Lecture 16: Relaxation methods

• Clever technique which begins with a first guess of the trajectory across the entire interval
  – Break the interval into M small steps:
    \[ x_1 = 0, \quad x_2, \quad \ldots, \quad x_M = L \]
  – Form a grid of points, \( y_{i,k} \)
    \[ i = 1,N \quad \quad k = 1,M \quad \Rightarrow \quad N \times M \text{ matrix} \]
Relaxation methods

• Now convert the system of equations
  \[ y' = f(x, y) \]

  into a set of difference equations
  \[ y_{i,k+1} - y_{i,k} = (x_{k+1} - x_k) f_i(\frac{1}{2}[x_{k+1} + x_k], (\frac{1}{2}[y_{k+1} + y_k]) \]

  \[ 0 = E_{i,k} \equiv y_{i,k+1} - y_{i,k} - (x_{k+1} - x_k)f_{i,k} \]

  Set of \( N(M-1) \) equations with \( N(M-1) \) unknowns (there are \( N \) b.c.'s)
Relaxation methods

• Can solve this problem iteratively by multidimensional Newton-Raphson, using

\[ 0 = E_{i,k}(y_{i,k+1} + \Delta y_{i,k+1}, y_{i,k} + \Delta y_{i,k}) \]

\[ = E_{i,k}(y_{i,k+1}, y_{i,k}) + \Delta y_{i,k+1} \frac{\partial E_{i,k}}{\partial \Delta y_{i,k+1}} + \Delta y_{i,k} \frac{\partial E_{i,k}}{\partial \Delta y_{i,k}} \]

to solve for the required \( \Delta y_{i,k} \)

For each iteration, we need to solve a MN x MN linear system to determine the required correction to \( y_{i,k} \) (but the system is fortunately a sparse one)
Relaxation methods

• The procedure is repeated until the trajectory relaxes to the correct one
Relaxation methods

• Grid size is critical ➔ put more points where the gradient is largest
  – If not known a priori, shooting methods may be better
  – Relaxation methods work best for smooth functions (use shooting methods for oscillatory functions)
  – Relaxation methods are favored when shooting methods are very unstable (e.g. in presence of a growing exponential solution)
Partial differential equations

*(Recipes, Chapter 19)*

• The Physical Universe is described by Partial Differential Equations
  
  – Maxwell’s equations
  – The Schrodinger Equation
  – The Navier-Stokes Equation
  – The Einstein Field equation
Partial differential equations

- PDEs are more complicated than ODEs to deal with analytically: not surprisingly, they are much more difficult to handle numerically
  - many more methods
  - could be the subject of an entire course
Partial differential equations

- We saw with ODEs that there was an important distinction between initial value problems and two point boundary problems.
- In PDEs, the very FORM of the equation determines where the bc’s can be specified.
Partial differential equations

Two key types of problem:

• *Initial value problems*:
  Given the state of the system at $t=0$, compute the time evolution

• *Boundary value problems*
  Find a static (time-independent) solution subject to boundary conditions on a surface enclosing a volume
Partial differential equations

Simplify the discussion by considering 2-D problems

• Examples of initial value problems:
  – Solution to the 1-(spatial)D wave equation, given $\phi(x,t)$ at time $t = 0$
    \[ \frac{\partial^2 \phi}{\partial x^2} - c^{-2} \frac{\partial^2 \phi}{\partial t^2} = 0 \]
  – Solution to 1-(spatial)D diffusion equation, given $\phi(x,t)$ at time $t = 0$
    \[ \kappa \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial \phi}{\partial t} = 0 \]
Partial differential equations

Simplify the discussion by considering 2-D problems

• Examples of boundary value problems:
  – Solution to Poisson’s equation,
    \[
    \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} - \rho = 0
    \]

    within some volume V enclosed by a boundary S on which the b.c.’s are specified
Boundary conditions

- In initial value problems, the boundary condition is typically specified at $t = 0$ and the solution is propagated forward in time, step by step.
Boundary conditions

