

Chapter 3

Review of Time-Stepping Algorithms for ODEs

CONTENTS

- Classification
- Examples: Leap-Frog, θ -Family, Multi-Step
- Equivalent Differential Equation
- Definition of Stability
- Stability for θ -Family
- Review of Lax's Equivalence Theorem
- Stability Studies – Characteristic Polynomials
- Rational Approximation Theorem; Examples
- Root Condition for Stability; Examples
- Stability Regions and Absolute Stability; Examples
- Stability of Stiff Equations
- Other Theorems on Multi-Step Methods

- Runge-Kutta Methods
- Summary – Choice of Method

Consider the IVP: $\frac{dU}{dt} = \mathcal{F}(U, t)$, where $U(t = 0) = U_0$. (If $\mathcal{F}(U)$ only, this is an autonomous ODE for which very efficient algorithms can be constructed.)

The discrete system has the form:

$$\frac{U^{n+1} - U^{n-k}}{(k+1)\Delta t} = \mathcal{F}(t, U^{n+1}, U^n, U^{n-1}, \dots) \text{ for } k \geq 0$$

where $U^n \equiv U(n\Delta t)$. An implicit scheme corresponds to $\mathcal{F}$ that depends on U^{n+1} , otherwise it is explicit. A multi-step scheme has $\mathcal{F}$ depending on several previous time levels of the solution, i.e. U^n, U^{n-1}, U^{n-2} , etc.

- To analyze the stability of various discretizations it is convenient to use the Eigenvalue-Model Problem: $\frac{dU}{dt} = -\lambda U$, $\lambda \in \mathcal{C}$ with $Re(\lambda) > 0$.

Example: The leap frog scheme

The model problem: $\frac{U^{n+1} - U^{n-1}}{2\Delta t} = -\lambda U^n$ is an explicit, two-step scheme, of second-order accuracy since the first-derivative is represented by central differencing.

Example: The θ -family (one-step)

$$\frac{U^{n+1} - U^n}{\Delta t} = -\lambda \{\theta U^{n+1} + (1 - \theta)U^n\}$$

- For $\theta = 0$: Euler-forward, (EF) explicit
- For $\theta = 1$: Euler-backward, (EB) implicit
- For $\theta = 1/2$: Crank-Nicolson, (CN) implicit

Note: Multi-step schemes can be either explicit or implicit. The general formula for a k -step scheme is:

$$\sum_{j=0}^k a_j U^{n+1-j} = \Delta t \sum_{j=0}^k \beta_j \mathcal{F}^{n+1-j}$$

where $\alpha_0 = 1$ (normalization); $\beta_0 = 0$ explicit. The physical analog is a “recursive digital filter.”

Examples:

- 2nd-order Adams-Bashforth: $\frac{U^{n+1}-U^n}{\Delta t} = \frac{3}{2}\mathcal{F}^n - \frac{1}{2}\mathcal{F}^{n-1}$
- 3rd-order Adams-Bashforth: $\frac{U^{n+1}-U^n}{\Delta t} = \frac{23}{12}\mathcal{F}^n - \frac{16}{12}\mathcal{F}^{n-1} + \frac{5}{12}\mathcal{F}^{n-2}$
- 3rd-order Backwards differentiation:

$$\frac{U^{n+1} - \frac{1}{11}(18U^n - 9U^{n-1} + 2U^{n-2})}{\Delta t} = \frac{6}{11}\mathcal{F}^{n+1}, \text{ implicit}$$

- 3rd-order Adams-Moulton method:

$$\frac{U^{n+1} - U^n}{\Delta t} = \frac{5}{12}\mathcal{F}^{n+1} + \frac{8}{12}\mathcal{F}^n - \frac{1}{12}\mathcal{F}^{n-1}$$

Typically, the coefficients of the Adams-Moulton (AM) methods are smaller than the coefficients of the Adams-Bashforth (AB) method, which means lower truncation errors and round-off. Also, for the same accuracy AM uses fewer points but it is implicit.

Equivalent (Modified) Differential Equation: $\frac{dU}{dt} = \mathcal{F}(U, t)$

θ -family: (expand $U^{n+1}, \mathcal{F}^{n+1}$, etc) *a la* Taylor

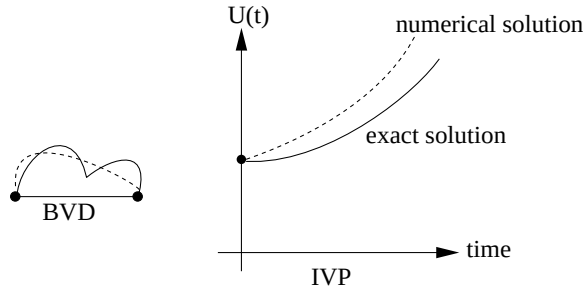
$$\begin{aligned} \left(\frac{dU^n}{dt} - \mathcal{F}^n \right) &= \Delta t \left(\theta \frac{d\mathcal{F}^n}{dt} - \frac{1}{2} \frac{d^2 U^n}{dt^2} \right) \\ &+ \Delta t^2 \left(\frac{\theta}{2} \frac{d^2 \mathcal{F}^n}{dt^2} - \frac{1}{6} \frac{d^3 U^n}{dt^3} \right) + \dots \text{ it satisfies consistency.} \end{aligned}$$

But $\frac{dU}{dt} = \mathcal{F}$, $\frac{d^2 U}{dt^2} = \frac{d\mathcal{F}^*}{dt}$, thus, $\left(\frac{dU^n}{dt} - \mathcal{F}^n \right) = \Delta t(\theta - 1/2)\frac{d^2 U}{dt^2} + \mathcal{O}(\Delta t^2)$ (* justified by expansion $U_0 + \Delta t U_1 + \Delta t^2 U_2 + \dots$). Thus, for $\theta = 0, 1$, we obtain 1st-order accuracy. For $\theta = 1/2$, 2nd-order accuracy. For $\theta \neq 1/2, 0, 1$ we obtain accuracy between first and second order.

