Computational Physics and Astrophysics

Partial Differential Equations: Diffusive Initial Value Problems

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Parabolic PDEs: Heat Equation

Consider the 1D heat equation

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

with D > 0 in the domain $0 \le x \le L$ and $t \ge 0$.

• Boundary conditions:

$$u(0,t) = c_1 u(L,t) = c_2$$

for $t \ge 0$

Initial conditions :

$$u(x,0)=f(x)$$

for $0 \le x \le L$.

Consider the following computational domain:



 $u(x,\!0)\!=\!f(x)$

Mesh spacing:

$$\Delta x = x_{i+1} - x_i = L/(M-1) \quad i = 1, \dots, M-1$$

$$\Delta t = t^{n+1} - t^n = ???$$

Consider the following approximations

$$\partial_t u_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{\Delta t}{2} \partial_t^2 u_i^n$$
$$\partial_x^2 u_i^n = \frac{u_{i+1}^n - 2 u_i^n + u_{i-1}^n}{\Delta x^2} - \frac{\Delta x^2}{12} \partial_x^4 u_i^n$$

Therefore, the heat equation

$$\partial_t u_i^n - D \,\partial_x^2 u_i^n = 0$$

is approximated as

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} - D \, \frac{w_{i+1}^n - 2 \, w_i^n + w_{i-1}^n}{\Delta x^2} = 0$$

Notice that u_i^t is the solution to the exact equations, and w_i^n is the solution to the corresponding finite-difference approximation.

Truncation and Solution Errors

• Solution Error:

$$\epsilon_i^n = w_i^n - u_i^n$$

• Truncation Error:

$$\begin{aligned} \tau_i^n &= \frac{u_i^{n+1} - u_i^n}{\Delta t} - D \frac{u_{i+1}^n - 2 u_i^n + u_{i-1}^n}{\Delta x^2} \\ &= \partial_t u_i^n + \frac{\Delta t}{2} \partial_t^2 u_i^n - D \left(\partial_x^2 u_i^n + \frac{\Delta x^2}{12} \partial_x^4 u_i^n \right) \\ &= \partial_t u_i^n - D \partial_x^2 u_i^n + \frac{\Delta t}{2} \partial_t^2 u_i^n - D \frac{\Delta x^2}{12} \partial_x^4 u_i^n \\ &= \frac{\Delta t}{2} \partial_t^2 u_i^n - D \frac{\Delta x^2}{12} \partial_x^4 u_i^n \end{aligned}$$

Solving for w_i^{n+1} in

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} - D \, \frac{w_{i+1}^n - 2 \, w_i^n + w_{i-1}^n}{\Delta x^2} = 0$$

one gets

$$\mathbf{w}_{i}^{n+1} = \left(1 - \frac{2D\Delta t}{\Delta x^{2}}\right)\mathbf{w}_{i}^{n} + \frac{D\Delta t}{\Delta x^{2}}\left(\mathbf{w}_{i+1}^{n} + \mathbf{w}_{i-1}^{n}\right)$$

or

$$\boldsymbol{w}_{i}^{n+1} = (1 - 2\alpha) \, \boldsymbol{w}_{i}^{n} + \alpha \left(\boldsymbol{w}_{i+1}^{n} + \boldsymbol{w}_{i-1}^{n} \right)$$

where

$$\alpha \equiv \frac{D\,\Delta t}{\Delta x^2}$$

Forward-time, Center-Space Updating

$$\boldsymbol{w}_{i}^{n+1} = (1 - 2\alpha) \, \boldsymbol{w}_{i}^{n} + \alpha \left(\boldsymbol{w}_{i+1}^{n} + \boldsymbol{w}_{i-1}^{n} \right)$$



In matrix notation this is equivalent to $\mathbf{w}^{(n+1)} = \mathbf{A} \cdot \mathbf{w}^{(n)}$, where