• In boundary value problems, the boundary condition is specified on some closed surface.
Boundary conditions

• The methods of solution are somewhat analogous to the case of ODEs:

• Initial value problems:
  – step forward in time, using derivatives determined by the PDEs

• Boundary value problems:
  – solve within the volume using relaxation methods
  – or, create a phony time-dependence and integrate to \( t \to \infty \)
Mathematical description

• It is usually fairly clear on physical grounds whether a problem is an *initial value problem* or a *boundary value problem*

Electro/magnetostatic problem: BVP
Time-indep. Schrodinger equation: BVP
Time-dependent Schrodinger equation: IVP
Wave equation: IVP
Diffusion equation: IVP
Mathematical description

• Note, however, that the type of b.c. is also determined by the FORM of the equation.

• For example, you can solve

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad \text{(Laplace’s equation)}$$

given arbitrary boundary conditions on a closed loop in the x-y plane.

• but you cannot solve

$$\frac{\partial^2 \phi}{\partial x^2} - c^{-2} \frac{\partial^2 \phi}{\partial t^2} = 0 \quad \text{(wave equation)}$$
Mathematical description

• Some PDEs (“hyperbolic” and “parabolic”) have “characteristic curves” on which arbitrary boundary conditions cannot be imposed
  – example: the wave equation

• Some PDEs (“elliptic”) do not have such curves
  – example: Laplace’s equation
Mathematical description

• For a 2\textsuperscript{nd}-order PDE in two variables:

\[ A \frac{\partial^2 \phi}{\partial x^2} + 2B \frac{\partial^2 \phi}{\partial x \partial y} + C \frac{\partial^2 \phi}{\partial y^2} + D \frac{\partial \phi}{\partial x} + E \frac{\partial \phi}{\partial y} + F \phi + G = 0 \]

the characteristic curves (if they exist) are given by

\[ \frac{dy}{dx} = \frac{B}{A} \pm \frac{1}{A} \sqrt{B^2 - AC} \]
Mathematical description

• Such PDEs are categorized according to the value of $B^2 - AC$

$B^2 - AC < 0 \Rightarrow \text{“elliptic eqn”}$
  - No characteristic curves

$B^2 - AC = 0 \Rightarrow \text{“parabolic eqn”}$
  - 1 family of characteristic curves

$B^2 - AC > 0 \Rightarrow \text{“hyperbolic eqn”}$
  - 2 families of characteristic curves
Mathematical description

• Examples:
  – Poisson/Laplace’s equation:
    \((A,B,C) = (1,0,1) \Rightarrow B^2 - AC < 0\)
    \(\Rightarrow\) elliptic
    \(\Rightarrow\) no characteristic curves
    \(\Rightarrow\) any boundary conditions allowed
Mathematical description

• Examples:
  – Diffusion equation:
    \[(A,B,C) = (k,0,0) \Rightarrow B^2 - AC = 0\]
    \(\Rightarrow\) parabolic
    \(\Rightarrow\) characteristic curves exist
    \(\Rightarrow\) not all boundary conditions allowed
Mathematical description

• Examples:
  – Wave equation:
    \[(A,B,C) = (1,0,-c^{-2}) \Rightarrow B^2 - AC = c^{-2} > 0\]
    \(\Rightarrow\) hyperbolic
    \(\Rightarrow\) 2 families of characteristic curve exist
    with \(dt/dx = \pm c^{-1}\)
    or \(dx/dt = \pm c\)
Mathematical description

• Characteristic curves for the wave equation: once a boundary condition is specified at one point on a characteristic curve, it cannot be arbitrarily specified at a 2nd point.
Mathematical description

• Information propagates along the characteristic curves (at speed $c$ in the $+x$ and $-x$ directions)
Mathematical description

• If the b.c.’s are determined at $t = 0$, the behavior for $t > 0$ is completely specified
Mathematical description

• We can’t arbitrarily specify $\phi$ on a boundary that crosses a given characteristic curve more than once