Numerical methods to solve differential equations

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Outline

Introduction to Numerical Methods

The bridge between theory and reality

What Are Numerical Methods?

From Continuous to Discrete

Numerical methods are computational techniques that approximate solutions to mathematical problems where exact methods often fail.

The Core Process

- **Discretization:** Converting continuous expressions (PDEs/ODEs) into manageable discrete forms.
- **Techniques:** Finite Differences (FDM), Finite Elements (FEM), Iterative Solvers.

The Philosophy

- Focus on **practicality** over pure symbolic elegance.
- Delivers answers with **controllable and quantifiable accuracy**.
- Invaluable for data-driven and computation-heavy environments.

Why Are They Indispensable?

1. Tackling Real-World Complexity

Analytical solutions are rare for nonlinear, coupled equations or complex boundary conditions.

- **Jet Engines:** Simulating heat transfer via Finite Difference methods.
- **Skyscrapers:** Modeling stress distribution using Finite Element Analysis (FEA).
- **Acoustics:** Solving the Wave Equation for concert hall design.

Why Are They Indispensable?

2. Scalability and Interdisciplinary Utility

Scalability

Handling massive systems of equations for:

- Climate simulations
- Large-scale Neural Networks
- Quantum simulations

Disciplines

- **Physics:** Chaotic systems and plasma dynamics.
- **Finance:** Option pricing via Stochastic Differential Equations.
- **Biology:** Disease spread and population dynamics.

Theoretical Underpinning

Beyond Pure Computation

The success of any numerical algorithm is grounded in three pillars:

- **Convergence:** Does the approximate solution v approach the exact solution u as $\Delta x, \Delta t \to 0$?
- **Stability:** Does the algorithm suppress errors (round-off/truncation) over time?
- **Consistency:** Does the numerical scheme truly represent the original PDE?

> **Lax Equivalence Theorem:** For a well-posed linear problem, Consistency + Stability = Convergence.

Challenges and the Path Forward

Precision vs. Cost

Current Hurdles

- **Trade-offs:** High accuracy vs. substantial computational resources.
- **Conditioning:** Managing ill-conditioned systems and truncation errors.
- **Design:** Adapting general methods to specific, creative problems.

The Future

- High-Performance Computing (HPC)
- Machine Learning-assisted solvers
- Adaptive Mesh Refinement (AMR)

Real-World Impact

Inspiration for Engineers and Scientists

🌉 **The Millau Viaduct:** Designed using FEM for maximum safety and efficiency.

🌊 **Tsunami Warnings:** Numerical propagation models providing life-saving early alerts.

🚀 **Space Exploration:** Runge-Kutta methods calculating spacecraft trajectories.

Some Thoughts

As Master's students, you are not just learning tools—**you are shaping the future.**

Numerical methods are the engine behind progress in science, engineering, and technology.

Go beyond the numbers: Solve problems, understand the world, and build the future.

Discretization

Differential Equations

Numerical methods to solve differential equations:

$$u_t = f(u,t) \qquad u_t = \frac{du}{dt}$$

Example:

$$u_t = A(t) \cdot u + B(t) \qquad u_t = A(t) \cdot u$$

Generally, we want to pass from N order differential equations to a system of N first order diff. equations:

$$\begin{cases} u_t &= v \\ v_t &= g(u,v,t) \end{cases}$$

Separation of variables

Given the Cauchy problem:

$$\begin{cases} u_t = Au \\ u(0) = u_0 \end{cases}$$

We are going to solve this system with the separation of variables:

$$\begin{aligned} \frac{du}{dt} &= Au \\ \Rightarrow \frac{du}{u} &= A\,dt \\ \Rightarrow \int_{u_0}^{u} \frac{du'}{u'} &= \int_0^t A\,dt \\ \Rightarrow \ln\left(\frac{u}{u_0}\right) &= At \\ \Rightarrow u(t) &= u_0 e^{At} \end{aligned}$$

Discretization of the Solution

Given the Cauchy problem:

$$\begin{cases} u_t = f(u,t) \\ u(0) = u_0 \end{cases}$$

Let's consider a temporal step $\Delta t = k$:

$$t_0 = 0; \quad t_1 = k; \quad t_2 = 2k; \quad \dots \quad t_k = nk; \qquad 0 \leq n \leq N$$

I want to obtain an approximation v^n of $u(t_n)$:

$$u(t_n) = u_n \simeq v^n \quad \Rightarrow \quad f(u_n, t_n) \simeq f(v^n, t_n) = f^n$$

Then I should find a criterion to build the sequence $v^0, v^1, \dots, v^n$ that furnishes the discrete representation of $u(t)$ in time. That will represent my **numerical solution**.

Finite Difference Quotient

I can apply the definition of derivative as **difference quotient**:

$$\frac{u(t_{n+1}) - u(t_n)}{t_{n+1} - t_n} \simeq u_t(t_n) \qquad \Rightarrow \qquad u_t(t_n) \simeq \frac{v^{n+1} - v^n}{k} = f^n$$

Obtaining then a recursive formula:

$$\begin{cases} v^{n+1} = v^n + kf^n \\ v^0 = u_0 \end{cases}$$

1. Starting from v^0, I evaluate $v^1 = v^0 + kf^0$ with $v^0 = u_0$ and $f^0 = f(u_0, 0)$.
2. Once found v^1, I calculate $f^1 = f(v^1, k)$.
3. ... and so on.

Explicit vs. Implicit Schemes

ACHTUNG!

I can have both:

$$\frac{v^{n+1} - v^n}{k} = f^n \quad \text{and} \quad \frac{v^{n+1} - v^n}{k} = f^{n+1}$$

Because I evaluate the derivative at endpoints of interest interval $[t_n; t_{n+1}]$.

I obtain then two recursive formulas:

$$v^{n+1} = v^n + k \cdot f^n$$ | **Explicit Euler**

$$v^{n+1} = v^n + k \cdot f^{n+1}$$ | **Implicit Euler**

Implicit because the f^{n+1} term contains v^{n+1}, a value that already appears at the first member.

↙

Slide: Central and Trapezium Schemes

I can also evaluate the derivative in a symmetrical point of the interval:

$$u_t(t_n) = \frac{u(t_{n+1}) - u(t_{n-1})}{t_{n+1} - t_{n-1}} = \frac{v^{n+1} - v^{n-1}}{2k}$$

→ $v^{n+1} = v^{n-1} + 2k \cdot f^n$ | **Central Value**

Taking the central value I cannot apply the formula to evaluate v^1: I have to use Euler for that.

