Poisson equation

$$\nabla^2 \phi(\vec{r}) = -4\pi\rho(\vec{r}) \quad \text{(CGS)}$$

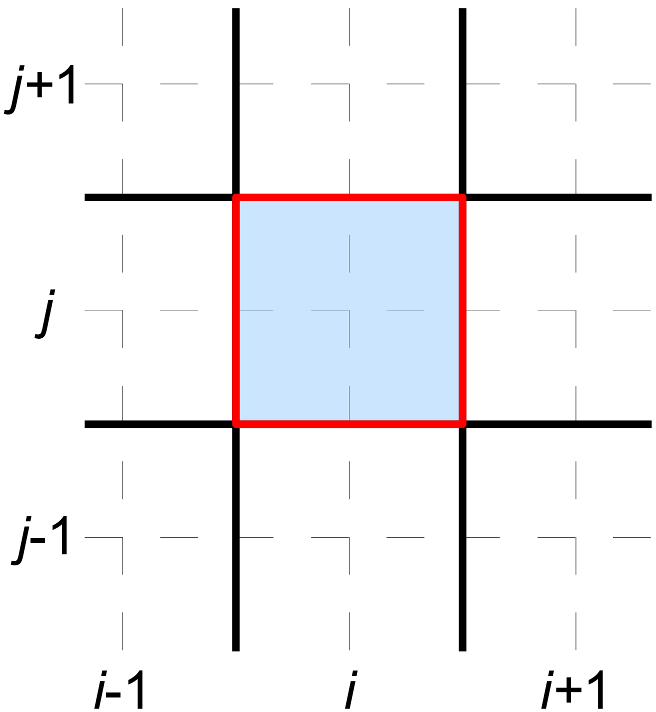
Finite volume method

General approach: divide the space into small volumes and look at the fluxes of some quantity between the volumes.

In electrostatics, we have Gauss theorem:

$$\oint_{\partial V} \vec{E}(\vec{r})\cdot\vec{n}\,dS = -\oint_{\partial V} \nabla\phi(\vec{r})\cdot\vec{n}\,dS = 4\pi\int_V \rho(\vec{r})\,dV$$

Consider division into small cubic volumes V_{ijk}. $\oint_{\partial V} \nabla\phi(\vec{r})\cdot\vec{n}\,dS = -4\pi Q_{ijk}$



$$\oint_{\partial V} \nabla\phi\cdot\vec{n}\,dS \approx$$

$$h^2\left(\frac{\partial\phi}{\partial x}(x_{i+1/2}, y_j, z_k) - \frac{\partial\phi}{\partial x}(x_{i-1/2}, y_j, z_k) + \frac{\partial\phi}{\partial y}(x_i, y_{j+1/2}, z_k) - \frac{\partial\phi}{\partial y}(x_i, y_{j-1/2}, z_k) + \frac{\partial\phi}{\partial z}(x_i, y_j, z_{k+1/2}) - \frac{\partial\phi}{\partial z}(x_i, y_j, z_{k-1/2})\right)$$

$$\oint_{\partial V} \nabla\phi\cdot\vec{n}\,dS \approx -h^2\left(\frac{\partial\phi}{\partial x}(x_{i+1/2},y_j,z_k)-\frac{\partial\phi}{\partial x}(x_{i-1/2},y_j,z_k)+\frac{\partial\phi}{\partial y}(x_i,y_{j+1/2},z_k)\right.$$
$$\left.-\frac{\partial\phi}{\partial y}(x_i,y_{j-1/2},z_k)+\frac{\partial\phi}{\partial z}(x_i,y_j,z_{k+1/2})-\frac{\partial\phi}{\partial z}(x_i,y_j,z_{k-1/2})\right)$$

