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Numerical Methods for Differential Equations in Physics

Temporal Discretization

$$\frac{du}{dt} = f(u) \qquad u, f \text{ in } \mathcal{R}^N$$

Goal: turn differential equation into difference equation

First order methods:

Forwards (Explicit) Euler:

$$u(t + \Delta t) = u(t) + \Delta t f(u(t))$$

explicit: "=" is an assignment statement

Backwards (Implicit) Euler:

$$u(t + \Delta t) = u(t) + \Delta t f(u(t + \Delta t))$$

implicit: "=" is an equation to be solved for $u(t + \Delta t)$

Taylor series:

$$u(t+\Delta t) = u(t) + \Delta t \frac{du}{dt} + \frac{\Delta t^2}{2}\frac{d^2u}{dt^2} + \ldots$$
$$= u(t) + \Delta t f(u(t)) + \frac{\Delta t^2}{2} f'(u(t)) f(u(t)) + \ldots$$

Forwards (Explicit) Euler:

$$u(t+\Delta t) = u(t) + \Delta t f(u(t))$$

Backwards (Implicit) Euler:

$$u(t+\Delta t) = u(t) + \Delta t f(u(t+\Delta t))$$
$$= u(t) + \Delta t \left(f(u(t)) + \Delta t f'(u(t)) f(u(t)) + \ldots\right)$$
$$= u(t) + \Delta t f(u(t)) + \Delta t^2 f'(u(t)) f(u(t)) + \ldots$$

First order: Δt terms match Taylor series but not Δt^2 terms

Second order methods:

Adams-Bashforth (explicit)

$$u(t+\Delta t) = u(t) + \Delta t \left(\frac{3}{2} f(u(t)) - \frac{1}{2} f(u(t-\Delta t)) \right)$$

Crank-Nicolson (implicit) also called trapezoidal

$$u(t+\Delta t) = u(t) + \Delta t \left(\frac{1}{2} f(u(t)) + \frac{1}{2} f(u(t+\Delta t)) \right)$$

Backwards Differentiation (implicit)

$$u(t+\Delta t) = \frac{4}{3} u(t) - \frac{1}{3} u(t-\Delta t) + \frac{2}{3} \Delta t f(u(t+\Delta t))$$

Second order: Δt, Δt^2 terms match Taylor series but not Δt^3

For fixed T, take $T/\Delta t$ steps

If one-step error is Δt^p,
total error at time T is $(T/\Delta t)\Delta t^p = T\Delta t^{p-1}$

First-order methods have one-step error Δt^2
and fixed-time error Δt

Second-order methods have one-step error Δt^3
and fixed-time error Δt^2

Have assumed $f(u(t))$, but can also have $f(u(t), t)$

Second or higher order differential equations:
Write $u_0 = u$, $u_1 = u_0'$, $u_2 = u_0''$, etc.

$$\frac{du}{dt} = f(u) \qquad u = (u_0, u_1, \ldots), f = (f_0, f_1, \ldots)$$

Stability: example of heat equation with periodic boundary conditions

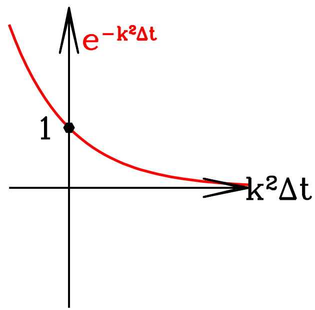
$$\partial_t u = \partial^2_{xx} u$$

$$u(x,t) = \sum_{k=1}^{k_{max}} \hat{u}_k(t) \sin kx$$

$$\partial_t \hat{u}_k = -k^2 \hat{u}_k$$

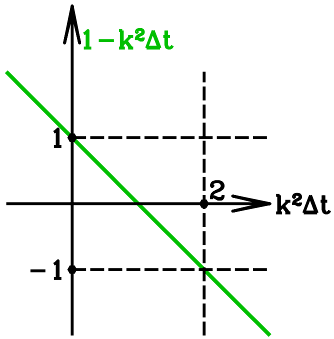
Exact solution

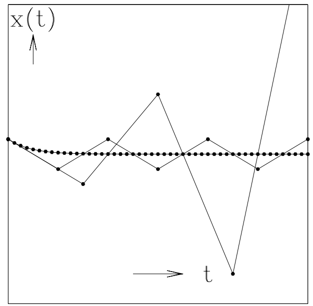
$$\hat{u}_k(t+\Delta t) = e^{-k^2 \Delta t} \hat{u}_k(t)$$