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & & & \\ \alpha & (1-2\alpha) & \alpha & & \\ & \alpha & (1-2\alpha) & \alpha & \\ & & & \vdots & \\ & \alpha & (1-2\alpha) & \alpha & \\ & & \alpha & (1-2\alpha) & \alpha & \\ & & & \alpha & 0 & 1 \end{pmatrix}$$
$$\mathbf{w}^{(n)} = \begin{pmatrix} w_1^n & & \\ w_2^n & & \\ w_3^n & & \\ \vdots & & & \\ w_{M-1}^n & & \\ w_M^n & & \end{pmatrix} \quad \mathbf{w}^{(0)} = \begin{pmatrix} c_1 & & \\ f_2 & & \\ f_3 & & \\ \vdots & & \\ f_{M-2} & & \\ f_{M-1} & & \\ c_2 & \end{pmatrix}$$

Stability

Consider a small error in the initial data. Let's investigate how this error propagates.

$$\mathbf{w}^{(1)} = \mathbf{A} \cdot \left(\mathbf{w}^{(0)} + \mathbf{e}^{(0)}\right) = \mathbf{A} \cdot \mathbf{w}^{(0)} + \mathbf{A} \cdot \mathbf{e}^{(0)}$$
$$\mathbf{w}^{(2)} = \mathbf{A} \cdot \mathbf{w}^{(1)} = \mathbf{A}^2 \cdot \mathbf{w}^{(0)} + \mathbf{A}^2 \cdot \mathbf{e}^{(0)}$$
$$\vdots$$
$$\mathbf{w}^{(n)} = \mathbf{A} \cdot \mathbf{w}^{(n-1)} = \mathbf{A}^n \cdot \mathbf{w}^{(0)} + \mathbf{A}^n \cdot \mathbf{e}^{(0)}$$

A method is said to be stable if

$$||\mathbf{A}^n \cdot \mathbf{e}^{(0)}|| \le ||\mathbf{e}^{(0)}||$$

Thus, we must require that

$$||\mathbf{A}^n|| \leq 1$$

Von Neumann Stability Analysis of FTCS

Substitute $w_i^n = \xi^n e^{l k i \Delta x}$ into

$$\boldsymbol{w}_{i}^{n+1} = (1 - 2\alpha) \, \boldsymbol{w}_{i}^{n} + \alpha \left(\boldsymbol{w}_{i+1}^{n} + \boldsymbol{w}_{i-1}^{n} \right)$$

So,

$$\xi^{n+1} e^{lk i \Delta x} = (1 - 2\alpha) \xi^n e^{lk i \Delta x} + \alpha \left(\xi^n e^{lk (i+1) \Delta x} + \xi^n e^{lk (i-1) \Delta x} \right)$$

$$\xi = (1 - 2\alpha) + \alpha \left(e^{lk \Delta x} + e^{-lk \Delta x} \right)$$

$$\xi = 1 - 2\alpha + 2\alpha \cos(k \Delta x) = 1 - 2\alpha \left[1 - \cos(k \Delta x) \right]$$

$$\xi = 1 - 4\alpha \sin^2(k \Delta x/2)$$

Then $|\xi| \leq 1$ implies

$$\begin{array}{rrrr} -1 & \leq & 1-4\,\alpha\,\sin^2\left(k\,\Delta x/2\right) \leq 1 \\ -2 & \leq & -4\,\alpha\,\sin^2\left(k\,\Delta x/2\right) \leq 0 \\ 1/2 & \geq & \alpha \geq \alpha\,\sin^2\left(k\,\Delta x/2\right) \geq 0 \end{array}$$

Von Neumann Stability Analysis of FTCS

That is, in order to be stable one requires that $alpha \le 1/2$. But since $\alpha \equiv D \Delta t / \Delta x^2$. This condition implies that

$$\Delta t \leq \frac{\Delta x^2}{2 D}$$

Notice that $\Delta t \propto \Delta x^2$; thus, halving the grid-spacing will decrease the time-step by a factor of 1/4. Also if

$$u(x, t) = u_0 e^{-pt} e^{-i k(x-q t)}$$

then

$$\partial_t u - D \,\partial_x^2 u = 0$$

yields $p = D k^2$ and q = 0. Thus,

$$u(x,t) = u_0 e^{-D k^2 t} e^{-i k x}$$

Notice that diffusion is stronger for large D or small scale features, i.e. large wave-numbers k.

