PY410 / 505
Computational Physics 1

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Partial Differential Equations

- Start looking at PDE's
  - http://en.wikipedia.org/wiki/Partial_differential_equation
- Just like ODE's, only harder! (Kidding)

- You should be familiar with the mathematics of PDE's
  - Poisson equation
  - Diffusion equation
  - Wave equation

- The general strategy is to look at finite derivatives (just like we did in ODE's), but now we have to look in multiple dimensions at once!

Partial Differential Equations

- First example : Elliptic PDEs

- Given an electric charge distribution rho(r), Poisson's equation is :

$$\nabla^2 V(\mathbf{r}) = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho(\mathbf{r})}{\epsilon_0}$$

- This determines the potential V(r) at each point r, provided boundary values are specified
  – Dirichlet : V(r) specified on boundary
  – Neumann : normal component $\hat{\mathbf{n}} \cdot \nabla V$ specified on boundary
    - For electrostatics, this specifies normal component of E-field in a conductor
  – Periodic : V(r) = V(r + dr) for some dr

Partial Differential Equations

- Why "elliptic"?
- Consider 2-d and let

$$V(x,y) \sim e^{ik_x x + ik_y y} .$$

- Then :

$$-\nabla^2 V(x,y) = (k_x^2 + k_y^2) V(x,y) .$$

- The kx, ky values in k-space of a given eigenvalue satisfy

$$(k_x^2 + k_y^2) = \text{constant}$$

- This is (of course) a circle, which is an ellipse
- We'll continue this "conic section" terminology, as you probably have done in your other courses

Partial Differential Equations

- Second case : parabolic PDEs

- Given a source S(r,t) and a diffusion coefficient D(r), the diffusion equation is :

$$\frac{\partial n(\mathbf{r},t)}{\partial t} - \nabla \cdot (D(\mathbf{r})\nabla n(\mathbf{r},t)) = S(\mathbf{r},t)$$

- This determines the concentration “n” in a closed space
  - Now need both initial conditions (t=t0) AND boundary conditions (Dirichlet, Neumann, periodic)

Partial Differential Equations

- Why “parabolic” ?
- Consider one spatial dimension, and a constant D, with

$$n(x,t) \sim e^{-\omega t + ikx} \; ,$$

- The differential operator on the LHS has the eigenvalue

$$-\omega + Dk^2 = \text{constant}$$

- which is a parabola in omega-k space

Partial Differential Equations

- The time-dependent Schroedinger equation is also a parabolic PDE :

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t) = \mathcal{H}\Psi(\mathbf{r},t)$$

- This can be viewed as a diffusion equation with imaginary diffusion constant $D = i\hbar/(2m)$, or mathematically as a diffusion equation in imaginary time with real diffusion constant $D = \hbar/(2m)$

Partial Differential Equations

- Third case : hyperbolic PDE’s
- The wave equation is :

$$\frac{1}{c^2}\frac{\partial^2 u(\mathbf{r},t)}{\partial t^2} - \nabla^2 u(\mathbf{r},t) = R(\mathbf{r},t)$$

- this is hyperbolic because the eigenvalues of the differential operator are :

$$-\frac{1}{c^2}\omega^2 + \mathbf{k}^2 = \mathrm{constant}$$

- These are hyperboloid surfaces in omega-k space

- Again need initial conditions (t=t0) and boundary conditions (Dirichlet, Neumann, Periodic)

Elliptic PDES

Partial Differential Equations

- Let's first take a look at the solution to the elliptic equation for Poisson's equation (solving Gauss's law for electrostatics)

- We have Gauss's law : $\nabla \cdot \mathbf{E} = \frac{\rho(x,y,z)}{\epsilon_0}$,

- The static electric field can be written as :

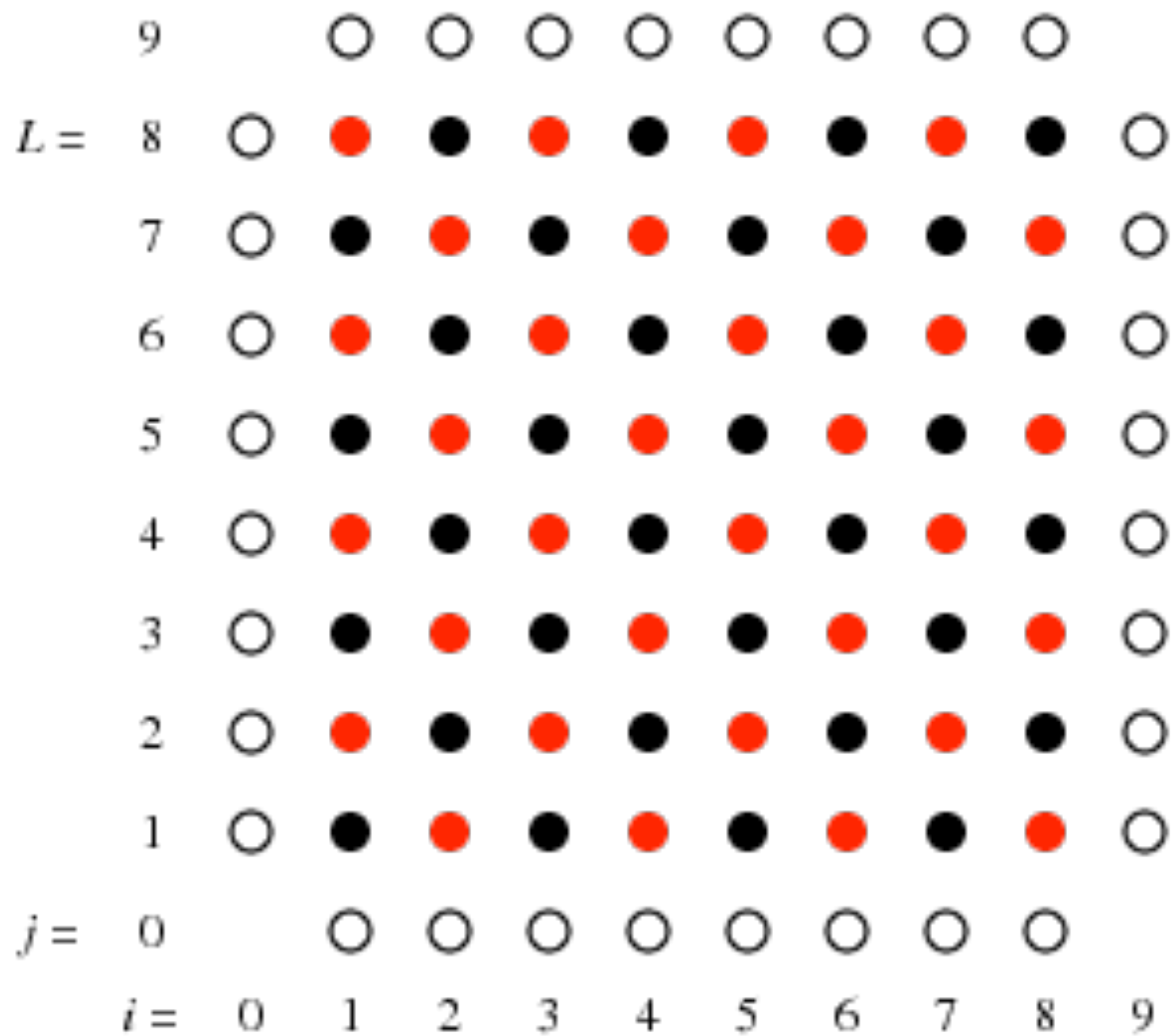
$$\mathbf{E} = -\nabla V \ ,$$

- And V(r) satisfies Poisson's equation:

$$\nabla^2 V = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) V = -\frac{\rho(x,y,x)}{\epsilon_0} \ .$$

Partial Differential Equations

- Now, we need to discretize the entire space
- Consider a 2-d space and discretize in 10x10 blocks:



Partial Differential Equations

- The 2-d Poisson's equation is :

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) V(x,y) = -\rho(x,y) \ ,$$

- Let's work in units with epsilon_0 = 1, and solve in the region of a square with length A=1.0
- The grid is :

$$x_i = ih \ , \quad i = 0, 1, \ldots L, L+1 \ , \qquad y_j = jh \ , \quad j = 0, 1, \ldots L, L+1 \ .$$

