

Time integration schemes: concepts of stability

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PDE vs ODE schemes

Numerical schemes for PDEs and ODEs were historically developed independantly.

PDE schemes:

- 1 discretize the PDE in full

$$\frac{\partial q}{\partial t} + \frac{\partial f_j(q)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\epsilon_{ij} \frac{\partial q}{\partial x_i} \right) \quad (1)$$

- 2 developed grid based methods, finite volumes, finite difference, etc.
- 3 heavily focused on spatial derivatives

ODE schemes:

- 1 discretize the derivative

$$\frac{\partial q}{\partial t} = f(q) \quad (2)$$

- 2 developed iterative solvers based on an update formula
- 3 provides a framework for any linear system

PDE vs ODE schemes

Using the *method of line* approach, the two approaches can be combined, utilizing the advantages of both.

PDE schemes:

- 1 discretize spatial derivatives

$$\frac{\partial q}{\partial t} = Lq \quad (3)$$

- 2 focus on the accuracy, representation and geometry

ODE schemes:

- 1 discretize the derivative

$$\frac{\partial q}{\partial t} = f(q) \quad (4)$$

- 2 focus on the stability of the system

Explicit time-integration

the basic linear ODE

For a quantity (or set of quantities) q , we consider the linear ODE (or linearized PDE)

$$\frac{\partial q}{\partial t} = Lq, \quad (5)$$

with an initial condition $q(0) = q^0$.

Explicit time-integration

the explicit update

When the time derivative is approximated (with finite difference), the quantity on the right-hand side (RHS) must be determined to obtain an update formula. For example, using a first order approximation

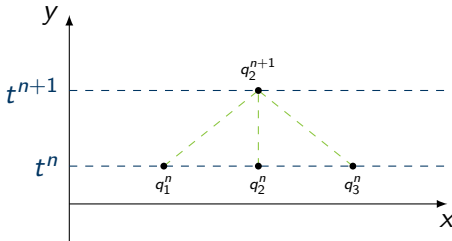
$$\frac{q^{n+1} - q^n}{\Delta t} = Lq^? + \mathcal{O}(\Delta t). \quad (6)$$

In this example, q^n is known. Choosing $q^? = q^n$ yields an explicit formula for q^{n+1} .

Explicit time-integration

Definition

Time-integration schemes written with an explicit update formula are referred to as explicit schemes.



We can visualize explicit schemes with time levels. Here, for example, q_2^{n+1} only requires solutions from the previous time level q_i^n .

Explicit time-integration: forward Euler

A lot of explicit time-integration schemes are defined based on the forward Euler step.

the forward Euler method

For a system of ODEs (5), the forward Euler step is the explicit update using a first order approximation

$$q^{n+1} = q^n + \Delta t L q^n + \mathcal{O}(\Delta t). \quad (7)$$

Explicit time-integration: advection with upwind

the forward Euler method

The advection equation

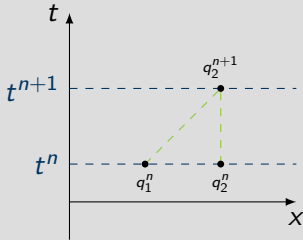
$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} = 0 \quad (8)$$

can be semi-discretized to a system of ODEs (5). Using the upwind scheme for $u > 0$,

$$L = \frac{u}{\Delta x} \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & \ddots & \ddots & & \\ & & -1 & 1 & \\ & & & & 1 \end{bmatrix}. \quad (9)$$

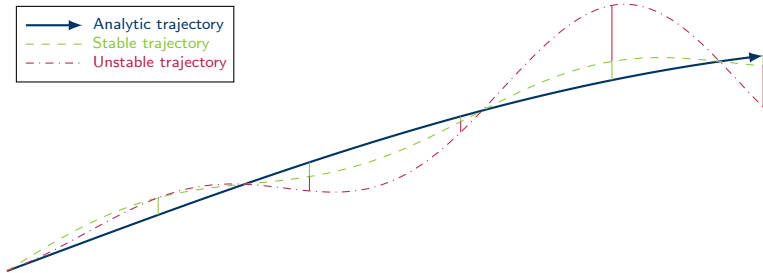
Explicit time-integration: advection with upwind

the forward Euler method



Visually, each solution point q_i^{n+1} , requires only the solution from the upstream, q_{i-1}^n .