Explicit Euler

$$\begin{aligned}\hat{u}_k(t+\Delta t) &= \hat{u}_k(t) - k^2 \Delta t \hat{u}_k(t) \\ &= (1 - k^2 \Delta t)\hat{u}_k(t)\end{aligned}$$





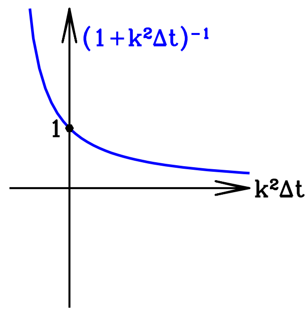
As $k_{max} \to \infty$, $\Delta t_{max} = \frac{2}{k^2_{max}} \to 0$

Implicit Euler

$$\begin{aligned}\hat{u}_k(t+\Delta t) &= \hat{u}_k(t) - k^2 \Delta t \hat{u}_k(t+\Delta t) \\ (1 + k^2\Delta t)\hat{u}_k(t+\Delta t) &= \hat{u}_k(t) \\ \hat{u}_k(t+\Delta t) &= (1 + k^2 \Delta t)^{-1}\hat{u}_k(t)\end{aligned}$$

Matrix version:

$$u(t+\Delta t) = (I - \Delta t L)^{-1} u(t)$$



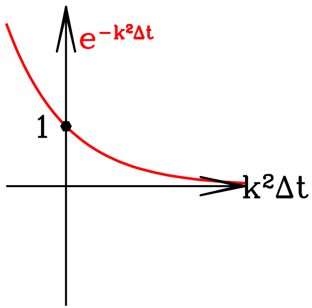
Crank-Nicolson:

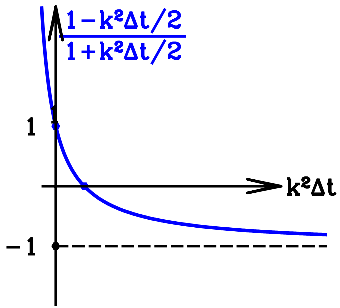
$$u(t+\Delta t) = u(t) + \frac{\Delta t}{2}\left(f(u(t)) + f(u(t+\Delta t))\right)$$

$$u(t+\Delta t) - \frac{\Delta t}{2} f(u(t+\Delta t)) = u(t) + \frac{\Delta t}{2} f(u(t))$$

$$\left(1 + \frac{k^2 \Delta t}{2}\right) \hat{u}_k(t+\Delta t) = \left(1 - \frac{k^2 \Delta t}{2}\right) \hat{u}_k(t)$$

$$\hat{u}_k(t+\Delta t) = \frac{1 - \frac{k^2 \Delta t}{2}}{1 + \frac{k^2 \Delta t}{2}} \quad \hat{u}_k(t)$$





|Amp. factor| < 1 but spurious large-k behavior: slow oscillatory decay

A-stable methods:

$$\frac{du}{dt} = -k^2 u \Longrightarrow \qquad u_{\text{exact}}(t) = e^{-k^2 t}$$

$$\Longrightarrow \qquad \lim_{t\to\infty} u_{\text{exact}}(t) = 0$$

$$\textbf{A-stable method} \Longrightarrow \qquad \lim_{t\to\infty} u_{\text{numerical}}(t) = 0$$