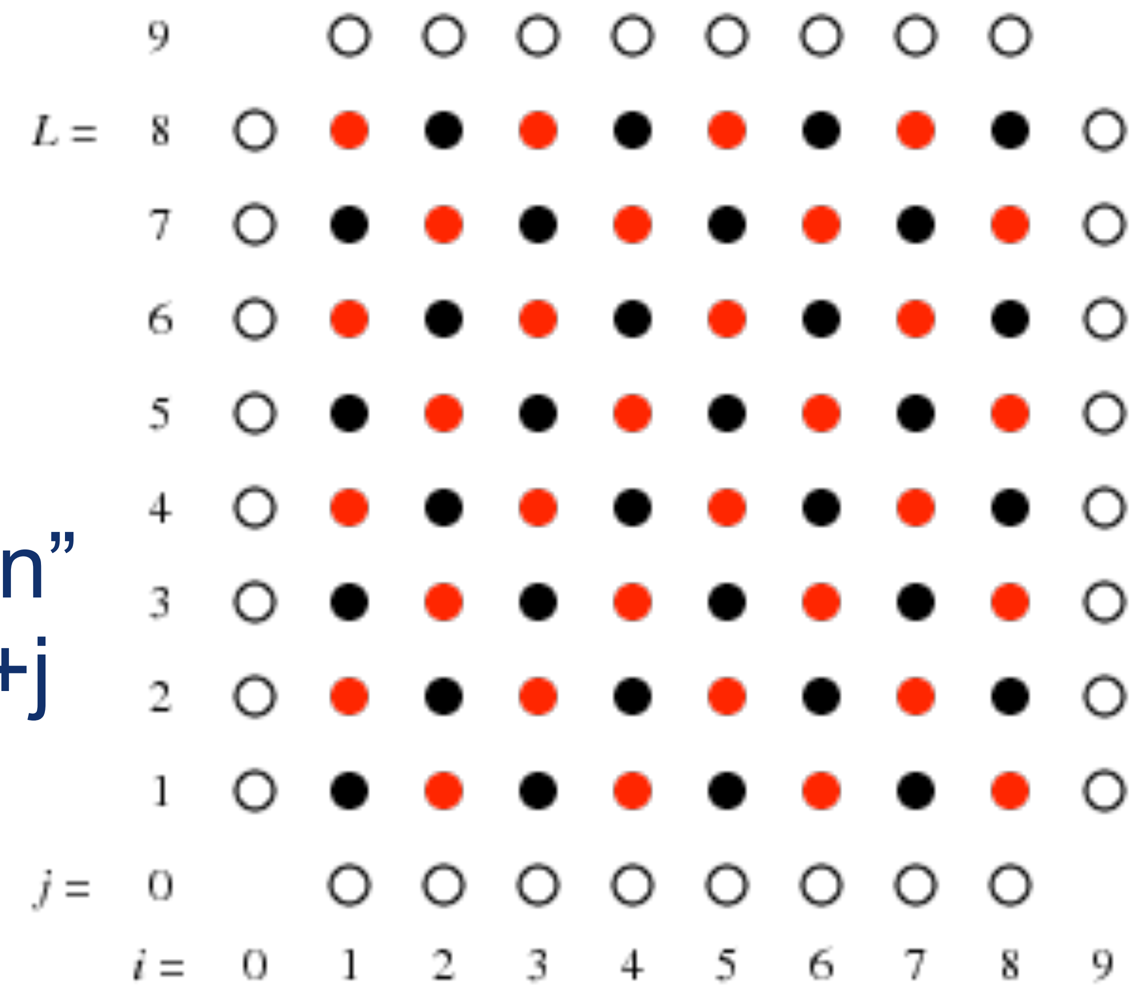
- The lattice spacing is h = 1/(L+1)
- Let $V(x_i, y_j) = V_{ij}, \ \ \rho(x_i, y_j) = \rho_{ij}$

- Now we need to discretize this

Partial Differential Equations

- The discretization is to look at an equivalent of Euler's formula, but now we have to do it in two dimensions:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) V(x_i, y_j) \simeq \frac{1}{h^2}\left[V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{i,j}\right]$$
$$= -\rho_{i,j} \ .$$



- Note the following :
  - The lattice is only connected to its four nearest neighbors
  - We will define "odd" and "even" sites depending on whether i+j is odd or even (red/black)
  - The boundaries are indicated with open circles

Partial Differential Equations

- First attempt : Jacobi's iterative method
- Suppose we have a solution of the discretized equation
- At each lattice site :

$$V_{i,j} = \frac{1}{4}\left[V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} + h^2 \rho_{i,j}\right] \ .$$

- If we knew the RHS, then we could compute the LHS
- But, the RHS pieces all have their own equations similar to this one!
- They all need to be solved simultaneously
- Instead of that, we try for a guess at each point, and then iteratively solve :

$$V_{i,j}^{n+1} = \frac{1}{4}\left[V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n} + h^2 \rho_{i,j}\right] \ , \quad n = 0, 1, 2, \ldots$$

Partial Differential Equations

- This should remind you a bit of the relaxation method for our ODE’s
  - We guess, then iterate until our boundary is solved and the equations are satisfied at the points
- But, all we know for sure are the boundary points
- Can instead iterate until our solution stops changing very much
- Usually “relaxes” to the right solution, but there are of course pathologies that can occur

Partial Differential Equations

- Next example : use the Gauss-Seidel method
- This is almost the same as the Jacobi method, but uses the updated neighbor sites
  - Remember the red/black? Red only talks to black, and vice versa
- Then we have :

$$V_{i,j}^{n+1} = \frac{1}{4}\left[V_{i+1,j}^{n} + V_{i-1,j}^{n+1} + V_{i,j+1}^{n} + V_{i,j-1}^{n+1} + h^2\rho_{i,j}\right]$$

- This converges faster than the Jacobi method

Partial Differential Equations

- Finally, consider the Successive Over-Relaxation (SOR) method

- Jacobi and Gauss-Seidel do not use V_ij at the same lattice point in updating V_ij
- If we use a linear combination of the old and new solutions, we can get better convergence :

$$V_{i,j}^{n+1} = (1-\omega)V_{i,j}^{n} + \frac{\omega}{4}\left[V_{i+1,j}^{n} + V_{i-1,j}^{n+1} + V_{i,j+1}^{n} + V_{i,j-1}^{n+1} + h^2\rho_{i,j}\right]$$

- Omega is called the “over-relaxation” parameter
  - Can be tuned for performance

Partial Differential Equations

- A few notes :
  - Converges only if 0 < omega < 2
  - Faster than Gauss-Seidel only if 1 < omega < 2
  - It converges fastest on a square lattice if

$$\omega \simeq \frac{2}{1+\frac{\pi}{L}} ,$$

    - Here, L is the number of lattice points

Partial Differential Equations

- For our strategy, we will use the red/black splitting to solve the equations faster :
  - First update the even sites, then update the odd sites
  - Can use the SOR method (or the others) with faster convergence in this case

- In Numerical Recipes 19.5, the iterations required to reduce the overall error by a factor of 10^{-p} for Laplace's equation is :

$$r \simeq \begin{cases} \frac{1}{2}pL^2 & \text{for Jacobi's method} \\ \frac{1}{4}pL^2 & \text{for the Gauss-Seidel method} \\ \frac{1}{3}pL & \text{for SOR with } \omega \simeq 2/(1+\pi/L) \end{cases} .$$

$$\begin{pmatrix} \frac{1}{2} \times 3 \times 50^2 = 3,750 \\ \frac{1}{4} \times 3 \times 50^2 = 1,875 \\ \frac{1}{3} \times 3 \times 50 = 50 \end{pmatrix}$$

Partial Differential Equations

- To solve for the convergence rates, let's look at the Poisson equation again:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -\frac{1}{\epsilon_0}\rho ,$$

- In matrix form, this is :

$$\mathbf{A}\mathbf{x} = \mathbf{b} ,$$

Discrete Poisson operator

Vij

Charge density

- Can break A into lower triangular, diagonal and upper triangular bits :

$$\mathbf{A} = \mathbf{L} + \mathbf{D} + \mathbf{U} ,$$

Partial Differential Equations

- Then, at each step, the Jacobi iteration is

$$\mathbf{D}\mathbf{x}^{(n)} = -(\mathbf{L} + \mathbf{U})\mathbf{x}^{(n-1)} + \mathbf{b} \; ,$$

$$\mathbf{x}^{(n)} = -\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})\mathbf{x}^{(n-1)} + \mathbf{D}^{-1}\mathbf{b} \; .$$

- The matrix :

$$-\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})$$

- This is the “iteration matrix”, and the magnitude of the largest eigenvalue is the “spectral radius” for the relaxation problem

Partial Differential Equations

- Spectral radius "ρ_s" should satisfy :
  - $0 < \rho_s < 1$ for the method to be stable
  - depends on the boundary conditions and the lattice spacing
  - approaches 1.0 as the number of lattice points increases

- For LxL square lattice with Dirichlet boundary conditions :

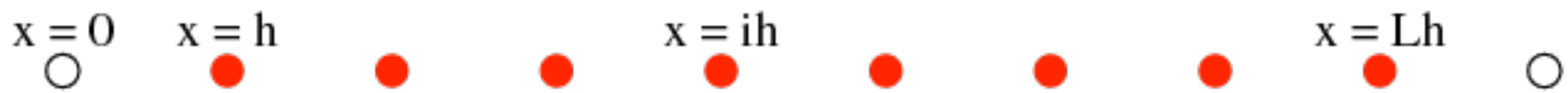
$$\rho_s \simeq 1 - \frac{\pi^2}{2L^2} \,.$$

Partial Differential Equations

- How to derive spectral radius ρ_s ?
- Let's just do it in 1-d
- The 1-d Laplace equation is :

$$\frac{d^2V}{dx^2} = 0\ .$$

- This can be discretized as :



$$\frac{V_{i+1} + V_{i-1} - 2V_i}{h^2} = 0\ .$$

- The Jacobi iteration is : $$V_i^{n+1} = \frac{1}{2}\left(V_{i+1}^n + V_{i-1}^n\right)\ .$$

- With Dirichlet BC's V(0)=V(L+1)=0, we see the eigenvectors are: $$u_i^{(k)} = \sin\left(\frac{\pi k i}{L+1}\right)\ , \qquad k = 1, 2, \ldots, L\ .$$

Partial Differential Equations

- Eigenvalues are determined by plugging in:

$$\frac{1}{2}\left(u_{i+1}^{(k)} + u_{i-1}^{(k)}\right) = \frac{1}{2}\left[\sin\left(\frac{\pi k(i+1)}{L+1}\right) + \sin\left(\frac{\pi k(i-1)}{L+1}\right)\right]$$

$$= \cos\left(\frac{\pi k}{L+1}\right) u_i^{(k)} \ .$$

- The spectral radius is given by the largest eigenvalue:

$$\rho_s = \cos\left(\frac{\pi}{L+1}\right) \simeq 1 - \frac{\pi^2}{2L^2} \ , \qquad \text{(for large L)}$$