Stability



Stability

Error growth

As the discrete problem evolves, the difference between analytic and numerical trajectories, $\tau^n = |q(t_n) - q^n|$, evolves according to

$$\tau_{\text{stable}}^{n+1} \leq C \tau_{\text{stable}}^n \quad \forall n. \quad (10)$$

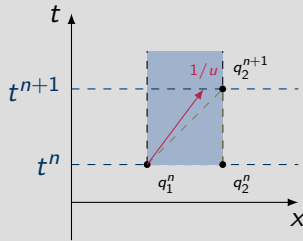
$$\exists N \text{ s.t., } \forall n > N, \tau_{\text{unstable}}^{n+1} > C \tau_{\text{unstable}}^n. \quad (11)$$

That is, the error (difference) in stable schemes is bounded, and the accuracy of the numerical solution is retained over time steps. On the other hand, for an unstable schemes, eventually, the error grows unboundedly, and the numerical solution is no longer accurate.

Stability: exploration through an example

From the advection example, we can utilize the time level figure to visualize the region of valid information. Adding to it the characteristic solution of advection, we can develop a criterion for stability.

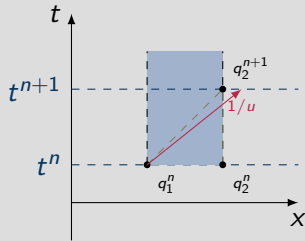
stable advection with upwind



Starting from q_1^n , the analytic solution follows the characteristic with slope $1/u$. The numerical solution follows a different trajectory with slope $\Delta t / \Delta x$. At time level t^{n+1} , if the analytic solution is within the region of valid information, the numerical solution can approximate it. So, the error is bounded, and the problem is stable.

Stability: exploration through an example

unstable advection with upwind



On the other hand, if the analytic trajectory falls outside the validity region, then, the numerical solution cannot represent the analytic one. Thus, it accumulates errors every time step, leading to unbounded error growth, and the problem is unstable.

Stability: The Courant–Fredrichs–Lewy condition

the CFL condition

Based on the advection example with upwind, we can define a criterion for stability based on the time step Δt . Since the problem was stable when the analytic trajectory was within the validity region, we can deduce that if

$$\frac{\Delta t}{\Delta x} \leq \frac{1}{u}, \quad (12)$$

then, the problem is stable.

Stability: The Courant–Fredrichs–Lewy condition

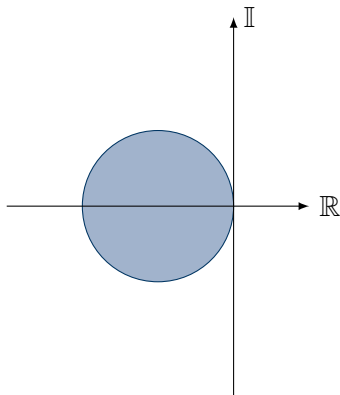
the CFL condition

More formally, the problem is stable if Δt satisfies the condition

$$\frac{u\Delta t}{\Delta x} \leq 1. \quad (13)$$

For general problems, the condition depends on the characteristic speed (for example, u for advection) and the geometry of the characteristic curve.

Stability: region of stability



The region of stability for forward Euler.

