Timestepping for Incompressible Navier-Stokes

- Here we will introduce a timestepping strategy that is appropriate for the unsteady incompressible Navier-Stokes equations.
- We will start with some basic considerations that guide the choices in developing the timestepper.
- The principal concerns are accuracy and stability—*not the same!*
  - **Accuracy**—requires accurate transport of the *modes of interest* (usually wavenumbers $k \ll k_{\max} = N/2$.)
  - **Stability**—all modes matter; $\Delta t \lambda_k$ must be inside the stability region for *all* values of k.

Euler-Forward

- Easiest example.

$$\text{ODE:} \qquad \frac{d\underline{u}}{dt} \;=\; L\underline{u} \qquad \textit{(Note change of sign from previous lecture!)} \tag{1}$$

$$\text{EF:} \qquad \frac{\underline{u}^n - \underline{u}^{n-1}}{\Delta t} \;=\; L\underline{u}^{n-1}. \tag{2}$$

- Solving for u^n,

$$\underline{u}^n \;=\; \underline{u}^{n-1} \;+\; \Delta t\, L\underline{u}^{n-1} \tag{3}$$

$$\;=\; \underbrace{\left[I \;+\; \Delta t L \right]}_{G} \underline{u}^{n-1}, \tag{4}$$

  we see that the update step only requires a multiplication by L plus a vector addition.

- Euler-Forward is an example of an *explicit method* in which one only applies the *forward* operator, not the inverse.

- We sometimes refer to G as the evolution (or growth) matrix.

- The spectral radius, $\rho(G) := \max |\,\lambda(G)\,|$, plays a critical role in the stability of EF and of timesteppers in general.

Modal Stability Analysis

- Consider the modal decomposition of the initial condition,

$$\underline{u}^0 = \sum_{k=1}^{m} \hat{u}_k^0 \, \underline{s}_k, \tag{5}$$

  where $\underline{s}_k$ is the kth eigenvector of G and assumed to satisfy $G\underline{s}_k = \mu_k \underline{s}_k$ with associated eigenvalue μ_k.

- Assume that μ_m is the eigenvalue of maximum modulus (i.e., $|\mu_m| > |\mu_k|$, $k \neq m$).

- If G is symmetric, the eigenvalues are real and there exist m orthogonal eigenvectors such that $\underline{s}_i^T \underline{s}_j = 0$ for $i \neq j$.

- As such, any vector in $\mathbb{R}^m$ admits a decomposition of the form (5).

- We refer to the set of coefficients $\{\hat{u}_k^0\}$ as the *spectrum* of the initial condition $\underline{u}^0$.

- Here, we assume that all of the coefficients $\hat{u}_k^0$ are nonzero.

- Even in cases where some coefficients are initially zero, the effect of round-off in the timestepping process tends to inject noise such that the solution invariably has a nontrivial contribution from each eigenmode.

- After n rounds of the Euler forward iteration, we find

$$
\begin{aligned}
\underline{u}^n &= G^n \underline{u}^0 && (6)\\
&= G^n \left(\sum_{k=1}^{m} \hat{u}_k^0 \, \underline{s}_k \right) && (7)\\
&= \left(\sum_{k=1}^{m} \hat{u}_k^0 \, G^n \underline{s}_k \right) && (8)\\
&= \left(\sum_{k=1}^{m} \hat{u}_k^0 \, \mu_k^n \, \underline{s}_k \right) && (9)\\
&= \mu_m^n \left[\hat{u}_m^0 \, \underline{s}_m + \sum_{k=1}^{m-1} \hat{u}_k^0 \left(\frac{\mu_k}{\mu_m} \right)^n \underline{s}_k \right]. && (10)
\end{aligned}
$$

- The final expression points to the behavior observed after several timesteps,

$$\underline{u}^n \sim \mu_m^n \hat{u}_m^0 \underline{s}_m. \tag{11}$$

- This asymptotic behavior emerges because $\left| \frac{\mu_k}{\mu_m} \right| < 1$ for $k \neq m$ and the remainder in (10) goes to zero as $n \longrightarrow \infty$.

- From (11), it is clear that we will have a growing, *unstable*, solution if $|\mu_m| > 1$ and a decaying, *stable*, solution if $|\mu_m| < 1$. If $|\mu_m| = 1$ we say the solution is *neutrally stable*.

- The growth factors $\mu_k = \mu_k(G)$ derive from two components, the eigenvalues of L and the design of our timestepper.