Approximate by centred differences:

$$\oint_{\partial V} \nabla\phi\cdot\vec{n}\,dS \approx h\big[\phi(x_{i+1},y_j,z_k)-\phi(x_i,y_j,z_k)-\phi(x_i,y_j,z_k)$$
$$+\phi(x_{i-1},y_j,z_k)+\phi(x_i,y_{j+1},z_k)-\phi(x_i,y_j,z_k)$$
$$-\phi(x_i,y_j,z_k)+\phi(x_i,y_{j-1},z_k)+\phi(x_i,y_j,z_{k+1})$$
$$-\phi(x_i,y_j,z_k)-\phi(x_i,y_j,z_k)+\phi(x_i,y_j,z_{k-1})\big]\approx -4\pi Q_{ijk}$$

$Q_{ijk}\approx h^3\rho(x_i,y_j,z_k)$ gives the standard discretization of the Poisson eq.

So what are the advantages?

1) the volumes don't need to be cubic – can have some arbitrary mesh, like in finite element methods;

2) easy treatment of discrete charges, surface charges, etc.

3) variable ε, including discontinuities: $\oint_{\partial V} \epsilon(\vec{r})\nabla\phi(\vec{r})\cdot\vec{n}\,dS = -4\pi Q_{ijk}$

Initial-value problems for PDEs

Parabolic equations

Diffusion equation: $\frac{\partial c(\vec{r},t)}{\partial t} = \nabla \cdot [D(\vec{r}) \nabla c(\vec{r},t)]$

c is the particle concentration

Can be obtained from Fick's first law: flux $\vec{J}(\vec{r},t) = -D(\vec{r}) \nabla c(\vec{r},t)$.

Boundary conditions for space variables:

$c(\vec{r},t)|_\Gamma = f(\vec{r},t)$ (Dirichlet) or $\left.\frac{\partial c(\vec{r},t)}{\partial n}\right|_\Gamma = f(\vec{r},t)$ (Neumann)

Initial condition for the time variable: $c(\vec{r},0) = c_0(\vec{r})$.

Total particle number $N(t) = \int c(\vec{r},t)\, dV$

$$\frac{dN(t)}{dt} = \frac{\partial \int c(\vec{r},t)\, dV}{\partial t} = \int \nabla \cdot [D(\vec{r}) \nabla c(\vec{r},t)]\, dV = \oint_{\partial V} D(\vec{r}) \vec{J}(\vec{r},t) \cdot \vec{n}\, dS$$
$$= \oint_{\partial V} \frac{\partial c(\vec{r},t)}{\partial n} dS.$$

For Neumann BC with f=0 N is conserved (reflecting BC). Dirichlet BC are also called absorbing.

$$\frac{\partial u(\vec{r},t)}{\partial t} = \nabla\cdot[D(\vec{r})\nabla u(\vec{r},t)] \qquad u(\vec{r},t)\big|_\Gamma = 0 \text{ or } \left.\frac{\partial u(\vec{r},t)}{\partial n}\right|_\Gamma = 0$$

Separation of variables $u(\vec{r},t) = R(\vec{r})T(t)$.

$$R(\vec{r})\frac{dT(t)}{dt} = T(t)\nabla\cdot[D(\vec{r})\nabla R(\vec{r})] \Rightarrow \frac{T'(t)}{T(t)} = \frac{\nabla\cdot[D(\vec{r})\nabla R(\vec{r})]}{R(\vec{r})}$$

$$T'(t) = -\lambda T(t) \Rightarrow T(t) = T_0 e^{-\lambda t}. \qquad \nabla\cdot[D(\vec{r})\nabla R(\vec{r})] = -\lambda R(\vec{r}).$$

Elliptic eigenvalue problem with the same boundary conditions. Suppose we know the solution. If the eigenvalues are λ_n and the corresponding eigenfunctions are $R_n(\vec{r})$, then the general solution is

$$u(\vec{r},t) = \Sigma_n C_n R_n(\vec{r}) e^{-\lambda_n t}. \qquad \int R_m(\vec{r}) R_n(\vec{r})\, dV = 0,\ \lambda_m \neq \lambda_n$$