Notice that the equivalent DE is consistent in that as Δt (discretization parameter) $\rightarrow 0$, we recover the exact DE.

Stability

Difference between BVP and IVP: Consistency for BVP is sufficient for convergence, not for IVP, we also need stability.



Stability-definition: ($\epsilon \equiv U_{ex}^n - U^n$)

- general stability $|\epsilon^n| < f(t_n)$, where $t_n = n\Delta t$, i.e. errors are bounded at a fixed time by a function that may depend on time! ($t_n = \text{fixed}, \Delta t \rightarrow 0, n \rightarrow \infty$)
- absolute stability: $|\epsilon^{n+1}| \leq |\epsilon^n|$ (“=”, weak stability; “<” strong). All components of error should be uniformly bounded.

Example: Euler-forward for $\frac{dU}{dt} = -\lambda U, \lambda > 0$

Then, error satisfies: $\epsilon^{n+1} = \epsilon^n(1 - \lambda\Delta t)$. But

$$|1 - \lambda\Delta t| < |1 + \lambda\Delta t| < e^{\lambda\Delta t},$$

thus

$$|\epsilon^{(n+1)}| < e^{\lambda\Delta t} |\epsilon^n| \leq (e^{\lambda\Delta t})^n |\epsilon^0| \Rightarrow |\epsilon| < e^{\lambda(n\Delta t)} |\epsilon^1|.$$

According to the above definition for *general stability*, this scheme is then stable! However, consider the counter example: $\left(\frac{dU}{dt} = -U, U(0) = 1\right)$ with $U_{ex} = e^{-t}$, then $U^{n+1} = -2U^n$, ($\Delta t = 3$), and we produce the sequence: $(1, -2, 4, -8, 16 \dots)$ which obviously does not converge to e^{-t} for $t = 12$!

We therefore need to apply the concept of *absolute stability*
 $\Rightarrow |1 - \lambda\Delta t| \leq 1 \Rightarrow \Delta t \leq 2/\lambda$, which we violated here.

For a general θ -scheme we obtain: $\epsilon^{n+1}(1 + \theta\lambda\Delta t) = \epsilon^n[1 - (1 - \theta)\lambda\Delta t]$
 so $\epsilon^{n+1} = \epsilon^n \frac{1 - (1 - \theta)\lambda\Delta t}{1 + \theta\lambda\Delta t}$, which is absolutely stable for

$$|1 - (1 - \theta)\lambda\Delta t| \leq 1 + \theta\lambda\Delta t, (\lambda > 0)$$

or

$$\begin{cases} 0 \leq \lambda\Delta t \forall \lambda, \Delta t \geq 0 \\ -1 - \theta\lambda\Delta t \leq 1 - (1 - \theta)\lambda\Delta t \\ \Rightarrow \boxed{(1 - 2\theta)\lambda\Delta t \leq 2} \end{cases}$$

- For $0 \leq \theta < 1/2 \Rightarrow \Delta t \leq \frac{2}{(1 - 2\theta)\lambda}$, conditional stability
- For $\theta \geq 1/2 \Rightarrow$ unconditional stability. e.g., Crank-Nicolson ($\theta = 1/2$) and Euler-back ($\theta = 1$) are unconditionally stable.

Note:

- General stability is useful for short-time integration only
- Stability is the property of a difference equation, not of the differential equation

Review of Lax's Equivalence Theorem: If a (linear) difference equation is consistent with a differential equation and stable, its solution will converge as $\Delta t \rightarrow 0$ to that of the differential equation (sufficient, also necessary)

Ref: Richtmyer, P.D. and Morton, K.W. (1967) *Difference Methods for Initial Value Problems*, 2nd edition, London, Wiley-Interscience.

The *Equivalence theorem of Lax* shows that in order to analyze an IVP, two tasks have to be performed:

- (1) *Analyze the consistency condition:* This leads to determining the order of accuracy of the scheme and the corresponding truncation error.
- (2) *Analyze the stability conditons:* This leads to determinig the frequency distribution of the error (e.g., eigenvalue-type analysis).

A stronger version of this theorem (surprisingly ignored by numerical analysis) was developed by G. Dahlquist in 1956. It applies to both linear or nonlinear initial value problems. It states that a multi-step formula is convergent if and only if it is consistent and stable. The Lax Equivalence theorem which was formulated for partial differential equations requires linearity.

Ref: G. Dahlquist, “Convergence and stability in the numerical integration of ordinary differential equations,” Math. Scand., **4**, p. 33–53, 1956.

