

Numerical methods to solve differential equations

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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 $\Delta x, \Delta t \rightarrow 0$?
- **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:

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

Example:

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

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 $\Delta t = k$:

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

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**:

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

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} :

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



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

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

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

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 time 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:

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

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

ANALYTICAL SOLUTION

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

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

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:

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

- 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
<ul style="list-style-type: none">▪ 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:

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

RECURSIVE STEP

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

Runge-Kutta 2 (RK2)

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

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]

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

[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]

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

[s]

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

BUTCHER TABLEAU

c	A
	b^T

General RK Structure

[END]

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

Runge–Kutta Coefficient Matrix (Butcher Tableau)

c_1				
c_2	α_{21}			
c_3	α_{31}	α_{32}		
\dots	\dots	\dots	\ddots	
c_s	α_{s1}	α_{s2}	\cdots	$\alpha_{s,s-1}$
	b_1	b_2	\cdots	b_{s-1}
				b_s

c_i : stage time coefficients

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

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)

0	$\frac{1}{2}$
$\frac{1}{2}$	0

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

0	
	1



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

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]

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

[Heun formula, 2nd order]

HEUN (RK3 VARIANT)

0	$\frac{1}{3}$	
$\frac{1}{3}$	0	$\frac{2}{3}$
$\frac{1}{4}$	0	$\frac{3}{4}$

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)

$$v^{n+1} = v^n + k(b_1f^n + b_2\tilde{f}^{n+c_2})$$

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)

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

(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)

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

STABILITY ANALYSIS

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

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

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 Constraints

General row-sum constraint (consistency):

$$\begin{aligned}\alpha_{21} &= c_2 \\ \alpha_{31} + \alpha_{32} &= c_3 \\ &\vdots \\ \alpha_{s1} + \cdots + \alpha_{s,s-1} &= c_s\end{aligned}$$



$$\sum_{j=1}^{i-1} \alpha_{ij} = c_i$$

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:

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

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

 Implicit Methods

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

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

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 non-zero. **Type:** Implicit.

Deep Dive: The Classical RK4

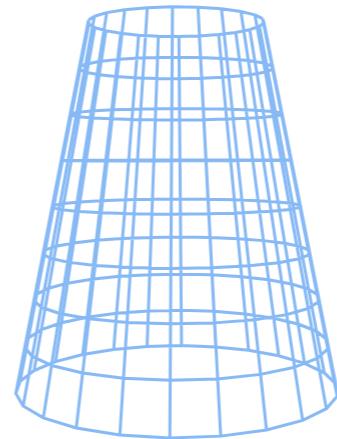
Verifying the structure

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)

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

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

Heun's Method (3rd Order)

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

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.

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

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.

$$\begin{array}{c|ccc} 0 & 1/6 & -1/6 & 0 \\ 1/2 & 1/6 & 1/3 & -1/6 \\ 1 & 1/6 & 5/6 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

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

$$\sum b_i = 1/2 + 1/3 + 1/3 + 1/2 = 5/3$$

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 $h \rightarrow 0$.
- **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:

$$\begin{aligned} \alpha_{n+1}v^{n+1} + \alpha_n v^n + \cdots + \alpha_{n-s+1}v^{n-s+1} &= \\ = k(\beta_{n+1}f^{n+1} + \beta_n f^n + \cdots + \beta_{n-s+1}f^{n-s+1}) \end{aligned}$$

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:

$$\left\{ \begin{array}{l} u_t = f(u, t) \\ u(0) = u_0 \end{array} \right.$$

Integral Formulation

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

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

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:

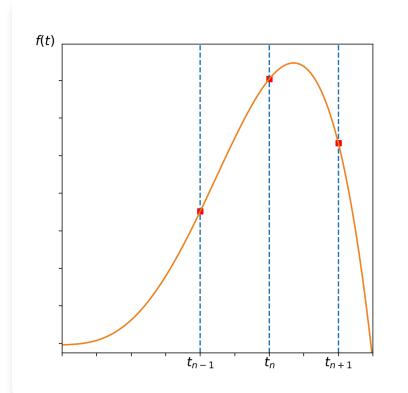
$$\begin{aligned} u(t_{n+1}) - u(t_n) &= \int_{t_n}^{t_{n+1}} f(t) dt \\ \Rightarrow v^{n+1} &= v^n + \int_{t_n}^{t_{n+1}} q(t) dt \end{aligned}$$

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:

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

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 $(t_{n+1}, v^{n+1}), (t_n, v^n), \dots$

