Introduction to Computational Physics

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Waves: a hyperbolic-advective process

Partial Differential Equations (PDE):
Most important in physics: *quasilinear PDEs of second order*:

$$a_{11}\frac{\partial^2 u}{\partial x^2} + 2a_{12}\frac{\partial^2 u}{\partial x \partial y} + a_{22}\frac{\partial^2 u}{\partial y^2} + f(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) \quad = \quad 0$$

hyperbolic:	$a_{11}a_{22} - a_{12}^2 < 0$	(e.g. $a_{12} = 0$, $a_{11}a_{22} < 0$)
parabolic:	$a_{11}a_{22} - a_{12}^2 = 0$	(or $a_{12} = 0$, $a_{11}a_{22} = 0$)
elliptic:	$a_{11}a_{22} - a_{12}^2 > 0$	(or $a_{12} = 0$, $a_{11}a_{22} > 0$)

Examples:

hyperbolic	$c^2\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} = f(x,t)$	Wave equation
	$c^2\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} - a\,\frac{\partial u}{\partial t} = f(x,t)$	Wave with damping
parabolic	$D\,\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} = f(x,t)$	Diffusion equation
	$\frac{\hbar^2}{2m}\,\frac{\partial^2 u}{\partial x^2} + i\hbar\,\frac{\partial u}{\partial t} - U(x)\,u = 0$	Schroedinger equation
elliptic	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(x,y)$	Potential equation
	$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{2m}{\hbar^2}\,U(x)\,u = 0$ (or $\ldots = \epsilon\,u$)	Schroedinger equation, stationary case

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hyperbolic parabolic	$\Longleftrightarrow$	initial value problems
elliptic	$\Longleftrightarrow$	boundary value problems

Conservative hyperbolic and parabolic equations, describing the transport of conserved quantities, may be written as

$$\boxed{\frac{\partial u}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{j}}$$

where $u(\mathbf{r}, t)$ (scalar or vector) is the density of a conserved quantity, and $\mathbf{j}(\mathbf{r}, t)$ the respective local "flux density", or "current density".

How come? $\Longrightarrow$

(1) Consider the electromagnetic wave equation in 2D:

$$\frac{\partial^2 E_y}{\partial t^2} \quad = \quad c^2 \frac{\partial^2 E_y}{\partial x^2}$$

which is equivalent to

$$\frac{\partial E_y}{\partial t} = c\,\frac{\partial B_z}{\partial x} \qquad\qquad \frac{\partial B_z}{\partial t} = c\,\frac{\partial E_y}{\partial x}$$

$\Longrightarrow$conservative-hyperbolic, with $u \equiv \mathbf{u} = (E_y, B_z)$, and $j \equiv \mathbf{j}(\mathbf{u}) = -c\,(B_z, E_y)$.

(2) Consider the diffusion equation in 1D:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \quad \equiv \quad \frac{\partial}{\partial x}(D\frac{\partial u}{\partial x})$$

$\Longrightarrow$conservative-parabolic, with $j \equiv j(\nabla u) = D\partial u/\partial x$.

Initial Value Problems I: Conservative-hyperbolic DE

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{\partial \mathbf{j}}{\partial x}$$

Best (i.e. most stable, exact, etc.): **Lax-Wendroff** technique

Approach via:

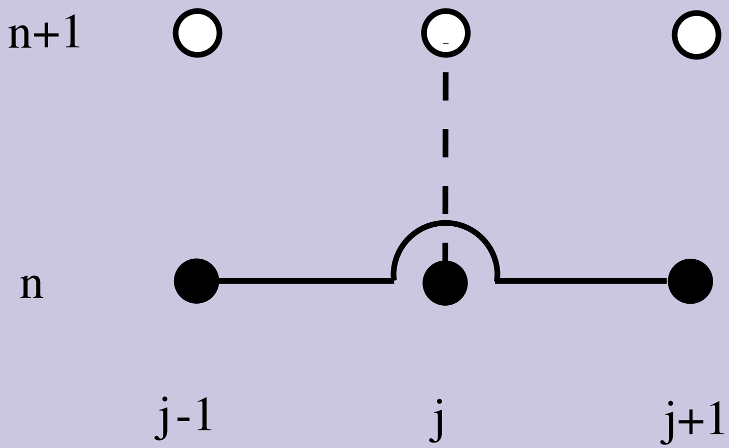
– **FTCS**
– **Lax**
– **Leapfrog**

FTCS Scheme; Stability Analysis

Writing $\mathbf{u}_j^n \equiv \mathbf{u}(x_j, t_n)$ and using DNGF for the time derivative (FT, "forward-time"), and DST for the space derivative (CS, for "centered-space"), we write $\partial\mathbf{u}/\partial t = -\partial\mathbf{j}/\partial x$ as