Stability studies—Characteristic polynomials

We can associate the polynomials $\rho(z)$ and $\sigma(z)$ to the k -step scheme $\sum_{j=0}^k \alpha_j U^{n+1-j} = \Delta t \sum_{j=0}^k \beta_j \mathcal{F}^{n+1-j}$ (a discrete model for $\frac{dU}{dt} = \mathcal{F}$):

$$\rho(z) = \sum_{j=0}^k \alpha_j z^{k-j}; \quad \sigma(z) = \sum_{j=0}^k \beta_j z^{k-j}$$

where degree $[\rho(z)] = k$; degree $[\sigma(z)] \leq k$, with the equal sign true for *implicit* schemes. For normalization we request: $\sum_{j=0}^k \beta_j = 1$.

Examples:

- Crank-Nicolson: $\rho(z) = z - 1$; $\sigma(z) = \frac{1}{2}(z + 1)$, implicit
- Leap-Frog: $\rho(z) = \frac{z^2 - 1}{2}$; $\sigma(z) = z$, explicit

Based on these polynomials several properties of the scheme can be deduced (see GEAR for proofs).

Rational Approximation Theorem: A multistep scheme with $\sigma(1) \neq 0$ has order of *accuracy* p if and only if:

As $z \rightarrow 1$

$$\begin{aligned} \frac{\rho(z)}{\sigma(z)} &= \log z + \mathcal{O}((z-1)^{p+1}) \\ &= [(z-1) - \frac{1}{2}(z-1)^2 + \frac{1}{3}(z-1)^3 - \dots] \\ &\quad + \mathcal{O}((z-1)^{p+1}) \end{aligned}$$

It is a *consistent* scheme if and only if

$$\begin{cases} \rho(1) = 0 \ (\Rightarrow p \geq 0) \\ \rho'(1) = \sigma(1) \ (\Rightarrow p \geq 1) \end{cases}$$

Proof: Let us first define a linear multistep difference operator acting on a continuously differentiable function $U(t)$

$$\mathcal{L} = E^{1-k}[\rho(E) - \Delta t \sigma(E)D]$$

where E is the shift operator (or displacement operator) $EU^n = U^{n+1}$. We also obtained in Chapter 2 that $\Delta t \cdot D = \log E$ where D is a time differentiation operator. Therefore,

$$\begin{aligned} \mathcal{L}[U(t^n)] &= \rho(E)U(t^{n+1-k}) - \Delta t \sigma(E)U_t(t^{n+1-k}) \\ &= \sum_{j=0}^k \{a_j U(t-j\Delta t) - \Delta t \beta_j U'(t-j\Delta t)\} \end{aligned}$$

The order of the operator $\mathcal{L}$ is p if

$$\mathcal{L}(U(t^n)) = \mathcal{O}(\Delta t^{p+1}) \text{ as } \Delta t \rightarrow 0 \quad (1)$$

For example, for the Euler we obtain

$$\begin{aligned} \mathcal{L}[U(t^n)] &= U^{n+1} - U^n - \Delta t \cdot U_t^n \\ &= \frac{\Delta t^2}{2} U_{tt}^n + \frac{\Delta t^3}{6} U_{ttt}^n + \dots \end{aligned}$$

Thus, $p = 1$ and the error constant $C_{p+1} = 1/2$.

Now consider the function $U(t) = e^t$, then

$$\mathcal{L}[e^{t^n}] = e^{\Delta t(n+1-k)}[\rho(e^{\Delta t}) - \Delta t \sigma(e^{\Delta t})] \quad (2)$$

Now, substitute in (1), $U(t^n) = e^{t^n}$ and since $e^{k\Delta t} = 1 + \mathcal{O}(\Delta t)$, we obtain

$$\mathcal{L}[e^{t^n}] = C_{p+1}(\Delta t)^{p+1} e^{\Delta t(n+1-k)} + \mathcal{O}(\Delta t^{p+2}) \quad (1A)$$

By comparing (1A) and (2) we obtain

$$\rho(e^{\lambda\Delta t}) - \lambda\Delta t \sigma(e^{\lambda\Delta t}) = C_{p+1}\Delta t^{p+1} + \mathcal{O}(\Delta t^{p+2}) \quad (3)$$

Let

$$\begin{aligned} \lambda\Delta t = \log(1+z) &= z - \frac{z^2}{2} + \frac{z^3}{3} \dots \\ &= z + \mathcal{O}(z^2) \end{aligned}$$

and substitute in (3):

$$\rho(1+z) - \log(1+z)\sigma(1+z) = C_{p+2}^* z^{p+1} + \mathcal{O}(z^{p+2}) \quad (3)$$

Therefore:

$$\frac{\rho(z)}{\sigma(z)} = \log z + \mathcal{O}(z-1)^{p+1}$$

which is a necessary condition for a method to have order p . It is also sufficient because the LHS = $\mathcal{L}[U(t)]$ for $U(t) = e^t$ but

$$\mathcal{L}[U(t)] = \sum_{n=0}^{\infty} C_n(\Delta t)^n e^t = \mathcal{O}(\Delta t^{p+1})$$

therefore $C_0 = C_1 = \dots = C_p = 0$ (by definition)

If we expand (3) in z we get

$$\begin{aligned} \{\rho(1) + z\rho'(1) + \mathcal{O}(z^2)\} - \{z + \mathcal{O}(z^2)\} \cdot \{\sigma(1) + \mathcal{O}(z)\} \\ = \rho(1) + z[\rho'(1) - \sigma(1)] + \mathcal{O}(z^2) \\ = C_{p+1} + z^{p+1} + \mathcal{O}(z^{p+2}) \end{aligned}$$

(Note $\sigma(1) = 1$ because of normalization $\sum_{j=0}^k p_j = 1$) For $p \geq 0 \Rightarrow \rho(1) = 0$. For $p \geq 1 \Rightarrow \rho'(1) = \sigma(1)$

We can interpret the condition (3) as follows: Since the displacement operator satisfies $\Delta t D = \log E$, equation (3) suggests that the multistep formula is such that the differentiation operator $\Delta t \cdot D$ is approximated by a rational function $\rho(E)/\sigma(E)$. This is a general concept in the method of *generating functions* and it is the basis of the method of stability analysis by *order stars* (A. Iserles and N. Nørsett, BIT, 1984).