The mode with the smallest $\lambda_n \equiv \lambda_1$ decays the slowest. Conversely, if we solve the parabolic equation corresponding to the given elliptic equation starting with an arbitrary initial condition, then, unless the initial condition has no "overlap" with R_1, at long times

$$u(\vec{r},t) \sim R_1(\vec{r}) e^{-\lambda_1 t}.$$

Numerical methods

$$\frac{\partial u(\vec{r},t)}{\partial t}=\nabla\cdot[D(\vec{r})\nabla u(\vec{r},t)]$$

Discretize in space, but not in time. Semi-discrete problem.

For simplicity, 1D, *D* = const. $$\frac{\partial u(x,t)}{\partial t}=D\frac{\partial^2 u(x,t)}{\partial x^2}$$

$$\frac{d u_m(t)}{d t}=D\frac{u_{m+1}(t)-2u_m(t)+u_{m-1}(t)}{h^2} \qquad u_0(t)=0,\ u_M(t)=0$$

A set of *M*-1 ODEs. In principle, can use standard methods for solving ODEs.

General principles: 1) different methods have different orders of accuracy; 2) explicit methods have a limited range of stability; 3) some implicit methods are always stable.

Particularly important, because the resulting system turns out to be stiff.

Method of lines.

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} \qquad u(x,t) = u(x)e^{-\lambda t} \qquad D\frac{d^2 u(x)}{d x^2} = -\lambda u(x)$$

$$u(x) = \sin kx \qquad \lambda = Dk^2 \qquad \text{For } u(0,t) = u(L,t) = 0,\ u_n(x) = \sin\frac{\pi n}{L}x$$

Semi-discrete equation

$$\frac{d u_m(t)}{d t} = D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{h^2}$$

Since this is a linear system with constant coefficients, there should also be solutions of the form $e^{-\lambda t}$.

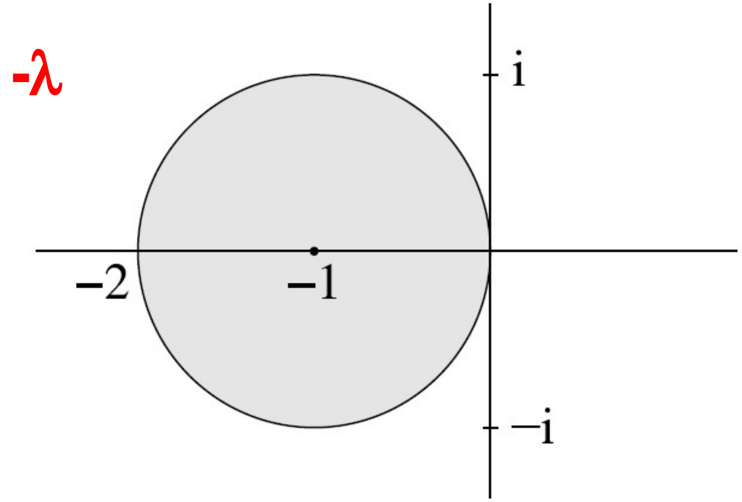
Guess: $u_m(t) = e^{ikhm - \lambda t}$. $\qquad -\lambda e^{ikhm-\lambda t} = \frac{D}{h^2}\left(e^{ikh(m+1)-\lambda t} - 2e^{ikhm-\lambda t} + e^{ikh(m-1)-\lambda t}\right)$

$$-\lambda = \frac{D}{h^2}\left(e^{ikh} - 2 + e^{-ikh}\right) \Rightarrow \lambda = \frac{2D}{h^2}(1 - \cos kh) = \frac{4D}{h^2}\sin^2\frac{kh}{2}$$

All modes decay.