$$\frac{1}{\Delta t}\left[\mathbf{u}_j^{n+1} - \mathbf{u}_j^n\right] \approx -\frac{1}{2\,\Delta x}\left[\mathbf{j}_{j+1}^n - \mathbf{j}_{j-1}^n\right]$$

$$\boxed{\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \frac{\Delta t}{2\Delta x}\left[\mathbf{j}_{j+1}^n - \mathbf{j}_{j-1}^n\right]}$$



Stability analysis (J. v. Neumann):

At time t_n, expand $u(x,t)$:

$$u_j^n = \sum_k U_k^n e^{ikx_j}$$

where $k = 2\pi l/L \ \ (l = 0, 1, \ldots)$. Insert this in $u_j^{n+1} = T[u_{j'}^n]$ to find each Fourier component's propagation law, $U_k^{n+1} = g(k)\, U_k^n$.

$\Longrightarrow$Stable if $|g(k)| \leq 1$ for all k.

Application to FTCS + advective equation with $j = c\,u$:

$$g(k)\, U_k^n e^{ikj\,\Delta x} = U_k^n e^{ikj\,\Delta x} - \frac{c\,\Delta t}{2\,\Delta x} U_k^n \left[e^{ik(j+1)\Delta x} - e^{ik(j-1)\Delta x}\right]$$

or

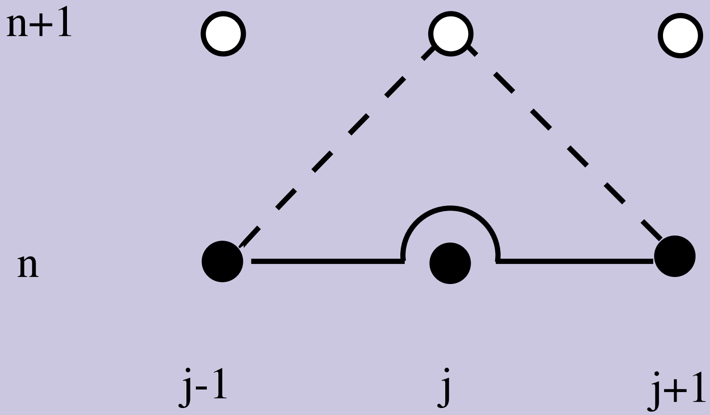
$$g(k) = 1 - \frac{ic\,\Delta t}{\Delta x} \sin k\Delta x$$

Obviously, $|g(k)| > 1$ for any k; the FTCS method is inherently unstable.

Lax Scheme

Replacing in the FTCS formula the term $\mathbf{u}_j^n$ by its spatial average $[\mathbf{u}_{j+1}^n + \mathbf{u}_{j-1}^n]/2$, we approximate $\partial \mathbf{u}/\partial t = -\partial \mathbf{j}/\partial x$ by

$$\boxed{\mathbf{u}_j^{n+1} = \frac{1}{2}\left[\mathbf{u}_{j+1}^n + \mathbf{u}_{j-1}^n\right] - \frac{\Delta t}{2\Delta x}\left[\mathbf{j}_{j+1}^n - \mathbf{j}_{j-1}^n\right]}$$



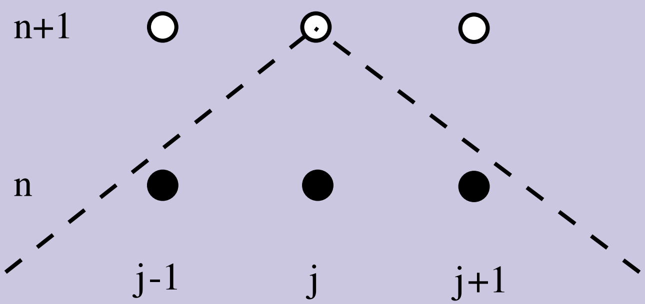
Stability / Friedrichs-Löwy condition:

