Initial Value Problems (IVP)

$$\left\{\begin{array}{llll} u_t = Lu & \text{in } \Omega\times]0,T[& \leftarrow & \text{PDE} \\ u = u_0 & \text{on } \Omega\times\{0\} & \leftarrow & \text{initial condition} \\ u = g & \text{on } \partial\Omega\times]0,T[& \leftarrow & \text{boundary condition} \end{array}\right\}$$

where L differential operator.

Ex.: (not done yet.)

- $L = \nabla^2$
  Poisson equation $\rightarrow$ heat equation
- $Lu = b \cdot \nabla u$
  advection equation
- $Lu = -\nabla^2(\nabla^2 u)$
  biharmonic equation $\rightarrow$ beam equation
- $Lu = F|\nabla u|$
  Eikonal equation $\rightarrow$ level set equation (nonlinear)
- etc.

Stationary solution of IVP: (if it exists)
$$\left\{\begin{array}{lll} Lu = 0 & \text{in} & \Omega \\ u = g & \text{on} & \partial\Omega \end{array}\right\}$$

Later:
second order problems $\Leftrightarrow$ systems

$u_{tt} = u_{xx}$ (wave equation)

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \frac{\partial}{\partial x}\begin{pmatrix} u \\ v \end{pmatrix}$$

Semi-Discretization

- In space (method of lines):
  Approximate $u(\cdot, t)$ by $\vec{u}(t)$
  Approximate Lu by $A \cdot \vec{u}$ (for linear problems) [FD, FE, spectral]
  $\rightarrow$ system of ODE: $\frac{d}{dt}\vec{u} = A \cdot \vec{u}$
- In time:
  Approximate time derivative by step:
  $\frac{d}{dt}u(x,t) \approx \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t}$ [explicit Euler]
  $\rightarrow$ Stationary problem:
  $u^{\text{new}}(x) = u(x) + \Delta t L u(x) = (I + \Delta t L)u(x)$
  Need to know about ODE solvers.

Numerical Methods for ODE

$$\left\{ \begin{array}{l} \dot{y}(t) = f(y(t)) \\ y(0) = \mathring{y} \end{array} \right\} \quad y(t) \in \mathbb{R}^d$$

$y^n \approx y(t),\ y^{n+1} \approx y(t + \Delta t)$

Linear approximation: $\dot{y} \approx \dfrac{y^{n+1} - y^n}{\Delta t}$

Explicit Euler (EE): $y^{n+1} = y^n + \Delta t \cdot f(y^n)$

Implicit Euler (IE): $y^{n+1} - \Delta t \cdot f(y^{n+1}) = y^n$

nonlinear system $\leftarrow$ Newton iteration.

Local truncation error (LTE):

EE: $\tau^n = y(t + \Delta t) - (y(t) + \Delta t f(y(t))) = \frac{1}{2}\ddot{y}(t)\Delta t^2 = O(\Delta t^2)$

IE: $\tau^n = O(\Delta t^2)$

Global truncation error (GTE):

Over $N = \dfrac{T}{\Delta t}$ time steps.

$E^n = y^n - y(t_n)$

$E^{n+1} = E^n + \Delta t(f(y^n) - f(y(t_n))) + \tau^n$

$\Longrightarrow |E^{n+1}| \leq |E^n| + \Delta t L |E^n| + |\tau^n|$

$\Longrightarrow |E^N| \leq e^{LT} \frac{T}{\Delta t} \max_n |\tau^n| = O(\Delta t)$

Time Stepping:

GTE = one order less than LTE.

Higher Order Time Stepping

- Taylor Series Methods:

  Start with EE, add terms to eliminate leading order error terms.
  PDE $\rightarrow$ Lax-Wendroff

- Runge-Kutta Methods:

  Each step = multiple stages

$$\begin{aligned} k_1 &= f(y^n + \Delta t \sum_j a_{ij} k_j) \\ &\vdots \\ k_r &= f(y^n + \Delta t \sum_j a_{rj} k_j) \\ y^{n+1} &= y^n + \Delta t \sum_j b_j k_j \end{aligned}$$

Butcher tableau: $(c_l = \sum_j a_{lj})$

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1r} \\ \vdots & \vdots & \ddots & \vdots \\ c_r & a_{r1} & \dots & a_{rr} \\ \hline & b_1 & \dots & b_r \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

EE: $\begin{array}{c|c} 0 & \\ \hline & 1 \end{array}$ $\qquad \begin{aligned} k_1 &= f(y^n) \\ y^{n+1} &= y^n + \Delta t k_1 \end{aligned}$

IE: $\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$ $\qquad k_1 = f(\overbrace{y^n + \Delta t \cdot k_1}^{=y^{n+1}})$, $\quad y^{n+1} = y^n + \Delta t \cdot k_1$

