Computational Methods for Astrophysical Applications

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Epilog

- **Advanced meshes**
  Multi-dimensional meshes : dimensionally split methods
  Non-cartesian meshes
  Adaptive Mesh Refinement
  Adaptive Time Stepping
- **Finite elements**
- **Parabolic & elliptic PDE**
- **Implicit methods**
- **Spectral methods**
- **Div B cleaning**
- **Workflow**
  Developing numerical codes
  Working on a cluster : job submission, etc
  Parallelization & vectorization
  Debugging & optimization

Integral form

- **useless?** Method is **consistent** since LTE vanish in limit $\Delta x \to 0$ and $\Delta t \to 0$
  - $\Rightarrow$ accuracy: 2nd order space, 1st order time $\to$ overall 1st
  - $\Rightarrow$ failure is related to numerical stability
- round-off errors should not grow during time progression
  - $\Rightarrow$ evaluate by **von Neumann method**
  - $\Rightarrow$ numerical solution = exact $+$ round-off error $\epsilon(x, t)$
  - $\Rightarrow$ represent $\epsilon(x, t)$ in Fourier series, analyse Fourier term

$$\epsilon_k(x, t) = \hat{\epsilon}_k \mathrm{e}^{\lambda t} \mathrm{e}^{\mathrm{i}kx}$$

- numerically stable scheme: for all spatial wavenumbers k

$$\left| \frac{\epsilon_k^{n+1}}{\epsilon_k^n} \right| = \left| \mathrm{e}^{\lambda \Delta t} \right| \leq 1$$

Differential and conservative forms

- FTCS scheme and von Neumann analysis yields

$$e^{\lambda \Delta t} = 1 - \frac{v \Delta t}{\Delta x} \frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2} = 1 - i \frac{v \Delta t}{\Delta x} \sin\left(k \Delta x\right)$$

$\Rightarrow$ scheme is **unconditionally unstable** since for all k

$$\left| \frac{\epsilon_k^{n+1}}{\epsilon_k^n} \right| > 1$$

- **three cures** to save stability
  - $\Rightarrow$ add ‘numerical diffusion’ to damp nonphysical instability
  - $\Rightarrow$ impose same space-time symmetry as original PDE
  - $\Rightarrow$ use implicit scheme

Conservative variables, fluxes, sources

- adding diffusion: advection-diffusion equation has form

$$\frac{\partial u}{\partial t} = -v\,\frac{\partial u}{\partial x} + \mathcal{D}\,\frac{\partial^2 u}{\partial x^2}$$

  $\Rightarrow$ diffusion coefficient $\mathcal{D}$

- replace u_i^n by spatial average between x_{i-1} and x_{i+1}, arrive at

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - v\,\frac{\Delta t}{\Delta x}\,\frac{u_{i+1}^n - u_{i-1}^n}{2}$$

  $\Rightarrow$ **Lax–Friedrichs scheme** (or Lax scheme)

  $\Rightarrow$ rearrange to form

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -v\,\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} + \frac{(\Delta x)^2}{2\Delta t}\,\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

  $\Rightarrow$ numerical dissipation with $\mathcal{D} \equiv \frac{(\Delta x)^2}{2\Delta t}$

Closure relation

- FTCS scheme and von Neumann analysis yields

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Linear advection equation

- perform von Neumann stability analysis for Lax–Friedrichs

$$e^{\lambda \Delta t} = \cos(k\Delta x) - i\,\frac{v\Delta t}{\Delta x}\,\sin(k\Delta x)$$

$\Rightarrow$ **conditional stability** requiring Courant number C

$$C \equiv \frac{|v|\Delta t}{\Delta x} \leq 1$$

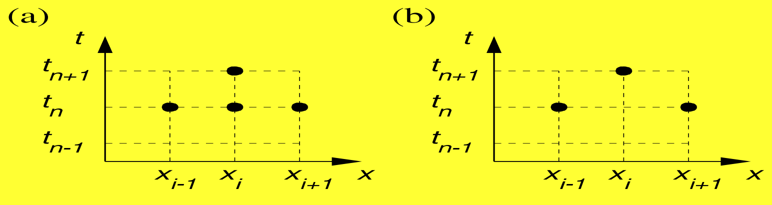
$\Rightarrow$ limitation of the time step Δt for a given resolution Δx

$\Rightarrow$ **Courant–Friedrichs–Lewy** condition (1928)

$\Rightarrow$ necessary (not sufficient) condition for stability!