Insert Fourier expanded $u(x)$ in Lax formula to find

$$g(k) = \cos k\Delta x - i\frac{c\Delta t}{\Delta x}\sin k\Delta x$$

The condition $|g(k)| \leq 1$ is tantamount to

$$\boxed{\frac{|c|\Delta t}{\Delta x} \leq 1}$$



Region below the dashed line: physically relevant for u_j^{n+1}, according to $x(t_{n+1}) = x(t_n) \pm |c|\,\Delta t$

Close scrutiny shows that LAX solves not the original PDE but

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

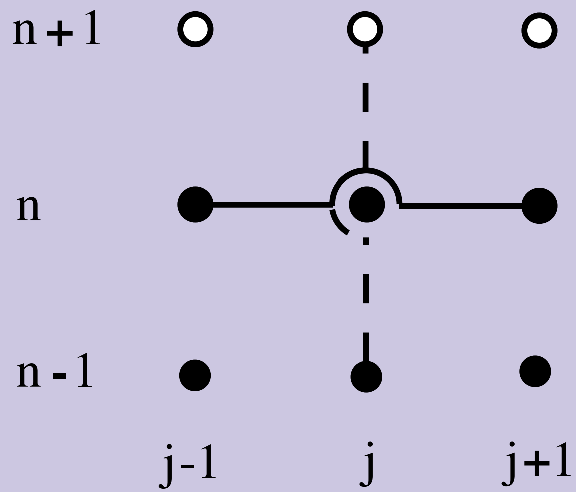
The additional diffusive term makes the method stable. However, it is an artefact and should be small:

$$|c|\Delta t \quad >> \quad \frac{\Delta x}{2}\frac{|\delta^2 u|}{|\delta u|}$$

Leapfrog Scheme (LF)

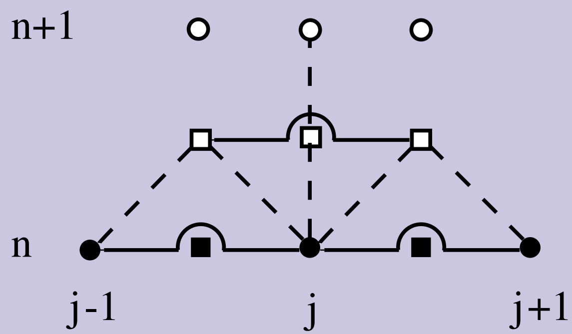
Use DST for $\partial/\partial t$: $\partial u/\partial t \approx (u^{n+1} - u^{n-1})/2\Delta t$ to find the *leapfrog* expression

$$\boxed{\mathbf{u}_j^{n+1} - \mathbf{u}_j^{n-1} = -\frac{\Delta t}{\Delta x}\left[\mathbf{j}_{j+1}^n - \mathbf{j}_{j-1}^n\right]}$$



Stability requires once more that $c\,\Delta t/\Delta x \leq 1$ (CFL condition)

Lax-Wendroff Scheme (LW):



- Lax method with half-step: $\Delta x/2$, $\Delta t/2$:

$$\mathbf{u}_{j+1/2}^{n+1/2} \;=\; \frac{1}{2}\left[\mathbf{u}_{j+1}^{n}+\mathbf{u}_{j}^{n}\right]-\frac{\Delta t}{2\Delta x}\left[\mathbf{j}_{j+1}^{n}-\mathbf{j}_{j}^{n}\right]$$

  and analogously for $\mathbf{u}_{j-1/2}^{n+1/2}$.

- Evaluation, e.g. for the advective case $\mathbf{j}=\mathbf{C}\cdot\mathbf{u}$:

$$\mathbf{u}_{j+1/2}^{n+1/2} \;\Longrightarrow\; \mathbf{j}_{j+1/2}^{n+1/2}$$

- *leapfrog* with half-step:

$$\mathbf{u}_{j}^{n+1} \;=\; \mathbf{u}_{j}^{n}-\frac{\Delta t}{\Delta x}\left[\mathbf{j}_{j+1/2}^{n+1/2}-\mathbf{j}_{j-1/2}^{n+1/2}\right]$$

Stability:

Once more assuming $j = cu$ and using the ansatz $U_k^{n+1} = g(k)U_k^n$ we find

$$g(k) \;=\; 1 - ia\,\sin k\Delta x - a^2(1 - \cos k\Delta x),$$

with $a = c\Delta t/\Delta x$. The requirement $|g|^2 \leq 1$ leads once again to the CFL condition, $c\,\Delta t/\Delta x \leq 1$.