Depending on the points selected, q will be a polynomial of $1^\circ, 2^\circ, \dots$ 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}) :

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

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

Backward Differentiation – Order 1

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

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

$$v^{n+1} = v^n + kf^n \quad (\textit{Explicit Euler})$$

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

$$v^{n+1} = v^n + kf^{n+1} \quad (\textit{Implicit Euler})$$

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:

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

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

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

(Explicit 2-step scheme)

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

\Rightarrow

$$v^{n+1} = -\frac{1}{3}v^{n-1} + \frac{4}{3}v^n + \frac{2}{3}k f^{n+1}$$

(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

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

$$\Delta x = h \quad (\text{spatial step})$$

Temporal Grid

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

$$\Delta t = k \quad (\text{temporal step})$$

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:

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

Commutative Property:

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

The spatial analog is defined similarly:

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

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:

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

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

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

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:

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

This yields the central difference for the second derivative:

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

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) .

The 1D Transport Equation

The foundation of Advection and Wave Propagation

Introduction

What is the Transport Equation?

The 1D Transport (or Advection) equation is a first-order partial differential equation that describes how a scalar quantity u is carried along by a velocity field a .

The Equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$

- $u(x, t)$: The quantity being transported (e.g., concentration, temperature).
- c : The constant velocity of propagation.

The Physical Meaning

It represents **pure translation**. The initial profile $u(x, 0)$ moves along the x-axis at speed c without changing its shape.

The Analytical Solution

Method of Characteristics

For the initial condition $u(x, 0) = \phi(x)$, the exact solution is:

$$u(x, t) = \phi(x - ct)$$

Key Observations:

1. **Constant Information:** The value of u is constant along the characteristic lines $x - ct = \text{constant}$.
2. **No Diffusion:** Unlike the heat equation, there is no smoothing; sharp edges remain sharp forever.

Challenges for Numerical Methods:

- **Numerical Diffusion:** Some methods "smear" the wave.
- **Numerical Dispersion:** Some methods create artificial oscillations (wiggles).

Discretizing the Domain

Setting the stage for Numerical Methods

To solve this numerically, we replace the continuous domain with a discrete computational grid:

- **Spatial step (Δx):** $x_j = j\Delta x$
- **Time step (Δt):** $t^n = n\Delta t$

$$u(x_j, t^n) \approx u_j^n$$

Target: Find a scheme for u_j^{n+1} using values from u^n

Preview: The CFL Condition

The Limit of Stability

For any explicit numerical method applied to the transport equation, stability is governed by the **Courant-Friedrichs-Lowy (CFL)** condition:

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

- ν : The Courant number.
- If $\nu > 1$, the numerical "information" travels slower than the physical wave, leading to total instability (the solution "blows up").
- **Physical interpretation:** The numerical domain of dependence must contain the physical domain of dependence.

Next Step:

Exploring Numerical Schemes

Upwind Scheme

Stable & Dissipative

Lax-Wendroff

2nd Order & Dispersive

Beam-Warming

Second-order Upwind

Numerical Schemes for Advection

Upwind vs. Lax-Friedrichs

UP-WIND (UW1)

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

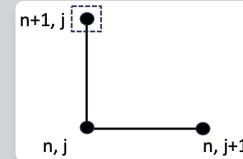
Starting from:

$$\delta^+ v_j^n = -c \delta^+ v_j^n$$

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

We obtain the update formula:

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



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

UP-WIND (UW2)

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

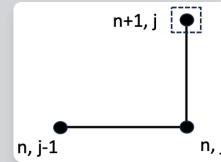
Starting from:

$$\delta^+ v_j^n = -c \delta^- v_j^n$$

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

We obtain the update formula:

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



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: $u_t + cu_x = 0$.

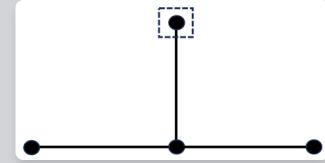
Starting from:

$$\delta^+ v_j^n = -c\delta_0 v_j^n$$

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

We obtain the update formula:

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



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

LEAP-FROG (LF)

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

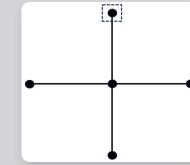
Starting from:

$$\delta^0 v_j^n = -c \delta_0 v_j^n$$

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

We obtain the update formula:

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



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

CRANK-NICHOLSON (CN)