Euler equations

- in (x, t) space, we identify **stencil** of a method
  - $\Rightarrow$ stencils visualizes discrete dependence of method



  - $\Rightarrow$ stencil for FTCS (a) versus Lax-Friedrichs (b)
- **hyperbolic** PDE and **physical characteristics**
  - $\Rightarrow$ the advection equation is hyperbolic as

$$\frac{\partial u}{\partial t} + \frac{\partial \left(\underbrace{vu}_{F} \right)}{\partial x} = 0$$

and Flux Jacobian $\frac{\partial F}{\partial u} = v$ is real number, 'characteristic speed'

Ideal Magneto-Hydrodynamics equations

- for second order wave equation

$$\frac{\partial^2 u}{\partial t^2} - v^2 \frac{\partial^2 u}{\partial x^2} = 0$$

$\Rightarrow$ factorizes to

$$\left(\frac{\partial}{\partial t} - v\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + v\frac{\partial}{\partial x}\right) u = 0$$

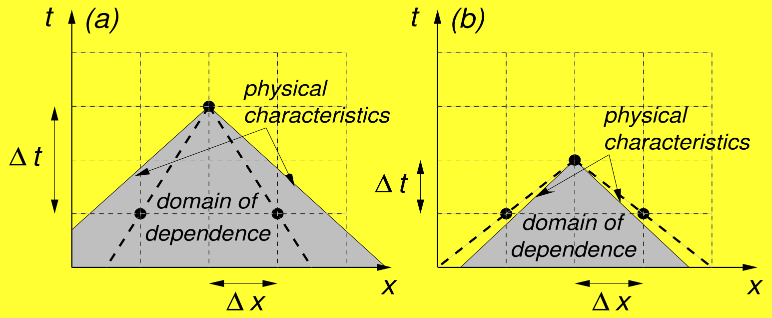
$\Rightarrow$ general solution has left and right going wave with

$$u = f(x - vt) + g(x + vt)$$

$\Rightarrow$ initial shapes $f(x)$, $g(x)$ combine

$\Rightarrow$ 2 characteristics $\frac{dx}{dt} = \pm v$

- illustrate CFL for second order wave equation: **the domain of dependence of the differential equation should be contained in the DOD of the discretised equations**



$\Rightarrow$ stability means physical DOD contained in stencil bounds (numerical DOD), hence Δt small enough (right case)

- note: linear advection + wave equation: DOD only involves 1 or 2 points from $t = 0 \leftrightarrow$ HD: DOD bounds set by $v \pm c_s$ with c_s sound speed, delimits $t = 0$ interval

- Second cure: maintain space-time symmetry of the PDE
  - $\Rightarrow$ use central discretisation for both x and t
  - $\Rightarrow$ obtain **leapfrog** scheme

$$u_i^{n+1} = u_i^{n-1} - \frac{\Delta t}{\Delta x}\left(F_{i+1}^n - F_{i-1}^n\right)$$

  - $\Rightarrow$ numerical flux function for advection is $F_i^n \equiv v u_i^n$
  - $\Rightarrow$ conditionally stable and second-order accurate
  - $\Rightarrow$ multiple time levels involved: $n-1$, n, $n+1$
  - $\Rightarrow$ potential problem: even/oneven time levels may ‘decouple’