Largest k is π/h; then repeats periodically. $\lambda = 4D/h^2$. Smallest k is π/h. $\lambda = \pi^2 D/L^2$. Ratio of the largest and smallest λ is $\sim L^2/h^2$. Stiff.

$$\lambda \approx \frac{2D}{h^2}\left((kh)^2/2 - (kh)^4/24 + \ldots\right) = Dk^2\left(1 + O\left((kh)^2\right)\right).$$



Gustafsson, Fundamentals of Scientific Computing

Even Euler method can be stable, if the time step is not too large.

$$\frac{d\,u_m(t)}{d\,t}=D\frac{u_{m+1}(t)-2u_m(t)+u_{m-1}(t)}{h^2}$$

$$\dot{\vec{u}}=\vec{f}(\vec{u}) \qquad \vec{u}^{n+1}=\vec{u}^n+\tau\vec{f}(\vec{u}^n)$$

$$u_m^{n+1}=u_m^n+\frac{D\tau}{h^2}\left(u_{m+1}^n-2u_m^n+u_{m-1}^n\right)$$

Forward-time centred-space (FTCS) scheme

For continuous time we had $u_m(t)=e^{ikhm-\lambda t}$. $\qquad u_m^n=e^{ikhm-\lambda\tau n}$

$$e^{ikhm-\lambda\tau(n+1)}=e^{ikhm-\lambda\tau n}+\frac{D\tau}{h^2}\left(e^{ikh(m+1)-\lambda\tau n}-2e^{ikhm-\lambda\tau n}+e^{ikh(m-1)-\lambda\tau n}\right)$$

$$e^{-\lambda\tau}=1+\frac{D\tau}{h^2}\left(e^{ikh}-2+e^{-ikh}\right) \Rightarrow \lambda=-\frac{1}{\tau}\ln\left[1-\frac{2D\tau}{h^2}\{1-\cos(kh)\}\right]$$

$$=-\frac{1}{\tau}\ln\left[1-\frac{4D\tau}{h^2}\sin^2(kh/2)\right].$$

Von Neumann stability analysis

Stability: Re λ ≥ 0 for all k.

$$\left|1-\frac{4D\tau}{h^2}\sin^2(kh/2)\right|\le 1 \Rightarrow \tau\le\frac{h^2}{2D}$$

Stability criterion $\tau \le \tau_{\max} = \dfrac{h^2}{2D}$. Rather stringent: quadratic in mesh step

$O(h^2) + O(\tau) = O(h^2)$ Does not really make sense to use a higher-order explicit method for time evolution: the stability ranges of all of them are not very different, so $\tau \sim h^2$ anyway, and then the time scheme is **too** accurate.

In fact, trying to be 2nd order in time can make things worse. Richardson (1910) – leapfrog method.

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

Take centred difference in time.

$$u_m^n = e^{ikhm - \lambda \tau n}$$

$$\frac{u_m^{n+1} - u_m^{n-1}}{2\tau} = D \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{h^2}$$

$$\frac{e^{-\lambda\tau} - e^{\lambda\tau}}{2\tau} = \frac{2D}{h^2}(\cos kh - 1)$$

Denote $e^{-\lambda\tau} \equiv G,\ b \equiv \dfrac{4D\tau}{h^2}(1 - \cos kh)$. $G - 1/G = -b \ \Rightarrow\ G = \dfrac{-b \pm \sqrt{b^2+4}}{2}$

For $b \neq 0$, one of the roots always has $|G|>1 \Rightarrow \lambda < 0$.

Unconditionally unstable!

On the other hand, going back to the FTCS scheme, since the error is

$O(h^2)+O(\tau)$ and τ has to be $O(h^2)$, these terms may cancel out

giving a higher-order method.

$$\lambda = -\frac{1}{\tau}\ln\left[1-\frac{2D\tau}{h^2}\{1-\cos(kh)\}\right]$$
$$= -\frac{1}{\tau}\ln\left[1-\frac{2D\tau}{h^2}\{(kh)^2/2-(kh)^4/24+O((kh)^6)\}\right]$$
$$= \frac{2D}{h^2}\{(kh)^2/2-(kh)^4/24+O((kh)^6)\}+\frac{D^2k^4\tau}{2} = Dk^2\left[1+(kh)^2\left(\frac{D\tau}{2h^2}-\frac{1}{12}\right)+O((kh)^4)\right]$$

When $\tau = \frac{h^2}{6D} = \frac{\tau_{max}}{3}$, the method is $O(h^4)$.