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

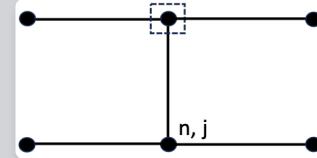
Starting from:

$$\delta^+ v_j^n = -\frac{c}{2} (\delta_0 v_j^n + \delta_0 v_j^{n+1})$$

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

We obtain the update formula:

$$v_j^{n+1} = v_j^n - \frac{1}{4} c \lambda (v_{j+1}^n - v_{j-1}^n + v_{j+1}^{n+1} - v_{j-1}^{n+1})$$



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

[implicit]

BACKWARD EULER (B-EU)

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

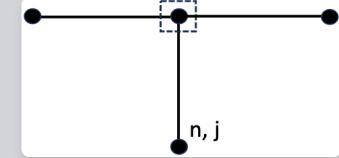
Starting from:

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

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

We obtain the update formula:

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



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

[implicit]

LAX-FRIEDRICH (LF)

A central scheme stabilized by replacing the local value with a spatial average.

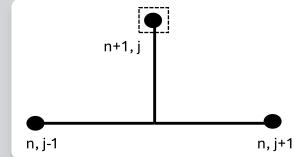
Starting from the centered approximation:

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

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

We obtain the update formula:

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



The update depends on the neighbors at time n , skipping the central node j .

LAX-WENDROFF (LW)

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

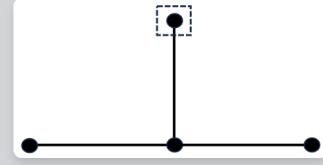
Starting from:

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

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

We obtain the update formula:

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



The Lax-Wendroff scheme adds numerical diffusion for stability.

BEAM-WARMING (BW)

A second-order accurate upwind scheme that utilizes a wider stencil to improve precision.

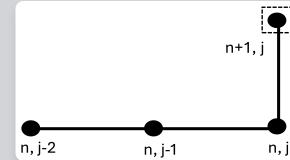
Starting from the second-order upwind discretization:

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

Where $\delta_- v_j^n = v_j^n - v_{j-1}^n$ is the backward difference operator (for $c > 0$) and $\nu = \frac{c\Delta t}{\Delta x}$.

We obtain the update formula:

$$v_j^{n+1} = v_j^n - \frac{\nu}{2} (3v_j^n - 4v_{j-1}^n + v_{j-2}^n) + \frac{\nu^2}{2} (v_j^n - 2v_{j-1}^n + v_{j-2}^n)$$



The stencil is fully biased upwind, requiring two points behind the current node.

Composition of Operators

By composing the backward operator δ_- with itself, we define $(\delta_-)^2$. This operator provides the second-order upwind spatial analog used in Beam-Warming:

Defining the second-order backward difference:

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

This is a purely upwinded operator, "looking" only at nodes j , $j - 1$, and $j - 2$.

Derivation via operator composition:

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

(j-2) --- (j-1) --- (j)

Unlike the central operator δ_X , this stencil is asymmetric and biased upstream.

The Upwind Scheme

Respecting the Physics of Flow ($c > 0$)

The Upwind scheme is the most intuitive approach: if the wind blows from the left, we look to the left to see what's coming.

The Formula

Using a **Forward in Time** and **Backward in Space** (FTBS) discretization:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + c \frac{u_j^n - u_{j-1}^n}{\Delta x} = 0$$

Solving for the future:

$$u_j^{n+1} = u_j^n - \nu(u_j^n - u_{j-1}^n)$$

where $\nu = \frac{c\Delta t}{\Delta x}$ is the Courant number.

Key Characteristics

- **First-order accurate** in time and space.
- **Stable** only if $0 \leq \nu \leq 1$.
- **Highly Dissipative:** It acts like "Numerical Diffusion," smoothing out sharp gradients and peaks.

The Lax-Friedrichs Scheme

Stability through Averaging

Standard central differences are unconditionally unstable for advection. Lax-Friedrichs fixes this by replacing u_j^n with a spatial average.

The Modification

Replace u_j^n with $\frac{1}{2}(u_{j+1}^n + u_{j-1}^n)$:

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{\nu}{2}(u_{j+1}^n - u_{j-1}^n)$$

The Stencil

It uses u_{j-1} and u_{j+1} , skipping the central point u_j at the current time step.

Pros & Cons

- **Pro:** Stable for $|\nu| \leq 1$ (works for both $c > 0$ and $c < 0$).
- **Con:** Extremely dissipative. The "averaging" term introduces massive artificial viscosity, which can ruin accuracy in long simulations.

