Explicit scheme

So far considered a **fully explicit** scheme to numerically solve the diffusion equation:

$$T_j^{n+1} = (1-2s)\,T_j^n + s(T_{j+1}^n + T_{j-1}^n) \qquad (1)$$

with $s = \frac{\kappa \Delta t}{(\Delta x)^2}$.
Only stable for $s < 1/2$. This scheme is sometimes referred to as FTCS (forward time centered space). It is fully explicit, since T_j^{n+1} can be computed from known quantities at time $n\Delta t$.

Advantage: Easy to solve numerically, because it's explicit.
Disadvantage: Usually interested in features of size $\lambda \gg \Delta x$. Let t_λ be the time to diffuse a distance λ, which is $\propto \lambda^2/\kappa$. In order to satisfy stability criterion, need
$\propto t_\lambda/\Delta t \propto (\lambda^2/\kappa)/(\Delta x^2/\kappa) \propto \lambda^2/\Delta x^2 \gg 1$ time steps before things happen on the scale of interest. Computationally expensive/prohibitive.

Notes

Fully implicit scheme

There are other ways to discretize the diffusion equation. Consider the following difference scheme:

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = \kappa \frac{T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1}}{(\Delta x)^2} \qquad (2)$$

This is very similar to FTCS, except that the spatial derivative on the RHS is evaluated at time step $(n+1)$, not n.

This scheme is called **fully implicit** or **backward time**. In contrast to the fully explicit scheme, $T_j^{n=1}$ cannot be solved purely in terms of function values at time step n

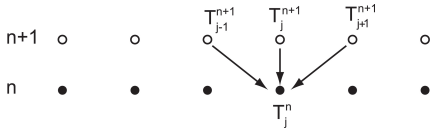
Notes

Fully implicit scheme

Why is it called *backward time* ? Rearranging yields

$$T_j^n = -sT_{j-1}^{n+1} + (1+2s)\,T_j^{n+1} - sT_{j+1}^{n+1} \qquad (3)$$

where $s = \kappa \Delta t/\Delta x^2$.



Therefore, one can obtain (explicitly) T_j^n in terms of values of the *next* time step $(n+1)$. This is not what we want, however.

Notes

Fully implicit scheme

In order to obtain the function values at time step $(n+1)$ need to solve a set of simultaneous linear equations (eq.(3)), which can be cast in matrix form:

$$\begin{pmatrix} -s & (1+2s) & -s & 0 & \cdots \\ 0 & -s & (1+2s) & -s & \cdots \\ \vdots & \ddots & \ddots & \cdots & \\ \vdots & \ddots & \ddots & \cdots & \\ & \cdots & -s & (1+2s) & -s \end{pmatrix} \begin{pmatrix} T_0^{n+1} \\ T_1^{n+1} \\ T_2^{n+1} \\ \vdots \\ T_J^{n+1} \end{pmatrix} = \begin{pmatrix} T_0^n \\ T_1^n \\ T_2^n \\ \vdots \\ T_J^n \end{pmatrix}$$

Notes

Fully implicit scheme

Do matrix inversion to obtain the function values at time step $(n+1)$.

$$\begin{pmatrix} T_0^{n+1} \\ T_1^{n+1} \\ T_2^{n+1} \\ \vdots \\ T_J^{n+1} \end{pmatrix} = \begin{pmatrix} -s & (1+2s) & -s & 0 & \cdots \\ 0 & -s & (1+2s) & -s & \cdots \\ \vdots & \ddots & \ddots & \cdots & \\ \vdots & \ddots & \ddots & \cdots & \\ & \cdots & -s & (1+2s) & -s \end{pmatrix}^{-1} \begin{pmatrix} T_0^{n} \\ T_1^{n} \\ T_2^{n} \\ \vdots \\ T_J^{n} \end{pmatrix}$$

Since matrix is *tridiagonal*, efficient algorithms exist to invert matrix. Also, if κ is a constant, s is constant and inversion only has to be done once.