M.V. Chubynsky and G.W. Slater, Phys. Rev. E 85, 016709.

$$u_m^{n+1} = u_m^n + \frac{D\tau}{h^2}\left(u_{m+1}^n(t) - 2u_m^n(t) + u_{m-1}^n(t)\right)$$

For $\tau = \tau_{\max} = \dfrac{h^2}{2D}$, $u_m^{n+1} = \dfrac{1}{2}\left(u_{m+1}^n + u_{m-1}^n\right)$

Suppose u_m^n is 1 for even *m* and 0 for odd *m*. Then u_m^{n+1} will be 0 for even *m* and 1 for odd *m*. Will oscillate forever. For larger τ this mode will grow.

Boundary conditions are implemented as before: fix u on the boundary for Dirichlet and introduce ghost sites for Neumann. FTCS does conserve the particle number for reflecting BC or in infinite space.

The small time step is needed to take care of short-wavelength modes. But they die down rapidly, so after a short while we don't care about them. But cannot ignore them, because if the method is unstable, they will grow back. As we know for ODEs, the way to deal with that is implicit schemes that are stable for arbitrarily large steps.

A trick that does not really work:

Unconditionally unstable leapfrog

$$\frac{u_m^{n+1}-u_m^{n-1}}{2\tau}=D\frac{u_{m+1}^n-2u_m^n+u_{m-1}^n}{h^2}$$

Try to remove the instability by making it implicit:

$$\frac{u_m^{n+1}-u_m^{n-1}}{2\tau}=D\frac{u_{m+1}^n-\left(u_m^{n+1}+u_m^{n-1}\right)+u_{m-1}^n}{h^2}$$

Dufort-Frankel scheme

It turns out it is unconditionally stable. Moreover, even though it looks implicit, it's a linear equation for u_m^{n+1}, so we can solve it. However,

$$\frac{u_{m+1}^n-\left(u_m^{n+1}+u_m^{n-1}\right)+u_{m-1}^n}{h^2}=\frac{u_{m+1}^n-2u_m^n+u_{m-1}^n}{h^2}-\frac{u_m^{n+1}-2u_m^n+u_m^{n-1}}{h^2}$$

$$\rightarrow\frac{\partial^2 u}{\partial x^2}-\frac{\tau^2}{h^2}\frac{\partial^2 u}{\partial t^2}$$

So it is only a correct representation of the diffusion equation, when $\tau \ll h$, and we have not gained anything.

$$\frac{d\,u_m(t)}{d\,t}=D\frac{u_{m+1}(t)-2u_m(t)+u_{m-1}(t)}{h^2}$$

Backward Euler: $\dot{\vec{u}}=\vec{f}(\vec{u})$ $\quad\vec{u}^{n+1}=\vec{u}^n+\tau\vec{f}(\vec{u}^{n+1})$

$$u_m^{n+1}=u_m^n+\frac{D\tau}{h^2}(u_{m+1}^{n+1}-2u_m^{n+1}+u_{m-1}^{n+1})$$

Backward-time centred-space (BTCS) scheme.