Visualizing Numerical Diffusion

Comparing the Exact vs. Numerical Profile

Numerical methods for transport equations often struggle to preserve the "shape" of the wave.

What you expect:

A square wave moving right, keeping its sharp corners ($u_t + cu_x = 0$).

What Upwind/Lax-F gives:

The corners round off and the wave spreads out, looking like the Heat Equation solution.

Image comparing exact solution vs numerical solution with numerical diffusion for advection

"Numerical diffusion is the price we pay for first-order stability."

Next Step: Higher Order

Can we achieve stability without the "Smearing"?

Enter: **Lax-Wendroff**

Second-order accuracy using a Taylor expansion in time.

High-Order Accuracy

Lax-Wendroff & Von Neumann Stability

The Lax-Wendroff Scheme

Second-order precision via Taylor Expansion

To avoid the excessive diffusion of Upwind, we use a second-order Taylor expansion in time: $u^{n+1} = u^n + \Delta t u_t + \frac{\Delta t^2}{2} u_{tt}$

The Strategy

Using the transport equation $u_t = -cu_x$, we find that $u_{tt} = c^2 u_{xx}$. Substituting these:

$$u_j^{n+1} = u_j^n - \frac{\nu}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{\nu^2}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

The Result: Dispersion

- **Pro:** Much less "smearing" (diffusion) than Upwind.
- **Con:** Introduces **Numerical Dispersion**. Sharp gradients create artificial "wiggles" (oscillations) behind the wave.

Von Neumann Stability Analysis

How to prove a method won't blow up

We assume the numerical error can be decomposed into a Fourier series. We test a single mode: $u_j^n = G^n e^{ikj\Delta x}$

The Amplification Factor (G)

After substituting the mode into our scheme, we solve for the ratio:

$$G = \frac{u^{n+1}}{u^n}$$

Stability Condition: The method is stable if and only if:

$$|G| \leq 1 \quad \forall \text{ wave numbers } k$$

For Advection Schemes:

- **Upwind:** Stable for $0 \leq \nu \leq 1$.
- **Lax-Wendroff:** Stable for $|\nu| \leq 1$.
- **Central Diff:** $|G| > 1$ (Always Unstable!)



Precision vs. Oscillations

Why we use 2nd-order schemes and how to fix them.

The Numerical Trade-off

Dissipation vs. Dispersion

In numerical methods, we are usually forced to choose between two types of errors:

1st Order (Upwind)

Numerical Dissipation

- **The "Smear":** Information is lost to artificial diffusion. The wave is smoothed out. Peaks lose height.
- **Physics:** High-frequency data (sharp edges) "melts" away.
- **Result:** No wiggles, but the solution vanishes over time.
- **No oscillations**

2nd Order (Lax-Wendroff)

Numerical Dispersion

- **The "Wiggle":** Different frequencies travel at different speeds (Phase errors).
- **Physics:** Energy and peak heights are conserved better. The wave keeps its height.
- **Result:** High precision, but trailing oscillations appear.

Why is 2nd-Order Superior?

Even with the Corners issues

If Upwind is so "clean," why bother with Lax-Wendroff?

- **Long-term Accuracy:** 1st-order schemes act as a low-pass filter. Over long distances, your signal will completely disappear.
- **Grid Efficiency:** To get the same accuracy as a 2nd-order grid of **100 points**, a 1st-order scheme might require **10,000 points**.
- **Conservation:** 2nd-order schemes maintain the "mass" and "peak" of your pulse much more effectively.

The Lesser of Two Evils: Most scientists prefer "wiggles" because they can see the data. When a solution is smeared, you don't know what you've lost.

Godunov's Theorem

The Fundamental Limit

Why can't we have a high-order linear scheme without wiggles?

Godunov's Theorem: "Linear numerical schemes for solving advection equations that do not create new under- or overshoots can be at most first-order accurate."

The Solution: Non-Linearity

To get high precision without oscillations, we must use **Non-linear Limiter Schemes**.

- Near smooth regions: **High Order (2nd)**
- Near sharp corners: **Low Order (1st)**

TVD & Flux Limiters

Total Variation Diminishing

We "blend" the schemes using a **Limiter Function** $\phi(r)$:

$$f_{j+1/2} = f_{Low} + \phi(r) \cdot (f_{High} - f_{Low})$$

Common Limiters

- **Min-Mod:** Conservative/Stable.
- **Superbee:** Aggressive/Sharp.
- **van Leer:** Smooth/Balanced.