Define $q \equiv -k^2 \Delta t$ **and generalize to** q **complex**

Define amplification factor $\Phi(q)$

Consider behavior for $\mathcal{R}e(q) < 0$

A-stable: $|\Phi(q)| < 1$

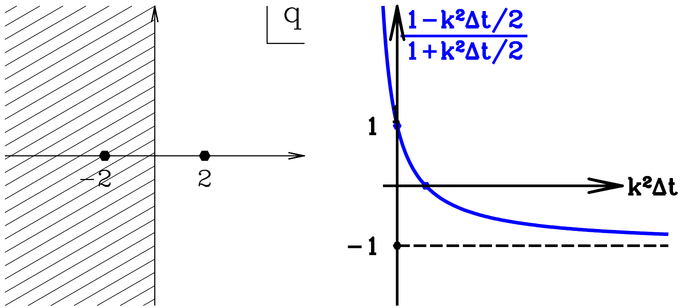
L-stable: $|\Phi(q)| \to 0$ **as** $q \to \infty$

Crank-Nicolson: seek stability region in complex plane, where

$$|\Phi(q)| \equiv \left|\frac{1+q/2}{1-q/2}\right| \leq 1$$

$$|1+q/2| \leq |1-q/2|$$

q is closer to -2 than to 2: q is in left half plane



A-stable $\Longleftrightarrow$ stability region contains negative real axis

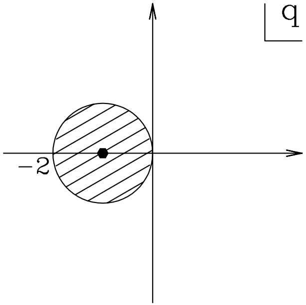
$\Longleftrightarrow$ **For $\mathcal{R}e(q) < 0$, have $|\Phi(q)| < 1$ ✓ YES**

L-stable $\Longleftrightarrow$ For $\mathcal{R}e(q) < 0$, have $|\Phi(q)| \to 0$ as $q \to \infty$

× NO

Forwards Euler

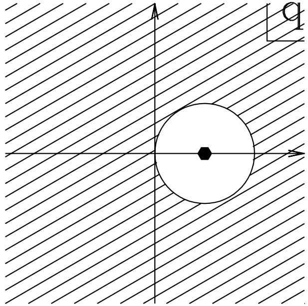
$$|1+q| < 1$$



Backwards Euler

$$1/|1-q| < 1$$

$$|1-q| > 1$$



For q real, require $-2 < q < 0$

All $q < 0$ in stability region

Adams-Bashforth:

$$u(t+\Delta t) = u(t) + \frac{\Delta t}{2}\left(3f(u(t)) - f(u(t-\Delta t))\right)$$
$$= u(t) + q\left(\frac{3}{2}u(t) - \frac{1}{2}u(t-\Delta t)\right)$$

$$\begin{pmatrix} u(t+\Delta t) \\ u(t) \end{pmatrix} = \begin{pmatrix} 1+\frac{3q}{2} & -\frac{q}{2} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u(t) \\ u(t-\Delta t) \end{pmatrix}$$

Require that both eigenvalues obey $|\lambda| < 1$

Eigenvalues λ obey characteristic polynomial

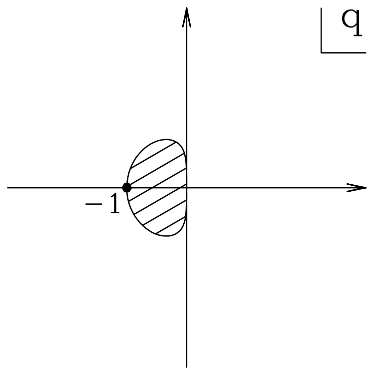
$$0 = \left(1 + \frac{3q}{2} - \lambda\right)(-\lambda) + \frac{q}{2}$$
$$= \lambda^2 - \lambda\left(1 + \frac{3q}{2}\right) + \frac{q}{2}$$
$$\frac{q}{2} = \frac{\lambda^2 - \lambda}{3\lambda - 1}$$