A tridiagonal set of equations for u_m^{n+1}

For FTCS we had: $\lambda=-\frac{1}{\tau}\ln\left[1-\frac{2D\tau}{h^2}\{1-\cos(kh)\}\right]$ $\quad u_m^n=e^{ikhm-\lambda\tau n}$

$$e^{ikhm-\lambda\tau(n+1)}=e^{ikhm-\lambda\tau n}+\frac{D\tau}{h^2}\left(e^{ikh(m+1)-\lambda\tau(n+1)}-2e^{ikhm-\lambda\tau(n+1)}+e^{ikh(m-1)-\lambda\tau(n+1)}\right)$$

$$1=e^{\lambda\tau}+\frac{D\tau}{h^2}\left(e^{ikh}-2+e^{-ikh}\right)\;\Rightarrow\;\lambda=\frac{1}{\tau}\ln\left[1+\frac{2D\tau}{h^2}\{1-\cos(kh)\}\right]$$

$\lambda \geq 0$ always. Unconditionally stable. But now 1st order accuracy is an issue.

$$\frac{du_m(t)}{dt} = D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{h^2}$$

Trapezoidal method: $\dot{\vec{u}} = \vec{f}(\vec{u})$ $\quad\quad$ $\vec{u}^{n+1} = \vec{u}^n + \frac{\tau}{2}[\vec{f}(\vec{u}^n) + \vec{f}(\vec{u}^{n+1})]$

$$u_m^{n+1} = u_m^n + \frac{D\tau}{2h^2}(u_{m+1}^{n+1} - 2u_m^{n+1} + u_{m-1}^{n+1} + u_{m+1}^n - 2u_m^n + u_{m-1}^n)$$

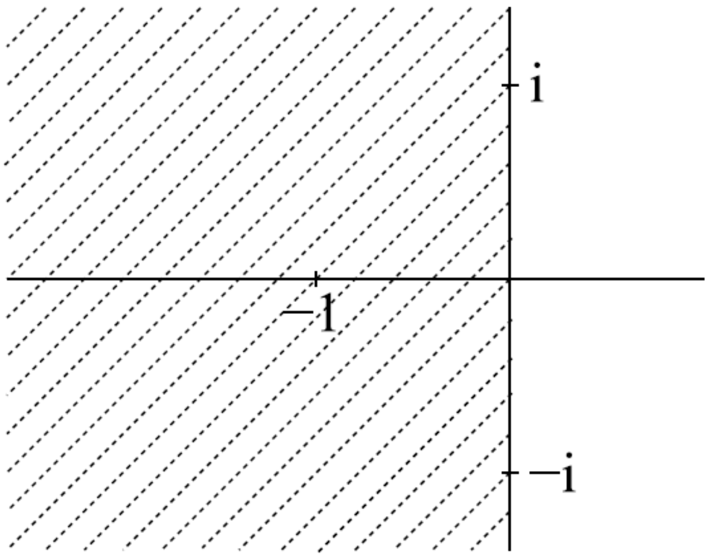
Crank-Nicolson scheme (often misspelled Nic**h**olson). 2^{nd} order in time as well

$$e^{ikhm - \lambda\tau(n+1)} = e^{ikhm - \lambda\tau n} + \frac{D\tau}{2h^2}\left(e^{ikh(m+1) - \lambda\tau(n+1)} - 2e^{ikhm - \lambda\tau(n+1)} + e^{ikh(m-1) - \lambda\tau(n+1)}\right)$$
$$+ \frac{D\tau}{2h^2}\left(e^{ikh(m+1) - \lambda\tau n} - 2e^{ikhm - \lambda\tau n} + e^{ikh(m-1) - \lambda\tau n}\right)$$

$$e^{-\lambda\tau} - 1 = \frac{D\tau}{h^2}(\cos kh - 1)(e^{-\lambda\tau} + 1) \quad\quad e^{-\lambda\tau} \equiv G \quad\quad \frac{D\tau}{h^2}(1 - \cos kh) \equiv b$$

$$G - 1 = -b(G + 1)$$

$$G = \frac{1 - b}{1 + b}$$ $\quad$ |G| < 1 for b > 0. $\quad$ Unconditionally stable.



Recall a nice property of the trapezoidal scheme: if an ODE has a solution $\sim e^{\lambda t}$ with purely imaginary λ, the trapezoidal scheme preserves this property.

