and partial differential equations
- Finite difference methods (FDM)
- Wave equation: vibrating string problem
- Heat equation: Steady state heat distribution problem

Example: Computer Model of Sea Surface Temperature in Atlantic Ocean



…there is a physical problem that is common to many fields, that is very old, and that has not been solved. Nobody in physics has really been able to analyze it mathematically satisfactorily in spite of its importance to the sister sciences. It is the analysis of circulating or turbulent fluids.
-Richard Feynman's Lectures on Physics

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

Calculating Continuous variables depending on continuous parameters

Weather can be thought of as a continuous function

```
[temperature, pressure, humidity, wind velocity(3)]
=
  Weather (longitude,latitude,elevation,time)
```

The state is thus a 6-tuple of continuous variables, each of which depends on 4 continuous parameters.

The governing equations are *partial differential equations (PDEs)*, which describes how each of the 6 variables changes as a function of all the others.

Other, simpler examples:
Heat flow (Temperature(position,time))
Diffusion (Concentration(position,time))
Electrostatic or Gravitational potential (Potential(position))
Electromagnetic field strength (Field(position,time))
Fluid flow (Velocity,Pressure,Density(position,time))
Semiconductor modeling (Electron_density(position,time))
Quantum Mechanics (Wave_function(position,time))
Elasticity (Stress,Strain(position,time)

An equation involving partial derivatives of an unknown function is called a PDE.

The laws of physics (conservation laws) are written in PDEs.

The order of a PDE is that of the highest order partial derivative. For example, second order equations have second-order derivatives, but no third-order derivatives.

A PDE is linear if only linear terms in the unknowns.

Widespread applications in engineering: **linear second-order equations.**

Classifying Linear Second-order PDEs

- Linear second-order PDEs are of the form

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Eu_x + Fu_y + Gu = H$$

where A - H are constants or functions of x and y only

- Elliptic PDEs: $B^2 - 4AC < 0$
  - steady state heat equations – no time derivatives
- Parabolic PDEs: $B^2 - 4AC = 0$
  - heat transfer equations – derivatives in space and time
- Hyperbolic PDEs: $B^2 - 4AC > 0$
  - wave equations – have 2nd-order time derivative

