Lecture 7: Simple PDEs

Supporting textbook chapters for week 8: Chapters 9.1 - 9.3

Topics:

- Classifying PDEs
- Elliptic equation solvers: Jacobi, Gauss-Seidel, overrelaxation
- Parabolic equation solver: Explicit FTCS (Forward Time, Centered Space)
- Parabolic and hyperbolic equation soliver: Implicit FTCS, Crank-Nicolson

Classification and General Approach

- Solving partial differential equations is one of the pinnacles of computational physics, bringing together many methods.
- Each type comes with design decisions on how to discretize and implement numerical methods,
- Stability is crucial.
- Accuracy is crucial too.

Recall conical equations in geometry:

$$\alpha x^2 + \beta xy + \gamma y^2 + \delta x + \varepsilon y = f,$$

classified using $\Delta = \beta^2 - 4\alpha\gamma$.

1. $\Delta = 0$: equation for a parabola,
2. $\Delta < 0$: equation for an ellipse,
3. $\Delta > 0$: equation for a hyperbola.

Similar for PDEs:

$$\alpha \frac{\partial^2 \phi}{\partial x^2} + \beta \frac{\partial^2 \phi}{\partial x \partial y} + \gamma \frac{\partial^2 \phi}{\partial y^2} + \delta \frac{\partial \phi}{\partial x} + \varepsilon \frac{\partial \phi}{\partial y} = f.$$

With $\Delta = \beta^2 - 4\alpha\gamma$,

1. $\Delta = 0$: parabolic PDE,
2. $\Delta < 0$: elliptic PDE,
3. $\Delta > 0$: hyperbolic PDE.

Physics Examples

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1. Canonical parabolic PDE: the diffusion equation, $\kappa\frac{\partial^2 T}{\partial x^2}-\frac{\partial T}{\partial t}=0$,
$$x\to x,\quad y\to t,\quad \alpha\to\kappa,\quad \varepsilon\to -1,\quad \beta,\gamma,\delta,f\to 0\quad\Rightarrow\quad \beta^2-4\alpha\gamma=0.$$
2. Canonical elliptic PDE: the Poisson equation, $\nabla^2\phi=\rho$,
$$x\to x,\quad y\to y,\quad \alpha,\gamma\to 1, f\to\rho,\beta,\delta,\varepsilon\to 0\quad\Rightarrow\quad \beta^2-4\alpha\gamma=-4<0.$$
   - e.g. 2D electrostatics, with electric potential ϕ s.t. $\vec{E}=\nabla\phi$, in the absence of charges ($\rho\equiv 0$), have Gauss' law: $\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$
3. Canonical hyperbolic PDE: the wave equation, $c^2\frac{\partial^2\phi}{\partial x^2}-\frac{\partial^2\phi}{\partial t^2}=0$.
$$x\to x,\quad y\to t,\quad \alpha\to c^2,\quad \gamma\to -1,\quad \beta,\delta,\varepsilon,f\to 0\quad\Rightarrow\quad \beta^2-4\alpha\gamma=4c^2>0.$$

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Note: we use these categorizations even when the spatial operator is $\nabla^2=\partial_x^2+\partial_y^2+\partial_z^2$, i.e., for 4D PDEs.

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General approach

- Discretize system spatially and temporally: can use finite difference, spectral coefficients, etc.
- $\Rightarrow$ set of coupled ODEs that you need to solve in an efficient way.
- Spatial derivatives bring information in from neighbouring points $\Rightarrow$ coupling,
- $\Rightarrow$ errors depend on space and time and can get wave-like characteristics.
- For 2nd derivatives, recall central difference calculation (§5.10.5, p.197):
$$f''(x)=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}-\frac{1}{12}h^2f^{(4)}(x)+\dots$$

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Elliptic Equations

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Start with simplest case of Gauss's Law with 2D Laplacian:
$$0=\nabla^2\phi=\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2},$$

On regular square grid of cell side length a, finite difference form is
$$\frac{\partial^2\phi}{\partial x^2}\approx\frac{\phi(x+a,y)-2\phi(x,y)+\phi(x-a,y)}{a^2},$$
$$\frac{\partial^2\phi}{\partial y^2}\approx\frac{\phi(x,y+a)-2\phi(x,y)+\phi(x,y-a)}{a^2}.$$
Gauss's law then becomes:
$$0\approx\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)-4\phi(x,y)$$
at each location (x,y).

- Put together a series of equations of the form
$$\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)-4\phi(x)=0$$
for each x and y, subject to boundary conditions.
- ϕ or derivative $\partial\phi/\partial\xi$ ($\xi=x,\ y$, or both) given on boundary.
- If ϕ given, use this value for adjacent points.
- If $\partial\phi/\partial\xi$ given, find algebraic relationship between points near to boundary using finite difference.
- Could solve using matrix methods $\mathbf{L}\phi=\mathbf{R}\phi$, but a simpler method is possible.

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Jacobi relaxation method

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$$\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)-4\phi(x)=0$$

- Iterate the rule $\phi_{new}(x,y)=\frac{1}{4}\left[\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)\right]$.
- Much like the relaxation method for finding solutions of $f(x)=x$,
- For this problem it turns out that Jacobi Relaxation is always stable and so always gives a solution!

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Overrelaxation method

$\phi_{new}(x,y)=$

$$(1+\omega)\left[\frac{\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)}{4}\right]-\omega\phi(x,y)$$

- When it works, it usually speeds up the calculation.
- Not always stable! How to choose ω is not always reproducible.
- see Newman's exercise 6.11 for a similar problem for finding $f(x)=x$.