- Let's suppose that L is an $m \times m$ matrix with a complete set of eigenvectors such that, for any $\underline{u} \in \mathbb{R}^m$, we can write

$$\underline{u} = \sum_k \hat{u}_k \underline{s}_k, \tag{12}$$

$$L\underline{s}_k = \lambda_k \, \underline{s}_k. \tag{13}$$

- Applying this decomposition to our EF timestepper, we have

$$\hat{u}_k^n = \underbrace{\left[1 + \Delta t \lambda_k\right]}_{g(\lambda \Delta t)} \hat{u}_k^{n-1}, \tag{14}$$

  where $g = g_{EF}(\lambda \Delta t)$ is the *growth factor* for EF.

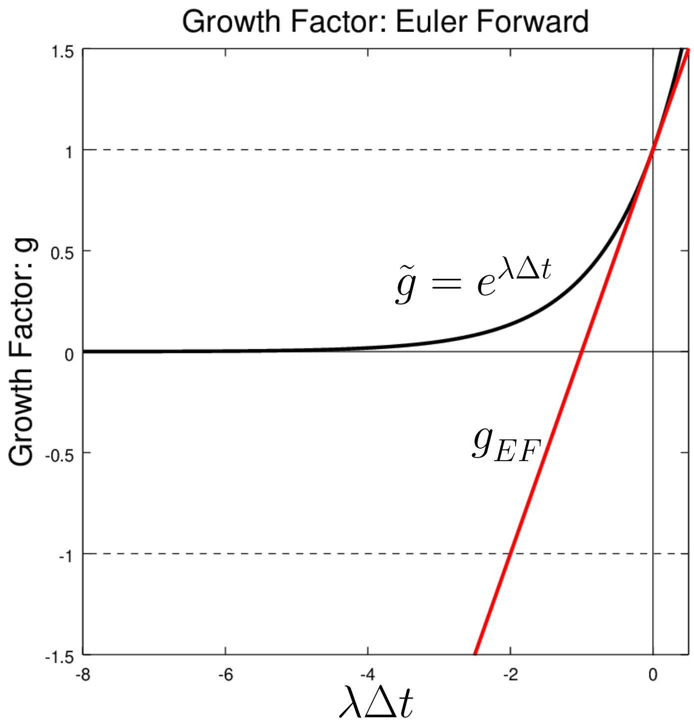
- We have a similar growth factor for our exact (analytical) timestepper.

- If we do not discretize in time, the Fourier coefficients satisfy

$$\hat{u}_k^n = \underbrace{e^{\lambda \Delta t}}_{\tilde{g}(\lambda \Delta t)} \hat{u}_k^{n-1}. \tag{15}$$

- Consider the case when λ is negative real.

- We plot g_{EF} and $\tilde{g}$ below.

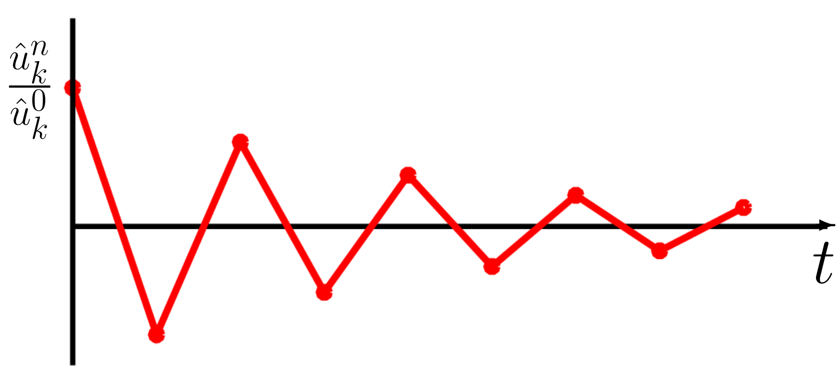


- For large $|\lambda \Delta t|$, the analytical solution decays very quickly:

$$e^{\lambda \Delta t} \ll 1 \tag{16}$$

- For EF, $|g| = |1 + \lambda \Delta t| < 1$ *iff* $-2 < \lambda \Delta t < 0$.

- Moreover, for $\lambda_k \Delta t < -1$, EF flips the sign of $\hat{u}_k^n$ on each timestep, particularly if $\lambda \Delta t \approx -2$.