Example: C-N is consistent since $\sigma(1) = \frac{1}{2}(z+1)|_{z=1} \neq 0$, $\rho(1) = (z-1) = 0$, $\rho'(1) = 1 = \sigma(1)$. To examine its accuracy we consider the ratio:

$$\begin{aligned} \frac{\rho(z)}{\sigma(z)} &= \frac{z-1}{\frac{1}{2}(z+1)} = \frac{z-1}{1+\frac{1}{2}(z-1)} = (z-1) \left[1 - \frac{z-1}{2} + \frac{(z-1)^2}{4} - \dots \right] \\ &= (z-1) - \frac{(z-1)^2}{2} + \frac{(z-1)^3}{4} - \dots \end{aligned}$$

Note that the last term is not $\frac{(z-1)^3}{3}$ (as in the log expansion) and thus it represents the truncation error. Thus, $p = 2$.

Example: Let $\rho(z) = z^2 - z$ and $k = 2$, then

$$\begin{aligned} \sigma(z) &= \frac{z^2 - z}{\log z} + \mathcal{O}((z-1)^3) = \frac{z(z-1)}{(z-1) - \frac{1}{2}(z-1)^2 + \frac{1}{3}(z-1)^3} + \mathcal{O}((z-1)^3) \\ &= \frac{z}{1 - \frac{1}{2}(z-1) + \frac{1}{3}(z-1)^2 \dots} + \mathcal{O}((z-1)^3) = z \left[1 + \frac{1}{2}(z-1) - \frac{1}{3}(z-1)^2 \right. \\ &\quad \left. + \frac{1}{4}(z-1)^4 \right] \\ &\quad + \mathcal{O}(\dots) = \frac{5}{12}z^2 + \frac{8}{12}z - \frac{1}{12} = \sigma(z) \end{aligned}$$

so we recover the 3rd-order Adams-Moulton method.

Example: Consider a multistep formula based purely on extrapolation of previous values, e.g., $U^{n+1} = 2U^n - U^{n-1}$ for which $\rho(z) = (z-1)^2$ and $\sigma(z) = 0$. We have that $\rho(1) = 0$ and $\rho'(1) = \sigma(1) = 0$. Notice that we need $\sigma(1) \neq 0$ for the rational approximation. Obviously, such

a formula cannot converge because we do not use at all the differential equation!

Root condition for stability: A multistep scheme is stable if and only if all the roots of $\rho(z)$ satisfy $|z| \leq 1$, and any root with $|z| = 1$ is simple.

Proof: The polynomial $\rho(z)$ has a total of k roots for which we can write (if they are distinct): $U^n = z^n$, where on the LHS n denotes superscript while on the RHS it denotes an exponent. For stability we require that the entire sequence $\{U^n, n = 1, 2, \dots\}$ be bounded and thus $|z| \leq 1$. However, for multiple roots, say of multiplicity m , we have the roots $U^n = nz^n, n^2z^n, \dots, n^{m-1}z^n$. In this case the requirement for boundness of the sequence U^n is $|z| < 1$.

An alternative proof can be formulated based on matrix theory as follows:

$$\begin{bmatrix} U^{n+2-k} \\ U^{n+3-k} \\ \vdots \\ U^{n+1} \end{bmatrix} = \begin{bmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & \ddots & \ddots \\ & & & 1 \\ \underbrace{-\alpha_k \quad \quad -\alpha_2 \quad -\alpha_1}_A \end{bmatrix} \begin{bmatrix} U^{n+1-k} \\ U^{n+2-k} \\ \vdots \\ U^n \end{bmatrix}$$

or $[U]^{n+1} = [A][U]^n$. Notice that the eigenvalues of $[A]$ are roots of polynomial $\rho(z)$. Thus, for boundness of $[U]^{n+1}$, we require that the eigenvalues of $[A]$ be smaller than 1 and those equal to 1 be simple. A rigorous proof requires to transform $[A]$ to its Jordan canonical form.

Example: Adams-Bashforth of k -order: $\rho(z) = z^k - z^{k-1} = z^{k-1}(z-1)$ with roots $\{1, 0, 0, \dots\} \Rightarrow$ stable.

Examples: (1) Most accurate 2-step explicit method ($p = 3$): $U^{n+1} = -4U^n + 5U^{n-1} + \Delta t(4\mathcal{F}^n + 2\mathcal{F}^{n-1})$ therefore, $\rho(z) = z^2 + 4z - 5$ with roots $\{1, -5\}$ unstable! (2-step, Adams method of 4th-order).

$$(2) \quad U^{n+1} = -\frac{3}{2}U^n + 3U^{n-1} - \frac{1}{2}U^{n-2} + 3\Delta t \cdot f^n$$

$$\rho(z) = 2z^3 + 3z^3 - 6z + 1 = (z-1)(2z^2 + 5\lambda - 1)$$

which has the roots 1.0, 0.186 and -2.686 and thus it is unstable.