In other words, the diffusion time τ across a spatial scale λ is

$$\partial_t u - D \partial_x^2 u = 0 \quad \Rightarrow \quad \frac{u}{\tau} - D \frac{u}{\lambda^2} \sim 0$$

thus,

Therefore, given the condition $\Delta t \leq \Delta x^2/D$, evolving scales $\lambda \gg \Delta x$ will require to take number of steps of order

 $\tau \sim \frac{\lambda^2}{D}$

$$rac{ au}{\Delta t}\sim rac{\lambda^2}{D\,\Delta t}\sim rac{\lambda^2}{\Delta x^2}\gg 1$$

which could be computationally prohibited.

Fully Implicit Evolution

Consider the following discretization

$$\frac{w_i^{n+1}-w_i^n}{\Delta t}-D\,\frac{w_{i+1}^{n+1}-2\,w_i^{n+1}+w_{i-1}^{n+1}}{\Delta x^2}=0$$



Solving for w_i^n , we get

$$(1-2\alpha) \mathbf{w}_i^{n+1} - \alpha \left(\mathbf{w}_{i+1}^{n+1} + \mathbf{w}_{i-1}^{n+1} \right) = \mathbf{w}_i^n$$

where again $\alpha \equiv \frac{D \Delta t}{\Delta x^2}$. A von Neumann stability analysis yields

$$\xi = \left[1 + 4\alpha \sin^2\left(k\,\Delta x/2\right)\right]^{-1}$$

That is, $|\xi| < 1$ for any step size Δt . The scheme is unconditionally stable

In matrix notation, the implicit update is equivalent to $\bm{A}\cdot\bm{w}^{(n+1)}=\bm{w}^{(n)},$ where

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & & & \\ -\alpha & (1-2\alpha) & -\alpha & & \\ & -\alpha & (1-2\alpha) & -\alpha & \\ & & & \vdots & \\ & -\alpha & (1-2\alpha) & -\alpha & \\ & & & -\alpha & (1-2\alpha) & -\alpha \\ & & & & 0 & 1 \end{pmatrix}$$
$$\mathbf{w}^{(n)} = \begin{pmatrix} w_1^n & & \\ w_2^n & & \\ w_3^n & & \\ \vdots & & \\ w_{M-1}^n & & \\ w_M^n & & \end{pmatrix} \qquad \mathbf{w}^{(0)} = \begin{pmatrix} c_1 & & \\ f_2 & & \\ f_3 & & \\ \vdots & & \\ f_{M-2} & & \\ f_{M-1} & & \\ c_2 & & \end{pmatrix}$$

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- Therefore, at every step, instead of updating the solution with w⁽ⁿ⁺¹⁾ = A · w⁽ⁿ⁾ (explicit update), now one needs to solve the system A · w⁽ⁿ⁺¹⁾ = w⁽ⁿ⁾ (implicit update)
- In spite of been able to take large steps, the implicit update could be quite expensive.
- In addition, the fully implicit method is still only first order accurate in time.
- Can we design a scheme that is second order accurate in both space and time with the stability properties of the implicit method?