- Similar analysis in 2-D gets the Numerical Recipes version for 2D

$$\rho_s = \frac{h_y^2 \cos\left(\frac{\pi}{L_x+1}\right) + h_x^2 \cos\left(\frac{\pi}{L_y+1}\right)}{h_x^2 + h_y^2}$$

Partial Differential Equations

- How many iterations does it take for the solution to be damped by a factor of 10^{-p}?
- Determined by the spectral radius!

$$10^{-p} = \rho_s^n \qquad \Rightarrow \qquad n = \frac{p \ln 10}{(-\ln \rho_s)} \simeq \frac{2pL^2 \ln 10}{\pi^2} \simeq \frac{1}{2} p L^2 \, .$$

- Jacobi method is not very efficient!
- If L = 1000, then n = 1M to improve to 1% of current value

Partial Differential Equations

- Gauss-Seidel does a little better

- Iteration matrix is

$$-(\mathbf{L}+\mathbf{D})^{-1}\mathbf{U} \, ,$$

- Then the spectral radius for the LxL Dirichlet lattice is :

$$\rho_s \simeq 1 - \frac{\pi^2}{L^2} \qquad \Rightarrow \qquad n \simeq \frac{1}{4} p L^2 \, .$$

- Only about twice as fast as Jacobi!

Partial Differential Equations

- What about SOR?

- Much better here, we have :

$$\rho_s \simeq 1 - \frac{2\pi}{L} \qquad \Rightarrow \qquad n \simeq \frac{1}{3} pL \; .$$

- So, if L=1000, need only n=667 iterations to improve to 1% of current value

Partial Differential Equations

- What about computational complexity?

- Jacobi and Gauss-Seidel update all interior lattice points per iteration
- So, for LxL 2-D lattice, we would have $\mathcal{O}(L^4)$

- For SOR, we would have $\mathcal{O}(L^3)$

- Neither of these are wonderful for very large L

Partial Differential Equations

- Can also use spectral analysis to solve our PDE's, just like you do in your math classes
- Here, "spectral analysis" is the FFT.
  - In 1D: $\frac{d^2V}{dx^2} = \rho(x)$.
- Then we express f and rho in terms of their Fourier transforms :

$$f(x) = \frac{1}{\sqrt{2\pi}} \int g(k) e^{ikx} dk \ , \qquad \rho(x) = \frac{1}{\sqrt{2\pi}} \int \sigma(k) e^{ikx} dk \ .$$

- This is diagonalized in k-space :

$$-k^2 g(k) = \sigma(k) \qquad \Rightarrow \qquad g(k) = -\frac{\sigma(k)}{k^2} \ .$$

- The solution is then the inverse FFT:

$$f(x) = -\frac{1}{\sqrt{2\pi}} \int \frac{\sigma(k)}{k^2} e^{ikx} dk \ .$$

- Two problems : 1. boundary conditions, 2. singularity at k=0

Partial Differential Equations

- Boundary conditions dictate the type of Fourier transform you want to use
  - Sometimes sine transforms are best, sometimes cosine, sometimes exponential
- Consider 1-D lattice 0 < x < L with N points

$$x_n = nL/N, n = 0, \ldots, N-1$$

- The complex FFT coefficients of f(x) are

$$g_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} W^{kn} f_n \,, \qquad W = e^{2i\pi/N} \,.$$

- The inverse will be periodic in xn with period L:

$$f_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} W^{-nk} g_k \,,$$

- So, if periodic conditions : use the complex FFT

Partial Differential Equations

- For Dirichlet conditions f(0) = f(L) = 0, then sine Fourier transform is best:

$$f_n = \sqrt{\frac{2}{N}} \sum_{k=1}^{N-1} \sin\left(\frac{\pi n k}{N}\right) g_k \,.$$

- For Neumann conditions use cosine Fourier transform:

$$f_n = \frac{1}{\sqrt{2N}} \left[g_0 + (-1)^n g_N\right] + \sqrt{\frac{2}{N}} \sum_{k=1}^{N-1} \cos\left(\frac{\pi n k}{N}\right) g_k \,.$$

- Note : These are not just the real and imaginary parts of the complex exponential transform!
  - Sine, Cosine, and exp(ikx) are all complete sets with different boundary conditions
  - Sine/Cosine are real, so also require 2x as many points

Partial Differential Equations

- Let's go back to Poisson's equation in 2d:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)V(x,y)$$
$$\simeq \frac{1}{h^2}\left[V_{j+1,k}+V_{j-1,k}+V_{j,k+1}+V_{j,k-1}-4V_{j,k}\right]$$
$$=-\rho_{j,k}$$

- Let's take an NxN grid in region 0 < x,y < 1
- Presume there is a point charge at the center
- Impose periodic BCs so we use the exponential FFT

- Since the FFT is linear, we can do it separately in the x and y directions, and it doesn't matter which order!

Partial Differential Equations

- The 2-D FFT coefficients are

$$\tilde{V}_{m,n} = \frac{1}{N}\sum_{j=0}^{N-1}\sum_{k=0}^{N-1} W^{mj+nk} V_{j,k} \,, \qquad \tilde{\rho}_{m,n} = \frac{1}{N}\sum_{j=0}^{N-1}\sum_{k=0}^{N-1} W^{mj+nk} \rho_{j,k} \,.$$

- The inverse transforms are :

$$V_{j,k} = \frac{1}{N}\sum_{m=0}^{N-1}\sum_{n=0}^{N-1} W^{-jm-kn} \tilde{V}_{m,n} \,, \qquad \rho_{j,k} = \frac{1}{N}\sum_{m=0}^{N-1}\sum_{n=0}^{N-1} W^{-jm-kn} \tilde{\rho}_{m,n} \,.$$

- So, if we plug these into our discretized equation and equating coefficients of W^{-mj-nk} we get :

$$\frac{1}{h^2}\left[W^m + W^{-m} + W^n + W^{-n} - 4\right]\tilde{V}_{m,n} = -\tilde{\rho}_{m,n} \,,$$

- IFFT gives the potential! $\tilde{V}_{m,n} = \dfrac{h^2\tilde{\rho}_{m,n}}{4 - W^m - W^{-m} - W^n - W^{-n}} \,.$

Partial Differential Equations

- In some sense, this is even easier than relaxation methods
- Take FFT of rows of rho
- Take FFT of columns of rho

$$\tilde{V}_{m,n} = \frac{h^2 \tilde{\rho}_{m,n}}{4 - W^m - W^{-m} - W^n - W^{-n}}$$

- Solve equation in Fourier domain

```
# Solve equation in Fourier space
V = cpt.Matrix(N, N)
W = cmath.exp(1.0j * 2 * math.pi / N)
Wm = Wn = 1.0 + 0.0j
for m in range(N):
    for n in range(N):
        denom = 4.0 - Wm - 1 / Wm - Wn - 1 / Wn
        if abs(denom) != 0.0:
            V[m][n] = rho[m][n] * h**2 / denom
        Wn *= W
    Wm *= W
```

- Take IFFT of rows of rho
- Take IFFT of columns of rho

Partial Differential Equations

- Since PDE's are done in higher dimensions, it is oftentimes beneficial to use "multigrid methods"
- General gist : start at a coarse scale, get close to the answer, then go to a finer scale
  - Similar to adaptive RK4 in philosophy
- For this, need an estimate of the error at each stage
- Described in Chapter 19 Section 6 of Numerical Recipes

Partial Differential Equations

- So let's again consider Poisson's equation in 2 D:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -f(x, y) ,$$

- Again let's impose this on a grid with units 0-1 and impose Dirichlet boundary conditions

- As before, the solution obeys :

$$u_{i,j} = \frac{1}{4} \left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} + h^2 f_{i,j} \right] .$$

Partial Differential Equations

- Then here is where things get different
- This uses a succession of ℓ lattices / grids
- This is the "multigrid"!

- Here's the trick : define the interior lattice points as a power of 2 so that :

$$L = 2^\ell + 2$$

- Thus the lattice spacing is

$$h = 1/(L-1)$$

- There are then sequentially coarser lattices with number of interior points as :

$$2^{\ell-1} \to 2^{\ell-2} \to \ldots \to 2^0 = 1$$

Partial Differential Equations

- Now to compute the error, we define the solution at any stage in the calculation as $u(x, y)$
- Also define the exact solution $u_{\text{exact}}(x, y)$
- The correction is

$$v = u_{\text{exact}} - u$$

- The "residual" or "defect" is defined as

$$r = \nabla^2 u + f \ .$$

- The correction and the residual are related by :

$$\nabla^2 v = \left[\nabla^2 u_{\text{exact}} + f\right] - \left[\nabla^2 u + f\right] = -r \ .$$

- So interestingly, this has the same form as Poisson's equation with v as the function u, and r being a known source function!