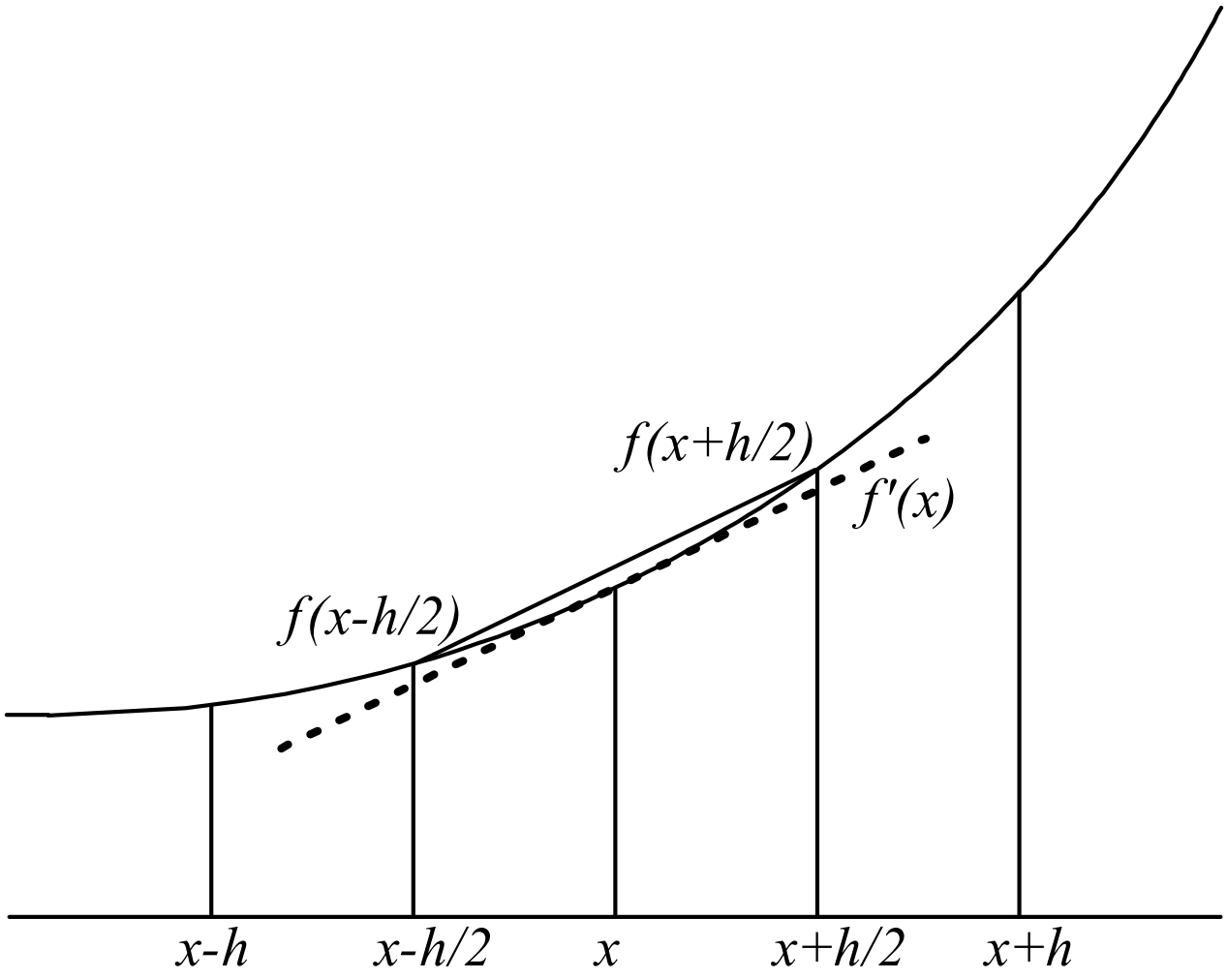
Solving PDEs - FEMs vs FDMs

- Finite element method

Computational method that subdivides a (CAD) model into very small but finite-sized elements of geometrically simple shapes. The collection is the so-called finite-element mesh.

- Finite difference method (our focus)
  - Direct approach that converts PDE into matrix equations - system over discrete basis elements
  - Result is usually a sparse matrix
  - Matrix-based algorithms represent matrices explicitly
  - Matrix-free algorithms represent matrix values implicitly (our focus)

Difference Quotients



Formulas for 1st, 2d Derivatives

$$f'(x) \approx \frac{f(x+h/2) - f(x-h/2)}{h}$$

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

Example of Finite Differences:

Let u(x) = sin x. We will approximate

$u'(1) = \cos 1 = .5403023$

Let us use finite difference quotients

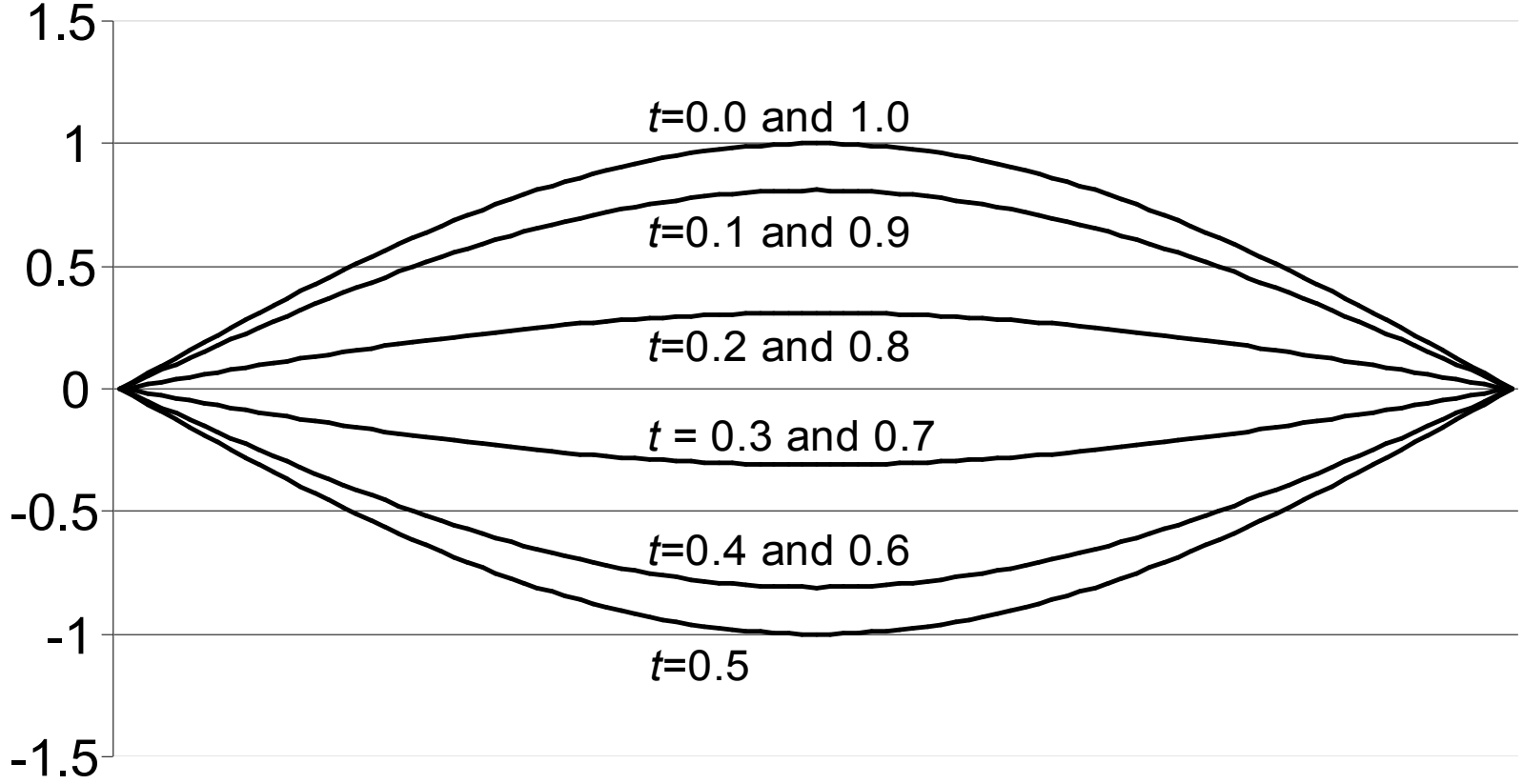
$\cos(1) \approx (\sin(1+h) - \sin(1-h))/2h$