←

Or I can also evaluate the average of f^n and f^{n+1}:

$$\frac{v^{n+1} - v^n}{k} = \frac{1}{2}\left(f^{n+1} + f^n\right)$$

→ $v^{n+1} = v^n + \frac{k}{2}\left(f^n + f^{n+1}\right)$ | **Trapezium**

Slide: Example - Explicit Euler

Example

Now let's apply the previous formulas to the Cauchy problem:

$$\begin{cases} u_t = f(u,t) = u \\ u(0) = u_0 \end{cases}$$

whose analytical solution is $u = u_0 \cdot e^t$.

$$[1] \quad v^1 = u_0 + u_0 \cdot k = u_0(1+k)$$

$$[2] \quad v^2 = v^1 + k \cdot f^1 = u_0(1+k)^2$$

$$[3] \quad v^3 = u_0(1+k)^3$$

$$[n] \quad v^n = u_0(1+k)^n$$

RECURSIVE STEP

$$v^{n+1} = v^n + k f^n$$

Explicit Euler

Slide: Example - Implicit

$$[1] \quad v^1 = v^0 + kv^1 \implies v^1 = \frac{1}{1-k} u_0$$

$$[2] \quad v^2 = v^1 + kv^2 \implies v^2 = \frac{1}{(1-k)^2} u_0$$

$$[3] \quad v^3 = u_0 (1-k)^{-3}$$

$$[n] \quad v^n = u_0 (1-k)^{-n}$$

RECURSIVE STEP

$$v^{n+1} = v^n + k f^{n+1}$$

Implicit Euler

Slide: Example - Trapezium

$$[1] \quad v^1 = v^0 + \frac{k}{2}(v^0 + v^1) \implies v^1 = u_0 \frac{1 + k/2}{1 - k/2}$$

$$[2] \quad v^2 = v^1 + \frac{k}{2}(v^1 + v^2) \implies v^2 = u_0 \frac{(1 + k/2)^2}{(1 - k/2)^2}$$

$$[3] \quad v^3 = u_0 \frac{(1 + k/2)^3}{(1 - k/2)^3}$$

$$[n] \quad v^n = u_0 \left(\frac{1 + k/2}{1 - k/2} \right)^n$$

RECURSIVE STEP

$$v^{n+1} = v^n + \frac{k}{2}(f^n + f^{n+1})$$

Trapezium Method

Slide: Comparison of Approximations (n=1)

Now let's try to understand which of the outlined methods better approximate the analytical solution. The latter, evaluated at time t_n, is: $u(t_n) = u_0 e^{nk}$. Let's consider the 4 formulas at the first tme step ($n = 1$).

Explicit:

$$\frac{v^1}{u_0} = 1 + k$$

Implicit:

$$\frac{v^1}{u_0} = \frac{1}{1-k} \approx 1 + k + k^2 + k^3 + \dots$$

Trapezium:

$$\frac{v^1}{u_0} = \frac{1 + k/2}{1 - k/2} \approx 1 + k + \frac{k^2}{2} + \frac{k^3}{4} + \dots$$

ANALYTICAL SOLUTION

$$\frac{u(t_1)}{u_0} = e^k$$

$$1 + k + \frac{k^2}{2} + \dots + \frac{k^m}{m!}$$

The trapezium method offers the best approximation, exact until the third term (second order in k). [The above formulas are obtained using Taylor expansions]

Explicit vs. Implicit Methods

Advantages, Disadvantages, and Applications

Choosing the right numerical approach

The choice between **Explicit** and **Implicit** schemes depends on the specific nature of the physical problem.

Explicit Methods

Compute the next state directly from current known values.

- **Analogy:** Looking at the current map to take the next step.

Implicit Methods

Compute the next state by solving a system of equations.

- **Analogy:** Solving a puzzle where the next step must satisfy a global balance.

Explicit Numerical Methods

Direct computation: $u^{n+1} = F(u^n)$

🟢 Advantages

- **Simplicity:** Straightforward implementation.
- **Memory:** Low requirements (no large matrices).
- **Efficiency:** Very fast per time step for high-resolution needs.

🔴 Disadvantages

- **Stability Constraints:** Must satisfy the **CFL Condition**:

$$c\frac{\Delta t}{\Delta x} \leq 1$$

- **Stiff Problems:** Inefficient; requires extremely small Δt to avoid "blowing up."

Example: The Wave Equation

Classical Explicit Application

The 1D Wave Equation describes propagation where information travels at a finite speed c:

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

Discretization:

$$u_j^{n+1} = 2u_j^n - u_j^{n-1} + C^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

where $C = c\frac{\Delta t}{\Delta x}$.

Implicit Numerical Methods

Coupled computation: $G(u^{n+1}, u^n) = 0$

🟢 Advantages

- **Unconditional Stability:** Allows much larger time steps Δt.
- **Stiff Systems:** The only viable choice for chemical kinetics or heavy diffusion.
- **Long-Term:** Efficient for long duration simulations.

🔴 Disadvantages

- **Complexity:** Requires solving a system of equations (Matrix Inversion).
- **Memory:** High; needs to store and solve large matrices.
- **Non-linear Problems:** Requires iterative solvers (e.g., Newton-Raphson).

Example: The Heat Equation

Implicit Mastery with Crank-Nicolson

Modeling heat conduction in a solid: $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

The **Crank-Nicolson** scheme is a popular implicit method:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\alpha}{2} \left[\delta_x^2 u_j^{n+1} + \delta_x^2 u_j^n \right]$$

- Results in a **Tridiagonal Matrix** system.
- **Unconditionally Stable:** You can pick Δt based on accuracy, not just to prevent crashes.

Summary Comparison

Feature	Explicit	Implicit
Computation	Direct (Algebraic)	Iterative/Matrix (System)
Stability	Conditional (CFL)	Often Unconditional
Time Step	Must be small	Can be large
Memory	Low	High
Best for...	Wave propagation, acoustics	Diffusion, chemical kinetics, stiffness

- **Use Explicit** for high-speed dynamics (Sound, Impact).
- **Use Implicit** for slow-evolving, diffusion-dominated systems (Heat, Groundwater).

Runge-Kutta methods

Runge-Kutta methods

Up to now, we have limited ourselves to evaluating the function only at the limits of each time step.
Now, given a time interval $[t_n, t_{n+1}]$, the idea is to also evaluate the function at intermediate points within this interval to improve accuracy.