Partial Differential Equations

- Now define the "Simple V-Cycle Algorithm"
- Define two grids (coarse and fine) with points:

$$L = 2^{\ell} + 2 \qquad L = 2^{\ell-1} + 2$$

- Need to move from one grid to another
- Given any function on the lattice, we need to :
  - –restrict the function from fine to coarse
  - –interpolate the function from coarse to fine

Partial Differential Equations

- If we have those, the multigrid V-cycle can be defined recursively :
  - $\ell = 0$, there is only one interior point, so solve exactly:

$$u_{1,1} = (u_{0,1} + u_{2,1} + u_{1,0} + u_{1,2} + h^2 f_{1,1})/4 .$$

  - Otherwise, calculate current $L = 2^\ell + 2$
  - Perform pre-smoothing iterations with a local algorithm (Gauss-Seidel, etc). This will damp out the short wavelength errors in the solution
  - Estimate correction $v = u_{\text{exact}} - u$ as :
    - Compute residual

$$r_{i,j} = \frac{1}{h^2}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}\right] + f_{i,j} .$$

    - Restrict residual r-> R to the coarser grid
    - Set the coarser grid correction V = 0 and improve it recursively
    - Prolongate the correction V-> v onto the finer grid
  - Correct u -> u + v
  - Perform post-smoothing Gauss-Seidel iterations and return improved u

Partial Differential Equations

- Is this worth it? What's the scaling with L?

- Recall that Jacobi / Gauss-Seidel iterations are the most time-consuming parts of the calculation.
  - Single step: $\mathcal{O}(L^2)$

- Now this gets performed on the sequence of grids with :

$$2^{\ell} \to 2^{\ell-1} \to 2^{\ell-2} \to \ldots \to 2^0 = 1$$

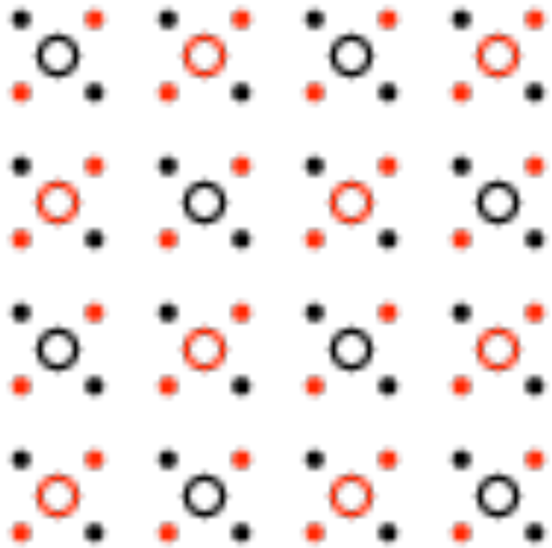
- So the total number is of order:

$$L^2 \sum_{n=0}^{\ell} \frac{1}{2^{2n}} \leq L^2 \frac{1}{1-\frac{1}{4}} \; .$$

- So in this, the TOTAL is $\mathcal{O}(L^2)$!!!!

Partial Differential Equations

- Details of restricting residual to coarser lattice:
- Define the coarser lattice H = 2h
- Set the value to the average of the values on the four corners:



$$R_{I,J} = \frac{1}{4}\left[r_{i,j} + r_{i+1,j} + r_{i,j+1} + r_{i+1,j+1}\right] \ , \ i = 2I - 1 \ , \ j = 2J - 1 \ .$$

Partial Differential Equations

- Details to prolong the correction to the finer lattice :
- Need to solve the equation

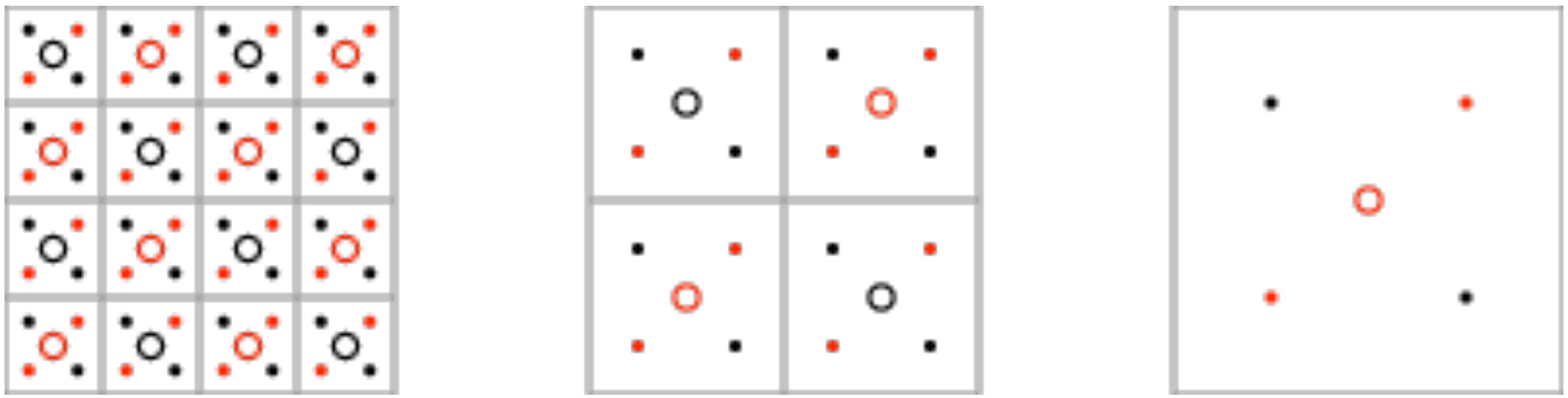
$$\nabla^2 V = -R(x, y) \ ,$$

- In the code this will be called “twoGrid”
- Then we copy the value of V(I,J) into the four neighboring points on the finer lattice v(i,j) :

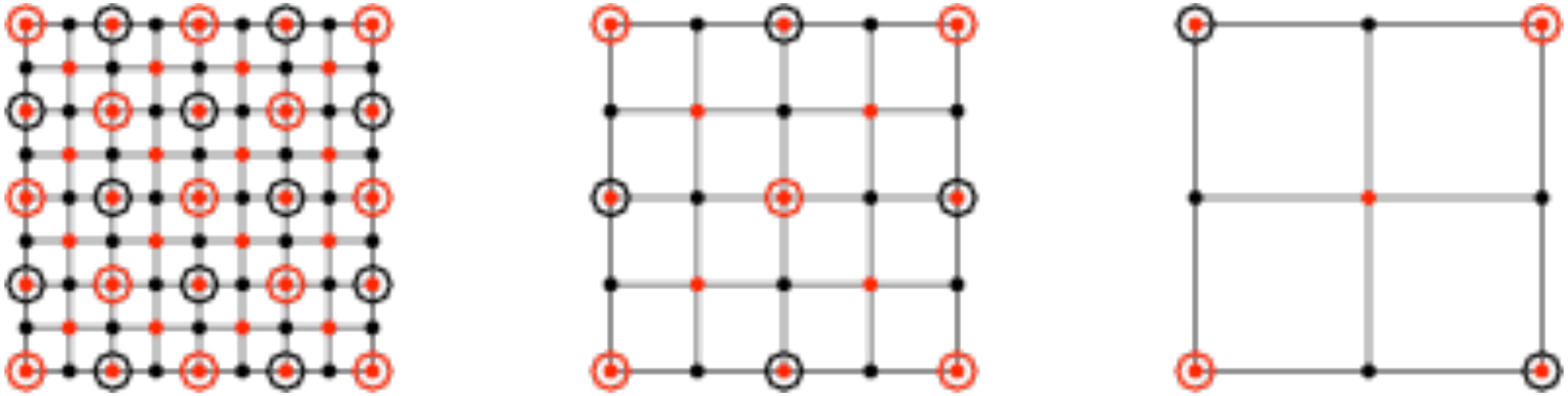
$$v_{i,j} = v_{i+1,j} = v_{i,j+1} = v_{i+1,j+1} = V_{I,J} \ , \quad i = 2I - 1 \ , \ j = 2J - 1 \ .$$

Partial Differential Equations

- Two possibilities :
  - Cell centered : $2^3 = 8 \rightarrow 2^2 = 4 \rightarrow 2^1 = 2 \rightarrow 2^0 = 1$.



  - Grid centered : $2^3 + 1 = 9 \rightarrow 2^2 + 1 = 5 \rightarrow 2^1 + 1 = 3$.



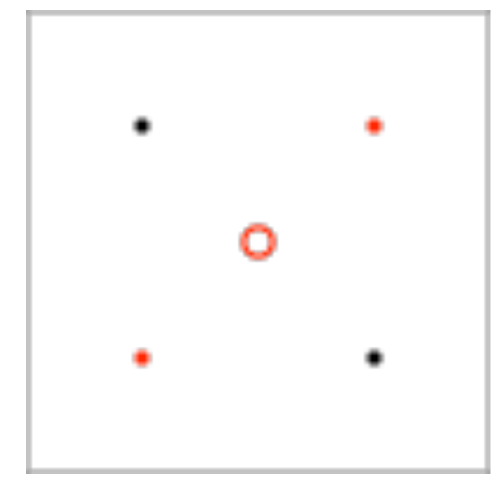
- Note : grid-centered needs to one more poit in each dimension

Partial Differential Equations

- The boundary points are specified as follows :
  - Cell-centered : Boundary points move in space toward the center of the region at each coarsening (so care must be taken here)
  - Vertex-centered : Boundary points do not move when lattice is coarsened
- A little more convenient to use vertex-centered