For any time-integration method with an update formula, applied to the modal problem

$$\frac{\partial q}{\partial t} = \lambda q, \quad (14)$$

we can visualize its region of stability based on the condition that its characteristic polynomial is bounded in absolute value by 1

$$\|q^{n+1}\| = |\mathcal{R}(\Delta t \lambda)| \|q^n\|, \quad (15)$$

$$|\mathcal{R}(\Delta t \lambda)| \leq 1. \quad (16)$$

Stability: region of stability

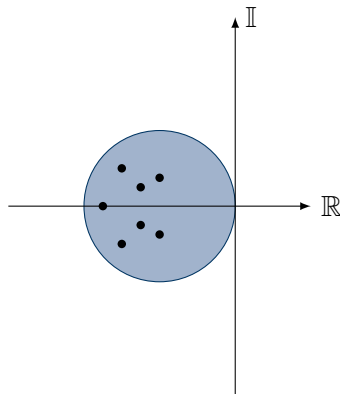
To assess the stability of a discretization, we compute the eigenvalues, λ_i of the linear operator L in

$$\frac{\partial q}{\partial t} = Lq, \quad (17)$$

and plot their value, $\Delta t \lambda_i$. If they all lie in the stability region, then the condition

$$|\mathcal{R}(\Delta t \lambda_i)| \leq 1 \quad (18)$$

is satisfied $\forall i$, and the problem is stable.



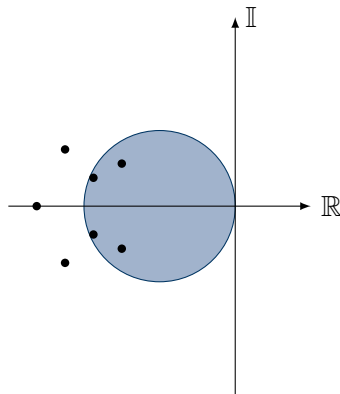
The region of stability for forward Euler.

Stability: region of stability

Because the eigenvalues are multiplied by Δt , it functions as a scaling to control whether they lie in or outside the region. If Δt is high enough that the condition

$$|\mathcal{R}(\Delta t \lambda_i)| \leq 1 \quad (19)$$

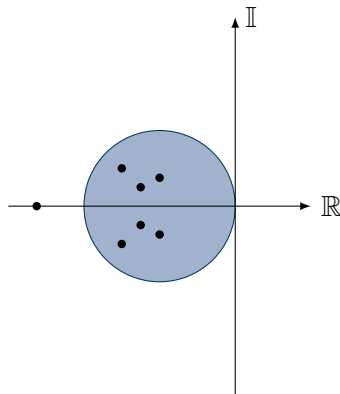
is not satisfied for at least one i , the problem is not stable.



The region of stability for forward Euler.

Stability: stiffness

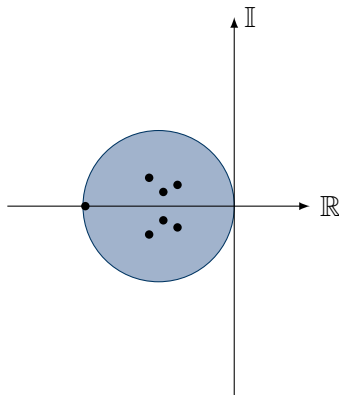
For a set of problems, called stiff problems, at least one eigen value is extremely far such that Δt is only large for this mode.



The region of stability for forward Euler.

Stability: stiffness

This constrains the whole problem to a very small Δt relative to most modes.



The region of stability for forward Euler.

Stability: stiffness

Convergence

For a scheme to be convergence, both the

- 1 accuracy, and
- 2 stability

requirements must be met.

Assuming a sufficient Δx was chosen for the semi-discrete problem, both requirements are controlled by Δt .

Stability: stiffness

Stiff vs non-stiff problems

In simple terms, we define the set of problems where Δt is sufficient for accuracy, but not stability as stiff problems (bound by stability).

On the other hand, problems where Δt is not bound by stability, are non-stiff.

How stiff?

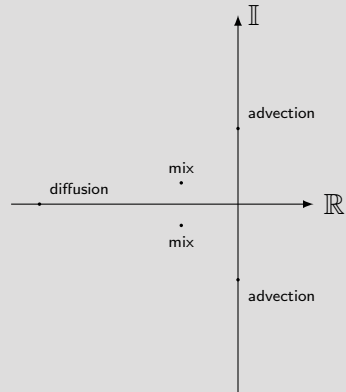
The higher the gap between a sufficient Δt for accuracy and a sufficient Δt for stability, the more stiff the problem is.