h=.1, .01, .001 .0001

approx= .539402, .540293,.540302,.540302

error=.0009,.000009,.00000009,.0000000009

Vibrating String Problem



Vibrating string modeled by a hyperbolic PDE

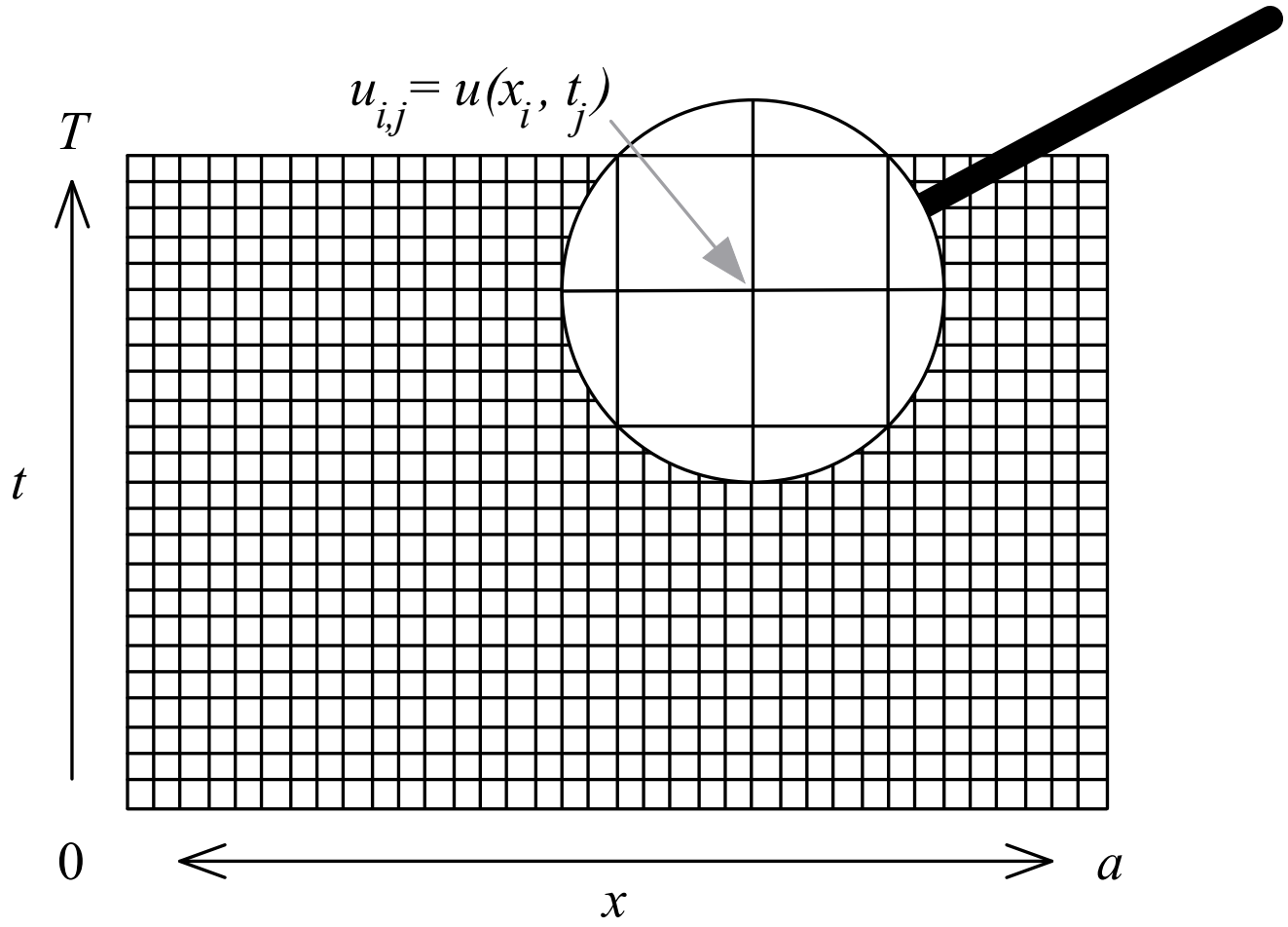
Derived from Newton's and Hooke's Laws

$$F = m\,a = -k\,y$$

Computer Solution Stored in 2-D Array

- 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

Discretized Space
Discretized Time Intervals
Displacement Values u(i,j) Stored in 2-D Array