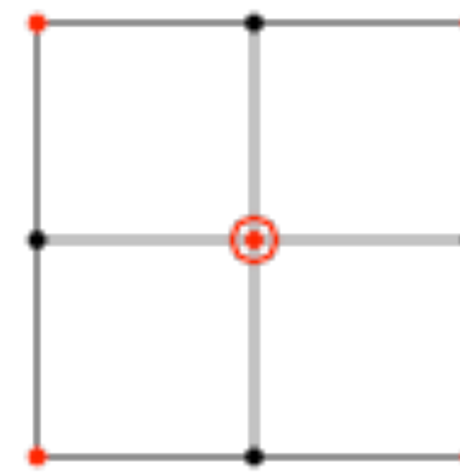
Partial Differential Equations

- What about restriction (fine->coarse) and prolongation (coarse->fine) operations?
- Cell-centered :
  - Prolongation : Set the values on the fine to the value from the coarse
  - Restriction : Average fine points to get coarse points



- Vertex-centered :
  - Prolongation : use bilinear interpolation at which value at F at a coarse grid point is copied to 9 neighboring fine-grid points with weights :

$$\begin{bmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & 1 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{bmatrix}.$$



  - Restriction : Adjoint of the prolongation

$$\begin{bmatrix} \frac{1}{16} & \frac{1}{8} & \frac{1}{16} \\ \frac{1}{8} & \frac{1}{4} & \frac{1}{8} \\ \frac{1}{16} & \frac{1}{8} & \frac{1}{16} \end{bmatrix}.$$

Partial Differential Equations

- Improvements are to use more than one cycle
  - Repeat the two-grid iteration more than once
  - Full multigrid starts with coarses grid, then proceeds to finer grids
  - Numerical Recipes Chapter 19 Section 6 goes over this
  - Can look into them at your leisure

Parabolic PDES

Partial Differential Equations

- Let's now turn to parabolic differential equations
  - Includes diffusion and time-dependent Schroedinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi \ .$$

  - Formal solution is:

$$\psi(x,t) = e^{-\frac{i}{\hbar}\mathcal{H}t}\psi(x,0) \ , \qquad \mathcal{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) = \mathcal{H}^\dagger \ ,$$

  - where H is the hermitian Hamiltonian operator

Partial Differential Equations

- Two separate strategies:
  - "Marching" in time
    - Similar to ODE technology, but now must account for derivatives in spatial dimension too!
  - Spectral analysis
    - Just like in your classes, we can also solve the PDE in the Fourier domain, and it is often more convenient

Will examine both solutions

Partial Differential Equations

- First: Marching

Partial Differential Equations

- The time-evolution is unitary, so the total probability is conserved :

$$\left(e^{-\frac{i}{\hbar}\mathcal{H}t}\right)^\dagger = \left(e^{-\frac{i}{\hbar}\mathcal{H}t}\right)^{-1} , \qquad \int |\psi(x,t)|^2 dx = \int |\psi(x,0)|^2 dx .$$

- Diffusion equations, on the other hand, are NOT unitary

$$\frac{\partial}{\partial t} n(x,t) = D \frac{\partial^2}{\partial x^2} n(x,t) + C n(x,t) .$$

- This leads to the characteristic damping
- Schroedinger's equation is mathematically equivalent to diffusion with an imaginary diffusion constant (or a real one, in imaginary time):

$$\frac{\partial \psi}{\partial (it)} = \frac{\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{1}{\hbar} V(x) \psi .$$

Partial Differential Equations

- We will look at a free particle as an instructive case:

$$\psi(x,t) \sim e^{i(px-Et)/\hbar}$$

- where the momentum is $p = \pm\sqrt{2mE}$
- Of course, the plane wave is not localized in space
  - Probability is not =1 over all space, so not a “real” particle solution
- Can instead construct a Gaussian state:

$$\phi(x) = \left(\frac{1}{\pi\sigma^2}\right)^{\frac{1}{4}} e^{-(x-x_0)^2/(2\sigma^2)}$$

  - But, this is stationary :

$$\langle p \rangle = \int_{-\infty}^{\infty} dx\, \phi^*(x) \left(\frac{\hbar}{i}\frac{d}{dx}\right) \phi(x) = 0\ .$$

Partial Differential Equations

- To get this to move, multiply by a phase factor:

$$\psi(x) = \phi(x)e^{ikx}$$

- then we have:

$$\begin{aligned}\langle\psi|p|\psi\rangle &= \int_{-\infty}^{\infty} dx\ \phi^*(x)e^{-ikx}\left(\frac{\hbar}{i}\frac{d}{dx}\right)e^{ikx}\phi(x)\\ &= \int_{-\infty}^{\infty} dx\ [\hbar k|\phi(x)|^2 - i\hbar\phi(x)\phi'(x)]\\ &= \hbar k\ .\end{aligned}$$

- Expectation value of the energy is:

$$\left\langle\psi\left|\frac{p^2}{2m}\right|\psi\right\rangle = \frac{\hbar^2}{2m}\left(k^2 + \frac{1}{2\sigma^2}\right)\ ,$$

- This is close to the classical result if the packet isn't too narrow

Partial Differential Equations

- Our wavepacket is :

$$\psi(x,0) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^{\frac{1}{4}} e^{ik_0 x - \frac{(x-x_0)^2}{4\sigma^2}}$$

- Moves to the right with speed hbar k0 / m
- Psi is approximated on a lattice by an N-component complex vector
- If potential is a function of space alone, can precompute the quantity

$$e^{-i\mathcal{V}(\S)\delta_t/(2\hbar)}$$

- which can be used to speed up computational times

Partial Differential Equations

- Also examine finite difference methods
- Start with a forward time-centered scheme (FTCS) :
  - Discretized equation :

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\delta_t} = -\frac{\hbar^2}{2m} \frac{\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n}{\delta_x^2} + V_j \psi_j^n \ ,$$

  - This can be solved explicitly for the solution at the next time step :

$$\psi_j^{n+1} = \psi_j^n - \frac{i\delta_t}{\hbar} \left[-\frac{\hbar^2}{2m} \frac{\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n}{\delta_x^2} + V_j \psi_j^n \right] \ .$$

  - If we introduce the column vector of values : $\Psi^n \equiv \begin{pmatrix} \psi_1^n \\ \psi_2^n \\ . \\ . \\ \psi_N^n \end{pmatrix} ,$
  - Then the equation is (in matrix form): $$\Psi^{n+1} = \left(\mathbf{I} - \frac{i\delta_t}{\hbar} \mathbf{H} \right) \Psi^n \ .$$

Partial Differential Equations

- Problem with this simplest scheme : always unstable
- For instance, for an eigenvector we have:

$$\mathbf{H}\Psi^1 = E\Psi^1 \ ,$$

- Then we'd compute:

$$\Psi^{n+1} = \left(1 - \frac{i\delta_t E}{\hbar}\right)\Psi^n = \left(1 - \frac{i\delta_t E}{\hbar}\right)^2 \Psi^{n-1} = \ldots = \left(1 - \frac{i\delta_t E}{\hbar}\right)^n \Psi^1 \ ,$$

- The magnitude of this is :

$$\left|\Psi^{n+1}\right| = \left(\sqrt{1 + \frac{\delta_t^2 E^2}{\hbar^2}}\right)^n \left|\Psi^1\right| \longrightarrow \infty \ , \qquad \text{as} \quad n \to \infty \ .$$

- Boooooo.

Partial Differential Equations

- What about backward time space centered (BTCS) implicit differencing?

$$i\hbar\frac{\psi_j^{n+1}-\psi_j^n}{\delta_t}=-\frac{\hbar^2}{2m}\frac{\psi_{j+1}^{n+1}+\psi_{j-1}^{n+1}-2\psi_j^{n+1}}{\delta_x^2}+V_j\psi_j^{n+1}\ ,$$

- Can't be solved exactly.
- Three unknown quantities on the LHS of

$$\psi_j^{n+1}+\frac{i\delta_t}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\psi_{j+1}^{n+1}+\psi_{j-1}^{n+1}-2\psi_j^{n+1}}{\delta_x^2}+V_j\psi_j^{n+1}\right]=\psi_j^n\ .$$

- If we solve all N equations at the same time, we get a matrix form: $\left(\mathbf{I}+\frac{i\delta_t}{\hbar}\mathbf{H}\right)\Psi^{n+1}=\Psi^n\ ,$
- with steps : $\Psi^{n+1}=\left(\mathbf{I}+\frac{i\delta_t}{\hbar}\mathbf{H}\right)^{-1}\Psi^n\ .$

Partial Differential Equations

- This one, on the other hand, is “stable”, but still wrong:

$$\Psi^{n+1} = \left(1 + \frac{i\delta_t E}{\hbar}\right)^{-1} \Psi^n = \left(1 + \frac{i\delta_t E}{\hbar}\right)^{-2} \Psi^{n-1}$$

$$= \ldots = \left(1 + \frac{i\delta_t E}{\hbar}\right)^{-n} \Psi^1 \,,$$

- Magnitude will be :

$$\left|\Psi^{n+1}\right| = \left(\sqrt{1 + \frac{\delta_t^2 E^2}{\hbar^2}}\right)^{-n} \left|\Psi^1\right| \longrightarrow 0 \,, \qquad \text{as} \quad n \to \infty \,.$$

- No probability conservation, still booooo.