Stability: stiffness

Practical setting

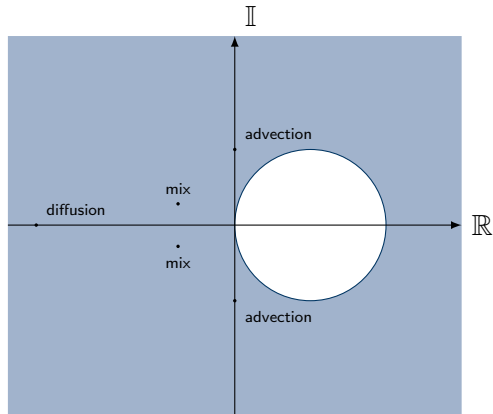
In practical terms, problems with a large negative real λ_i are stiff. This distinction is helpful, because we can categorize the modes based on the physics of the system.

Modes that are attributed to pure diffusion (viscosity, dissipation) are purely large negative real numbers. Modes that are attributed to pure advection (inviscid, convection) are purely imaginary numbers.



Implicit time-integration

To overcome the restrictions of stiff problems, implicit time integration schemes are used. Implicit schemes provide stability regions that encompass all the eigenvalues of stiff problems inside the stability region.



The region of stability for backward Euler.

Implicit time-integration

the implicit update

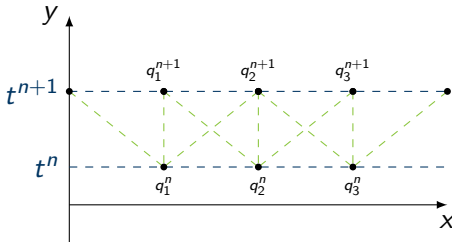
When the time derivative is approximated (with finite difference), the quantity on the right-hand side (RHS) is chosen at the new time level,

$$\frac{q^{n+1} - q^n}{\Delta t} = Lq^{n+1} + \mathcal{O}(\Delta t). \quad (20)$$

Implicit time-integration

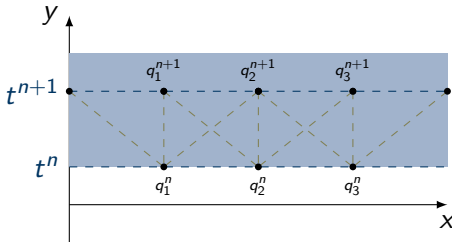
Definition

Time-integration schemes written with an implicit update formula are referred to as implicit schemes.



We can visualize implicit schemes with time levels. Here, all the points in the new time level, q_i^{n+1} are coupled to the solutions from the previous time level q_i^n .

Implicit time-integration: unconditional stability



We immediately notice that the region of valid information is the whole domain! Thus, these schemes are unconditionally stable (no CFL condition).

Literature

- Masatsuka, Katate. "I do like CFD, VOL. 1, version 2.6." (2018). pp. 45-46
- LeVeque, Randal. "Finite volumes method for hyperbolic problems".

Summary of Concepts

Equations of motion

Equation	Form	Examples
Mass flow	$\frac{\partial \psi}{\partial t} + \frac{\partial f(\psi)}{\partial x} = 0$	Advection, Burgers, Continuity
Momentum	$\frac{\partial \rho \psi}{\partial t} + \frac{\partial \rho \psi u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\mu \tau_{ij}) + F$	Navier–Stokes
Energy		

Summary of concepts

Types of PDEs

Type	Form	Examples
Hyperbolic	$\frac{\partial^2 \psi}{\partial t^2} - w^2 \frac{\partial^2 \psi}{\partial x^2} = 0$	Advection, Burgers
Parabolic	$\frac{\partial \psi}{\partial t} + \frac{\partial f(\psi)}{\partial x} = \epsilon \frac{\partial^2 \psi}{\partial x^2}$	Heat
Elliptic	$\epsilon \frac{\partial^2 \psi}{\partial x^2} = 0$	Heat (at $t \rightarrow \infty$), Pressure term (in NS)

Thanks for your attention!

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