Resume: Conservative-hyperbolic DE

$$\frac{\partial \mathbf{u}}{\partial t} \;=\; -\frac{\partial \mathbf{j}}{\partial x}$$

– **Use Lax-Wendroff!**

– **If not, use at least Lax**, but see that in addition to CFL,

$$|c|\Delta t \;>>\; \frac{\Delta x}{2}\frac{|\delta^2 u|}{|\delta u|}$$

– **Forget FTCS and Leapfrog!**

Initial Value Problems II: Conservative-parabolic DE

Diffusion:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(\lambda \frac{\partial u}{\partial x}) \qquad \text{or} \qquad \frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2}$$

Best: 2 second-order schemes

– **Crank-Nicholson**
– **Dufort-Frankel**

But: first-order algorithms perform well, too

– **FTCS** (one up for old Leonhard E.!)
– **Implicit** (even better – good enough for many purposes!)

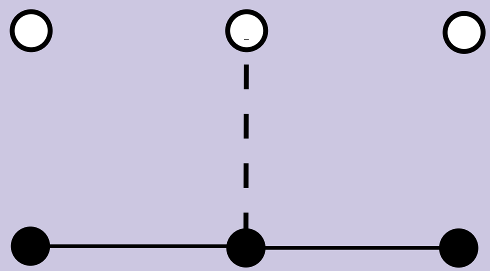
FTCS Scheme:

In $\partial u/\partial t = \lambda \partial^2 u/\partial x^2$, replace $\partial u/\partial t$ by DNGF and $\partial^2 u/\partial x^2$ by DDST formula:
$\Longrightarrow$ "forward time-centered space" algorithm,

$$\frac{1}{\Delta t}\left[u_j^{n+1} - u_j^n\right] \quad = \quad \frac{\lambda}{(\Delta x)^2}\left[u_{j+1}^n - 2u_j^n + u_{j-1}^n\right]$$

Using $a \equiv \lambda \Delta t/(\Delta x)^2$ this is

$$\boxed{u_j^{n+1} = (1-2a)u_j^n + a(u_{j-1}^n + u_{j+1}^n)}$$



Stability:

For the k-dependent growth factor we find $g(k) = 1 - 4a \sin^2 \frac{k\Delta x}{2}$, which tells us that for stability the condition is

$$\Delta t \quad \leq \quad \frac{(\Delta x)^2}{2\lambda} \equiv \tau$$

where τ is the characteristic time for the diffusion over a distance Δx (i.e. one lattice space).

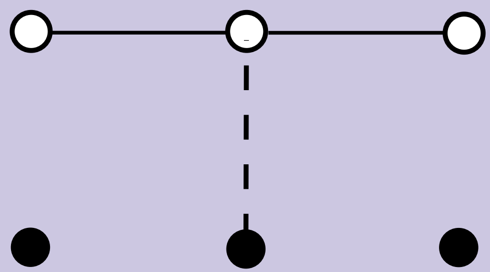
The FTCS scheme is simple and stable, but inefficient.

Exercise: Remember the thermal conduction problem we considered earlier? If you haven't done it then, do it now, using FTCS. Interpret the behavior of the solution for varying time step sizes in the light of the above stability considerations.

Implicit Scheme of First Order:

Take the second spatial derivative *at time* t_{n+1} instead of t_n:

$$\frac{1}{\Delta t}\left[u_j^{n+1} - u_j^n\right] = \frac{\lambda}{(\Delta x)^2}\left[u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right]$$



Again defining $a \equiv \lambda \Delta t/(\Delta x)^2$, we find, for each space point x_j $(j = 1, 2, ..N - 1)$,

$$\boxed{-a u_{j-1}^{n+1} + (1 + 2a) u_j^{n+1} - a u_{j+1}^{n+1} = u_j^n}$$

Let the boundary values u_0 and u_N be given; the set of equations may then be written as

$$\mathbf{A} \cdot \mathbf{u}^{n+1} \quad = \quad \mathbf{u}^{n}$$

with

$$\mathbf{A} \quad \equiv \quad \begin{pmatrix} 1 & 0 & 0 & . & . & 0 \\ -a & 1+2a & -a & 0 & . & 0 \\ 0 & . & . & . & 0 & . \\ . & . & . & . & . & . \\ . & . & . & -a & 1+2a & -a \\ . & . & . & 0 & 0 & 1 \end{pmatrix}$$

$\Longrightarrow$Solve by Recursion!