Crank-Nicholson

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} = \frac{D}{2} \left[\frac{w_{i+1}^{n+1} - 2w_i^{n+1} + w_{i-1}^{n+1}}{\Delta x^2} + \frac{w_{i+1}^n - 2w_i^n + w_{i-1}^n}{\Delta x^2} \right]$$

2 $(1 + \alpha) w_i^{n+1} - \alpha \left(w_{i+1}^{n+1} + w_{i-1}^{n+1} \right) = -2 (1 - \alpha) w_i^n + \alpha \left(w_{i+1}^n + w_{i-1}^n \right)$



u(x,0) = f(x)

Thin Accretion Disks

- An accretion disk formes when by diffuse material orbits a central body.
- Gravity and losses in angular momentum causes the material ito spiral inward towards the central body.
- Gravitational forces compress the material causing the emission of electromagnetic radiation.
- Accretion disks of young stars and protostars radiate in the infrared; those around neutron stars and black holes in the x-ray.



Accretion condition:

 $\begin{array}{rcl} \mbox{central object} & \leftarrow & \mbox{mass flow} \\ \mbox{central object} & \Rightarrow & \mbox{angular momentum flow} \end{array}$

Angular momentum per unit mass:

$$j = r^2 \omega$$

Kepler's 3th law:

$$\omega = \sqrt{\frac{GM}{r^3}}$$

• Therefore,

$$j = \sqrt{GMr}$$

Disk Model



• We will use cylindrical coordinates $\{t, r, \phi, z\}$.

• We will not include the central object in the computation. That is $r_{min} \le r \le r_{max}$

Basic Assumptions:

- The viscosity in the disk drives the flow of angular momentum outwards.
- The size of the disk is much larger than its thickness, i.e. thin disk
- All physical properties are independent of ϕ

 z-dependences will be integrated over the disk thickness. For example,

$$\sigma = \int_{-\infty}^{\infty} \rho \, dz \qquad \text{surface mass density}$$

Keplerian disk

$$m{v}_{\phi} = m{r}\,\omega \qquad ext{where} \qquad \omega = \sqrt{rac{G\,M}{r^3}}$$

Mass of the disk is much smaller than the mass of the central object.

$$2\pi\int_0^\infty \sigma \, r \, dr \ll M$$

• The orbital speed of a fluid element in the disk is much larger than the thermal speed.

$$\mathbf{v}_{\phi} = \mathbf{r}\,\omega \gg \sqrt{\frac{\mathbf{k}t}{m}}$$

- Mass Density: ρ or σ
- Fluid Velocity: $\vec{v} = (v_r, v_{\phi}, v_z) = (v_r, r \, \omega, 0)$
- Energy Density: ignored
- Gas pressure: ignored
- Disk viscosity: ν
- Disk self-gravity: ignored
- Central object gravity: *M*/*r*

Mass Conservation

Also known as the continuity equation

$$\partial_t
ho +
abla \cdot (
ho \, ec{m{v}}) = \mathbf{0}$$

In cylindrical coordinates, it reads

$$\partial_t \rho + \frac{1}{r} \partial_r (\rho \, r \, v_r) + \partial_\phi (\rho \, v_\phi) + \partial_z (\rho \, v_z) = 0$$

$$\partial_t \rho + \frac{1}{r} \partial_r (\rho \, r \, v_r) = 0$$

$$\int_{-\infty}^{\infty} \left[\partial_t \rho + \frac{1}{r} \partial_r (\rho \, r \, v_r) \right] dz = 0$$

Then

$$\partial_t \sigma + \frac{1}{r} \partial_r (\sigma \, r \, v_r) = 0$$

Angular Momentum Conservation

$$\partial_t(\rho j) + \frac{1}{r} \partial_r(r \rho j v_r) = -\frac{1}{r} \partial_r(r \Pi_{r\rho})$$

where
$$\Pi_{r\phi} = -\nu \rho r^2 \frac{d\omega}{dr}$$

Integration across the *z*-direction and substitution mass conservation equation yields

$$\partial_t j + v_r \partial_r j = \frac{1}{r \sigma} \partial_r \left(r^3 \nu \sigma \frac{d\omega}{dr} \right)$$

Recall, $j = \sqrt{GMr}$ and $\omega = \sqrt{GM/r^3}$.