Notes

Fully implicit scheme

Is it stable? Let's do von Neumann stability analysis:
Substitute $T_j^n = \xi^n e^{ikj\Delta x}$ into the difference scheme:

$$\begin{aligned} T_j^n &= -sT_{j-1}^{n+1} + (1+2s)T_j^{n+1} - sT_{j+1}^{n+1} \\ \xi^n e^{ikj\Delta x} &= -s\xi^{n+1}e^{ik(j-1)\Delta x} + (1+2s)\xi^{n+1} - s\xi^{n+1}e^{ik(j+1)\Delta x} \\ 1 &= -s\xi e^{-ik\Delta x} + (1+2s)\xi - s\xi e^{ik\Delta x} \\ \xi &= \frac{1}{1+2s-s(e^{ik\Delta x}+e^{-ik\Delta x})} \\ \xi &= \frac{1}{1+2s(1-\cos(k\Delta x))} \\ \xi &= \frac{1}{1+4s(\sin(k\Delta x/2))^2} \end{aligned}$$

Since $\sin^2 \geq 0$, $\xi \leq 1$ for all k, the fully implicit scheme is **unconditionally stable**.

Notes

Improving upon the implicit scheme

Even though the fully implicit scheme is unconditionally stable, the accuracy has not improved. While it is second order accurate in the spatial part, it is only first order accurate in the temporal part.

We can improve the fully implicit scheme by *averaging* the explicit and implicit difference scheme:

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = \frac{\kappa}{2}[(\delta^2 T)_j^{n+1} + (\delta^2 T)_j^n] \tag{4}$$

where

$$(\delta^2 T)_j^n = \frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{(\Delta x)^2}$$

Both the LHS and RHS are now centered around $(n+1/2)$, which makes the scheme *second order accurate in time*.
This scheme is known as the **Crank Nicholson scheme**.

Notes

Stability of Crank-Nicholson

How stable is it? Substituting $T_j^n = \xi^n e^{ikj\Delta x}$ into the difference scheme yields an amplification factor

$$\xi = \frac{1 - 2s\left(\sin(\frac{k\Delta x}{2})\right)^2}{1 + 2s\left(\sin(\frac{k\Delta x}{2})\right)^2} \tag{5}$$

which is ≤ 1 for all k.

So the Crank-Nicholson scheme has unconditional stability just like the fully implicit scheme. *In addition it is second order accurate in both time and space.*
Is therefore the recommended method for these types of PDE's.

Notes

Computational implementation

Since the scheme is not fully explicit, we need to solve a set of coupled linear equations.

$$\begin{aligned}\frac{T_j^{n+1}-T_j^n}{\Delta t} &= \frac{\kappa}{2}[(\delta^2 T)_j^{n+1}+(\delta^2 T)_j^n] \\ \frac{T_j^{n+1}-T_j^n}{\Delta t} &= \frac{\kappa}{2}\left[\frac{(T_{j+1}^{n+1}-2T_j^{n+1}+T_{j-1}^{n+1})+(T_{j+1}^n-2T_j^n+T_{j-1}^n)}{(\Delta x)^2}\right]\end{aligned}$$

Regrouping the terms yields

$$-\frac{s}{2}T_{j-1}^{n+1}+(1+s)T_j^{n+1}-\frac{s}{2}T_{j-1}^{n+1}=\frac{s}{2}T_{j-1}^n+(1-s)T_j^n+\frac{s}{2}T_{j-1}$$

Notes

Computational implementation

Again, we can cast the coupled equations into a matrix:

$$\begin{pmatrix} -\frac{s}{2} & (1+s) & -\frac{s}{2} & 0 & \cdots \\ 0 & -\frac{s}{2} & (1+s) & -\frac{s}{2} & \cdots \\ \vdots & \ddots & \ddots & \cdots & \\ \vdots & \ddots & \ddots & \cdots & \\ & \cdots & -\frac{s}{2} & (1+s) & -\frac{s}{2} \end{pmatrix} \begin{pmatrix} T_0^{n+1} \\ T_1^{n+1} \\ T_2^{n+1} \\ \vdots \\ T_J^{n+1} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{s}{2} & (1-s) & \frac{s}{2} & 0 & \cdots \\ 0 & \frac{s}{2} & (1-s) & \frac{s}{2} & \cdots \\ \vdots & \ddots & \ddots & \cdots & \\ \vdots & \ddots & \ddots & \cdots & \\ & \cdots & \frac{s}{2} & (1-s) & \frac{s}{2} \end{pmatrix} \begin{pmatrix} T_0^n \\ T_1^n \\ T_2^n \\ \vdots \\ T_J^n \end{pmatrix}$$

Multiplying by the inverse of the first matrix allows us to compute the T_j^{n+1}.