Stability:

We find

$$g = \frac{1}{1 + 4a \sin^2(k\Delta x/2)}$$

Since $|g| \leq 1$ under all circumstances, we have here an *unconditionally stable* algorithm!

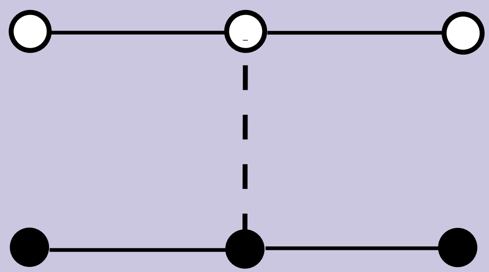
Exercise: Apply the implicit technique to the thermal conduction problem discussed before. Consider the efficiency of the procedure as compared to FTCS. Relate the problem to the Wiener-Levy *random walk*.

Crank-Nicholson Scheme (CN):

As before, replace $\partial u/\partial t$ by $\Delta_n u/\Delta t \equiv (u^{n+1} - u^n)/\Delta t$.

Noting that this approximation is in fact centered at $t_{n+1/2}$, introduce the same kind of time centering on the right-hand side: taking the mean of $\delta_j^2 u^n$ (= FTCS) and $\delta_j^2 u^{n+1}$ (= implicit scheme) we write

$$\frac{1}{\Delta t}\left[u_j^{n+1} - u_j^n\right] = \frac{\lambda}{2(\Delta x)^2}\left[(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (u_{j+1}^n - 2u_j^n + u_{j-1}^n)\right]$$



The *Crank-Nicholson* formula is of *second* order in Δt.

Defining $a \equiv \lambda \Delta t / 2(\Delta x)^2$ we may write CN as

$$\boxed{-a u_{j-1}^{n+1} + (1+2a) u_j^{n+1} - a u_{j+1}^{n+1} = a u_{j-1}^{n} + (1-2a) u_j^{n} + a u_{j+1}^{n}}$$

or

$$\mathbf{A} \cdot \mathbf{u}^{n+1} \quad = \quad \mathbf{B} \cdot \mathbf{u}^{n}$$

with

$$\mathbf{A} \equiv \begin{pmatrix} 1 & 0 & 0 & . & . & 0 \\ -a & 1+2a & -a & 0 & . & 0 \\ 0 & . & . & . & 0 & . \\ . & . & . & . & . & . \\ . & . & . & -a & 1+2a & -a \\ . & . & . & 0 & 0 & 1 \end{pmatrix} \quad \mathbf{B} \equiv \begin{pmatrix} 1 & 0 & 0 & . & . & 0 \\ a & 1-2a & a & 0 & . & 0 \\ 0 & . & . & . & 0 & . \\ . & . & . & . & . & . \\ . & . & . & a & 1-2a & a \\ . & . & . & 0 & 0 & 1 \end{pmatrix}$$

Tridiagonal $\Longrightarrow$ *Solve by Recursion!*

Stability of CN:

The amplification factor is

$$g(k) \quad = \quad \frac{1 - 2a\ \sin^2(k\Delta x/2)}{1 + 2a\ \sin^2(k\Delta x/2)} \leq 1\ ,$$

which makes the CN method unconditionally stable.

Example: The time-dependent Schroedinger equation,

$$\frac{\partial u}{\partial t} = -iHu\,, \quad \text{with } H \equiv \frac{\partial^2}{\partial x^2} + U(x)$$

when rewritten à la Crank-Nicholson, reads

$$\begin{aligned}\frac{1}{\Delta t}[u_j^{n+1} - u_j^n] &= -\frac{i}{2}[(Hu)_j^{n+1} + (Hu)_j^n] \\ &= -\frac{i}{2}\left[\frac{\delta_j^2 u_j^{n+1}}{(\Delta x)^2} + U_j u_j^{n+1} + \frac{\delta_j^2 u_j^n}{(\Delta x)^2} + U_j u_j^n\right]\end{aligned}$$

With $a \equiv \Delta t/2(\Delta x)^2$ and $b_j \equiv U(x_j)\Delta t/2$ this leads to

$$\begin{aligned}(ia)u_{j-1}^{n+1} + (1 - 2ia + ib_j)u_j^{n+1} \;&+\; (ia)u_{j+1}^{n+1} = \\ &= (-ia)u_{j-1}^n + (1 + 2ia - ib_j)u_j^n + (-ia)u_{j+1}^n\end{aligned}$$

Again, we have a tridiagonal system which may be inverted very efficiently by recursion.