(3) All one-step methods $U^{n+1} = U^n + \Delta t \mathcal{F}^n$ are stable because: $\rho(z) = z - 1 \Rightarrow \text{root} = 1$.

Stability Regions and Absolute Stability

Consider the ODE: $\frac{dU}{dt} = \lambda U + q(t)$ where $\lambda \in \mathbf{C}$ with $\text{Re}(\lambda) < 0$. The corresponding error ϵ^n of the discrete solution is given by $\sum_{j=0}^k (\alpha_j - \Delta t \lambda \beta_j) \epsilon^{k-j} = 0$ independently of the inhomogeneity of $q(t)$.

To compute the solution of this difference equation, we introduce $\epsilon^n = z^n$ (where n on LHS denotes superscript but on RHS an exponent) and thus: $\sum_{j=0}^k (\alpha_j - \Delta t \lambda \beta_j) z^{k-j} = 0$. Therefore, the z are roots of the polynomial $\Pi(z) \equiv \rho(z) - \lambda \Delta t \cdot \sigma(z) = 0 \Rightarrow z_j$.

If all the roots are distinct, then the general solution for the error ϵ^n is: $\epsilon^n = \sum_{j=1}^k c_j z_j^n$, (k roots). If z_j is an m -fold root, then the term $(c_j + c_{j+1}n + c_{j+2}n^2 + \dots + c_{j+m-1}n^{m-1})z_j^m$ is present. Therefore, for any $|z_j| \geq 1$, disturbances are amplified irrespective of Δt .

In general $z_j = z_j(\lambda \Delta t)$. Therefore, if $|z_j(0)| < 1 \Rightarrow \exists \Delta t^*: |z_j(\lambda \Delta t)| \leq 1$ in the neighborhood with radius Δt^*

Expanding $z_j(\lambda \Delta t)$ we obtain: $z_j(\lambda \Delta t) = z_j(0) + \mathcal{O}(\Delta t \lambda)$. Thus,

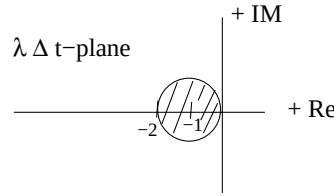
$$|z_j^n(\lambda \Delta t)| \leq |z_j(0) + \mathbf{C} \Delta t|^n \leq |1 + \mathbf{C} \Delta t|^n \leq e^{\mathbf{C} n \Delta t} \leq e^{\mathbf{C} t}$$

i.e., if $|z_j(0)| \leq 1$ then the roots of $\Pi(z)$ are less than 1, which implies stability. This explains how the roots of $\rho(z) = \Pi(0)$ are related to

stability of the scheme. For *strong stability* we require that the roots of $\Pi(z)$ are ≤ 1 in absolute value, i.e., we have to find $\lambda\Delta t$: $|z_j(\lambda\Delta t)| \leq 1$.

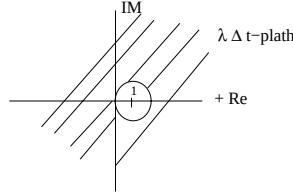
Examples:

(1) **Euler-forward:** $\Pi_{EF} = (z - 1) - \lambda\Delta t \cdot 1 = z - (1 + \lambda\Delta t)$, then
 Root: $z = 1 + \lambda\Delta t \Rightarrow -1 \leq 1 + \lambda\Delta t \leq 1$ or $|\lambda\Delta t - (-1)| \leq 1 \Rightarrow$
 $\Delta t \leq -2/\lambda$, $\lambda \in \mathbb{C}$. (Also, $\lambda\Delta t \leq 0$ for the exact modes to decay.)



(2) **Euler-backward:** $\Pi_{EB} = (z - 1) - \lambda\Delta t \cdot z = (1 - \lambda\Delta t)z - 1$ and
 therefore $|\lambda\Delta t - 1| \geq 1$, if

$$\begin{cases} \lambda \leq 0, \text{ stability } \forall \Delta t > 0 \\ \lambda\Delta t > 1, \text{ stability } \forall \Delta t > 2/\lambda \text{ (is not physical!)} \end{cases}$$

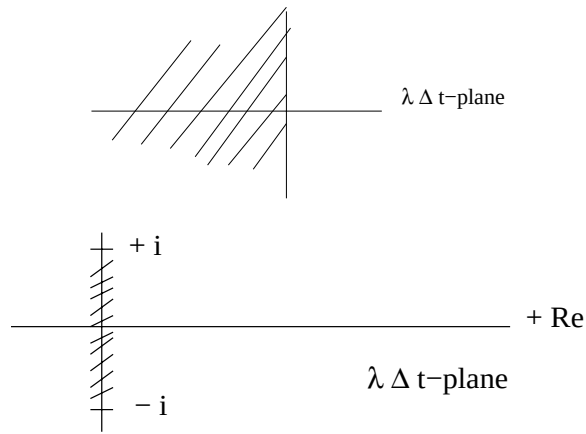


Note: EB damps high frequency rapidly

(3) **Crank-Nicolson:** $\Pi_{CN} = (z - 1) - \frac{\lambda\Delta t}{2}(z + 1) = (1 - \frac{1}{2}\lambda\Delta t)z - (1 + \frac{1}{2}\lambda\Delta t) \Rightarrow z = \frac{1+1/2\lambda\Delta t}{1-1/2\lambda\Delta t} = \frac{2+\lambda\Delta t}{2-\lambda\Delta t}$. For $Re(\lambda) \leq 0$, we obtain absolute stability.