Notes

Summary

FTCS (fully explicit):First order accurate in time, second order accurate in space.*Conditionally stable:* $\kappa\Delta t/\Delta x^2 \leq 1/2$.Even though easy to implement, the stability criterion imposes small time steps, which is computationally extensive.

Fully implicit:*Unconditionally stable*, but accuracy is the same as for FTCS.

Crank Nicholson:Combines the fully implicit and explicit scheme.The spatial and time derivative are both centered around $n+1/2$.Therefore, the method is second order accurate in time (and space).*Unconditionally stable*.

Crank Nicholson is the recommended method for solving diffusive type equations due to accuracy and stability.

Notes

Higher dimensions

So far considered only one spatial dimension for simplicity. Extensions to higher dimensions is straightforward.Consider the diffusion equation in two dimensions:

$$\frac{\partial T}{\partial t}=\kappa\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)$$

Approximating $T(x,y,t)\approx T(j\Delta x, l\Delta y, n\Delta t)$ and implementing the Crank-Nicholson scheme gives us

$$\frac{T_{j,l}^{n+1}-T_{j,l}^n}{\Delta t}=\frac{\kappa}{2}[(\delta_x^2 T)_{j,l}^n+(\delta_x^2 T)_{j,l}^{n+1}+(\delta_y^2 T)_{j,l}^n+(\delta_y^2 T)_{j,l}^{n+1}]$$

where

$$(\delta_x^2 T)_{j,l}^n=\frac{T_{j+1,l}^n-2T_{j,l}^n+T_{j-1,l}^n}{(\Delta x)^2}$$

and similarly for $(\delta_y^2 T)_{j,l}^n$

Notes

Higher dimensions

Note: Even though the coupled linear equations can be cast into a matrix that is sparse, it is not tridiagonal anymore as for the one dimensional case.

Therefore, computation time can increase significantly.

Note: Methods exits to circumvent this problem (see Numerical recipes book).

Notes

Numerically solving the time-dependent Schrodinger equation

The time-dependent Schrödinger equation has similar structure as the diffusion equation.However, it is not diffusive, but *dispersive*. Solution tends to break up into oscillatory wave packets.

In one spatial dimension the equation reads (with $\hbar = 1$ and $m = 1/2$)

$$i\frac{\partial \psi}{\partial t} = H\psi \tag{6}$$

where $H = -\frac{\partial^2}{\partial x^2} + V(x)$.
If one is given the (*normalized*) initial wave packet $\psi(x, t = 0)$, we may use the finite difference scheme we developed for the diffusion equation.(e.g. BC is that $\psi \to 0$ as $x \to \pm\infty$).We then numerically integrate the Schrödinger's equation in order to find the wave function $\psi(x, t)$ at later times.

Notes

Implicit scheme for the Schrödinger equation

Analogous to the heat equation we can apply the implicit difference scheme.

$$i\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = -\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta x)^2} + V_j\psi_j^{n+1} \tag{7}$$

The von Neumann stability analysis yields

$$\xi = \frac{1}{1 + i\left[\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_j\Delta t\right]} \tag{8}$$

Therefore,

$$|\xi| = \frac{1}{\sqrt{1 + \left[\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) + V_j\Delta t\right]^2}} \leq 1 \tag{9}$$

Notes

Implicit scheme for the Schrödinger equation

Despite the unconditional stability of the implicit scheme, it is not appropriate for solving the Schrödinger equation.

The reason is that the wave function ψ needs to *remain normalized* at all times during the time evolution:

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 1 \tag{10}$$

If the initial condition/wave function $\psi(x, t = 0)$ is normalized, then the Schrödinger equation ensures this normalization condition during the time evolution of the wave packet.