STEP 1: Intermediate Value (Euler)

$$\tilde{v}^{n+\frac{1}{2}} = v^n + \frac{k}{2} f^n$$

STEP 2: Evaluation

$$\tilde{f}^{n+\frac{1}{2}} = f(\tilde{v}^{n+\frac{1}{2}}, t_{n+\frac{1}{2}})$$

FINAL STEP:

$$v^{n+1} = v^n + k\tilde{f}^{n+\frac{1}{2}}$$

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*The **Midpoint** method uses an intermediate estimate to improve the slope accuracy.*

RECURSIVE STEP

$$v^{n+1} = v^n + k f^{n+\frac{1}{2}}$$

Runge-Kutta 2 (RK2)

Two-Stage Intermediate Time Integration

We consider two intermediate times within the interval $[t_n, t_{n+1}]$, namely $t_{n+\frac{1}{3}}$ and $t_{n+\frac{2}{3}}$. Starting from the known values (t_n, v^n, f^n), we can define intermediate estimates as follows:

[1] First Stage:

$$\tilde{v}^{n+\frac{1}{3}} = v^n + \frac{k}{3} f^n, \quad \tilde{f}^{n+\frac{1}{3}} = f(\tilde{v}^{n+\frac{1}{3}}, t_{n+\frac{1}{3}})$$

[2] Second Stage:

$$\tilde{v}^{n+\frac{2}{3}} = v^n + \frac{2k}{3} \tilde{f}^{n+\frac{1}{3}}, \quad \tilde{f}^{n+\frac{2}{3}} = f(\tilde{v}^{n+\frac{2}{3}}, t_{n+\frac{2}{3}})$$

[3] Final Step:

$$v^{n+1} = v^n + \frac{k}{2} \left(\tilde{f}^{n+\frac{1}{3}} + \tilde{f}^{n+\frac{2}{3}} \right)$$

MULTI-STAGE STEP

$$v^{n+1} = v^n + \sum c_i f_i$$

Runge-Kutta Variant

The idea is to divide the interval into intermediate times (in principle, we could use more stages), and recursively construct $\tilde{v}^{n+c_i}$ and $\tilde{f}^{n+c_i}$ for $0 < c_i < 1$. This approach improves the accuracy by incorporating multiple evaluations of the derivative function $f(v, t)$ within each time step.

General Recursive Formula

Starting from $c_1 = 0$, let α_{ij} denote the intermediate coefficients and b_i the final weights.

[1]

$$\text{Known} \quad v^{n+c_1} \quad \text{and} \quad f^{n+c_1} = f(v^{n+c_1}, t_{n+c_1})$$

[2]

$$\tilde{v}^{n+c_2} = v^n + k\,\alpha_{21} f^{n+c_1}; \quad \tilde{f}^{n+c_2} = f(\tilde{v}^{n+c_2}, t_{n+c_2})$$

[3]

$$\tilde{v}^{n+c_3} = v^n + k\left(\alpha_{31} f^{n+c_1} + \alpha_{32} f^{n+c_2}\right); \quad \tilde{f}^{n+c_3} = f(\tilde{v}^{n+c_3}, t_{n+c_3})$$

[s]

$$\tilde{v}^{n+c_s} = v^n + k\left(\alpha_{s1} f^{n+c_1} + \cdots + \alpha_{s,s-1} f^{n+c_{s-1}}\right)$$

[END]

$$v^{n+1} = v^n + k \sum_{i=1}^{s} b_i f^{n+c_i}$$

BUTCHER TABLEAU

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

General RK Structure

Runge–Kutta Coefficient Matrix (Butcher Tableau)

$$
\begin{array}{c|ccccc}
c_1 & & & & & \\
c_2 & \alpha_{21} & & & & \\
c_3 & \alpha_{31} & \alpha_{32} & & & \\
\cdots & \cdots & \cdots & \ddots & & \\
c_s & \alpha_{s1} & \alpha_{s2} & \cdots & \alpha_{s,s-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}
$$

c_i: stage time coefficients

α_{ij}: intermediate weights, $i = 1, \ldots, s, j = 1, \ldots, i-1$

b_i: final weights

Runge–Kutta of Order 1 (Midpoint Method)

[1]

$$\tilde{v}^{n+\frac{1}{2}} = v^n + \frac{k}{2} f^n \quad \Rightarrow \quad \tilde{f}^{n+\frac{1}{2}}$$

[2]

$$v^{n+1} = v^n + k\, \tilde{f}^{n+\frac{1}{2}}$$

MIDPOINT (RK2)

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

The simple Euler method can be viewed as a Runge–Kutta method of order zero, with matrix:

$$\begin{array}{c|c} 0 & \\ \hline & 1 \end{array} \quad \rightarrow \quad v^{n+1} = v^n + k f^n$$

From Matrix to Implementation

[1]

$$\tilde{v}^{n+\frac{1}{3}} = v^n + \frac{k}{3} f^n \Rightarrow \tilde{f}^{n+\frac{1}{3}}$$

[2]

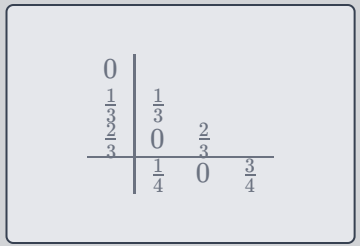
$$\tilde{v}^{n+\frac{2}{3}} = v^n + k\left(0 \cdot f^n + \frac{2}{3}\tilde{f}^{n+\frac{1}{3}}\right) \Rightarrow \tilde{f}^{n+\frac{2}{3}}$$

[END]

$$v^{n+1} = v^n + \frac{k}{4}\left(f^n + 3f^{n+\frac{2}{3}}\right)$$

[Heun formula, 2nd order]

HEUN (RK3 VARIANT)



Application Example

(1)

Initial state: t_n, v^n, f^n

(2)

$$\tilde{v}^{n+c_2} = v^n + k\alpha_{21} f^n \quad \Rightarrow \quad \tilde{f}^{n+c_2}$$

(3)

$$v^{n+1} = v^n + k(b_1 f^n + b_2 f^{n+c_2})$$

GENERAL 2-STAGE RK

0		
c_2	α_{21}	
	b_1	b_2

Apply this to the Cauchy problem:

$$\begin{cases} u_t = u \\ u(0) = u_0 \end{cases}$$

→

Analytical Solution:

$$u(t) = u_0 e^t$$

Order Conditions

(1)

$$t_0 = 0,\ v^0 = u_0,\ f^0 = u_0$$

(2)

$$\tilde{v}^{c_2} = u_0 + k\alpha_{21}u_0 = u_0(1 + k\alpha_{21}) \quad \Rightarrow \quad \tilde{f}^{c_2} = \tilde{v}^{c_2}$$

(3)

$$v^1 = u_0\left[1 + k(b_1 + b_2) + k^2 b_2 \alpha_{21}\right]$$

STABILITY ANALYSIS

$$u(t_1) = u_0 e^k$$

$$u_0(1 + k + \tfrac{1}{2}k^2 + \dots)$$

Comparing with the exact solution, for **second-order accuracy** we require:

$$\begin{cases} b_1 + b_2 = 1 \\ \alpha_{21} b_2 = \frac{1}{2} \end{cases}$$

Two equations for three unknowns (b_1, b_2, α_{21}).