Explicit midpoint: $\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array}$

Heun's: $\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$

RK4: $\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & & \frac{1}{2} & & \\ 1 & & & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$

Implicit trapezoidal: $\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$ $\qquad$ PDE $\to$ Crank-Nicolson

- Multistep Methods:

$$\sum_{j=0}^{r} \alpha_j y^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(y^{n+j})$$

Explicit Adams-Bashforth:

$$\begin{aligned} y^{n+1} &= y^n + \Delta t f(y^n) & &= \text{EE} \quad O(\Delta t) \\ y^{n+2} &= y^{n+1} + \Delta t \cdot [\tfrac{3}{2} f(y^{n+1}) - \tfrac{1}{2} f(y^n)] & & \quad O(\Delta t^2) \\ &\vdots \end{aligned}$$

Implicit Adams-Moultion:

$$\begin{aligned} y^{n+1} &= y^n + \Delta t \cdot (\tfrac{1}{2} f(y^n) + \tfrac{1}{2}(y^{n+1})) & &= \text{trapezoidal} \quad O(\Delta t^2) \\ y^{n+2} &= y^{n+1} + \Delta t \cdot (\tfrac{5}{12} f(y^{n+2}) + \tfrac{8}{12} f(y^{n+1}) - \tfrac{1}{12} f(y^n)) & & \quad O(\Delta t^3) \\ &\vdots \end{aligned}$$

BDF (backward differentiation):

$$\begin{aligned} y^{n+1} &= y^n + \Delta t f(y^{n+1}) \quad = \text{IE} \quad O(\Delta t) \\ 3y^{n+2} - 4y^{n+1} + y^n &= 2\Delta t f(y^{n+2}) \quad O(\Delta t^2) \\ &\vdots \end{aligned}$$

Linear ODE Systems

$$\begin{cases} \dot{y} = A \cdot y \\ y(0) = \mathring{y} \end{cases}$$

solution: $y(t) = \exp(tA) \cdot \mathring{y}$

solution stable, if $\mathrm{Re}(\lambda_i(A)) < 0 \ \forall i$.

$$\begin{array}{lll} \text{EE:} & y^{n+1} = & \overbrace{(I + \Delta t \cdot A)}^{= \mathrm{M_{EE}}} \cdot y^n \\ \text{IE:} & y^{n+1} = & \underbrace{(I - \Delta t \cdot A)^{-1}}_{= \mathrm{M_{IE}}} \cdot y^n \end{array}$$

Iteration $y^{n+1} = M \cdot y^n$ stable, if $|\lambda_i(M)| < 1 \ \forall i$

λ_i eigenvalue of A

$$\Rightarrow \left\{ \begin{array}{ll} 1 + \Delta t \cdot \lambda_i & \text{eigenvalue of } \mathrm{M_{EE}} \\ \dfrac{1}{1 - \Delta t \cdot \lambda_i} & \text{eigenvalue of } \mathrm{M_{IE}} \end{array} \right\} \qquad \begin{array}{l} |1 + \Delta t \cdot \lambda_i| < 1 \text{ if } \Delta t < \dfrac{2}{|\lambda_i|} \\ \left| \dfrac{1}{1 - \Delta t \cdot \lambda_i} \right| < 1 \text{ always} \end{array}$$

EE conditionally stable: $\Delta t < \dfrac{2}{\rho(A)}$

IE unconditionally stable

<u>Message</u>: One step implicit is more costly than one step explicit.

<u>But</u>: If $\underbrace{\rho(A) \text{ large}}_{\text{stiffness}}$, then implicit pays!

<u>Ex.</u>: Different time scales

$$A = \begin{bmatrix} -50 & 49 \\ 49 & -50 \end{bmatrix}, \ \mathring{y} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

Solution: $y(t) = \underbrace{e^{-t} \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix}}_{\text{behavior}} + \underbrace{e^{-99t} \cdot \begin{bmatrix} -1 \\ 1 \end{bmatrix}}_{\text{restricts } \Delta t \text{ for EE}}$

<u>Ex.</u>:

$$A = \frac{1}{(\Delta x)^2} \cdot \underbrace{\begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}}_{-4 < \lambda_i < 0} \quad \boxed{\text{heat equation}} \quad \Rightarrow \rho(A) < \frac{4}{(\Delta x)^2}$$

EE stable if $\Delta t < \dfrac{(\Delta x)^2}{2}$.

OTOH: Crank-Nicolson

$$\left(I - \frac{\Delta t}{2} A \right) \cdot y^{n+1} = \left(I + \frac{\Delta t}{2} A \right) \cdot y^n$$

Unconditionally stable.