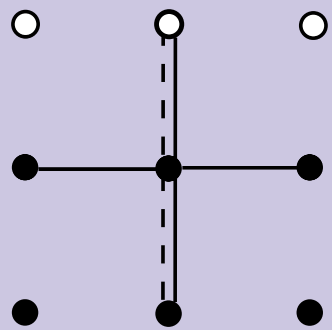
Dufort-Frankel Scheme (DF):

DST in time and space, but in place of $-2u_j^n$ use $-(u_j^{n+1} + u_j^{n-1})$:

$$\frac{1}{2\Delta t}\left[u_j^{n+1} - u_j^{n-1}\right] = \frac{\lambda}{(\Delta x)^2}\left[u_{j+1}^n - (u_j^{n+1} + u_j^{n-1}) + u_{j-1}^n\right]$$

or, with $a \equiv 2\lambda\Delta t/(\Delta x)^2$,

$$\boxed{u_j^{n+1} = \frac{1-a}{1+a}u_j^{n-1} + \frac{a}{1+a}\left[u_{j+1}^n + u_{j-1}^n\right]}$$



The DF algorithm is of second order in Δt. In contrast to CN, it is an *explicit* expression for u_j^{n+1}.

Stability:

$$g = \frac{1}{1+a}\left[a \cos k\Delta x \pm \sqrt{1 - a^2 \sin^2 k\Delta x}\right]$$

Considering in turn the cases $a^2 \sin^2 k\Delta x \geq 1$ and $\ldots < 1$ we find that $|g|^2 \leq 1$ always; the method is unconditionally stable.

Resume: Conservative-parabolic DE

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

– **Use Crank-Nicholson!** (2nd order implicit scheme; needs recursion)
– **If too lazy for implicit scheme, use Dufort-Frankel** (2nd order explicit)
– **If 1st order is sufficient, use implicit scheme**

Boundary Value Problems: Elliptic DE

Standard problem: two-dimensional potential equation,

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

For general $\rho(x, y)$ this is Poisson's equation; if $\rho \equiv 0$ it is called Laplace's equation.

Assuming $\Delta y = \Delta x \equiv \Delta l$ we have

$$\frac{1}{(\Delta l)^2}\left[\delta_i^2 u_{i,j} + \delta_j^2 u_{i,j}\right] = -\rho_{i,j}$$

or

$$\frac{1}{(\Delta l)^2}\left[u_{i+1,j} - 2u_{i,j} + u_{i-1,j} + u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right] = -\rho_{i,j}$$
$$(i = 1, 2, \ldots N; \;\; j = 1, 2, \ldots M)$$

Construct a vector $\mathbf{v}$ of length $N.M$ by linking together the *rows* of the matrix $\{u_{i,j}\}$:

$$v_r \;=\; u_{i,j}\,, \quad \text{with} \;\; r = (i-1)M + j$$

The potential equation then reads

$$v_{r-M} + v_{r-1} - 4v_r + v_{r+1} + v_{r+M} = -(\Delta l)^2 \rho_r$$

or

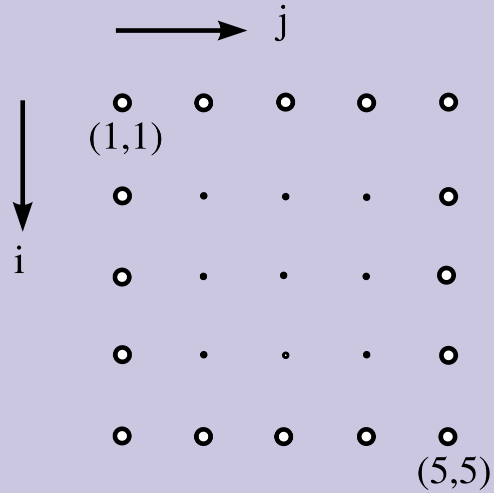
$$\mathbf{A} \cdot \mathbf{v} \;=\; \mathbf{b}$$

with $\mathbf{b} \equiv -(\Delta l)^2 \{\rho_1, \ldots \rho_{N.M}\}^T$ and

$$\mathbf{A} \;\equiv\; \begin{pmatrix} -4 & 1 & \ldots & 1 & & \\ 1 & -4 & 1 & & \ddots & \\ \vdots & \ddots & \ddots & \ddots & & \\ 1 & & & & & \\ & \ddots & & & & \end{pmatrix}$$