We add the common constraint relating coefficients of the same row.

Consistency Contraints

General row-sum constraint (consistency):

$$
\begin{aligned}
\alpha_{21} &= c_2 \\
\alpha_{31} + \alpha_{32} &= c_3 \\
&\vdots \\
\alpha_{s1} + \cdots + \alpha_{s,s-1} &= c_s
\end{aligned}
\quad \Rightarrow \quad
\boxed{\sum_{j=1}^{i-1} \alpha_{ij} = c_i}
$$

IMPOSING THE CONSTRAINT FOR OUR CASE:

$$
\begin{cases}
b_1 + b_2 = 1 \\
c_2 b_2 = \frac{1}{2}
\end{cases}
$$

These conditions ensure second-order accuracy by reducing the number of independent unknowns.

ORDER 2 CONDITIONS

$s = 2$

THE RESULTING R-K MATRIX IS:

$$\begin{array}{c|cc} 0 & & \\ c_2 & c_2 & \\ \hline & 1-\frac{1}{2c_2} & \frac{1}{2c_2} \end{array}$$

PARAMETRIC FORM

General solution for 2nd order accuracy with $s = 2$

In general, it also holds that:

$$\sum_{i=1}^{s} b_i = 1$$

For specific choices of coefficients, canonical reference matrices exist.

Butcher Tableaux

The DNA of Runge-Kutta Methods

The Anatomy of the Table

Systematic representation of coefficients

A **Butcher Tableau** provide a compact way to represent the coefficients of Runge-Kutta (RK) methods:

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array}$$

- $\mathbf{A} = [a_{ij}]$: Matrix of coefficients for intermediate stages.
- $\mathbf{c} = [c_i]$: Nodes (time offsets).
- $\mathbf{b} = [b_i]$: Weights for the final update.

Explicit vs. Implicit: The Matrix Test

Identifying the scheme type at a glance

🔵 Explicit Methods

Condition: $\mathbf{A}$ is **strictly lower triangular**.

- $a_{ij} = 0$ for all $j \geq i$.
- Stage k_i depends only on $k_1, \ldots, k_{i-1}$.
- **Result:** Direct evaluation, no iterative solvers needed.

🟠 Implicit Methods

Condition: $\mathbf{A}$ has **nonzero entries** on or above the diagonal.

- $a_{ij} \neq 0$ for some $j \geq i$.
- Stage k_i depends on itself or future stages.
- **Result:** Requires solving algebraic equations (e.g., Newton's method).

Comparative Examples

Case studies in matrix structure

Explicit Euler

$$\begin{array}{c|c} 0 & \mathbf{0} \\ \hline & 1 \end{array}$$

Diagnosis: Strictly lower triangular. **Type:** Explicit.

Implicit Euler

$$\begin{array}{c|c} 1 & \mathbf{1} \\ \hline & 1 \end{array}$$

Diagnosis: Nonzero diagonal. **Type:** Implicit.

Trapezoidal Rule

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & \mathbf{1/2} \\ \hline & 1/2 & 1/2 \end{array}$$

Diagnosis: Diagonal entry (a_{22}) is nonzero. **Type:** Implicit.

Deep Dive: The Classical RK4

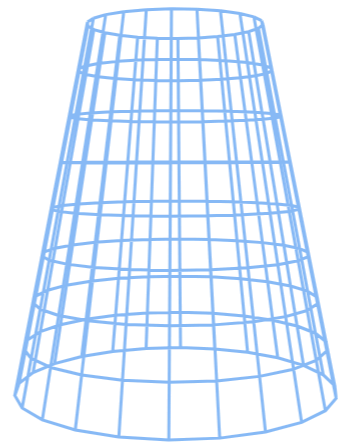
Verifying the structure

Let's examine the standard fourth-order Runge-Kutta matrix $\mathbf{A}$:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- **Diagonal check:** All a_{ii} are 0.
- **Upper triangle check:** All a_{ij} (where $j > i$) are 0.
- **Conclusion:** The matrix is strictly lower triangular.
- **Final Verdict:** RK4 is an **explicit** method.

Butcher Tableaux Examples



1. First & Third Order Methods

From Euler to Heun

Explicit Euler (1st Order)

0	0
	1

Formula: $y_{n+1} = y_n + hf(t_n, y_n)$

Heun's Method (3rd Order)

0	0	0	0
1/3	1/3	0	0
2/3	0	2/3	0
	1/4	0	3/4

Formula: $y_{n+1} = y_n + h(\frac{1}{4}k_1 + \frac{3}{4}k_3)$

2. Strong Stability Preserving

SSPRK3 (3rd Order Explicit)

Often used for hyperbolic PDEs to avoid oscillations.

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 \\
1/2 & 1/4 & 1/4 & 0 \\
\hline
 & 1/6 & 1/6 & 2/3
\end{array}
$$

Why it matters: SSPRK3 ensures that the solution does not grow in norm, making it ideal for non-linear conservation laws.

3. Fourth-Order Explicit Methods

The Gold Standard

Classical RK4

0	0	0	0	0
$1/2$	$1/2$	0	0	0
$1/2$	0	$1/2$	0	0
1	0	0	1	0
	$1/6$	$1/3$	$1/3$	$1/6$

The most widely used integrator.

3/8-Rule

0	0	0	0	0
$1/3$	$1/3$	0	0	0
$2/3$	$-1/3$	$1/3$	0	0
1	1	-1	1	0
	$1/8$	$3/8$	$3/8$	$1/8$

An alternative with different stability properties.

4. Implicit Schemes: Lobatto IIIC

Stability for Stiff Problems

Unlike explicit methods, the A matrix is dense, requiring a system solver.

0	$1/6$	$-1/6$	0
$1/2$	$1/6$	$1/3$	$-1/6$
1	$1/6$	$5/6$	$1/6$
	$1/6$	$2/3$	$1/6$

Analyzing an Invalid Table

Case Study in Consistency

Consider this provided table:

0	0	0	0	0
$1/2$	$1/2$	0	0	0
$1/2$	$1/2$	1	0	0
1	0	0	1	0
	$1/2$	$1/3$	$1/3$	$1/2$

❌ Row Sum Violation

For $c_3 = 1/2 : 1/2 + 1 = 3/2 \neq 1/2$ **Result:** Violation of consistency.