Set $\lambda = e^{i\theta}$:

$$\frac{q}{2} = \frac{\lambda^2 - \lambda}{3\lambda - 1} = \frac{e^{2i\theta} - e^{i\theta}}{3e^{i\theta} - 1} = \frac{\cos 2\theta - \cos\theta + i(\sin 2\theta - \sin\theta)}{(3\cos\theta - 1) + 3i\sin\theta}$$

$$= \frac{(\cos 2\theta - \cos\theta)\,(3\cos\theta - 1) + (\sin 2\theta - \sin\theta) 3\sin\theta}{(3\cos\theta - 1)^2 + (3\sin\theta)^2}$$

$$+\, i\,\frac{(\cos 2\theta - \cos\theta)\,(-3\sin\theta) + (\sin 2\theta - \sin\theta)(3\cos\theta - 1)}{(3\cos\theta - 1)^2 + (3\sin\theta)^2}$$



not A-stable

Backwards Differentiation:

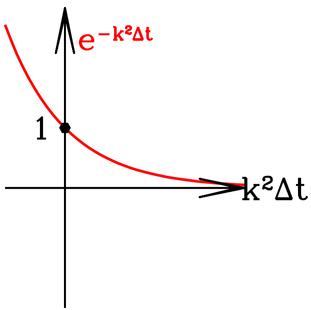
$$\begin{aligned}
u(t+\Delta t) &= \frac{4}{3}u(t) - \frac{1}{3}u(t-\Delta t) + 2\Delta t f(u(t+\Delta t)) \\
&= \frac{4}{3}u(t) - \frac{1}{3}u(t-\Delta t) + 2qu(t+\Delta t) \\
(1-2q)u(t+\Delta t) &= \frac{4}{3}u(t) - \frac{1}{3}u(t-\Delta t) \\
u(t+\Delta t) &= \frac{1}{1-2q}\left(\frac{4}{3}u(t) - \frac{1}{3}u(t-\Delta t)\right) \\
\begin{pmatrix} u(t+\Delta t) \\ u(t) \end{pmatrix} &= \begin{pmatrix} \frac{4/3}{1-2q} & -\frac{1/3}{1-2q} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u(t) \\ u(t-\Delta t) \end{pmatrix}
\end{aligned}$$

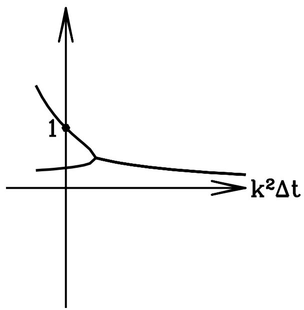
Eigenvalues λ obey characteristic polynomial

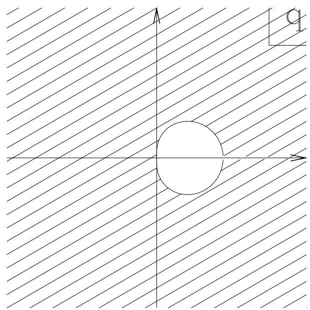
$$\begin{aligned}
0 &= \left(\frac{4/3}{1-2q} - \lambda\right)(-\lambda) + \frac{1/3}{1-2q} \\
3(2q-1) &= -\frac{4}{\lambda} + \frac{1}{\lambda^2}
\end{aligned}$$

Require that both eigenvalues obey $|\lambda| < 1$ so set $\lambda = e^{i\theta}$

$$
\begin{aligned}
3(2q-1) &= -\frac{4}{e^{i\theta}} + \frac{1}{e^{2i\theta}} \\
&= -4(\cos\theta - i\sin\theta) + (\cos 2\theta - i\sin 2\theta) \\
q &= \frac{1}{6}\left(3 - 4\cos\theta + \cos 2\theta + i[4\sin\theta - \sin 2\theta]\right)
\end{aligned}
$$







A-stable

General formalism:

$$\sum_{j=0}^{s} \alpha_j u^{n+1-j} = \Delta t \sum_{j=0}^{s} \beta_j f(u^{n+1-j})$$

Degrees of freedom $\{\alpha_j\}$, $\{\beta_j\}$ allow many routes to order-p accuracy.
Scale by setting $\alpha_0 = 1$. Explicit $\Longleftrightarrow$ $\beta_0 = 0$:

$$u^{n+1} = \sum_{j=1}^{s} \left(-\alpha_j u^{n+1-j} + \Delta t \beta_j f(u^{n+1-j})\right)$$

