(25.10.30) Computational Physics B

class 1

- implicit method (continued)
  - $\vec{y}^{n+1} = \vec{y}^n + \Delta t \cdot \vec{f}(t^{n+1}, \vec{y}^{n+1})$
  - guess a solution first, $\vec{y}_0^{n+1}$, and then $\vec{y}^{n+1} = \vec{y}_0^{n+1} + \Delta \vec{y}_0$, and do Taylor expansion:
  - $\vec{f}(t^{n+1}, \vec{y}^{n+1}) = \vec{f}(t^{n+1}, \vec{y}_0^{n+1}) + \frac{\partial \vec{f}}{\partial \vec{y}}\Big|_{\vec{y}_0^{n+1}} \Delta \vec{y}_0 + ...$
  - then substitute into the implicit equation:
  - $\vec{y}_0^{n+1} + \Delta \vec{y}_0 = \vec{y}^n + \Delta t \left[\vec{f}(t^{n+1}, \vec{y}_0^{n+1}) + \frac{\partial \vec{f}}{\partial \vec{y}}\Big|_{\vec{y}_0^{n+1}} \Delta \vec{y}_0 \right]$ and solve for $\Delta \vec{y}_0$.
  - then we can get a better approximation of $\vec{y}^{n+1}$, and repeat the process until $|\frac{\Delta \vec{y}_k}{\vec{y}_k}| < \epsilon$.
- How to solve PDE?
  - linear advection
    - $\frac{\partial a}{\partial t} + u \frac{\partial a}{\partial x} = 0$
    - solution: $a(x,t) = a(x - ut, 0)$, this depicts a wave moving to the right without changing its shape, so it's "linear", and the solution consists of a straight line in the x-t plane -- characteristics.
  - 1st order finite difference method (FDM)
    - $\frac{a_i^{n+1} - a_i^n}{\Delta t} + u \frac{a_i^n - a_{i-1}^n}{\Delta x} = 0$ -- explicit method
      - where n is time step and i is spatial index.
    - numerical stability
      - define Courant number $c = \frac{u \Delta t}{\Delta x}$, then $a_i^{n+1} = a_i^n + c_{i-1}^n$
      - Conside a single Fourier mode: $a_i^n = A^n e^{I i \theta}$, where $\theta = k \Delta x$, and k is the wavenumber.
      - then $A^{n+1} = A^n((1 - c + c\cos\theta) - (Ic\sin\theta))$, then the magnitude of the amplification is $|\frac{A^{n+1}}{A^n}| = \sqrt{(1 - c + c\cos\theta)^2 + (c\sin\theta)^2} = \sqrt{1 - 2c(1-c)(1-\cos\theta)}$
      - the error increases monotonically without bound and will cause numerical instability if $|\frac{A^{n+1}}{A^n}| > 1$. And to avoid this instability, we need $c \leq 1$, which is the Courant-Friedrichs-Lewy (CFL) condition.
      - This means physically that the wave cannot travel more than one grid cell in one time step. The maximum wave speed sets the upper limit on the time step Δt.

- As a simple example, if we doubles the spatial resolution in a 3D simulation, the computational cost increases by a factor of 16: 2^3 from the number of grid cells and another factor of 2 from the CFL condition on the time step.

class 2

- method revisited
  - "upwind" scheme
    - $\frac{a_i^{n+1}-a_i^n}{\Delta t}+u\frac{a_i^n-a_{i-1}^n}{\Delta x}=0$, for $u>0$
    - $\frac{a_i^{n+1}-a_i^n}{\Delta t}+u\frac{a_{i+1}^n-a_i^n}{\Delta x}=0$, for $u<0$
    - we need to consider the direction of "information flow", if we do not do this way, the numerical simulation may crush.
  - 2nd order finite difference method
    - time forward, centered space (FTCS) -- $\frac{\partial a}{\partial x}\sim\frac{a_{i+1}-a_{i-1}}{2\Delta x}$
    - stability analysis shows that this method is unconditionally unstable for linear advection equation since it mixes upwind and downwind information flow. Therefore, this will cause unphysical oscillations.
- second and higher order advection equation with finite-volume method (FVM)
  - advantages
    - conservation is ensured
    - shocks are accurately treated -- so almost all astrophysical fluid simulation codes employ FVM
  - basic equation
    - $\frac{\partial}{\partial t}<a_i>=-\frac{F(a)_{i+1/2}-F(a)_{i-1/2}}{\Delta x}$, the volume-averaged quantity depends on the flux through the boundary of the zone.
  - second-order predictor-corrector scheme
    - $\frac{a_i^{n+1}-a_i^n}{\Delta t}=-\frac{F(a)_{i+1/2}^{n+1/2}-F(a)_{i-1/2}^{n+1/2}}{\Delta x}$ -- predictor step
      - where flux at the half time step is equal to state at half time step: $F(a)_{i+1/2}^{n+1/2}=F(a_{i+1/2}^{n+1/2})$, while the state can be calculated by Taylor expansion
        - $a_{i+1/2,l}^{n+1/2}=a_i^n+\frac{\Delta x}{2}\left(\frac{\partial a}{\partial x}\right)_i^n+\frac{\Delta t}{2}\left(\frac{\partial a}{\partial t}\right)_i^n$
        - $a_{i+1/2,r}^{n+1/2}=a_{i+1}^n-\frac{\Delta x}{2}\left(\frac{\partial a}{\partial x}\right)_{i+1}^n+\frac{\Delta t}{2}\left(\frac{\partial a}{\partial t}\right)_{i+1}^n$
        - the core question now turns to how to calculate the spatial derivative $\frac{\partial a}{\partial x}$, and we can use "reconstruction" method to do this.