❌ Weight Violation

$\sum b_i = 1/2 + 1/3 + 1/3 + 1/2 = \mathbf{5/3}$

Requirement: $\sum b_i = 1$ **Result:** Incorrect total step size.

Conclusion: Why Validity Matters

A Butcher table is **invalid** if it fails consistency and order conditions.

- **Non-Convergence:** If $\sum b_i \neq 1$, the error does not vanish as $h \to 0$.
- **Stability:** Inconsistent c_i values lead to unphysical phase shifts.
- **Accuracy:** Higher-order terms will accumulate, causing the solution to diverge rapidly.

> **Takeaway:** Always verify row sums and weight sums before implementing a custom tableau.

Linear Multistep Methods

Linear Multistep

A general form of a linear multistep scheme is given by:

$$\alpha_{n+1} v^{n+1} + \alpha_n v^n + \cdots + \alpha_{n-s+1} v^{n-s+1} = \\ = k \left(\beta_{n+1} f^{n+1} + \beta_n f^n + \cdots + \beta_{n-s+1} f^{n-s+1} \right)$$

This class of schemes is called a **Linear Multistep Method (LMM)**.

Unlike Runge–Kutta methods, which use multiple function evaluations within one step, LMMs use several past time levels to advance the solution.

We start again from the Cauchy problem:

$$\begin{cases} u_t &= f(u,t) \\ u(0) &= u_0 \end{cases}$$

Integral Formulation

We discretize time as $t_n = nk$ and define:

$$v^n = u(t_n), \qquad f^n = f(v^n, t_n)$$

Integrating between two consecutive time levels:

$$\int_{t_n}^{t_{n+1}} u_t \, dt = \int_{t_n}^{t_{n+1}} f(u,t) \, dt$$

Let $q(t)$ be a polynomial that interpolates f within $[t_n, t_{n+1}]$.
Then:

$$u(t_{n+1}) - u(t_n) = \int_{t_n}^{t_{n+1}} f(t) \, dt$$

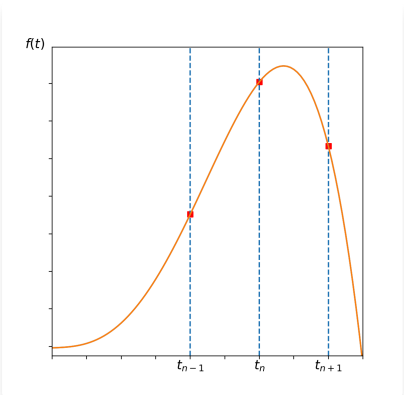
$$\Rightarrow \quad v^{n+1} = v^n + \int_{t_n}^{t_{n+1}} q(t) \, dt$$

Polynomial Interpolation and Implicitness

If $f(t)$ is known at several points, we can build higher-order interpolating polynomials $q(t)$.

Depending on whether f^{n+1} is included in $q(t)$, the resulting scheme is:

- **Explicit**, if f^{n+1} is not included.
- **Implicit**, if f^{n+1} appears in $q(t)$.



Interpolation of $f(t)$ at multiple time levels.

Adams-Bashforth Methods

Consider $q_{AB}(t)$ as the interpolating polynomial. We seek the solution in the time interval $[t_n, t_{n+1}]$.

1st ORDER

Supposing we know the function at t_n: $q_{AB}(t) = f^n$.
Applying $t_{n+1} - t_n = k$:

$$v^{n+1} = v^n + \int_{t_n}^{t_{n+1}} f^n dt$$

$\Rightarrow$ $v^{n+1} = v^n + kf^n$ | ADAMS-BASHFORTH, 1°

Adams–Bashforth Methods

2nd ORDER

Suppose we know the function at f^{n-1} and f^n. Then $q_{AB}(t)$ is the line passing through the points (t_{n-1}, f^{n-1}) and (t_n, f^n):

$$q_{AB}(t) = f^{n-1} + \frac{f^n - f^{n-1}}{t_n - t_{n-1}}(t - t_{n-1})$$

Integrating between t_n and t_{n+1} yields:

$$v^{n+1} = v^n + \frac{k}{2}(3f^n - f^{n-1})$$

ADAMS-BASHFORTH, 2° ORDER

Adams–Moulton Methods

Including also f^{n+1} in the interpolation makes the scheme **implicit**. We are interested in the solution in $[t_n, t_{n+1}]$.

1st ORDER

Supposing we know the function at t_{n+1}: $q_{AM}(t) = f^{n+1}$.
Integrating between t_n and t_{n+1} gives:

$$v^{n+1} = v^n + kf^{n+1}$$

ADAMS–MOULTON, 1° ORDER

Adams–Moulton Methods

2nd ORDER

Suppose $q_{AM}(t)$ is the linear interpolant passing through (t_n, f^n) and (t_{n+1}, f^{n+1}):

$$q_{AM}(t) = f^n + \frac{f^{n+1} - f^n}{t_{n+1} - t_n}(t - t_n)$$

Integrating between t_n and t_{n+1} yields:

$$v^{n+1} = v^n + \frac{k}{2}(f^{n+1} + f^n)$$

ADAMS-MOULTON, 2° ORDER

Trapezoidal Rule: This 2nd order implicit scheme is famously known as the Trapezoidal method. At the 3° ORDER I will have a parabola instead.

Backward Differentiation Methods

Backward Differentiation

We now approximate the solution $u(t)$ itself with an interpolating polynomial $q(t)$ passing through known points $(t_{n+1}, v^{n+1}), (t_n, v^n), \ldots$

Depending on the points selected, q will be a polynomial of 1°, 2°, ... order.

Note: Approximating q as a constant at v^{n+1} results in a zero derivative, which is a too low order approximation.

If q is of **degree 1**, it passes through (t_n, v^n) and (t_{n+1}, v^{n+1}):

$$q_{BD}(t) = v^n + \frac{v^{n+1} - v^n}{k}(t - t_n)$$

$$\Rightarrow \quad \dot{q}_{BD}(t) = \frac{v^{n+1} - v^n}{k}$$

Backward Differentiation – Order 1

We can now evaluate $\dot{q}_{BD}(t)$ at different time levels:

- In t_n: $\frac{v^{n+1}-v^n}{k} = f^n$

  $$\boxed{v^{n+1} = v^n + k f^n}$$ *(Explicit Euler)*

- In t_{n+1}: $\frac{v^{n+1}-v^n}{k} = f^{n+1}$

  $$\boxed{v^{n+1} = v^n + k f^{n+1}}$$ *(Implicit Euler)*

These represent the simplest members of the Backward Differentiation family.