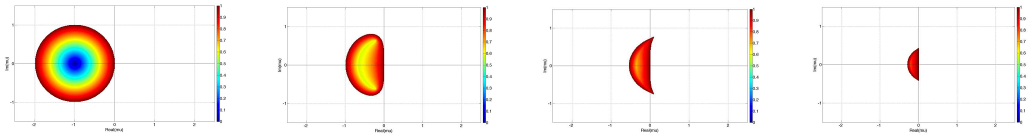
Adams-Bashforth (explicit): $\alpha_0 = 1, \alpha_1 = -1, \alpha_{j\geq 2} = 0, \beta_0 = 0$
Select $\beta_{1\leq j\leq p}$ to achieve p-order accuracy.

Adams-Moulton (implicit): $\alpha_0 = 1, \alpha_1 = -1, \alpha_{j\geq 2} = 0$
Select $\beta_{0\leq j\leq p-1}$ to achieve p-order accuracy.

Backwards-Differentiation (implicit): $\alpha_0 = 1, \beta_{j\geq 1} = 0$

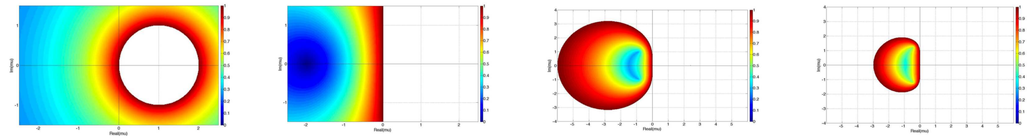
Select $\beta_0, \alpha_{1\leq j\leq p}$ to achieve p-order accuracy.

Stability regions of Adams-Bashforth formulas:



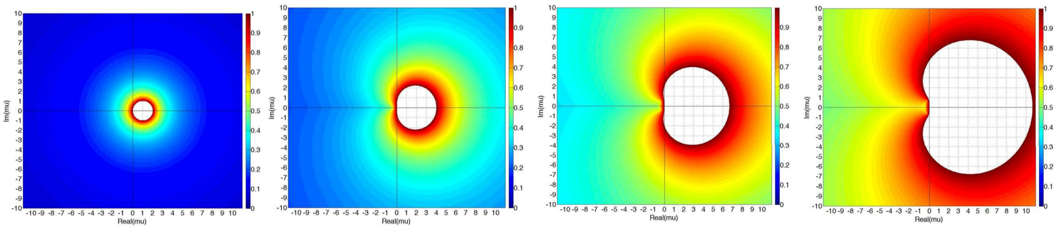
Forwards Euler

Stability regions of Adams-Moulton formulas:



Backwards Euler **Crank-Nicolson**

Stability regions of Backwards Differentiation formulas:



Backwards Euler

order 1 **order 2** **order 3** **order 4**

In general, increasing accuracy $\Longrightarrow$ decreasing stability

A-stable methods must be implicit and at most second order.

Explicit methods approximate exponential by polynomial:
Necessarily grow as $q \rightarrow \pm\infty$

Implicit methods approximate the exponential by a rational.

What about using the exponential itself?

This is sometimes possible if the operator:
–is linear
–can be cheaply diagonalized

Exponential of a matrix with real eigenvalues

$$
\begin{aligned}
e^{Lt} &= I + tL + \frac{t^2}{2}L^2 + \ldots \\
&= VV^{-1} + tV\Lambda V^{-1} + \frac{t^2}{2}V\Lambda V^{-1}\, V\Lambda V^{-1} + \\
&= V\left[I + t\Lambda + \frac{t^2}{2}\Lambda^2 + \ldots\right]V^{-1} = V e^{\Lambda t} V^{-1} \\
\Lambda^2 &= \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{pmatrix} \\
e^{t\Lambda} &= \begin{pmatrix} 1 + t\lambda_1 + \frac{(t\lambda_1)^2}{2} + \ldots & 0 \\ 0 & 1 + t\lambda_2 + \frac{(t\lambda_2)^2}{2} + \ldots \end{pmatrix} \\
&= \begin{pmatrix} e^{t\lambda_1} & 0 \\ 0 & e^{t\lambda_2} \end{pmatrix}
\end{aligned}
$$