Flux Jacobian

- von Neumann stability analysis for BTCS scheme

$$\left|\mathrm{e}^{\lambda \Delta t}\right| = \frac{1}{\left|1 + \mathrm{i}\frac{v\Delta t}{\Delta x}\sin\left(k\Delta x\right)\right|} < 1 \qquad \text{for all } k$$

$\Rightarrow$ **unconditionally stable**, any (large) time step Δt allowed

- note: **stability does not imply accuracy**

  $\Rightarrow$ large Δt affects accuracy, defines time resolution:
  behavior may involve physical timescale that needs to be resolved!
- implicit backward Euler: first order in time

Eigenvalues & eigenvectors

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Hyperbolic, parabolic and elliptic PDE

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Linear, non-linear & quasi-linear

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Explicit

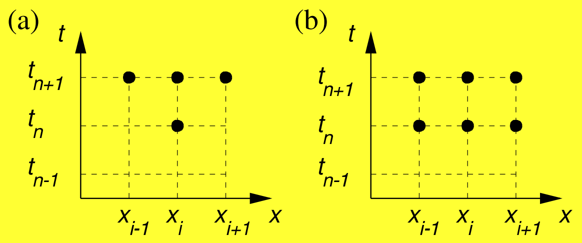
- spatial differences as average of n-th and $(n+1)$-th time step

$$u_i^{n+1} = u_i^n - \frac{1}{4} v \frac{\Delta t}{\Delta x} \left(u_{i+1}^{n+1} + u_{i+1}^n - u_{i-1}^{n+1} - u_{i-1}^n \right)$$

$\Rightarrow$ second order **Crank–Nicolson method**

$\Rightarrow$ **Exercise**: show that this scheme is unconditionally stable, 2nd order accurate

- stencils for BTCS (left) and Crank-Nicolson (right)



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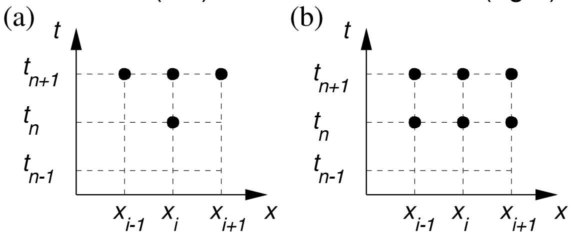

Properties

- many practical implementations use ‘method of lines’
  - $\Rightarrow$ vector $\mathbf{u}$ of unknowns after first spatial discretization
  - $\Rightarrow$ obtain ODE system

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u})$$

  - $\Rightarrow$ RHS vector function $\mathbf{f}$ could even be nonlinear in $\mathbf{u}$

- discretize ODE in time using parameter α in

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \left[\alpha \mathbf{f}(\mathbf{u}^{n+1}) + (1-\alpha)\mathbf{f}(\mathbf{u}^n) \right]$$

  - $\Rightarrow$ note case $\alpha = 0$: explicit (unstable) forward Euler method

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Stencils, domain of dependence, range of influence

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The Riemann problem

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \left[\alpha \mathbf{f}(\mathbf{u}^{n+1}) + (1-\alpha)\mathbf{f}(\mathbf{u}^n)\right]$$

- $\alpha = 1$ is **implicit backward Euler**
- $\alpha = 1/2$ gives second-order accuracy, **trapezoidal method**

  $\Rightarrow$ Crank-Nicolson for central discretization of flux in $\mathbf{f}$

- when $\mathbf{f}$ nonlinear: linearize using

$$\mathbf{f}(\mathbf{u}^{n+1}) \approx \mathbf{f}(\mathbf{u}^n) + \frac{\partial \mathbf{f}^n}{\partial \mathbf{u}} (\mathbf{u}^{n+1} - \mathbf{u}^n)$$

$\Rightarrow$ introduces matrix $\dfrac{\partial \mathbf{f}^n}{\partial \mathbf{u}}$ called ***"Jacobian matrix"*** of $\mathbf{f}$