Finite Difference Approximation

Central difference approximations

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_\ell) \approx \frac{u_{i-1}^\ell - 2u_i^\ell + u_{i+1}^\ell}{\Delta x^2},$$
$$\frac{\partial^2 u}{\partial t^2}(x_i, t_\ell) \approx \frac{u_i^{\ell-1} - 2u_i^\ell + u_i^{\ell+1}}{\Delta t^2}$$

Inserted into the equation:

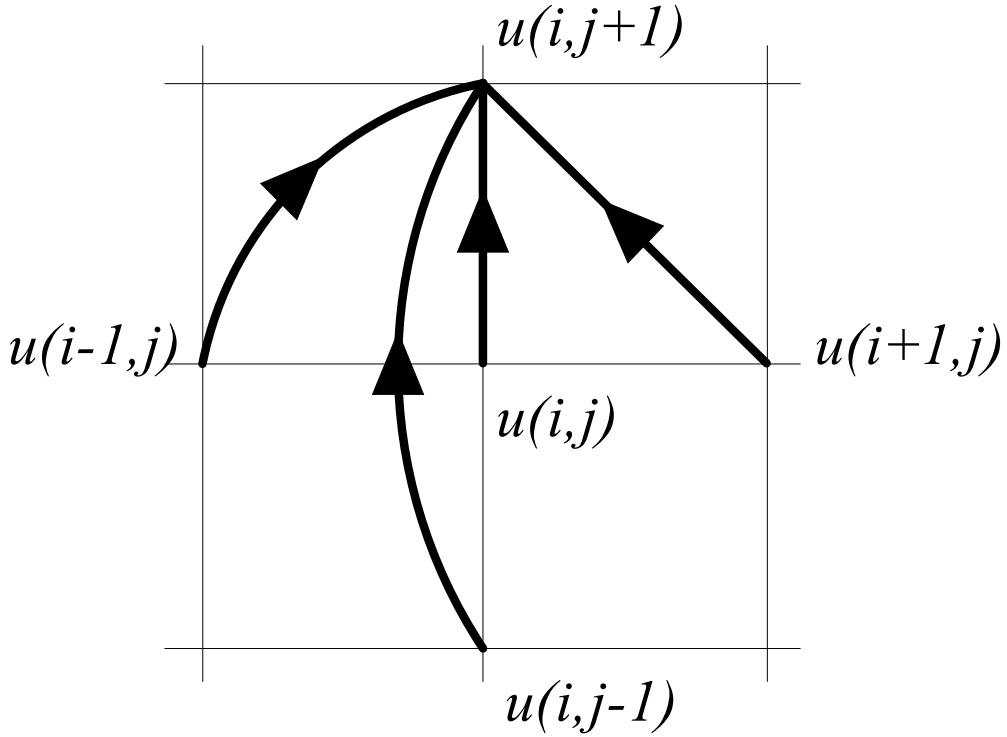
$$\frac{u_i^{\ell-1} - 2u_i^\ell + u_i^{\ell+1}}{\Delta t^2} = \gamma^2 \frac{u_{i-1}^\ell - 2u_i^\ell + u_{i+1}^\ell}{\Delta x^2}$$

Solve for $u_i^{\ell+1}$. Then the difference equation reads

$$u_i^{\ell+1} = 2u_i^\ell - u_i^{\ell-1} + C^2 \left(u_{i-1}^\ell - 2u_i^\ell + u_{i+1}^\ell \right)$$

Heart of Sequential C Program

```
u[j+1][i] = 2.0*u[j][i] - u[j-1][i]
   + C2*(u[j][i+1] - 2.0*u[j][i] + u[j][i-1])
```

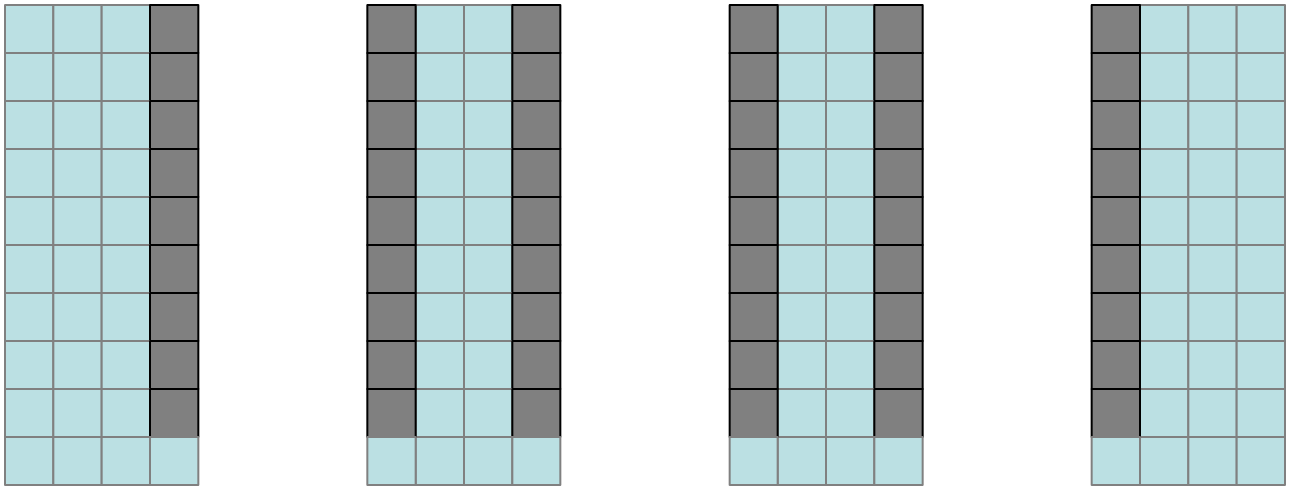


Parallel Program Design

- Associate primitive task with each element of matrix
- Examine communication pattern
- Agglomerate tasks: thread per column
- Static number of identical tasks
- Regular communication pattern
- Strategy: agglomerate columns into blocks
- Difficulty: sharing information across blocks