Treating the boundaries:

Assume $u_{i,j} = u^0_{i,j}$ to be given along the sides: $\Longrightarrow v_1 = u^0_{1,1}$ etc.



At the interior points we have

$$-4v_7 + v_8 + v_{12} \quad = \quad -(\Delta l)^2 \rho_{2,2} - u^0_{2,1} - u^0_{1,2}$$

etc., yielding a modified system matrix $\mathbf{A}$ and vector $\mathbf{b}$.

Relaxation and Multigrid Techniques

Now apply any one of the iterative techniques to solve for the vector $\mathbf{v}$. In particular, the Jacobi scheme reads

$$\mathbf{v}^{n+1} = \left[\mathbf{I} + \frac{1}{4}\mathbf{A}\right] \cdot \mathbf{v}^{n} + \frac{(\Delta l)^2}{4}\boldsymbol{\rho}$$

$\mathbf{A}$ sparsely populated $\Longrightarrow$Gauss-Seidel, SOR

To speed up convergence, use the *multigrid* method:

– Relax the small-wavelength modes of u on the fine grid
– Double the grid width (coarsening) to get faster relaxation for the long modes
– Interpolate to recover the fine grid

Of course, this is done in a *cascade*, going back and forth between very coarse and fine grids.

ADI Method for the Potential Equation

Alternating Direction Implicit technique: In addition to $\mathbf{v}$, construct another long vector $\mathbf{w}$ by linking together the *columns* of the matrix $\{u_{i,j}\}$:

$$w_s = u_{i,j}\,, \quad \text{with } s = (j-1)N + i$$

The discretized potential equation is then

$$w_{s+1} - 2w_s + w_{s-1} + v_{r+1} - 2v_r + v_{r-1} = -(\Delta l)^2 \rho_{i,j}$$

or

$$\mathbf{A}_1 \cdot \mathbf{v} + \mathbf{A}_2 \cdot \mathbf{w} = \mathbf{b}$$

with *tridiagonal* matrices $\mathbf{A}_1$ and $\mathbf{A}_2$: $\Longrightarrow$Recursion method

Fourier Transform Method (FT)

Let $u_{0,l} = u_{M,l}$ and $u_{k,0} = u_{k,N}$ (periodic boundary conditions.) Then we may write

$$u_{k,l} = \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} U_{m,n} e^{-2\pi i\, km/M} e^{-2\pi i\, nl/N}$$

with

$$U_{m,n} = \sum_{k=0}^{M-1} \sum_{l=0}^{N-1} u_{k,l} e^{2\pi i\, km/M} e^{2\pi i\, nl/N}$$

A similar expansion is used for the charge density $\rho_{k,l}$:

$$R_{m,n} = \sum_{k=0}^{M-1} \sum_{l=0}^{N-1} \rho_{k,l} e^{2\pi i\, km/M} e^{2\pi i\, nl/N}$$

Inserting these expressions in

$$u_{k+1,l} - 2u_{k,l} + u_{k-1,l} + u_{k,l+1} - 2u_{k,l} + u_{k,l-1} \quad = \quad -(\Delta l)^2 \rho_{k,l}$$

we find

$$U_{m,n} \quad = \quad \frac{-R_{m,n}(\Delta l)^2}{2[\cos 2\pi m/M + \cos 2\pi n/N - 2]}$$

FT method for periodic boundary conditions:

- Determine $R_{m,n}$ by Fourier analysis of $\rho_{k,l}$
- Compute $U_{m,n}$ from $R_{m,n}$ according to the above equation
- Insert $U_{m,n}$ in the Fourier series for $u_{k,l}$

Use Fast Fourier Transform! (N ln N operations instead of N^2.)

Variants of the method cover other than periodic boundary conditions.