Stability Diagram in the Complex Plane

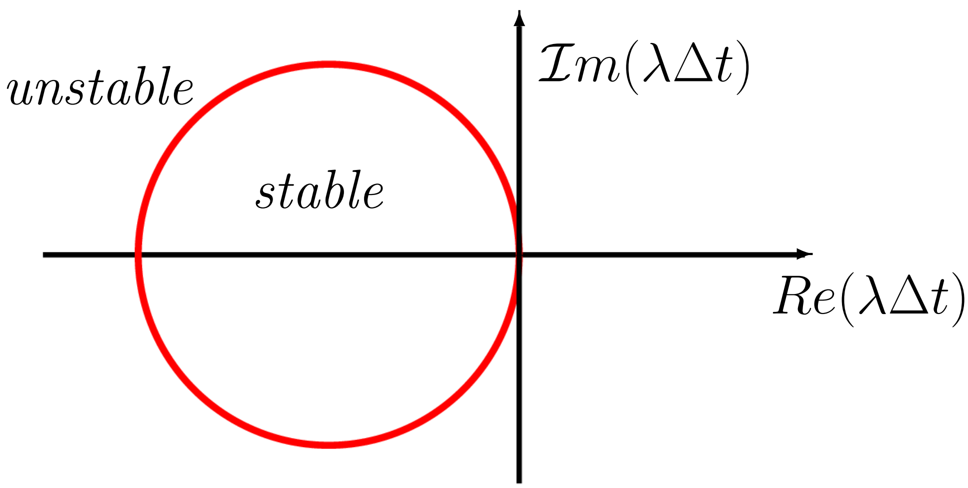
- Consider the situation where $\lambda \in \mathbb{C}$.

$$|\, g_{EF}(\lambda \Delta t)\,| \;=\; |\,1 + \lambda \Delta t\,| \;\leq\; 1. \tag{17}$$

- Suppose $|\, g\,| \;=\; 1$ (neutral stability curve).

$$1 + \lambda \Delta t \;=\; e^{i\theta} \;\;\text{(circle of radius 1 in}\,\mathbb{C}\text{)}. \tag{18}$$

$$\Longrightarrow \;\lambda \Delta t \;=\; e^{i\theta} - 1. \tag{19}$$



- For *advection*, $\lambda \Delta t \in \mathcal{I}m$, which is not inside the stability region *for any* $\lambda \Delta t$.
- Need something better.

Alternatives to Euler-Forward

- Many possibilities:

$$\left.\begin{array}{l}\circ \text{ Explicit} \\ \circ \text{ Implicit}\end{array}\right\} \quad \text{multiphysics} \longrightarrow \textit{semi-implicit.}$$

- We will look at two:
  - Crank-Nicolson (*aka* trapezoid-rule)
    - implicit
    - not L-stable :(
  - BDFk/EXTk
    - semi-implicit
    - L-stable

Euler-Backward

- Recall Euler-Forward (EF):

$$\underline{u}^n = \underline{u}^{n-1} + \Delta t\, L\underline{u}^{n-1}. \tag{20}$$

- This scheme is *explicit* because we simply need to *apply* L in a forward fashion (i.e., as a matrix-vector product), rather than *solve* a system involving L.

- We also have Euler-Backward (EB):

$$\underline{u}^n = \underline{u}^{n-1} + \Delta t\, L\underline{u}^n \tag{21}$$

$$\Longrightarrow \underbrace{(I - \Delta t L)}_{H}\,\underline{u}^n = \underline{u}^{n-1} \tag{22}$$

$$\underline{u}^n = H^{-1}\underline{u}^{n-1}. \tag{23}$$

- EB is *implicit*—we have to solve a system involving L.

- Impact on stability, from Fourier (von Neumann analysis):

$$\underline{\hat{u}}_k^n \;=\; \left(\frac{1}{1-\Delta t\lambda_k}\right)\underline{\hat{u}}_k^{n-1} \;=\; g\,\underline{\hat{u}}_k^{n-1}. \tag{24}$$

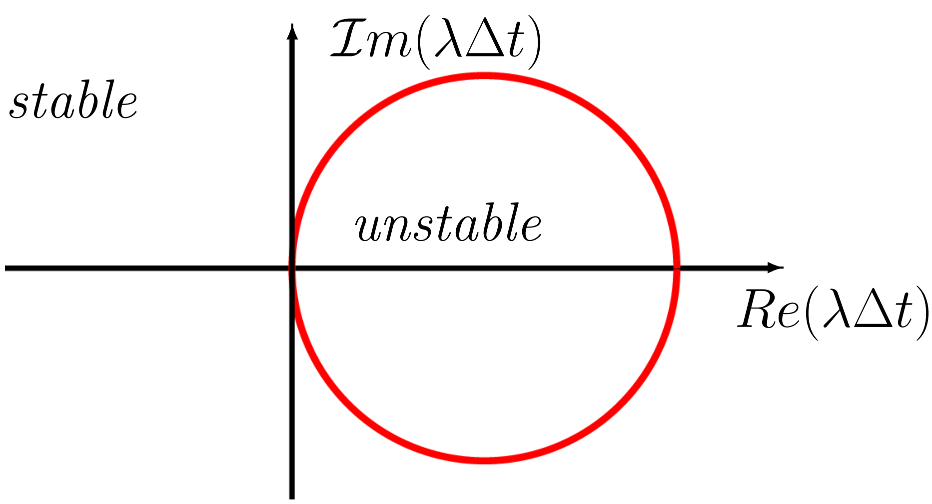
- Neutral stability curve:

$$g(\lambda\Delta t) \;=\; (1\;-\;\lambda\Delta t)^{-1} \;=\; e^{i\theta}. \tag{25}$$