Communication Still Needed

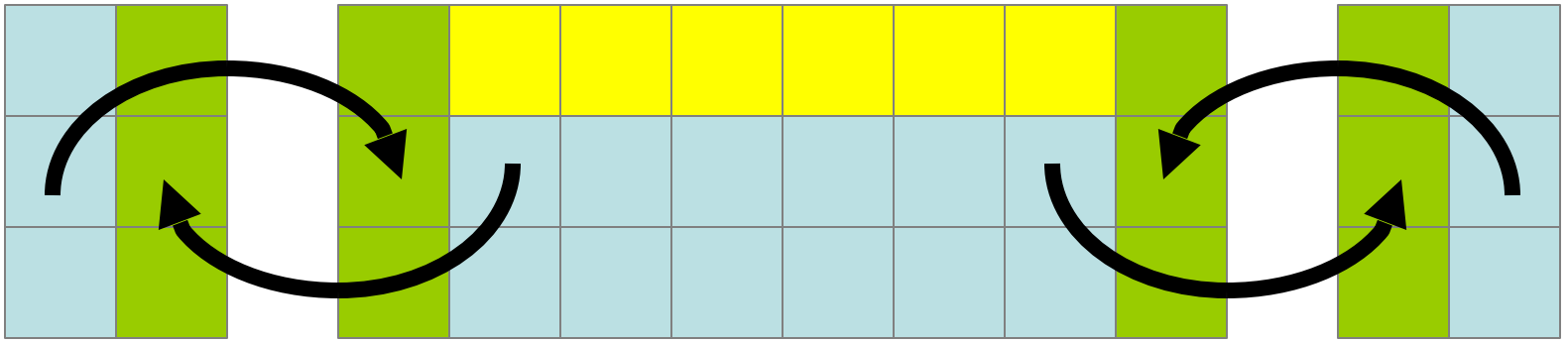
- Initial values (in lowest row) are computed without communication
- Values in black cells cannot be computed without access to values held by other tasks



Ghost Points

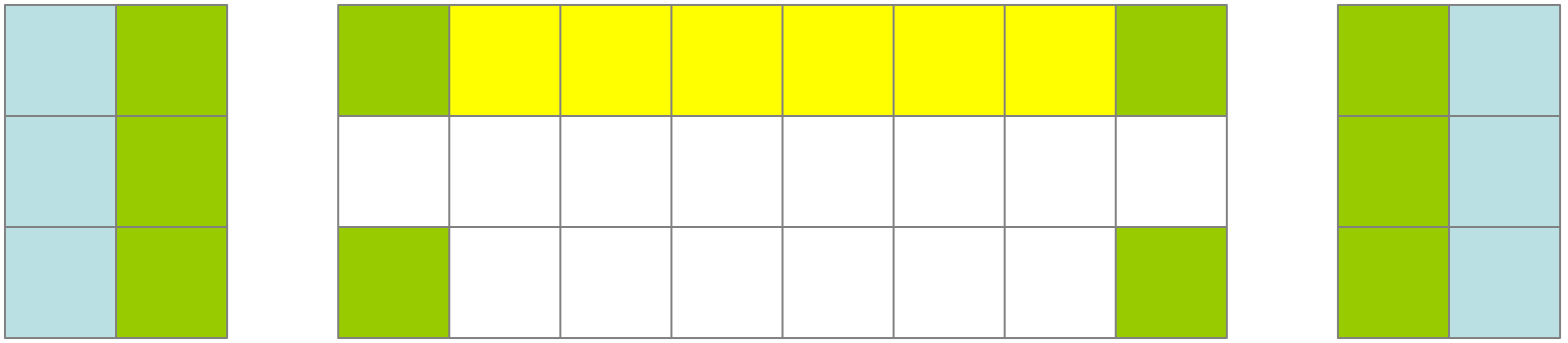
- Ghost points: memory locations used to store redundant copies of data held by neighboring processes
- Allocating ghost points as extra columns simplifies parallel algorithm by allowing same loop to update all cells