Partial Differential Equations

- Symmetric time space centered (STCS) differencing does the trick (Crank-Nicolson):

$$\Psi^{n+1} = \Psi^n - \frac{i\delta_t}{2\hbar}\mathbf{H}\left(\Psi^n + \Psi^{n+1}\right) \ ,$$

- Matrix solution : $$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\delta_t}{2\hbar}\mathbf{H}\right)^{-1}\left(\mathbf{I} - \frac{i\delta_t}{2\hbar}\mathbf{H}\right)\Psi^n \ .$$
  - This is unitary : $$\Psi^{n+1} = \left[\frac{1 - \frac{i\delta_t E}{2\hbar}}{1 + \frac{i\delta_t E}{2\hbar}}\right]^n \Psi^1 \ ,$$
  - And conserves probability at each step : $$\left|\Psi^{n+1}\right| = \left|\Psi^1\right| \ .$$

Partial Differential Equations

- As you'd naively guess, this is also more accurate than the forward and backward only versions (by an order of magnitude)

- To show explicitly, write the exact evolution operator for one time step:

$$e^{-\frac{i}{\hbar}\mathcal{H}\delta_t} \equiv e^{-z} = 1 - z + \frac{z^2}{2} - \frac{z^3}{6} + \ldots,$$

- Here, we have $z = \mathcal{O}(\delta_t)$

- Backward scheme : $\frac{1}{1+z} = 1 - z + z^2 - z^3 + \ldots = e^{-z} + \mathcal{O}(\delta_t^2)$,

- Crank-Nicolson scheme:

$$\frac{1}{1+\frac{z}{2}}\left(1 - \frac{z}{2}\right) = \left(1 - \frac{z}{2} + \frac{z^2}{4} - \frac{z^3}{8} + \ldots\right)\left(1 - \frac{z}{2}\right)$$

$$= 1 - z + \frac{z^2}{2} - \frac{z^3}{4} + \ldots = e^{-z} + \mathcal{O}(\delta_t^3) .$$

Partial Differential Equations

- We have the Schroedinger equation :

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi\ .$$

- Solved using Crank-Nicolson algorithm :

$$\Psi^{n+1} = \left(\mathbf{I} + \frac{i\delta_t}{2\hbar}\mathbf{H}\right)^{-1}\left(\mathbf{I} - \frac{i\delta_t}{2\hbar}\mathbf{H}\right)\Psi^n\ .$$

- And this is basically a matrix inversion problem!
- Is it tractable?
  - Incidentally, yes! It's a sparse matrix!

Partial Differential Equations

- For instance, impose Dirichlet BC's , and we get :

$$\left(\frac{\partial^2\psi}{\partial x^2}\right)_j^n = \frac{1}{\delta_x^2}\begin{cases} \psi_2^n - 2\psi_1^n \ , & \text{for } j = 1 \\ \psi_{j-1}^n + \psi_{j+1}^n - 2\psi_j^n \ , & \text{for } 1 < j < N \\ \psi_{N-1}^n - 2\psi_N^n \ , & \text{for } j = N \end{cases} .$$

- if N=5 then we get :

$$\mathbf{H}_{\text{Dirichlet}} = -\frac{\hbar^2}{2m\delta_x^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix}$$

$$+ \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 & 0 \\ 0 & 0 & V_3 & 0 & 0 \\ 0 & 0 & 0 & V_4 & 0 \\ 0 & 0 & 0 & 0 & V_5 \end{pmatrix} .$$

Partial Differential Equations

- Imposing periodic BC's we get:

$$\left(\frac{\partial^2 \psi}{\partial x^2}\right)_j^n = \frac{1}{\delta_x^2}\begin{cases} \psi_N^n + \psi_2^n - 2\psi_1^n\,, & \text{for } j = 1 \\ \psi_{j-1}^n + \psi_{j+1}^n - 2\psi_j^n\,, & \text{for } 1 < j < N \\ \psi_{N-1}^n + \psi_1^n - 2\psi_N^n\,, & \text{for } j = N \end{cases} .$$

- if N=5 then we get :

$$\mathbf{H}_{\text{Periodic}} = -\frac{\hbar^2}{2m\delta_x^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 1 & -2 \end{pmatrix}$$

$$+\begin{pmatrix} V_1 & 0 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 & 0 \\ 0 & 0 & V_3 & 0 & 0 \\ 0 & 0 & 0 & V_4 & 0 \\ 0 & 0 & 0 & 0 & V_5 \end{pmatrix} .$$

Partial Differential Equations

- So both of these are tridiagonal, so we can use our Matrix Methods from earlier in the semester to solve this very quickly

- Explicitly :
  - Note that $$\left(\mathbf{I} + \frac{i\delta_t}{2\hbar}\mathbf{H}\right)^{-1}\left(\mathbf{I} - \frac{i\delta_t}{2\hbar}\mathbf{H}\right) = \mathbf{Q}^{-1} - \mathbf{I}\,,$$
  - where : $$\mathbf{Q} = \frac{1}{2}\left(\mathbf{I} + \frac{i\delta_t}{2\hbar}\mathbf{H}\right)$$
  - So, we solve the linear equation: $$\mathbf{Q}\chi = \Psi^n\,, \qquad \chi = \mathbf{Q}^{-1}\Psi^n\,,$$
  - We get an intermediate “chi”, which we can use to solve: $$\Psi^{n+1} = \chi - \Psi^n\,.$$

Partial Differential Equations

- Second : spectral analysis

Partial Differential Equations

- To solve this ‘exactly’, can look at the exact solution in the Fourier domain (and keep in mind that we’re going to do the FFT later)
- Write the S.E. as

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial^2 x^2} + V(x)\psi(x,t) \equiv (\mathcal{T}+\mathcal{V})\psi(x,t) \ ,$$

- Here, T is a differential operator and V is a multiplicative operator in position space
- In Fourier domain :

$$\tilde{\psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\ e^{-ipx/\hbar}\psi(x,t) \ ,$$

- then we’d have:

$$i\hbar\frac{\partial\tilde{\psi}(p,t)}{\partial t} = \frac{p^2}{2m}\tilde{\psi}(p,t) + \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dq\ \tilde{V}(p-q)\tilde{\psi}(q,t) \ .$$

Partial Differential Equations

- Here, the kinetic operator T is multiplicative, while the potential operator V is a convolution
  - So, this is an integral equation in the Fourier domain
- Formal solution :

$$\psi(x,t) = e^{-i(\mathcal{T}+\mathcal{V})(t-t_0)/\hbar}\psi(x,t_0) \ ,$$

- Where :

$$e^{\mathcal{A}} \equiv 1 + \mathcal{A} + \frac{1}{2!}\mathcal{A}\mathcal{A} + \frac{1}{3!}\mathcal{A}\mathcal{A}\mathcal{A} + \cdots$$

- T and V do not commute here, so exponential is not amenable to numerical evaluation

Partial Differential Equations

- To make the discrete time approximation, we use a small time step delta t :

$$\psi(t+\delta_t) = e^{-i(\mathcal{T}+\mathcal{V})\delta_t/\hbar}\psi(x,t)$$

- In this case, T and V can be disentangled (linear approximation ===> they commute)

- Can use Baker-Campell-Hausdorff formula :
  - http://en.wikipedia.org/wiki/Baker-Campbell-Hausdorff_formula
  - This states that : $e^{\mathcal{A}}e^{\mathcal{B}} = e^{\mathcal{C}}$
  - if and only if : $\mathcal{C} = \mathcal{A} + \mathcal{B} + \frac{1}{2}[\mathcal{A},\mathcal{B}] + \cdots$

Partial Differential Equations

- Commutator is :

$$[\mathcal{T},\mathcal{V}] = -\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2}, V(x)\right] = -\frac{\hbar^2}{2m}V''(x) - \frac{\hbar^2}{m}V'(x)\frac{d}{dx} \neq 0\ .$$

- So, the simplest factorization has an error of $\mathcal{O}(\delta_t^2)$:

$$e^{-i(\mathcal{T}+\mathcal{V})\delta_t/\hbar} \approx e^{-i\mathcal{T}\delta_t/\hbar}e^{-i\mathcal{V}\delta_t/\hbar}\ ,$$

- The symmetric factorization, however, has an error $\mathcal{O}(\delta_t^3)$:

$$e^{-i(\mathcal{T}+\mathcal{V})\delta_t/\hbar} \approx e^{-i\mathcal{V}\delta_t/(2\hbar)}e^{-i\mathcal{T}\delta_t/\hbar}e^{-i\mathcal{V}\delta_t/(2\hbar)}$$

  – In addition, this is unitary so preserves the normalization of the wavefunction

Partial Differential Equations

- Split the time evolution operator into a symmetric factorization
- Evolve by :
  - Multiply by first half-step : $\psi(x,t) \to \psi_1(x) = e^{-iV(x)\delta_t/(2\hbar)}\psi(x,t)$. (diagonal in position space)
  - Fourier transform to p-space : $\tilde{\psi}_1(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar}\psi_1(x)$.
  - Multiply by kinetic evolution (diagonal in momentum space) $\tilde{\psi}_1(p) \to \tilde{\psi}_2(p) = e^{-ip^2\delta_t/(2m\hbar)}\tilde{\psi}_1(p)$.
  - Fourier transform back to x-space : $\psi_2(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{ipx/\hbar}\tilde{\psi}_2(p)$.
  - Multiply by the second half step evolution operator (diagonal in position space) $\psi(x,t+\delta_t) = e^{-iV(x)\delta_t/(2\hbar)}\psi_2(x)$.