Useful for solving the time-dependent Schrödinger equation

Rescale *t* and *x* to get $i\frac{\partial\psi}{\partial t}=-\frac{\partial^2\psi}{\partial x^2}+V(x)\psi$ $\qquad i\frac{\partial\psi}{\partial t}=\hat{H}\psi$

If *V*(*x*) = 0 and there are no boundaries, we can still look for a solution of the form $\psi(x,t)=\exp(-\lambda t+ikx)$. $\qquad -i\lambda=k^2 \;\Rightarrow\; \lambda=ik^2$.

The wave function preserves its norm; the evolution operator is unitary.

$$\int|\psi(x,t)|^2 dx=\text{const} \qquad \psi(x,t)=e^{-i\hat{H}t}\psi(x,0)$$

Need $\psi_j^{n+1}=\hat{U}\psi_j^n,\; \hat{U}^H\hat{U}=\hat{I}$ $\qquad \int(U\psi)^*(U\psi)\,dx=\int\psi^*(U^H U\psi)\,dx=\int\psi^*\psi\,dx$

$$\frac{\partial \psi}{\partial t} = -i\left(-\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi\right) = -i\hat{H}\psi$$

$$\hat{H}\psi = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$ Discretized $$\hat{\tilde{H}}\psi_m^n = -\frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{h^2} + V_m \psi_m^n$$

Forward Euler method is unstable for purely imaginary λ. For FTCS,

$$\psi_m^{n+1} = \psi_m^n - i\tau\hat{\tilde{H}}\psi_m^n \qquad \psi_m^{n+1} = (1 - i\tau\hat{\tilde{H}})\psi_m^n$$

$$(1 - i\tau\hat{\tilde{H}})^H (1 - i\tau\hat{\tilde{H}}) = (1 + i\tau\hat{\tilde{H}})(1 - i\tau\hat{\tilde{H}}) = 1 + \tau^2\hat{\tilde{H}}^2 \neq 1$$

In Backward Euler method modes with purely imaginary λ decay. For BTCS,

$$\psi_m^{n+1} = \psi_m^n - i\tau\hat{\tilde{H}}\psi_m^{n+1} \qquad \psi_m^{n+1} = (1 + i\tau\hat{\tilde{H}})^{-1}\psi_m^n$$

$$(1 + i\tau\hat{\tilde{H}})^{-H}(1 + i\tau\hat{\tilde{H}})^{-1} = [(1 + i\tau\hat{\tilde{H}})(1 - i\tau\hat{\tilde{H}})]^{-1} = (1 + \tau^2\hat{\tilde{H}}^2)^{-1} \neq 1$$

$$\frac{\partial \psi}{\partial t}=-i\left(-\frac{\partial^2 \psi}{\partial x^2}+V(x)\psi\right)=-i\hat{H}\psi$$

$$\hat{H}\psi=-\frac{\partial^2 \psi}{\partial x^2}+V(x)\psi$$ Discretized $$\hat{\tilde{H}}\psi_m^n=-\frac{\psi_{m+1}^n-2\psi_m^n+\psi_{m-1}^n}{h^2}+V_m\psi_m^n$$

In the trapezoidal method, the oscillations do not grow nor decay.

For Crank-Nicolson,

$$\psi_m^{n+1}=\psi_m^n-(i\tau\hat{\tilde{H}}/2)(\psi_m^n+\psi_m^{n+1})$$ $$(1+i\tau\hat{\tilde{H}}/2)\psi_m^{n+1}=(1-i\tau\hat{\tilde{H}}/2)\psi_m^n$$

$$\psi_m^{n+1}=(1+i\tau\hat{\tilde{H}}/2)^{-1}(1-i\tau\hat{\tilde{H}}/2)\psi_m^n$$

$$[(1+i\tau\hat{\tilde{H}}/2)^{-1}(1-i\tau\hat{\tilde{H}}/2)]^H(1+i\tau\hat{\tilde{H}}/2)^{-1}(1-i\tau\hat{\tilde{H}}/2)=$$

$$(1-i\tau\hat{\tilde{H}}/2)^{-1}(1+i\tau\hat{\tilde{H}}/2)(1+i\tau\hat{\tilde{H}}/2)^{-1}(1-i\tau\hat{\tilde{H}}/2)=1$$