Imaginary Eigenvalues

$$L = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix} \qquad \lambda_\pm = \pm i\omega$$

$$L^2 = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}\begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix} = \begin{pmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{pmatrix}$$

$$L^3 = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}\begin{pmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{pmatrix} = \begin{pmatrix} 0 & \omega^3 \\ -\omega^3 & 0 \end{pmatrix}$$

$$e^{Lt} = I + tL + \frac{t^2}{2}L^2 + \frac{t^3}{6}L^3 + \ldots$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + t\begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix} + \frac{t^2}{2}\begin{pmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{pmatrix} + \frac{t^3}{6}\begin{pmatrix} 0 & \omega^3 \\ -\omega^3 & 0 \end{pmatrix}$$

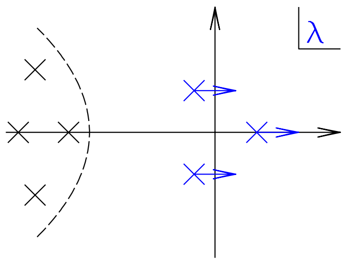
$$= \begin{pmatrix} 1 - \frac{1}{2}(t\omega)^2 + \ldots & -t\omega + \frac{1}{6}(t\omega)^3 + \ldots \\ t\omega - \frac{1}{6}(t\omega)^3 + \ldots & 1 - \frac{1}{2}(t\omega)^2 + \ldots \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{pmatrix}$$

Complex Eigenvalues:

$$\exp\left[t\begin{pmatrix}\mu & -\omega\\ \omega & \mu\end{pmatrix}\right] = e^{\mu t}\begin{pmatrix}\cos(\omega t) & -\sin(\omega t)\\ \sin(\omega t) & \cos(\omega t)\end{pmatrix}$$

Mixed spectrum:



$$\Lambda = \begin{bmatrix}\lambda_1 & 0 & 0 & 0\\ 0 & \mu & -\omega & 0\\ 0 & \omega & \mu & 0\\ 0 & 0 & 0 & \lambda_4\end{bmatrix}$$

$$Re(\lambda_1) \geq Re(\lambda_2) = Re(\lambda_3) \geq Re(\lambda_4)$$

$$\exp(\Lambda t) = \begin{bmatrix}e^{\lambda_1 t} & 0 & 0 & 0\\ 0 & e^{\mu t}\cos(\omega t) & -e^{\mu t}\sin(\omega t) & 0\\ 0 & e^{\mu t}\sin(\omega t) & e^{\mu t}\cos(\omega t) & 0\\ 0 & 0 & 0 & e^{\lambda_4 t}\end{bmatrix}$$

Holds for any analytic function $f(L)$

$$
\begin{aligned}
f(L) &= \sum_j \frac{1}{j!} f^{(j)}(0) L^j \\
&= \sum_j \frac{1}{j!} f^{(j)}(0) \left(V \Lambda V^{-1}\right)^j \\
&= V \left[\sum_j \frac{1}{j!} f^{(j)}(0) \Lambda^j \right] V^{-1} = V f(\Lambda) V^{-1}
\end{aligned}
$$

where

$$
f(\Lambda) = f \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix} = \begin{pmatrix} f(\lambda_1) & & & \\ & f(\lambda_2) & & \\ & & \ddots & \\ & & & f(\lambda_N) \end{pmatrix}
$$