Hyperbolic PDES

Partial differential equations

- We now turn to the final chapter in our investigation of PDE's : hyperbolic waves

- This class covers a wide range of physical phenomena :
  - Light waves
  - Sound waves
  - Water waves
  - etc
- The wave equation is

Source term

$$\frac{1}{c^2}\frac{\partial^2 u(\mathbf{r},t)}{\partial t^2} - \nabla^2 u(\mathbf{r},t) = R(\mathbf{r},t) \ ,$$

Wave speed

Hyperbolic (+dt^2 - dx^2)

Partial differential equations

- There is a unique solution if
  - the initial values of $u(\mathbf{r}, t_0)$ and $\partial u(\mathbf{r}, t)/\partial t|_{t=t_0}$ are specified
  - the boundary values are specified on a closed region

- So examine the 1-d equation with no source term:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} ,$$

- This factorizes into simpler first-order equations:

$$\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} = \left(\frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial t} - c \frac{\partial}{\partial x} \right) .$$

Partial differential equations

- Solutions to this equation are given by a superposition of left- and right-moving waves:

$$u(x,t) = g(x+ct) + f(x-ct) \; ,$$

$$\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right) g(x+ct) = 0 \; , \quad \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right) f(x-ct) = 0 \; ,$$

- Here, g and f are determined from initial conditions

Partial differential equations

- Examine one of the equations ("right-moving" one):

$$\frac{\partial u(x,t)}{\partial t} = -c\frac{\partial u(x,t)}{\partial x} \ ,$$

- The analytical solution here is :

$$u(x,t) = f_0(x - ct) \ ,$$

- where f0(x) is the initial condition at t=0
- This basically means the initial shape simply propagates with a velocity c
  - This is called "advection"
- Contrast with cases where the wave shape depends on position
  - This is "convection" (hot fluid rising, colder fluid sinking, for instance)

Partial differential equations

- In the advective case, the flux is conserved:

$$\frac{\partial \vec{u}}{\partial t} = -\frac{\partial \vec{F}(\vec{u})}{\partial x} \ ,$$

- Here, u(x,t) is a vector of functions, and the vector F is the conserved flux of u
- Now, suppose that u(x,t) is the density at point x and time t
- Total amount (mass) of fluid in a boundary is:

$$M(t) = \int_{x_L}^{x_R} u(x,t)\, dx \ .$$

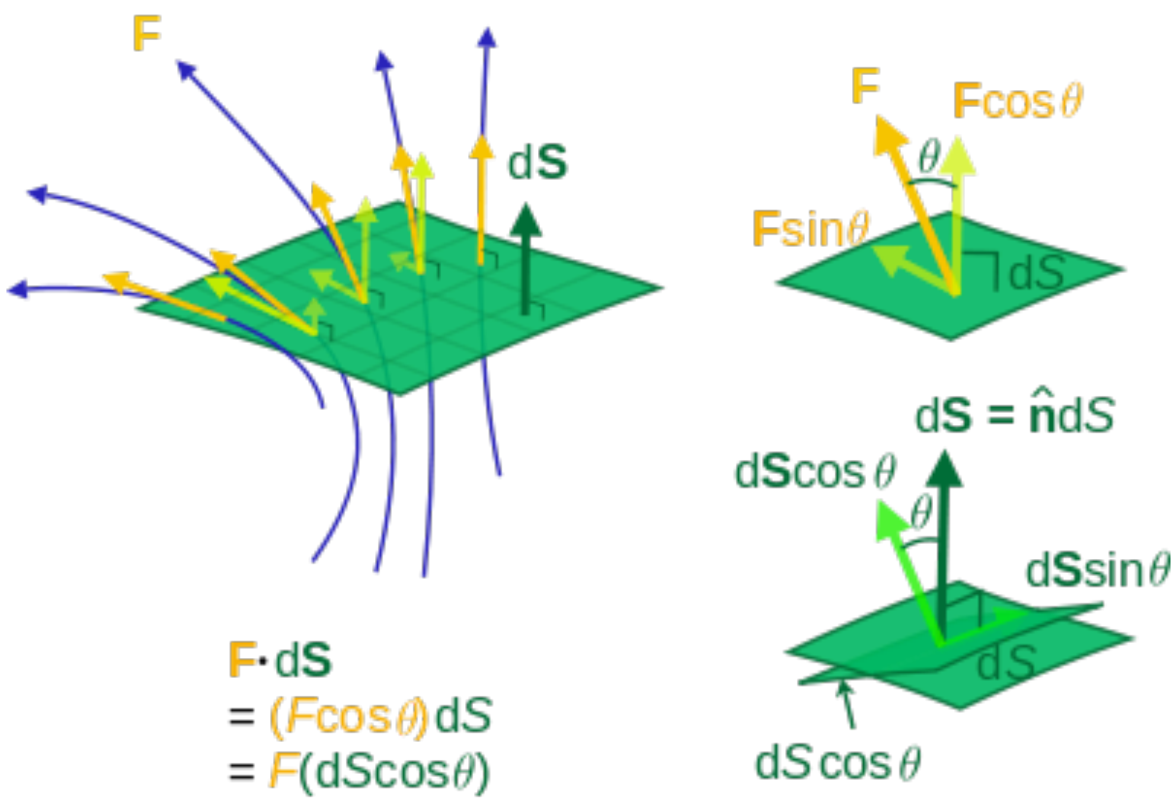
- The rate of change of fluid in the region is:

$$\frac{d}{dt} M(t) = \frac{d}{dt} \int_{x_L}^{x_R} u(x,t)\, dx = \int_{x_L}^{x_R} \frac{\partial u(x,t)}{\partial t}\, dx$$

$$= -\int_{x_L}^{x_R} \frac{\partial F(u(x,t))}{\partial x}\, dx = F(u(x_L,t)) - F(u(x_R,t)) \ ,$$

Partial differential equations

- This should remind you of your vector calculus (Stoke’s theorem, etc)
  - http://en.wikipedia.org/wiki/Flux
  - http://en.wikipedia.org/wiki/Stokes'_theorem



Partial differential equations

- In 1-d, should be clear how we may discretize this
- Again can try the forward time-centered solution as we did last lecture (generalized Euler's method!)

$$u_j^{n+1} = u_j^n - \frac{c\delta_t}{2\delta_x}\left(u_{j+1}^n - u_{j-1}^n\right) .$$

- So we try the FTCS :

$$u_j^{n+1} = u_j^n - \frac{c\delta_t}{2\delta_x}\left(u_{j+1}^n - u_{j-1}^n\right) .$$

- The spatial derivative was approximated by a symmetric difference : $\frac{\partial u(x,t)}{\partial x} \simeq \frac{u_{j+1}^n - u_{j-1}^n}{2\delta_x} .$
- As we saw last class, the "bare bones" Euler-step-like solution is unconditionally unstable

$$e^{ikj\delta_x} - \frac{c\delta_t}{2\delta_x}\left(e^{ik(j+1)\delta_x} - e^{ik(j-1)\delta_x}\right)$$

- If $u_j^n \sim e^{ikj\delta_x}$: modes amplified by: $= \left(1 - i\frac{c\delta_t}{\delta_x}\sin(k\delta_x)\right) e^{ikj\delta_x} \equiv \xi e^{ikj\delta_x} .$

Partial differential equations

- Instead, try the "Lax" method:

$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{c\delta_t}{2\delta_x}\left(u_{j+1}^n - u_{j-1}^n\right) .$$

- The mode amplification factor in this case is:

$$\xi = \frac{1}{2}\left(e^{ik\delta_x} + e^{-ik\delta_x}\right) - \frac{c\delta_t}{2\delta_x}\left(e^{ik\delta_x} - e^{-ik\delta_x}\right) ,$$

$$|\xi|^2 = \cos^2(k\delta_x) + \left(\frac{c\delta_t}{\delta_x}\right)^2 \sin^2(k\delta_x) .$$

- If we choose $\delta_t = \delta_x / c$ then flux is exactly conserved

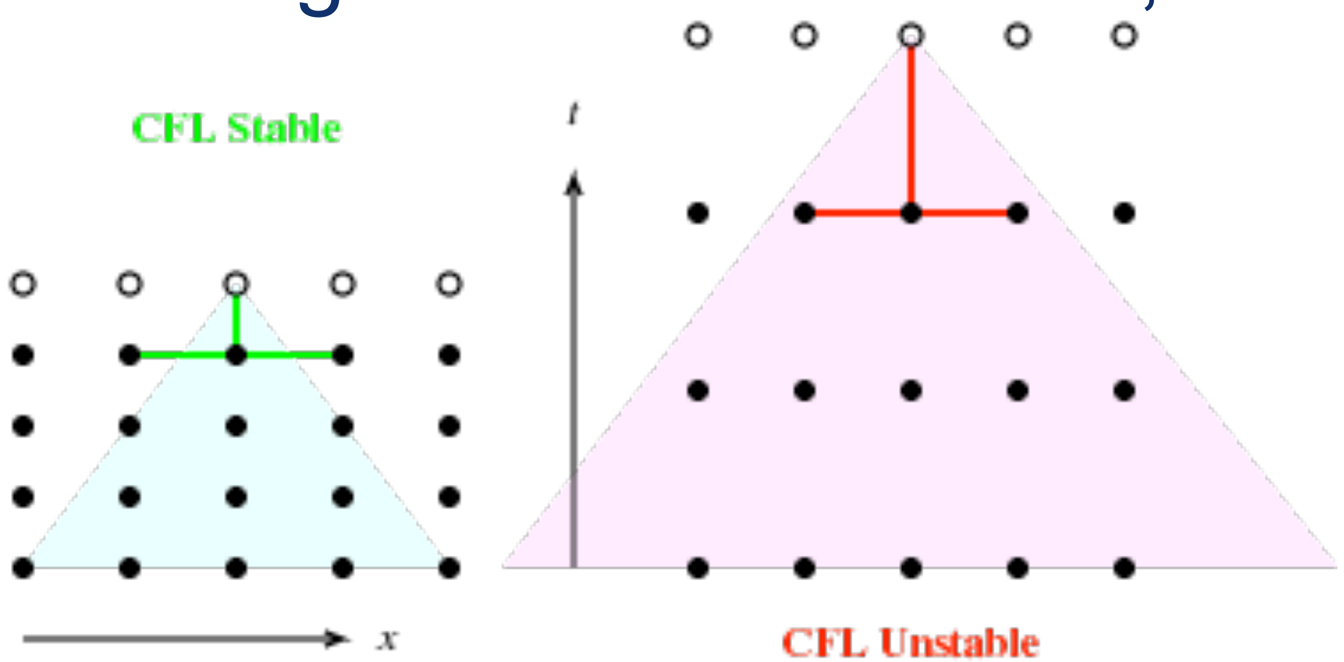
- Any other choice of delta t will make this either decay or grow without bound