Can also see from von Neumann analysis. We had

$$e^{-\lambda\tau}\equiv G \qquad G=\frac{1-b}{1+b} \qquad b\rightarrow ib \qquad \left|\frac{1-ib}{1+ib}\right|=1$$

Another, explicit possibility is, surprisingly, the leapfrog method

$$\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2\tau}=-i\,\hat{\tilde{H}}\,\psi_m^n \;\Rightarrow\; \psi_m^{n+1}=\psi_m^{n-1}-2i\tau\,\hat{\tilde{H}}\,\psi_m^n$$

$$e^{-\lambda\tau}\equiv G,\; b\equiv\frac{4D\tau}{h^2}(1-\cos kh). \qquad G=\frac{-b\pm\sqrt{b^2+4}}{2}$$

$$b\to ib \;\Rightarrow\; G=\frac{-i|b|\pm\sqrt{-|b|^2+4}}{2} \qquad |G|=\frac{\sqrt{4-|b|^2+|b|^2}}{2}=1,\; |b|<2$$

Need $\psi_m^1=e^{-i\tau\hat{H}}\psi_m^0\approx\sum_{j=0}^2\frac{(-i\tau\,\hat{\tilde{H}})^j}{j!}\psi_m^0$

Higher dimensions

Of course, the explicit methods (FTCS for diffusion eq. and leapfrog for Schrodinger eq.) can be generalized straightforwardly.

$$\frac{\partial u(x,y,t)}{\partial t}=D\left(\frac{\partial^2 u(x,y,t)}{\partial x^2}+\frac{\partial^2 u(x,y,t)}{\partial y^2}\right)+D f(x,y)$$

$$u_{j,l}^{n+1}=u_{j,l}^{n}+\frac{D\tau}{h^2}(u_{j+1,l}^{n}+u_{j-1,l}^{n}+u_{j,l+1}^{n}+u_{j,l-1}^{n}-4u_{j,l}^{n})+\tau D f_{j,l}$$

In this case, $\tau_{\max}=h^2/4D$

$$u_{j,l}^{n+1}=\frac{1}{4}(u_{j+1,l}^{n}+u_{j-1,l}^{n}+u_{j,l+1}^{n}+u_{j,l-1}^{n})+\frac{h^2}{4}f_{j,l}$$

This is exactly the Jacobi iteration for the elliptic problem

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

Higher dimensions

It is possible in principle to use the Crank-Nicolson method in higher dimensions, but the matrix will not be tridiagonal, but rather will have a structure similar to that we encountered for elliptic equations.

Alternating direction implicit (ADI) method: split each step into 2 substeps, treating 1 direction implicitly and the other explicitly in each substep.

$$u_{j,l}^{n+1/2}=u_{j,l}^{n}+\frac{D\tau}{2h^2}\left(u_{j+1,l}^{n+1/2}-2u_{j,l}^{n+1/2}+u_{j-1,l}^{n+1/2}+u_{j,l+1}^{n}-2u_{j,l}^{n}+u_{j,l-1}^{n}\right)$$

$$u_{j,l}^{n+1}=u_{j,l}^{n}+\frac{D\tau}{2h^2}\left(u_{j+1,l}^{n+1/2}-2u_{j,l}^{n+1/2}+u_{j-1,l}^{n+1/2}+u_{j,l+1}^{n+1}-2u_{j,l}^{n+1}+u_{j,l-1}^{n+1}\right)$$

A particular case of general operator splitting methodology (if there are several terms, each can be treated in a separate substep), although with a slightly different twist.

Nonlinear equations

Straightforward with explicit methods. Hard with implicit methods. Lagging nonlinear coefficients, iteration, Newton's method.