Communication in an Iteration



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

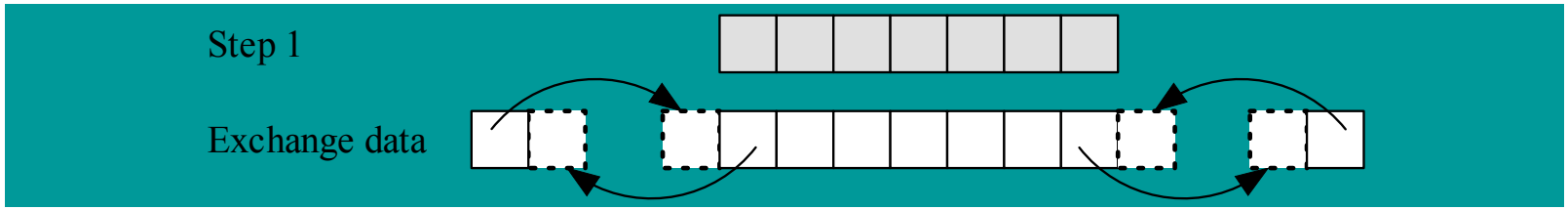
Computation in an Iteration



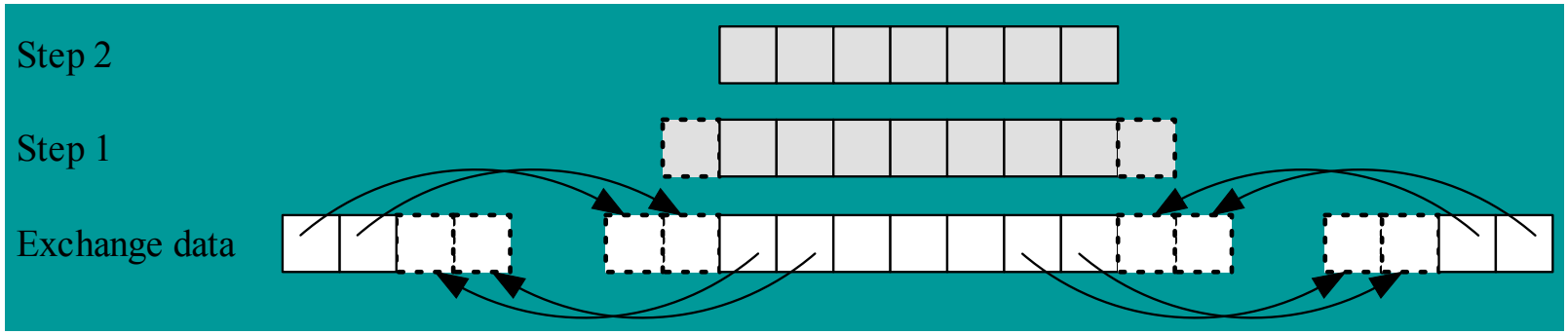
This iteration the process is responsible for computing the values of the yellow cells. The striped cells are the ones accessed as the yellow cell values are computed.

Replicating Computations

Without replication:

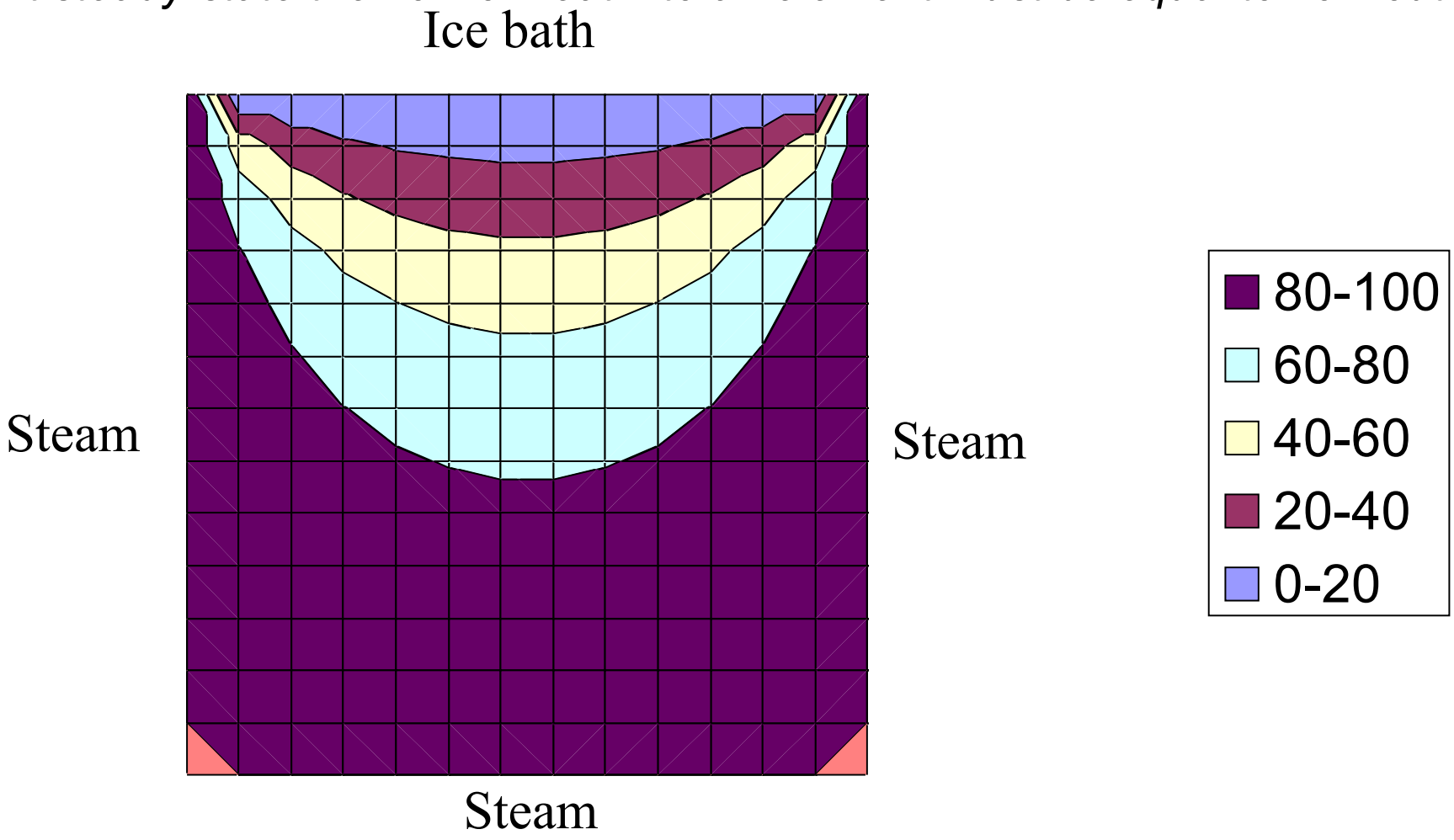


With replication:



Case: The Laplace Equation
Steady State Heat Distribution Problem

At steady-state the flow of heat into an element must be equal to flow out.



Solving the Problem

- Underlying PDE is the Poisson equation

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

- When f = 0 called Laplace equation
- This is an example of an elliptical PDE
- Will create a 2-D grid
- Each grid point represents value of state state solution at particular (*x, y*) location in plate

Laplace Difference Equation

- Let h = grid interval
- Txx = T(i+1,j) – 2T(i,j) + T(i-1,j)/ h^2
- Tyy = T(i, j+1,) – 2T(i,j) + T(i,j-1)/ h^2
- So collecting terms
- T(i+1,j)+T(i-1,j)+T(i, j+1,)+T(i,j-1)– 4T(i,j) = 0

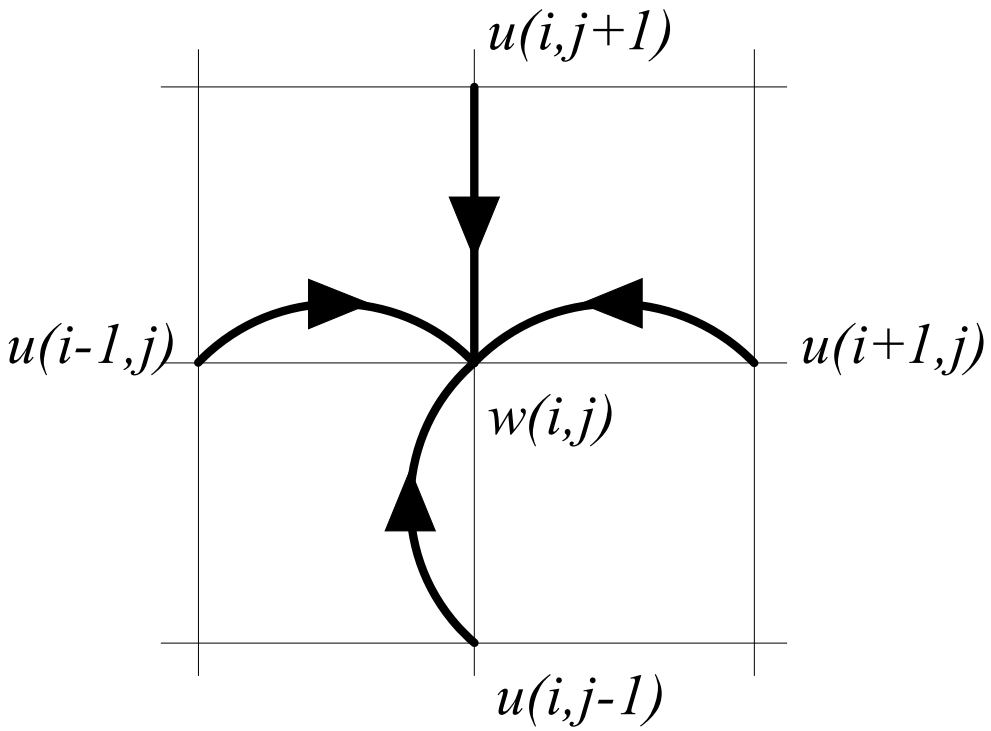
- Dirichlet boundary condition: all boundary temps are fixed at constant.