Notes

Unitary requirement

Formally, this can be shown. Let's integrate the Schrödinger equation,

$$i\frac{\partial \psi}{\partial t} = H\psi \tag{11}$$

where the Hamiltonian operator is $H = -\frac{\partial^2}{\partial x^2} + V(x)$.

The formal solution is simply

$$\begin{aligned} \psi(x,t) &= e^{-iHt}\psi(x,0) \\ |\psi(t)\rangle &= e^{-i\hat{H}t}|\psi(0)\rangle \text{ bra-ket notation} \\ \langle\psi(t)| &= \langle\psi(0)|e^{i\hat{H}t} \text{ the conjugate} \end{aligned}$$

Note, that $\hat{H}$ is self-adjoint $\hat{H}^+ = \hat{H}$ and unitary $HH^+ = H^+H = I$

Notes

Unitary requirement

Normalization is guaranteed, since the time evolution operator $e^{-i\hat{H}t}$ is **unitary**.

$$\begin{aligned} \int_{-\infty}^{+\infty} |\psi|^2 dx &= \langle\psi(t)|\psi(t)\rangle \\ &= \langle\psi(0)|e^{i\hat{H}t}e^{-i\hat{H}t}|\psi(0)\rangle \\ &= \langle\psi(0)|\psi(0)\rangle = 1 \end{aligned}$$

The implicit scheme approximates the time evolution $\psi(x,t) = e^{-iHt}\psi(x,0)$ as

$$\begin{aligned} \psi(x,t) &= \frac{1}{e^{iHt}}\psi(x,0) \\ \psi_j^{n+1} &\approx \frac{1}{1+iH\Delta t}\psi_j^n \end{aligned}$$

But the approximation of the time evolution operator $(1+iH\Delta t)^{-1}$ is **not unitary**.

Notes

Unitary requirement

Let's show briefly that this approximation is indeed the implicit scheme:

$$\begin{aligned} (1+iH\Delta t)\psi_j^{n+1} &= \psi_j^n \\ \frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} &= -iH\psi_j^{n+1} \end{aligned}$$

where

$$H\phi_j^n = -\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{(\Delta x)^2} + V_j\psi_j^n$$

Therefore, we have

$$i\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = -\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta x)^2} + V_j\psi_j^{n+1}$$

which is equivalent to eq. (7)

Notes

Caley's form

The FTCS scheme suffers from the same problem. Here, the time evolution is approximated as

$$\begin{aligned} \psi(x,t) &= e^{-iHt}\psi(x,0) \\ \psi_j^{n+1} &\approx (1-iH\Delta t)\psi_j^n \end{aligned}$$

Again, $(1-iH\Delta t)$ is **not unitary**.

We can remedy this problem by using *Caley's form* for the finite difference approximation of e^{-iHt}:

$$\begin{aligned} \psi(x,t) &= e^{-iHt}\psi(x,0) \\ \psi(x,t) &= \frac{e^{-iHt/2}}{e^{iHt/2}}\psi(x,0) \\ \psi_j^{n+1} &\approx \frac{(1-iH\Delta t/2)}{(1+iH\Delta t/2)}\psi_j^n \end{aligned}$$

Notes

Caley's form

The approximation of the time evolution operator

$$e^{-iHt} \approx \frac{(1 - iH\Delta t/2)}{(1 + iH\Delta t/2)}$$

is unitary.

The difference scheme is then

$$(1 + iH\Delta t/2)\psi_j^{n+1} = (1 - iH\Delta t/2)\psi_j^n \qquad (12)$$

which is unconditionally stable, unitary and and second order accurate in space and time. In fact it is the Crank-Nicholson scheme. Rearranging yields

$$i\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \frac{1}{2}(H\psi_j^{n+1} + H\psi_j^n) \qquad (13)$$

Notes

Summary

The Schrödinger equation is an example where stability of the numerical solution alone is not sufficient to obtain good results.

We also want the numerical scheme to obey the unitarity requirement, such that the total probability remains 1.

It happens that the Crank-Nicholson scheme does just that. It interpolates the Hamiltonian between time step n (FTCS) and $(n + 1)$ (implicit).
Example - applet:

`http://www.lifelong-learners.com/pde/com/SYL/s2node7.php`

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