The Result

We achieve **High Resolution** on the plateaus and **Sharp Corners** without the dispersive wiggles. *This is the standard approach in modern CFD solvers.*

Comprehensive Comparison of Advection Schemes

Scheme	Order	Stability (ν)	Behavior at "Spigoli"	Main Error	Best Use Case
Upwind	1st	$0 \leq \nu \leq 1$	Smears / Melts	Dissipation	Simple tests, robust stability
Lax-Friedrichs	1st	$\nu \leq 1$	Heavy Smearing	Dissipation	General robust 1st-order solver
Lax-Wendroff	2nd	$\nu \leq 1$	Trailing Wiggles	Dispersion	Standard 2nd-order benchmark
Beam-Warming	2nd	$0 \leq \nu \leq 2$	Leading Wiggles	Dispersion	Purely directional upwind flows

Numerical Dissipation (1st Order): Information is lost as the wave "melts." The energy of the signal decreases over time, rounding off all sharp features.

Numerical Dispersion (2nd Order): Information is conserved, but the phase is shifted. Different wavelengths travel at different speeds, causing "wiggles."

"The choice of scheme is a trade-off between losing information (Diffusion) and distorting information (Dispersion)."

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:

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

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:

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

Therefore:

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

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:

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

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:

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

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 $c\lambda$:

$$0 \leq c\lambda \leq 1$$

This is the CFL (Courant-Friedrichs-Lowy) 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:

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

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:

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

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:

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

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:

$$x' = x_j - c\Delta t$$

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

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

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:

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

CFL principle:

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

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:

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

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 $x_j, j = 1, \dots, N$, 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):

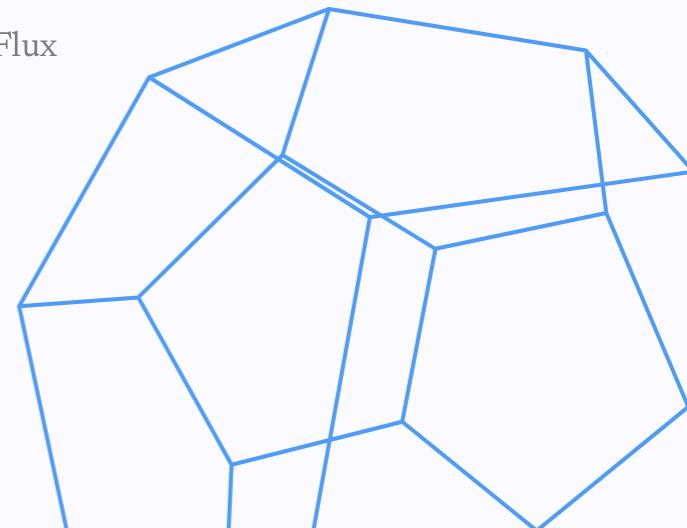
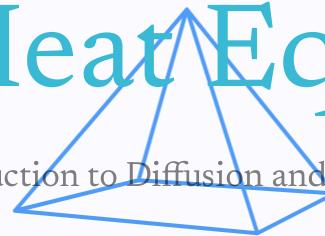
$$\begin{cases} v_1^n = g(t_n) & \text{(inflow)} \\ v_j^{n+1} = v_j^n - c\lambda(v_j^n - v_{j-1}^n), & j \geq 2 \end{cases}$$

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

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

The Heat Equation

An Introduction to Diffusion and Thermal Flux



Physical Motivation

What is Heat Diffusion?

The Heat Equation describes how temperature $u(x, t)$ distributes itself in a medium over time. It is based on two fundamental physical principles:

1. Fourier's Law

Heat flux \vec{q} is proportional to the negative gradient of temperature:

$$\vec{q} = -k \nabla u$$

Heat flows from hot to cold.

2. Conservation of Energy

The change in internal energy in a volume must equal the heat flux through its boundaries:

$$\rho c_p \frac{\partial u}{\partial t} = -\nabla \cdot \vec{q}$$

Energy is not created or destroyed.

The Mathematical Model

From Physics to PDE

By combining Fourier's Law and Energy Conservation, we derive the **Parabolic** PDE:

The Standard Form:

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

$$u_t = Du_{xx}$$

Where:

- $u(x, t)$ is the Temperature
- t is Time
- x is Space
- D is the **Thermal Diffusivity** ($D = \frac{k}{\rho c_p}$)

The second spatial derivative acts as a "smoothing" operator.