Backward Differentiation – Order 2

Now consider three points: (t_{n-1}, v^{n-1}), (t_n, v^n), and (t_{n+1}, v^{n+1}).

The quadratic interpolant (a parabola) is:

$$\begin{aligned} q_{BD}(t) = & v^{n-1} + (t - t_{n-1}) \frac{v^n - v^{n-1}}{k} \\ & + \frac{(t - t_n)(t - t_{n-1})}{2k^2} (v^{n+1} - 2v^n + v^{n-1}) \end{aligned}$$

Differentiating with respect to time:

$$\dot{q}_{BD}(t) = \frac{v^n - v^{n-1}}{k} + \frac{v^{n+1} - 2v^n + v^{n-1}}{2k^2} (2t - t_n - t_{n-1})$$

Backward Differentiation – Evaluation

Evaluating the derivative $\dot{q}_{BD}(t)$ at different time levels:

- **In t_n:** $\dot{q}_{BD}(t_n) = f^n$

  $\Rightarrow$ $\boxed{v^{n+1} = v^{n-1} + 2kf^n}$ *(Explicit 2-step scheme)*

- **In t_{n+1}:** $\dot{q}_{BD}(t_{n+1}) = f^{n+1}$

  $\Rightarrow$ $\boxed{v^{n+1} = -\frac{1}{3}v^{n-1} + \frac{4}{3}v^n + \frac{2}{3}kf^{n+1}}$ *(Implicit 2-step scheme / BDF2)*

Spatial-temporal discretization

Spatial-temporal discretization

Suppose we know the solution at discrete points (x_j, t_n). We define v_j^n as the numerical approximation: $v_j^n \simeq u(x_j, t_n)$.

Spatial Grid

$$x_{j+1} = x_j + h$$

$\Delta x = h$ (spatial step)

Temporal Grid

$$t_{n+1} = t_n + k$$

$\Delta t = k$ (temporal step)

Let's introduce a series of **discrete operators**. Those acting on the **time** coordinate use a **superscript** (n), while those for the **spatial** coordinate use a **subscript** (j).

Discrete Operators

Temporal (Time)

$$\delta^+ v_j^n = \frac{1}{k}(v_j^{n+1} - v_j^n)$$
$$\delta^- v_j^n = \frac{1}{k}(v_j^n - v_j^{n-1})$$
$$\delta^0 v_j^n = \frac{1}{2k}(v_j^{n+1} - v_j^{n-1})$$

Spatial (Space)

$$\delta_+ v_j^n = \frac{1}{h}(v_{j+1}^n - v_j^n)$$
$$\delta_- v_j^n = \frac{1}{h}(v_j^n - v_{j-1}^n)$$
$$\delta_0 v_j^n = \frac{1}{2h}(v_{j+1}^n - v_{j-1}^n)$$

Properties:

$$\delta^- v_j^{n+1} = \delta^+ v_j^n$$
$$\delta^0 = \frac{1}{2}(\delta^- + \delta^+)$$

$$\delta_- v_{j+1}^n = \delta_+ v_j^n$$
$$\delta_0 = \frac{1}{2}(\delta_- + \delta_+)$$

Composition of Operators

Consider the composition of the two operators δ^- and δ^+. By defining $\delta^X = \delta^- \cdot \delta^+$, we obtain the second-order central difference:

$$\delta^X v_j^n = \frac{1}{k^2}\left(v_j^{n+1} - 2v_j^n + v_j^{n-1}\right)$$

Commutative Property:

$$\delta^X = \delta^- \cdot \delta^+ = \delta^+ \cdot \delta^-$$

The spatial analog is defined similarly:

$$\delta_X v_j^n = \frac{1}{h^2}\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right)$$

Geometric Interpretation

If I know the solution near v_j^n, I could know it everywhere interpolating with a straight line:

$$u(x,t_n) = v_j^n + \frac{v_{j+1}^n - v_j^n}{h}(x - x_j) \quad [\text{line by } v_j^n; v_{j+1}^n]$$

The slope of the straight line is given by:

$$\delta_+ v_j^n = \frac{1}{h}(v_{j+1}^n - v_j^n) \quad \Rightarrow \quad \boxed{\delta_+ v_j^n = \tfrac{\partial}{\partial x} u(x,t_n)}$$

The same holds for δ_- interpolating between x_{j-1} and x_j:

$$\delta_- v_j^n = \frac{1}{h}(v_j^n - v_{j-1}^n) \quad \Rightarrow \quad \boxed{\delta_- v_j^n = \tfrac{\partial}{\partial x} u(x,t_n)}$$

Higher Order Interpolation

Now suppose we interpolate with a parabola passing through $v_{j-1}^n, v_j^n, v_{j+1}^n$. After some passages, we arrive at the second order derivative:

$$\frac{\partial^2}{\partial x^2} u(x, t_n) = \frac{1}{h^2} \left(v_{j+1}^n - 2v_j^n + v_{j-1}^n \right) = \delta_X v_j^n$$

This yields the central difference for the second derivative:

$$\Rightarrow \boxed{\frac{\partial^2 u}{\partial x^2} = \delta_X v_j^n}$$ *curvature of the parabola*

Summary of approximations:

- Interpolating polynomial 1° degree: $D^{(1)} = \delta_\pm$
- Interpolating polynomial 2° degree: $D^{(1)} = \delta_0$; $D^{(2)} = \delta_X$

It is possible to achieve the same result by expanding in a **Taylor series** around (x_j, t_n).

UP-WIND (UW1)

Let's start from the transport equation: $u_t + cu_x = 0$.

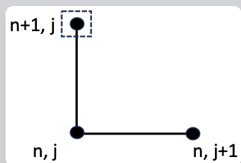
Starting from:

$$\boxed{\delta^+ v_j^n = -c\delta^+ v_j^n}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{h}\left(v_{j+1}^n - v_j^n\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - c\lambda\left(v_{j+1}^n - v_j^n\right)}$$



Two points at the base allow to find the upper one.

UP-WIND (UW2)

Starting from the transport equation: $u_t + cu_x = 0$.

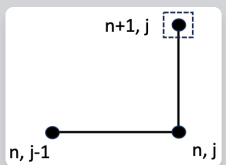
Starting from:

$$\boxed{\delta^+ v_j^n = -c\delta^- v_j^n}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{h}\left(v_j^n - v_{j-1}^n\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - c\lambda\left(v_j^n - v_{j-1}^n\right)}$$



The backward spatial stencil uses points $j-1$ and j.

UP-WIND Choice

But how can I choose between the previous formulas?