$$\frac{du}{dt} = Lu \Longrightarrow u(t) = e^{Lt}u(0)$$

$$u(0)$$

$$\downarrow \qquad \textbf{multiply by matrix } V^{-1}$$

$$V^{-1}u(0)$$

$$\downarrow \qquad \textbf{multiply by diagonal matrix } e^{\Lambda t}$$

$$e^{t\Lambda}V^{-1}u(0)$$

$$\downarrow \qquad \textbf{multiply by matrix } V$$

$$Ve^{t\Lambda}V^{-1}u(0) = e^{Lt}u(0)$$

Example: Heat Equation

$$\partial_t u = \partial^2_{xx} u$$

$$u(x,t) = \sum_{k=1}^{k_{max}} \hat{u}_k(t) \sin kx$$

$$\partial_t \hat{u}_k = -k^2 \hat{u}_k$$

Begin with $u(x_j, t=0)$ **on a grid of values** $\{x_0, x_1, \ldots x_n\}$

Take Fourier transform: $\{u(x_j, t=0)\} \Longrightarrow \{\hat{u}_k(t=0)\}$

$$\hat{u}_k(t) = e^{-k^2 t} \hat{u}_k(t=0)$$

Take inverse Fourier transform: $\{\hat{u}_k(t)\} \Longrightarrow \{u(x_j, t)\}$

Complete answer valid for all time.

Not usually possible, since most problems are:

–not linear

–not easily diagonalized

but exponential integration can be combined with other ideas

Time-splitting for $\frac{du}{dt} = Lu + N(u)$

Backwards Euler / Forwards Euler:

$$\begin{aligned} u(t+\Delta t) &= u(t) + \Delta t L u(t+\Delta t) + \Delta t N(u(t)) \\ (I - \Delta t L) u(t+\Delta t) &= u(t) + \Delta t N(u(t)) \\ u(t+\Delta t) &= (I - \Delta t L)^{-1} \left[u(t) + \Delta t N(u(t) \right] \end{aligned}$$

Exponential / Forwards Euler:

$$u(t+\Delta t) = e^{L\Delta t} \left[u(t) + \Delta t N(u(t)) \right]$$

Exponential / Adams-Bashforth:

$$u(t{+}\Delta t) = e^{L\Delta t} \left[u(t) + \Delta t \left(\frac{3}{2} N(u(t)) - \frac{1}{2} N(u(t - \Delta t) \right) \right]$$

Runge-Kutta Methods

RK2 (two evaluations of f per timestep, order 2)

$$U_1 = u(t)$$
$$U_2 = u(t) + \Delta t f(U_1)$$
$$u(t+\Delta t) = u(t) + \frac{\Delta t}{2}\left(f(U_1) + f(U_2)\right)$$

RK4 (four evaluations of f per timestep, order 4)

$$U_1 = \Delta t f(u(t))$$
$$U_2 = \Delta t f\left(u(t) + \frac{U_1}{2}\right)$$
$$U_3 = \Delta t f\left(u(t) + \frac{U_2}{2}\right)$$
$$U_4 = \Delta t f\left(u(t) + U_3\right)$$
$$u(t+\Delta t) = u(t) + \frac{1}{6}\left(U_1 + 2U_2 + 2U_3 + U_4\right)$$

Many, many others

For conservative (Hamiltonian, area-preserving) systems, numerical method should also preserve area.

Oscillator:

$$\frac{d^2u}{dt^2} = -\omega^2 u \Longleftrightarrow \begin{cases} \frac{du}{dt} = -\omega v \\ \frac{dv}{dt} = \omega u \end{cases}$$

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

or

$$\frac{d}{dt}(u + iv) = i\omega(u + iv)$$

Set $q = i\omega\Delta t$ **and consider** $|\Phi(q)|$

Forwards Euler:

$$\Phi(i\omega\Delta t) = 1 + i\omega\Delta t$$

$$|\Phi(i\omega\Delta t)|^2 = 1 + (\omega\Delta t)^2 > 1$$

Increases area

Backwards Euler:

$$\Phi(i\omega\Delta t) = \frac{1}{1 + i\omega\Delta t}$$

$$|\Phi(i\omega\Delta t)|^2 = \frac{1}{1 + (\omega\Delta t)^2} < 1$$

Decreases area

Crank-Nicolson:

$$\Phi(i\omega\Delta t) = \frac{1 + i\omega\Delta t/2}{1 - i\omega\Delta t/2}$$

$$|\Phi(i\omega\Delta t)|^2 = \frac{1 + (\omega\Delta t/2)^2}{1 + (\omega\Delta t/2)^2} = 1$$

Preserves area