Properties of the Heat Equation

Qualitative Behavior

The Heat Equation is "Nature's Blur Tool." It has distinct mathematical properties:

1. Smoothing Effect

Even if the initial condition $u_0(x)$ is "sharp" (like a box or a spike), for any $t > 0$, the solution becomes **infinitely differentiable (C^∞)**.

2. Maximum Principle

The temperature inside the domain will never exceed the maximum temperature of the initial state or the boundaries. *No "spontaneous" hot spots.*

Infinite Speed of Propagation: A disturbance at one point is felt (theoretically) everywhere else instantly, though the magnitude decreases exponentially with distance.

Boundary Conditions (BCs)

Defining the Environment

To solve the Heat Equation on a finite domain $[0, L]$, we must specify what happens at the ends:

Type	Name	Physical Meaning
Dirichlet	$u(0, t) = T_0$	Fixed Temperature (e.g., end in ice water)
Neumann	$u_x(0, t) = 0$	Insulated End (no heat flux)
Robin	$u_x + \alpha u = g$	Convection (heat exchange with surroundings)

Stability of the Heat Equation

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

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

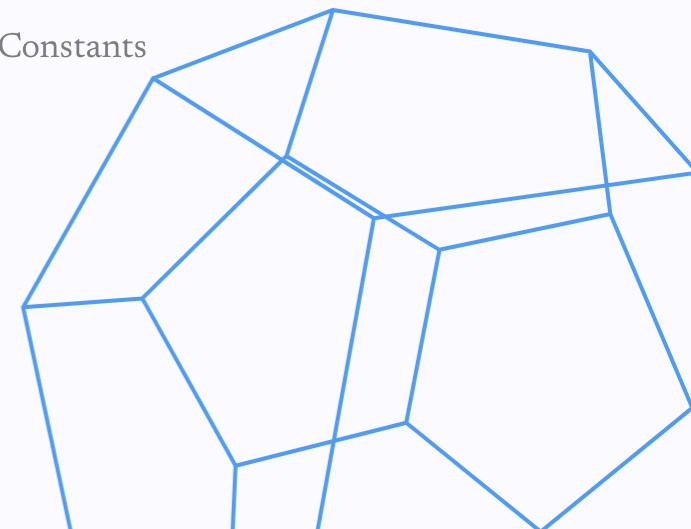
- The CFL condition cannot be derived via characteristics
- Stability must be studied purely by von Neumann analysis

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

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

The Diffusion Equation Solution

Solving with Fourier Transforms & Dimensional Constants



Introduction: The Diffusion Model

We consider the one-dimensional diffusion equation with a diffusion coefficient $D > 0$.

The Governing System:

$$\begin{cases} u_t = Du_{xx}, & x \in \mathbb{R}, t > 0 \\ u(x, 0) = u_0(x), & x \in \mathbb{R} \end{cases}$$

The solution evolves as a convolution with the **Gaussian Kernel**:

$$G(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

Spreading and smoothing effects are controlled by the coefficient D .

General Solution

Inverse Transform & Convolution

Returning to the physical domain via the Inverse Fourier Transform:

Substituting $\hat{u}(k, t)$ into $u(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(k, t) e^{ikx} dk$:

$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} u_0(y) e^{-\frac{(x-y)^2}{4Dt}} dy$$

The solution is a **convolution** of the initial state $u_0(x)$ with the Gaussian kernel. As $t \rightarrow \infty$, the initial features are smoothed out.

Case 1: Dirac Delta $\delta(x)$

The Fundamental Solution

If the initial condition is a concentrated pulse at the origin: $u_0(x) = \delta(x)$.

$$u(x, t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

Key Property:

$$\text{Variance } \sigma^2 = 2Dt$$

Using the sifting property $\int \delta(y) f(y) dy = f(0)$, the Gaussian kernel **is** the solution for a point source.

Case 2: The Box Function

Diffusion of a Rectangular Pulse

Consider the initial condition $u_0(x) = U$ for $-L \leq x \leq L$, and 0 elsewhere.

Solving the integral $u(x, t) = \frac{U}{\sqrt{4\pi Dt}} \int_{-L}^L e^{-\frac{(x-y)^2}{4Dt}} dy$:

$$u(x, t) = \frac{U}{2} \left[\operatorname{erf}\left(\frac{x+L}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{x-L}{\sqrt{4Dt}}\right) \right]$$

Where the Error Function is defined as: $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$

The corners of the box are immediately rounded as time progresses.