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Gauss-Seidel method

- Replace function on the fly as in
$$\phi(x,y)\leftarrow\frac{\phi(x+a,y)+\phi(x-a,y)+\phi(x,y+a)+\phi(x,y-a)}{4}.$$
- Crucial difference: the LHS is ϕ, not ϕ_{new}: we use newer values as they are being computed (Jacobi used only old values to compute new one).
- This can be shown to run faster.
- Can be combined with overrelaxation.

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Parabolic PDEs

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- Consider the 1D heat equation:
$$\frac{\partial T}{\partial t}=\kappa\frac{\partial^2 T}{\partial x^2},$$
- B.Cs.:
$$T(x=0,t)=T_0,\quad T(x=L,t)=T_L.$$
- I.C.:
$$T(x,t=0)=T_0+(T_L-T_0)\left(\frac{f(x)-f(0)}{f(L)-f(0)}\right)$$

Explicit Forward Time Centred Space method

Step 1: Discretize in space

$$x_m = \frac{m}{M}L = am, \quad m = 0 \ldots M, \quad a = \frac{L}{M},$$

$$T_m(t) = [T_0(t), \ldots, T_M(t)]$$

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{x=x_m,t} \approx \frac{T_{m+1} - 2T_m + T_{m-1}}{a^2} \quad \text{("centred space", CS)}$$

Step 2: Discretize in time

$$\frac{dT_m}{dt} \approx \kappa \frac{T_{m+1} - 2T_m + T_{m-1}}{a^2}, \quad m = 1 \ldots, M-1$$

Let $t_n = nh$, h the time step. Let $T_m(t_n) \equiv T_m^n$.

$$\Rightarrow \left.\frac{\partial T}{\partial t}\right|_{x=ma,t=nh} \approx \frac{T_m^{n+1} - T_m^n}{h} \equiv \kappa \frac{T_{m+1}^n - 2T_m^n + T_{m-1}^n}{a^2} \text{ ("Forward Time", FT).}$$

⇒ **Explicit FTCS method:**

$$\boxed{T_m^{n+1} = T_m^n + \frac{\kappa h}{a^2}\left(T_{m+1}^n - 2T_m^n + T_{m-1}^n\right)}.$$

It may be easier to understand by writing the problem as a set of ODEs

$$\frac{\partial \phi_m}{\partial t} = \psi_m, \quad \text{and} \quad \frac{\partial \psi_m}{\partial t} = \frac{c^2}{a^2}(\phi_{m+1} - 2\phi_m + \phi_{m-1})$$

and the discretization in time as:

$$\begin{bmatrix} \phi_m^{n+1} \\ \psi_m^{n+1} \end{bmatrix} = \begin{bmatrix} 1 & +h \\ -\frac{2hc^2}{a^2} & 1 \end{bmatrix} \begin{bmatrix} \phi_m^n \\ \psi_m^n \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{c^2 h}{a^2}\left(\phi_{m+1}^n + \phi_{m-1}^n\right) \end{bmatrix}$$

Implicit FTCS Method

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Evaluate the RHS of the above at time $t+h$ instead of t

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- first do $h \to -h$ (from the current time step, compute the *previous* one):

$$\phi_m^{n-1} = \phi_m^n - h\psi_m^n,$$
$$\psi_m^{n-1} = \psi_m^n - h\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right),$$

- Then, $n \to n+1$ (one shift forward in time):

$$\phi_m^n = \phi_m^{n+1} - h\psi_m^{n+1},$$
$$\psi_m^n = \psi_m^{n+1} - h\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right),$$

or

$$\begin{bmatrix}\phi_m^n \\ \psi_m^n\end{bmatrix} = \begin{bmatrix}1 & -h \\ +\frac{2hc^2}{a^2} & 1\end{bmatrix}\begin{bmatrix}\phi_m^{n+1} \\ \psi_m^{n+1}\end{bmatrix} - \begin{bmatrix}0 \\ \frac{c^2h}{a^2}\left(\phi_{m+1}^{n+1} + \phi_{m-1}^{n+1}\right)\end{bmatrix}$$

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"Implicit": we now have a set of simultaneous equations relating the values of $\phi,\ \psi$ at t to their values at $t+h$.

Why bother solving these simultaneous equations, rather than using an "explicit" expression for the values of $\phi,\ \psi$ at $t+h$ given their values at t ?

Because in certain cases, this is numerically stable while the explicit FTCS is not! (More about this later)

Note, it does often suffer from accuracy issues, where solutions decay to 0 over time.

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Crank-Nicolson

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Average of explicit and implicit methods.

Explicit ('forward'):

$$\phi_m^{n+1} = \phi_m^n + h\psi_m^n, \qquad \psi_m^{n+1} = \psi_m^n + h\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right).$$

Implicit ('backward'):

$$\phi_m^{n+1} - h\psi_m^{n+1} = \phi_m^n, \qquad \psi_m^n = \psi_m^{n+1} - h\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right).$$

Crank-Nicholson (C-N):

$$\phi_m^{n+1} - \frac{h}{2}\psi_m^{n+1} = \phi_m^n + \frac{h}{2}\psi_m^n$$
$$\psi_m^{n+1} - \frac{h}{2}\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right) = \psi_m^n + \frac{h}{2}\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right).$$

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C-N is 2nd-order accurate in time, while both explicit and implicit methods are 1st-order accurate. So, C-N often solves the 'decaying to 0' issues encountered with the implicit method.

Hyperbolic PDEs

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Explicit FTCS is always unstable. Use C-N, or spectral methods (next time)