A-stable: half-left plane. (Dahlquist (1963): A multi-step method that is A-stable cannot have order greater than two.)

(4) **Leap-Frog:** $\Pi_{LF} = z^2 - 2\lambda\Delta t z - 1$ and therefore $|z_1| \leq 1, |z_2| \geq 1$. For stability the only possibility is $|z_1| = |z_2| = 1 \Rightarrow$ the region of stability is the region on the imaginary axis between $(-i, i)$.



Note:

- LF is good for problems with purely imaginary eigenvalues, e.g., advection in a periodic domain.
- non-dissipative scheme

In general, to obtain the stability regions of multi-step schemes we construct the curve $\lambda \Delta t = \frac{\rho(z)}{\sigma(z)}$, with $z = e^{i\theta}$, $\theta \in [0, 2\pi]$ in the complex $\lambda \Delta t$ plane.

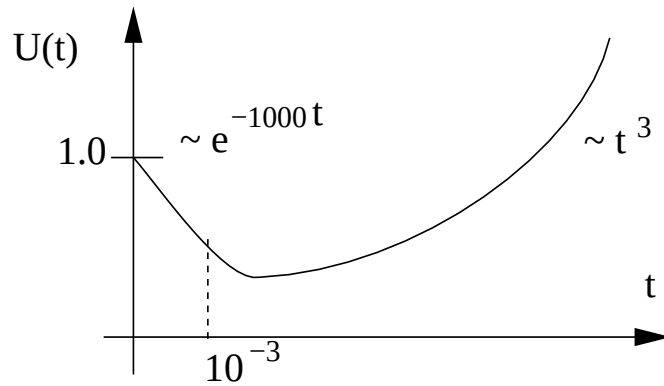
The region of stability for the implicit Adams-Moulton is larger by a factor of 10 than that of Adams-Bashforth.

Stability of stiff ODEs:

A “stiff” equation has a slowly varying solution combined with rapidly decaying transients. Typically, of interest is the long term solution, however the initial transients cause severe problems in stability, e.g., aeroacoustics, combustion, etc.

Example:

$$\left. \begin{aligned} \frac{dU}{dt} &= -1000(U - t^3) + 3t^2 \\ U(0) &= 1 \end{aligned} \right\} U_{ex}(t) = e^{-1000t} + t^3$$



A boundary layer of thickness 0.001 is present.

Use of explicit scheme (EF): $U^{n+1} = U^n - 1000\Delta t(U^n - (t^n)^3) + 3\Delta t(t^n)^2$ with error: $\epsilon^{n+1} = \epsilon^n(1 - 1000\Delta t)$. If $\Delta t = 0.1 \Rightarrow \epsilon^{n+1} = 99\epsilon^n$, thus we lose two decimal points in each time step. Yet the scheme is generally stable, i.e.,

$$\epsilon^n = (1 - 1000\Delta t)^n \epsilon^0 < e^{1000\Delta t n} |\epsilon^0|$$

or

$$\epsilon^n < e^{1000t} |\epsilon^0|, \forall \Delta t.$$

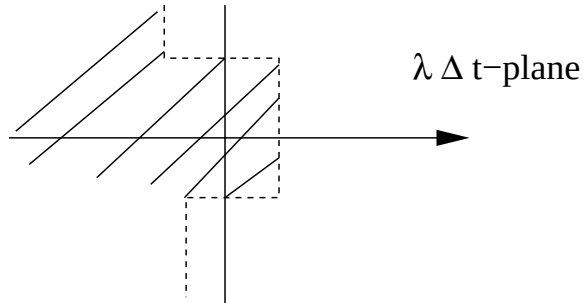
However, the error bound constant e^{1000t} is so large at $t = 1$ that this discretization is totally impractical even though it is stable. For useful results we require absolute stability, i.e., $|1 - 1000\Delta t| < 1 \Rightarrow \Delta t =$



0.002, that is we require a very small Δt to resolve the transient e^{1000t} rather than the long-term solution t^3 .

Use of implicit scheme (EB): $U^{n+1} = U^n - 1000\Delta t(U^{n+1} - (t^{n+1})^3) + 3\Delta t(t^{n+1})^2$ with error $\epsilon^{n+1} = \epsilon^n / (1 + 1000\Delta t)$. If $\Delta t = 0.1$ then $\epsilon^{n+1} = \epsilon^n / 101$, thus the error is decreasing as rapidly as it increases for the EF method. For large Δt the boundary layer is inaccurate but we capture the long-term solution. An A -stable scheme would solve the stiffness problem; however it is too stringent. Ideally, for these problems we require:

- absolute stability for transients
- general stability for long-term



General stiffly stable schemes (due to GEAR):

$$U^{n+1} = \sum_{j=0}^k \alpha_{j+1} U^{n-j} + \Delta t \beta_0 \mathcal{F}^{n+1}$$

k	2	3	4
β_0	2/3	6/11	12/25
α_1	4/3	18/11	48/25
α_2	-1/3	-9/11	-36/25
α_3	—	2/11	16/25
α_4			-3/25

For stiffly stable schemes stability studies are more complicated as the $\rho(z)$ polynomials are non-trivial. For example the 3rd-order

$$\begin{aligned}\rho(z) &= \frac{1}{11}(11z^3 - 18z^2 + 9z - 2) \\ \sigma(z) &= \frac{6}{11}z^3\end{aligned}$$

They are stable for $1 \leq k \leq 6$ and generally unstable for $6 < k < 12$ (with exceptions). They are definitely unstable for $k \geq 12$ (proof by Hairer and Wanner, 1983).