Gauss-Seidel/Liebmann Method

- An nxn grid leads to n^2 linear algebraic equations (each with max of 5 unknowns)
- Direct methods like Gaussian elimation are infeasible
- Iteration to solve for each T(i,j)
- T(i,j)= ¼ T(i+1,j)+T(i-1,j)+T(i, j+1,)+T(i,j-1)
- Iteration is repeated (with overrelaxation) until relative errors (changes) are all below threshold

Heart of Sequential C Program

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



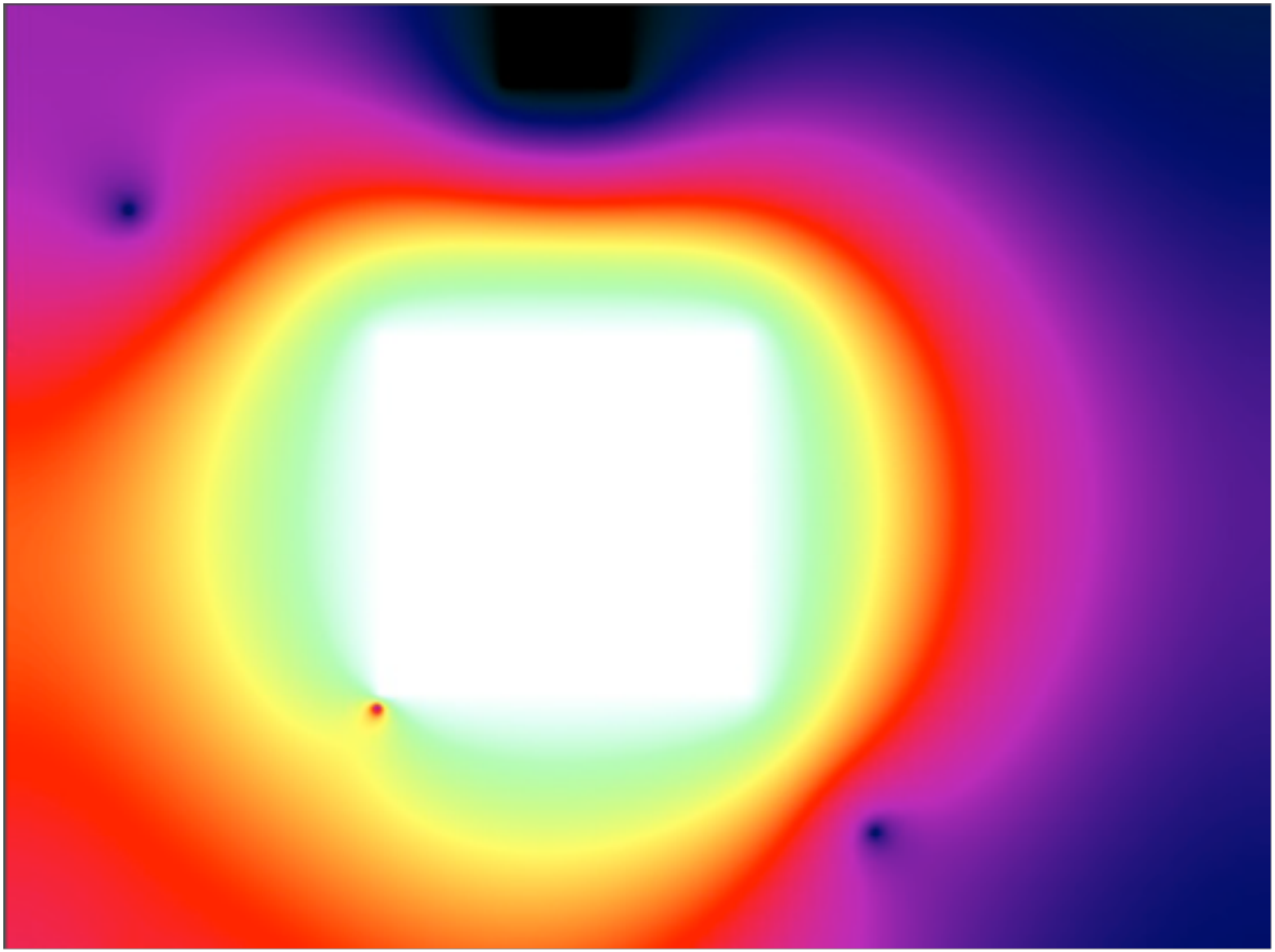
//Cuda Kernel Code that updates temperatures based on difference with average of neighbors
// T-new= T-old + k [Sum(Neighbors) – 4T-old]

```
__global__ void blend_kernel
   ( float *outSrc, const float *inSrc ) {
// map from threadIdx/BlockIdx to pixel position
int x = threadIdx.x + blockIdx.x * blockDim.x;
int y = threadIdx.y + blockIdx.y * blockDim.y;
int offset = x + y * blockDim.x * gridDim.x;


int left = offset - 1;  int right = offset + 1;
if (x == 0) left++;  if (x == DIM-1) right--;


int top = offset - DIM; int bottom = offset + DIM;
if (y == 0) top += DIM; if (y == DIM-1) bottom -=
   DIM;


outSrc[offset] = inSrc[offset] + SPEED * ( inSrc[top] +
```



Optimized Implementation

- Method 1: use ghost points around 2-D blocks, but requires extra copying steps

- Method 2: use “texture memory” in CUDA which provides for fast access – spatially localized cache. Global, constant, and texture memory spaces are persistent across kernels called by the same application.