$$v_r = \frac{1}{r\sigma} \left(\frac{dj}{dr}\right)^{-1} \partial_r \left(r^3 \nu \sigma \frac{d\omega}{dr}\right)$$

$$v_r = \frac{-3}{r^{1/2}\sigma} \partial_r \left(r^{1/2} \nu \sigma \right)$$

We then have

$$\partial_t \sigma + \frac{1}{r} \partial_r (\sigma \, r \, v_r) = 0$$
$$v_r = \frac{-3}{r^{1/2} \sigma} \partial_r \left(r^{1/2} \, \nu \, \sigma \right)$$

to solve for σ and v_r given a viscosity model for $\nu = \nu(\sigma, r, t)$. Notice that the second equation trivially gives a way to compute the drift velocity.

Substitution of v_r in the mass conservation equation yields

$$\partial_t \sigma - \frac{3}{r} \partial_r \left[r^{1/2} \partial_r \left(r^{1/2} \nu \sigma \right) \right] = 0$$

What type of equation is

$$\partial_t \sigma - \frac{3}{r} \partial_r \left[r^{1/2} \partial_r \left(r^{1/2} \nu \sigma \right) \right] = 0$$

Define $x \equiv 2 r^{1/2}$ and $\mu \equiv \nu \sigma r^{1/2}$. One gets,

$$\partial_t \mu - \frac{12\nu}{x^2} \partial_x^2 \mu = 0$$

This is a diffusion equation with diffusion coefficient

$$D = \frac{12\nu}{x^2}$$

On the tidal interaction between protoplanets and the protoplanetary disk, D.N.C. Lin and John Paapaloizou, Astrophysical Journal, vol 309, p 846, y 1986.

- Viscosity model for solar disks $\nu = \sigma^2$
- Tidal interaction

$$v_r = \frac{-3}{r^{1/2}\sigma} \partial_r \left(r^{1/2} \nu \sigma \right) + 3 \Lambda r^{1/2}$$

where Λ is the injection rate of angular momentum by tidal interaction with the protoplanet.

$$\Lambda = \operatorname{sign}(r - r_p) \frac{A}{r} \left(\frac{r}{\delta_p}\right)^4$$

where r_p is the radial position of the protoplanet, *A* is the strength of tidal effects and $\delta_p = Max(H, |r - r_p|)$

Therefore

$$\partial_t \sigma = -\frac{1}{r} \partial_r (\sigma r v_r)$$
 and $v_r = \frac{-3}{r^{1/2} \sigma} \partial_r \left(r^{1/2} \sigma^3 \right) + 3 \Lambda r^{1/2}$

yields

$$\partial_t \sigma = \frac{3}{r} \partial_r \left[r^{1/2} \partial_r \left(r^{1/2} \sigma^3 \right) - \Lambda \sigma r^{3/2} \right]$$

or

$$\partial_t \sigma = \frac{3}{r} \partial_r \left[r^{1/2} \partial_r \left(r^{1/2} \sigma^3 \right) - \operatorname{sign}(r - r_p) A \sigma r^{1/2} \left(\frac{r}{\delta_p} \right)^4 \right]$$

We need the equation of motion for the protoplanet. In the absence of the disk, we will assume that the planet moves in circular orbits. That is, $\frac{dr_p}{dt} = 0$.

The presence of the disk modifies the protoplanet orbital dynamics as follows:

$$rac{d r_{
ho}}{dt} = -3 B A r_{
ho}^{1/2} \int_{r_{min}}^{r_{max}} \operatorname{sign}(r - r_{
ho}) \sigma \, \left(rac{r}{\delta_{
ho}}
ight)^4 dr$$

where B is the mass ratio of the disk to the protoplanet.

We will consider the following parameters

$$A = 10^{-3} B = 20 r_{min} = 0 r_{max} = 2 r_{p} = 0.8 \sigma = e^{-r^{2}/2}$$
at $t = 0 H = 0.05$



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