Typical stability regions for order $p = 1 - 6$ are shown in the figure.

Other Theorems on Multi-Step Methods

1. First Dahlquist Stability Barrier

The order of accuracy p of a stable k -step (linear) multi-step formula satisfies

$$p \leq \left\{ \begin{array}{ll} k+2, & k \text{ even} \\ k+1, & k \text{ odd} \\ k, & \text{explicit form} \end{array} \right\}$$

For example: The 4th-step Adams-Moulton formula corresponds to 6th-order; The Crank-Nicolson 1-step method is of second-order; The explicit 3-step Adams Bashforth method is of 3rd- order.

Notice that the highest order accuracy obtainable with a k -step method is $2k$; however, that method is unstable. An elegant proof of this theorem is given by Iserles and Norsett (BIT, 1986) based on the concept of order stars.

II. Second Dahlquist Stability Barrier

The order of accuracy of an explicit A -stable multi-step formula satisfies $p \leq 2$. An explicit multi-step formula cannot be A -stable.

Notice that of all second-order A -stable methods, the one with the smallest truncation error is the trapezoidal rule, i.e., Crank-Nicolson scheme. It is also possible to get around the restriction $p \leq 2$ for A -stability by use of Richardson's extrapolation.

We will prove next that no explicit methods (such as the Adams Bashforth methods) are A -stable.

Consider $U' = \lambda U$ (where $Re(\lambda) < 0$), then

$$\sum_{j=0}^k \alpha_j U^{n+1-j} = \lambda \Delta t \sum_{j=1}^k \beta_j U^{n+1-j}, \quad (\beta_0 = 0)$$

or (let $\alpha_0 = 1$)

$$\begin{aligned} U^{n+1} &= -\alpha_1 U^n + \dots \alpha_k U^{n+1-k} + \lambda \Delta t [\beta_1 U^n + \dots \\ &+ \beta_k U^{n+1-k}] \end{aligned}$$

Let us substitute: $U^n = z^n$, where on the LHS (n) denotes superscript but on the RHS is power exponent.

$$z^k = -\alpha_1 z^{k-1} \dots - \alpha_k + \lambda \Delta t \beta_1 z^{k-1} + \dots + \lambda \Delta t \beta_k$$

For the scheme to be A -stable we require that $|z| \leq 1 \quad \forall \quad \lambda \Delta t$, where $Re(\lambda) < 0$. Let us assume that $\beta_1 \neq 0$ and that $|\lambda \Delta t| \gg |\alpha_j|, |\lambda \Delta t| \gg |\beta_j|$ also $|\lambda \Delta t \beta_1| > |\alpha_j|, |\lambda \Delta t \beta_1| > |\beta_j|$. From dominant balance arguments we obtain:

$$z^k \sim \lambda \Delta t \beta_1 z^{k-1}$$

and thus $z \sim \lambda \Delta t \beta_1$, which means $|z| > 1$ is a large root, which will violate the A -stability condition. However, to complete the proof we

have to demonstrate consistency with the assumptions, i.e., $|\alpha_j z^{k-j}| \ll |\lambda \Delta t \beta_j|^k$ and similarly for the β_j -terms.

But

$$\begin{aligned} |\alpha_j z^{k-j}| &= |\alpha_j (\lambda \Delta t \beta_1)^{k-j}| \\ &= |\lambda \Delta t \beta_1|^k \frac{|\alpha_j|}{|\lambda \Delta t \beta_1|^j} \ll |\lambda \Delta t \beta_1|^k \end{aligned}$$

for $j = 1, \dots, k$

Similarly,

$$\begin{aligned} |\lambda \Delta t \beta_j z^{k-j}| &= |\lambda \Delta t \beta_j (\lambda \Delta t \beta_1)^{k-j}| \\ &\ll |\lambda \Delta t \beta_1|^{k-j+1} \\ &\leq |\lambda \Delta t \beta_1|^k \end{aligned}$$

for $j = 2, \dots, k$

Notice that in the case of the implicit Adams-Moulton scheme, there is an extra term on the RHS $\lambda \Delta t \beta_0 z^k$ which would dominate all other terms (including the LHS since $\lambda \Delta t$ is large) and thus it cannot be balanced. Therefore, in this case we conclude that there are not necessarily large roots and the method is not guaranteed to be unstable for large $\lambda \Delta t$.

Runge-Kutta Methods: (Runge, 1895; Heun, 1900; Kutta, 1901)

Unlike the Adams family and the backwards-differentiation schemes, Runge-Kutta methods are a single step methods. The basic idea is to create a weighted sum of corrections ΔU^k to the solution at several stages within the time step, i.e.,

$$U^{n+1} = U^n + C_1 \Delta U^1 + C_2 \Delta U^2 + C_3 \Delta U^3 + \dots$$

The coefficients C_k are determined by matching with the corresponding expansion by Taylor series. Other parameters are also introduced to accommodate different stages, e.g.,

$$\begin{aligned} \Delta U^1 &= \Delta t \mathcal{F}^n(t^n, U^n) \quad (\text{Euler Forward}) \\ \Delta U^2 &= \Delta t \mathcal{F}(t^n + \alpha \Delta t, U^n + \beta \Delta U^1) \\ &\vdots \end{aligned}$$

They tend to be non-unique due to the large number of parameters introduced. In the recent literature the objective is to minimize storage levels as shown in the following examples. For hyperbolic systems it is important to produce RK schemes which are TVD.