CASE 1 **If $c > 0$:**

The wave propagates backward, and it is useful to use the first formula:

$$\delta^{+} v_j^n = c\delta_{+} v_j^n$$

CASE 2 **If $c < 0$:**

The wave propagates forward, and it is useful to use the second one:

$$\delta^{+} v_j^n = c\delta_{-} v_j^n$$

> *Note: The choice of the spatial operator depends on the **direction of information flow** (characteristic direction).*

EULER (EU)

Starting from the transport equation: $u_t + cu_x = 0$.

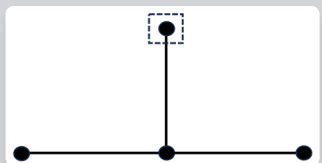
Starting from:

$$\boxed{\delta^+ v_j^n = -c\delta_0 v_j^n}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{2h}\left(v_{j+1}^n - v_{j-1}^n\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - \tfrac{1}{2}c\lambda\left(v_{j+1}^n - v_{j-1}^n\right)}$$



The two points at the base allow to find the upper one.

LEAP-FROG (LF)

Starting from the transport equation: $u_t + cu_x = 0$.

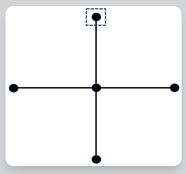
Starting from:

$$\boxed{\delta^0 v_j^n = -c\delta_0 v_j^n}$$

$$\frac{1}{2k}\left(v_j^{n+1} - v_j^{n-1}\right) = -\frac{c}{2h}\left(v_{j+1}^n - v_{j-1}^n\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^{n-1} - c\lambda\left(v_{j+1}^n - v_{j-1}^n\right)}$$



The leap-frog scheme uses the time level $n-1$ *to find* $n+1$.

CRANK-NICHOLSON (CN)

Starting from the transport equation: $u_t + cu_x = 0$.

Starting from:

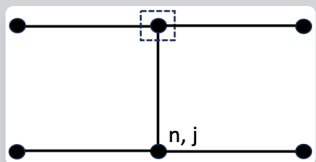
$$\boxed{\delta^+ v_j^n = -\tfrac{c}{2}\left(\delta_0 v_j^n + \delta_0 v_j^{n+1}\right)}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{4h}\left(v_{j+1}^n - v_{j-1}^n + v_{j+1}^{n+1} - v_{j-1}^{n+1}\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - \tfrac{1}{4}c\lambda\left(v_{j+1}^n - v_{j-1}^n + v_{j+1}^{n+1} - v_{j-1}^{n+1}\right)}$$

[implicit]



The Crank-Nicholson stencil involves points at both time levels n and $n+1$.

BACKWARD EULER (B-EU)

Starting from the transport equation: $u_t + cu_x = 0$.

Starting from:

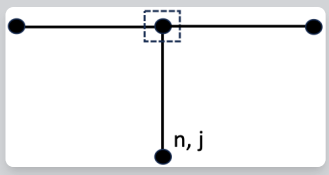
$$\boxed{\delta^+ v_j^n = -c\delta_0 v_j^{n+1}}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{2h}\left(v_{j+1}^{n+1} - v_{j-1}^{n+1}\right) \qquad \text{setting } \lambda = \frac{k}{h}$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - \tfrac{1}{2}c\lambda\left(v_{j+1}^{n+1} - v_{j-1}^{n+1}\right)}$$

[implicit]



The Backward Euler scheme evaluates the spatial derivative at the future time level $n+1$.

LAX-WENDROFF (LF)

It was born as an attempt to stabilize Euler: it adds a 2° order term to Euler's formula. [some like $u_t = -cu_x + \frac{c^2}{2}u_{xx}$]

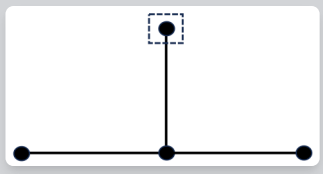
Starting from:

$$\boxed{\delta^+ v_j^n = c\left(-\delta_0 v_j^n + c\frac{k}{2}\delta_X v_j^n\right)}$$

$$\frac{1}{k}\left(v_j^{n+1} - v_j^n\right) = -\frac{c}{2h}\left(v_{j+1}^n - v_{j-1}^n\right) + \frac{c^2 k}{2h^2}\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right)$$

We obtain the update formula:

$$\boxed{v_j^{n+1} = v_j^n - \tfrac{1}{2}c\lambda\left(v_{j+1}^n - v_{j-1}^n\right) + \tfrac{1}{2}c^2\lambda^2\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right)}$$



The Lax-Wendroff scheme adds numerical diffusion for stability.

Stability of the Solution

Stability of the solution

We study the stability of discrete solutions for the transport equation:

Starting from the IVP (Initial Value Problem) with constant velocity $c > 0$:

$$\begin{cases} u_t + cu_x = 0, \\ u(x,0) = u_0(x). \end{cases}$$

We consider the Upwind (UW) scheme:

$$\boxed{v_j^{n+1} = v_j^n - c\lambda \left(v_j^n - v_{j-1}^n \right)}$$

where $\lambda = \frac{\Delta t}{\Delta x}$ is the mesh ratio.

Von Neumann Hypothesis

Assume a harmonic solution of the form:

$$v_j^n = A_n e^{i\xi x_j}$$

Then:

$$v_{j-1}^n = A_n e^{i\xi(x_j - h)} = v_j^n e^{-i\xi h}$$

Define the amplification factor:

$$\boxed{z = \frac{A_{n+1}}{A_n}}$$

Amplification Factor

Substituting the von Neumann ansatz into the upwind scheme:

$$\begin{aligned} z v_j^n &= v_j^n - c\lambda \left(v_j^n - v_{j-1}^n \right) \\ &= v_j^n - c\lambda \left(1 - e^{-i\xi h} \right) v_j^n \end{aligned}$$

Therefore:

$$\boxed{z = 1 - c\lambda \left(1 - e^{-i\xi h} \right)}$$

Let $\theta = \xi h$

Since z does not depend on n:

$$v_j^n = z^n v_j^0 = z^n u_0(x_j)$$

Real and Imaginary Parts of z

Using Euler's formula: $e^{-i\theta} = \cos\theta - i\sin\theta$, we obtain:

$$
\begin{aligned}
z &= 1 - c\lambda + c\lambda(\cos\theta - i\sin\theta) \\
&= \underbrace{(1 - c\lambda + c\lambda\cos\theta)}_{\Re(z)} - i\,\underbrace{(c\lambda\sin\theta)}_{\Im(z)}
\end{aligned}
$$

> This decomposition allows us to analyze the **magnitude** $|z|$, which must be ≤ 1 for stability.