Partial differential equations

- This is the Courant-Freidrichs-Lewy condition:

$$\frac{c\delta_t}{\delta_x} \leq 1 \qquad \text{(CFL number)}$$

- Consider the domain of dependency
- For any differencing scheme, the domain consists of the set of points in the “past cone”
- If the differencing domain is wider in x than the domain of dependency, then this is stable
- If the differencing domain is narrower, then unstable



Partial differential equations

- Can also add terms of order δ_t^2 in the discretization
- Using $\partial u/\partial t = -c\partial u/\partial x$ then we get:

$$u(x,t+\delta_t) = u(x,t) + \delta_t \frac{\partial u}{\partial t} + \frac{\delta_t^2}{2}\frac{\partial^2 u}{\partial t^2} + \ldots$$
$$\simeq u(x,t) - c\delta_t \frac{\partial u}{\partial x} + \frac{c^2\delta_t^2}{2}\frac{\partial^2 u}{\partial x^2} \,,$$
$$u_j^{n+1} = u_j^n - \frac{c\delta_t}{2\delta_x}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{c^2\delta_t^2}{2\delta_x^2}\left(u_{j+1}^n + u_{j-1}^n - 2u_j^n\right) \,.$$

- This is the “Lax-Wendroff” method
- The stability is the same CFL condition as before in the Lax method
- Note that the added term is a discretized diffusive term

$$\frac{\partial n(x,t)}{\partial t} = D\frac{\partial^2 n(x,t)}{\partial x^2} \,, \qquad n_i^{n+1} = n_i^n + \frac{D\delta_t}{\delta_x^2}\left(n_{i+1}^n + n_{i-1}^n - 2n_i^n\right) \,.$$

- General feature : diffusive terms in recurrence formulae have damping effects on the amplitude

Partial differential equations

- Can also consider nonlinear wave equations
  - Don't preserve shape in general
  - Linear wave equation has linear dispersion!
- Dispersion is the relation between wave number and frequency.
  - Plane wave : $u(x,t) \sim e^{i(kx-\omega t)}$ $\Rightarrow \quad (-i\omega - ick)(-i\omega + ick) = 0$

    $\Rightarrow \quad \omega = \pm ck \ .$

    - Here, all the modes move with the same velocity c
    - Wave velocity is omega / k
- What if the velocity depends on the wave number?
  - Example: $$\frac{\partial u(x,t)}{\partial t} = -c\frac{\partial u(x,t)}{\partial x} - d\frac{\partial^3 u(x,t)}{\partial x^3} \ .$$
  - Plugging in $e^{ikx-i\omega t}$ (plane wave), we get a dispersion: $\omega = ck - dk^3 \ .$ Wave velocity depends on k!

Partial differential equations

- Now let's go back to advection equation and add a diffusive term

$$\frac{\partial u(x,t)}{\partial t} = -c\frac{\partial u(x,t)}{\partial x} + D\frac{\partial^2 u(x,t)}{\partial x^2} \ ,$$

- From plane wave, we get the dispersion relation:

$$\omega = ck - iDk^2 \quad \Rightarrow \quad e^{ik(x-ct)-Dk^2 t} \ ,$$

Partial differential equations

- Some nonlinear equations can have traveling waves
- Example is Burgers' equation:
  - http://en.wikipedia.org/wiki/Burgers'_equation

$$\frac{\partial u}{\partial t} = -\alpha \frac{\partial u}{\partial x} - \beta u \frac{\partial u}{\partial x} ,$$

- The last term is nonlinear in the wave amplitude
- Can solve by calculating partial derivatives:

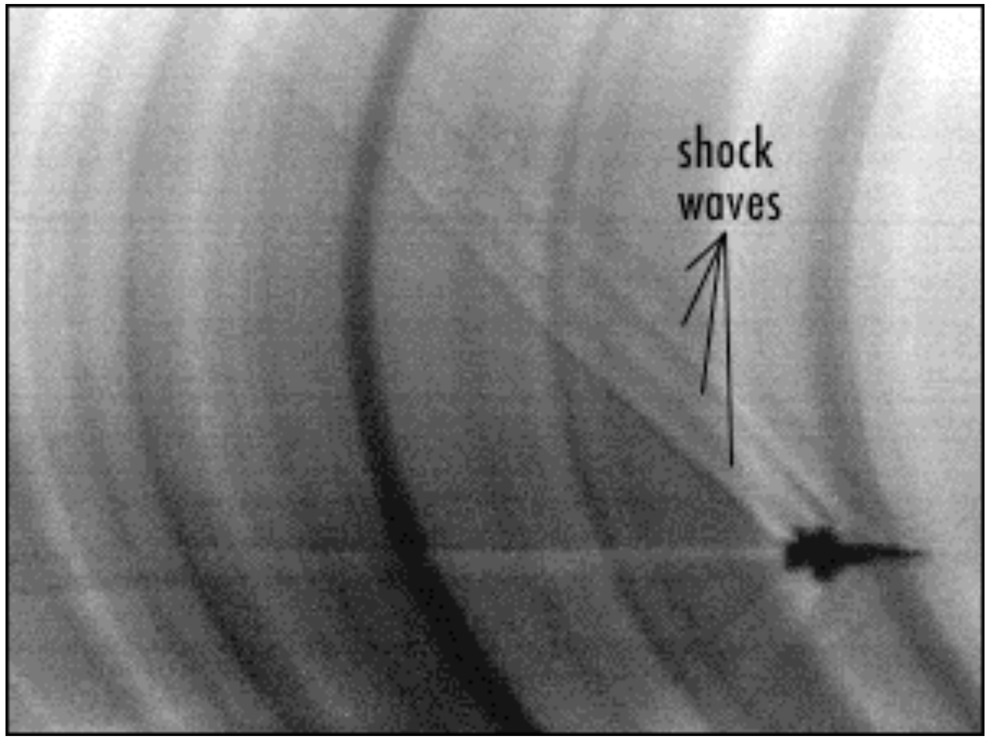
$$\frac{\partial u}{\partial t} = -(\alpha + \beta u) f' - \beta f' t \frac{\partial u}{\partial t} \quad \Rightarrow \quad \frac{\partial u}{\partial t} = -(\alpha + \beta u) f' / (1 + \beta f' t) ,$$

$$\frac{\partial u}{\partial x} = f' - \beta f' t \frac{\partial u}{\partial x} \quad \Rightarrow \quad \frac{\partial u}{\partial t} = f' / (1 + \beta f' t) .$$

- This is solved if we have a right-moving wave with functior $u(x,t) = f\left(x - (\alpha + \beta u)t\right)$,
- This wave moves with velocity $c = \alpha + \beta u(x,t)$

Partial differential equations

- Here, the velocity depends on the density of the wave!
- This leads to breaking and shock fronts:



Partial differential equations

- The Burgers' equation was introduced in 1948 as a simple model of shock propagation   J.M. Burgers, Adv. Appl. Mech. **1**, 171 (1948)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} ,$$

- First, set nu = 0 and we get

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 .$$

- Compare to the linear wave equation:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 ,$$

- Schematically the speed is equal to "u"!
- Peaks travel faster than troughs in the wave
- Eventually we get breaking, which we cannot represent as a function since it is multi-valued
- Passes through a shock front (solution is discontinuous)

Partial differential equations

- This kind of PDE was studied by Godunov in 1959

S.K. Godunov, Mat. Sb. **47**, 271 (1959)

- This is a class of "Riemann problem"
  - IVP for a PDE which has a piecewise constant initial value function, with a discontinuity (like a step function)
- Need to find an exact or approximate algorithm for this
  - called a "Riemann solver"

$$u_j^{n+1} = u_j^n - \frac{\tau}{h}\left[F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}\right] + \frac{\nu\tau}{h^2}\left[u_{j+1} + u_{j-1} - 2u_j\right] \ ,$$

- Here, $F_{j\pm\frac{1}{2}}$ is the average flux on the cells to the left and right of the lattice point j, respectively
- Solve these from Riemann problems in the cells to the right and left of j using "upwind" initial data:

$$u_j^{(+)} = \begin{cases} u_j & \text{if } u_j > 0 \\ 0 & \text{otherwise} \end{cases} \qquad u_j^{(-)} = \begin{cases} u_j & \text{if } u_j < 0 \\ 0 & \text{otherwise} \end{cases}$$

Partial differential equations

- The solution in the left cell is :

$$F_{j-\frac{1}{2}} = \max\left\{\frac{1}{2}(u_{j-1}^{(+)})^2, \frac{1}{2}(u_j^{(-)})^2\right\} \;,$$

- and on the right it is :

$$F_{j+\frac{1}{2}} = \max\left\{\frac{1}{2}\left(u_j^{(+)}\right)^2, \frac{1}{2}\left(u_{j+1}^{(-)}\right)^2\right\} \;.$$