(1) *Second-order RK2 with two levels of storage*

Set:

$$\begin{aligned} X &= U^n \\ Y &= \mathcal{F}(U, t^n) \end{aligned}$$

Compute:

$$\begin{aligned} X &= X + \alpha \cdot \Delta t Y \\ Y &= aY + \mathcal{F}(X, t^n + \alpha \Delta t) \end{aligned}$$

Update: $U^{n+1} = X + \frac{\Delta t}{2\alpha} Y$

where $a = -1 + 2\alpha - \alpha^2$

Note that for $\alpha = 1/2$ we obtain the modified Euler method and for $\alpha = 1$ we obtain the classical Heun method.

(2) *Classical Fourth-Order RK4*

Compute:

$$\begin{aligned} X_1 &= \mathcal{F}(U^n, t^n) \\ X_2 &= \mathcal{F}(U^n + \frac{1}{2}X_1\Delta t, t^n + \frac{1}{2}\Delta t) \\ X_3 &= \mathcal{F}(U^n + \frac{1}{2}X_2\Delta t, t^n + \frac{1}{2}\Delta t) \\ X_4 &= \mathcal{F}(U^n + X_3\Delta t, t^n + \Delta t) \end{aligned}$$

Update:

$$U^{n+1} = U^n + \frac{1}{6}\Delta t[X_1 + 2X_2 + 2X_3 + X_4]$$

An alternative implementation (due to Blum, 1962, Math. Comp., vol. 16) requires only 3 levels of storage.

Stage I: $X = U^n; Y = X; Z = \mathcal{F}(X, t^n)$

Stage II: $X = X + \frac{1}{2}\Delta t Z; Y = Z; Z = \mathcal{F}(X, t^n + \frac{1}{2}\Delta t)$

Stage III: $X = X + \frac{1}{2}\Delta t(Z - Y); Y = \frac{1}{6}Y; Z = \mathcal{F}(X, t^n + \frac{1}{2}\Delta t) - \frac{1}{2}Z$

Stage IV: $X = X + \Delta t Z; Y = Y - Z; Z = \mathcal{F}(X, t^n + \Delta t) + 2Z$

Update:

$$U^{n+1} = X + \Delta t \left(Y + \frac{1}{6}Z \right)$$

- (3) *For an autonomous ODE, i.e., $\mathcal{F} = \mathcal{F}(U)$ only, the following version due to Jameson, Schmidt and Turkel (1981) produces a RK method of order p with only 3 levels of storage.*

Set $X = U^n$

For $k = p, 1, -1$

$$X = U^n + \frac{1}{k}\Delta t \mathcal{F}(X)$$

End For

Update: $U^{n+1} = X$

- (4) *Third-Order Runge-Kutta*

A. Low storage schemes (Wray) [not written yet]

B. TVD schemes (Shu) [not written yet]

- *Stability of Runge-Kutta Methods*

As an example let us consider the equation

$$\frac{dU}{dt} = \lambda U$$

and examine the stability of $RK4$. We compute:

$$\begin{aligned} X_1 &= \lambda U^n \\ X_2 &= \lambda(U^n + \frac{1}{2}\lambda U^n \Delta t) \\ &\vdots \end{aligned}$$

and therefore

$$U^{n+1} = U^n + \frac{1}{6}\Delta t[X_1 + X_2 + 2X_3 + X_4]$$

or

$$U^{n+1} = U^n \left[1 + \lambda\Delta t + \frac{\lambda^2\Delta t^2}{2} + \frac{\lambda^3\Delta t^3}{6} + \frac{\lambda^4\Delta t^4}{24} \right]$$

The growth factor

$$G = \left[1 + \dots + \frac{\lambda^4\Delta t^4}{24} \right]$$

and we require $|G| \leq 1$. By setting $\mu \equiv \lambda\Delta t$, we solve:

$$1 + \mu + \frac{\mu^2}{2} + \frac{\mu^3}{6} + \frac{\mu^4}{24} = e^{i\theta}, \quad \theta \in [0, 2\pi]$$

and determine (numerically) $\mu(\theta)$

Notice that unlike the multistep methods in RK methods the stability regions increase with order!

Summary of Time-Stepping Schemes: Choice of Method

- The **Rung-Kutta** method is the easiest to use and is often a good choice, although somewhat inefficient. Low storage and TVB schemes are useful in practice. Boundary conditions at intermediate stages may be an issue as they may affect accuracy.
- **Multi-step** methods (e.g., Adams-Bashforth) are often used in formulations of Navier-Stokes equations for discretizing convective contributions. They require a lot of memory but they are efficient. The high-order versions exhibit very low dispersion errors. If unstable the error is oscillatory.
- **Leap-frog** schemes are good for problems with complex eigenvalues.
- **Predictor-corrector** methods are good except when it is necessary to change the step size. It is also easy to estimate time errors. They are less stable than implicit.
- Stiff equations require implicit methods. For efficiency **stiffly stable** methods (i.e., backwards differentiation) is recommended.
- The truncation error of a k -order stiffly stable method is $(1/k)$ compared to the corresponding Adams-Moulton method.
- Typical instabilities appear in a spontaneous (explosive) way – it only takes a few time steps for the solution to blow up!