Modulus of the Amplification Factor

For a complex number $z = a + ib$, the modulus is defined as:

$$|z| = \sqrt{a^2 + b^2}, \qquad |z|^2 = a^2 + b^2$$

Thus, for our specific amplification factor:

$$|z|^2 = (1 - c\lambda + c\lambda \cos\theta)^2 + (c\lambda \sin\theta)^2$$

Simplification of $|z|^2$

Expanding the terms and using the identity $\sin^2\theta + \cos^2\theta = 1$:

$$|z|^2 = (1 - c\lambda)^2 + 2c\lambda(1 - c\lambda)\cos\theta + (c\lambda)^2$$

Rewriting the expression:

$$\boxed{|z|^2 = 1 - 2c\lambda(1 - c\lambda)(1 - \cos\theta)}$$

Stability Condition

Since we know that $1 - \cos\theta \geq 0$ for all θ, the stability condition $|z| \leq 1$ (or $|z|^2 \leq 1$) becomes:

$$2c\lambda(1 - c\lambda) \geq 0$$

Hence, we find the required range for $c\lambda$:

$$\boxed{0 \leq c\lambda \leq 1}$$

*This is the **CFL (Courant-Friedrichs-Lewy)** condition for the upwind scheme.*

Exact Solution Comparison

For a harmonic initial condition:

$$u_0(x) = Ae^{i\xi x}$$
$$u(x,t) = Ae^{i\xi(x-ct)}$$

The exact amplification factor over one time step Δt is:

$$\boxed{z_{\text{exact}} = e^{-i\xi c\Delta t}, \qquad |z_{\text{exact}}| = 1}$$

> The ideal numerical scheme should satisfy $|z| = 1$ to preserve the amplitude of the solution.

Effect of the Amplification Factor

The discrete solution can be expressed as:

$$\boxed{v_j^n = |z|^n e^{in\phi} e^{i\xi x_j}}$$

The behavior of the scheme depends on the magnitude of z:

- $|z| < 1$: stable but **numerically diffusive** (amplitude decreases)
- $|z| = 1$: stable and **amplitude-preserving**
- $|z| > 1$: **unstable** (amplitude grows exponentially)

Stability of Common Schemes (Von Neumann)

Summary of stability conditions for the 1D transport equation:

- **Upwind:** stable $\iff 0 \leq c\lambda \leq 1$
- **Forward Euler (FTCS):** always unstable
- **Backward Euler:** unconditionally stable (diffusive)
- **Crank–Nicolson:** $|z| = 1$ (neutrally stable)
- **Lax–Friedrichs:** stable $\iff c\lambda \leq 1$
- **Lax–Wendroff:** stable $\iff c\lambda \leq 1$

Note: Unconditionally stable schemes allow for larger time steps, but they may introduce significant numerical dissipation.

CFL Condition

CFL Condition: Characteristics

We consider the linear transport equation:

$$u_t + cu_x = 0, \qquad c \in \mathbb{R}$$

The exact solution is constant along characteristic curves $x - ct = \alpha$:

$$u(x,t) = u_0(x - ct)$$

> *The value of the solution at a point (x,t) depends only on values taken along the same characteristic line at previous times.*

Mathematical Domain of Dependence

Let x_j be a grid point and $t_{n+1} = t_n + \Delta t$. Tracing the characteristic backward in time:

$$x' - ct_n = x_j - ct_{n+1}$$

Which gives:

$$\boxed{x' = x_j - c\Delta t}$$

Thus, the value $u(x_j, t_{n+1})$ depends on the interval:

$$\boxed{I_{\text{MAT}} = [x_j - c\Delta t,\ x_j]}$$

This is the mathematical domain of dependence.

Numerical Domain of Dependence

The numerical domain of dependence is the set of grid points used to compute v_j^{n+1}. For the upwind scheme ($c > 0$):

$$v_j^{n+1} = v_j^n - c\lambda(v_j^n - v_{j-1}^n)$$

The numerical domain of dependence is:

$$\boxed{I_{\text{NUM}} = [x_{j-1},\, x_j]}$$

CFL principle:

$$\boxed{I_{\text{NUM}} \supseteq I_{\text{MAT}}}$$

CFL Condition

From the domains of dependence:

$$x_j - c\Delta t \geq x_{j-1} = x_j - \Delta x$$

This implies $c\Delta t \leq \Delta x$, or equivalently:

$$\boxed{c\lambda \leq 1, \qquad \lambda = \frac{\Delta t}{\Delta x}}$$

This is the CFL condition for the upwind scheme.

Remark on the CFL Condition

The CFL condition is a **necessary** condition for stability, but in general it is **not sufficient**.

- Some unstable schemes satisfy CFL (e.g. FTCS for transport)
- Stability must be verified by von Neumann analysis

> The CFL condition ensures that numerical information propagates at least as fast as physical information.

Physical Interpretation

The CFL number $c\lambda = c\frac{\Delta t}{\Delta x}$ represents the distance traveled by a wave during one time step, measured in units of the spatial grid size.

- $c\lambda < 1$: wave travels less than one cell per time step
- $c\lambda = 1$: wave travels exactly one cell
- $c\lambda > 1$: numerical scheme cannot capture the propagation

Boundary Conditions

In addition to initial conditions, boundary conditions are required. Let x_j, $j = 1, \ldots, N$, be grid points with spacing Δx.

Boundary conditions must be imposed only where characteristics **enter** the computational domain.

Direction of Propagation

Consider again the transport equation: $u_t + cu_x = 0$.

- **If $c > 0$:** information travels from left to right
- **If $c < 0$:** information travels from right to left

Boundary conditions are needed only at the **inflow boundary**.

Upwind Boundary Conditions

Case $c > 0$ (right-moving wave):

$$\begin{cases} v_1^n = g(t_n) \quad \text{(inflow)} \\ v_j^{n+1} = v_j^n - c\lambda(v_j^n - v_{j-1}^n), \quad j \geq 2 \end{cases}$$

Case $c < 0$ (left-moving wave):

$$\begin{cases} v_N^n = g(t_n) \quad \text{(inflow)} \\ v_j^{n+1} = v_j^n - c\lambda(v_{j+1}^n - v_j^n), \quad j \leq N-1 \end{cases}$$

Heat Equation

Consider the heat equation: $u_t = b^2 u_{xx}$.

> *This equation has **no characteristics**, since information propagates instantaneously.*

- The CFL condition cannot be derived via characteristics
- Stability must be studied purely by von Neumann analysis

Explicit schemes will impose a restrictive stability condition of the form:

$$\boxed{\Delta t \leq C \Delta x^2}$$