- Solve for $\lambda\Delta t$ from (25):

$$1\;-\;\lambda\Delta t \;=\; e^{-i\theta} \tag{26}$$

$$\lambda\Delta t \;=\; 1\;+\;e^{-i\theta} \quad \text{(unit circle centered at (1,0) in } \mathbb{C}\text{).} \tag{27}$$



- Notices that the full imaginary axis is inside the stable region.
- In fact, a fair amount of the imaginary axis is *far from the neutral stability curve,* which means that using EB for advection will generally lead to decaying modes.

Crank-Nicolson

- We consider a *splitting* of L into an explicit part and an implicit part:

$$\frac{\underline{u}^n - \underline{u}^{n-1}}{\Delta t} \;=\; \frac{1}{2}\left(L\underline{u}^{n-1} \,+\, L\underline{u}^n\right) \,+\, \underline{f} \tag{28}$$

$$\underbrace{\left(I \,-\, \frac{\Delta t}{2}L\right)}_{H_L}\underline{u}^n \;=\; \underbrace{\left(I \,+\, \frac{\Delta t}{2}L\right)}_{H_R}\underline{u}^{n-1} \,+\, \underline{f} \tag{29}$$

$$\underline{u}^n \;=\; H_L^{-1}\left(\,H_R\,\underline{u}^{n-1} \,+\, \Delta t\underline{f}\right). \tag{30}$$

- Here, we have included an inhomogeneous term, $\underline{f}$, just to illustrate how it is included in the CN update step.

- For stability analysis, we neglect the inhomogeneous term.

- As with EB, Crank-Nicolson requires a system solve, so the cost of CN and EB is essentially the same.

- Following our standard von Neumann procedure, we find the growth factor for the individual eigenmodes,

$$\underline{\hat{u}}_k^n = \underbrace{\left(\frac{1 + \frac{1}{2}\lambda\Delta t}{1 - \frac{1}{2}\lambda\Delta t}\right)}_{g}. \tag{31}$$

- If $\lambda \in \mathcal{I}m$, then the modulus yields,

$$|1 + \frac{1}{2}\lambda\Delta t| = |1 - \frac{1}{2}\lambda\Delta t|, \tag{32}$$

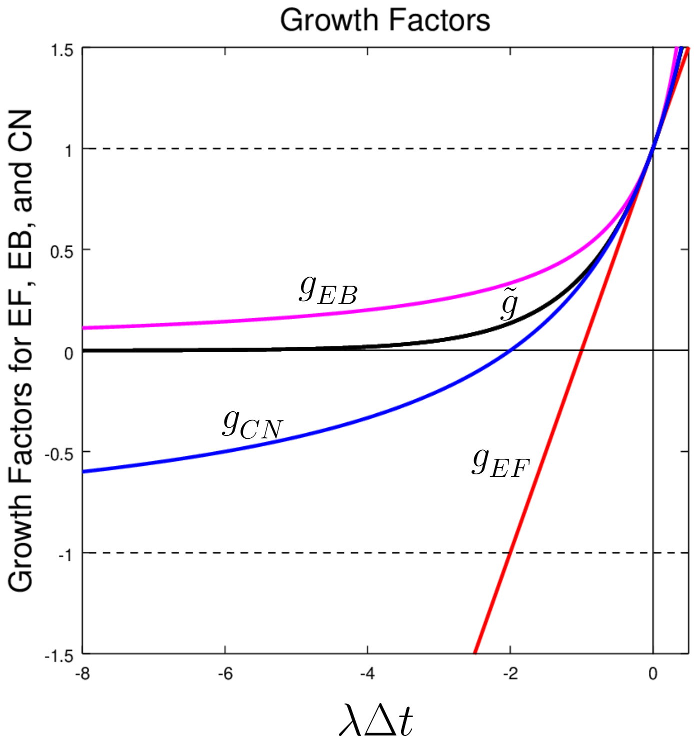
  so the neutral stability curve *is* the imaginary axis, just as it is for the analytical case.

- $\therefore$ No decay for If $\lambda \in \mathcal{I}m$, but phase error will still exist.

L-Stability of Crank-Nicolson

- Unfortunately, CN is not L-stable.

- Consider once again $\lambda < 0$ (negative real) and return to $g(\lambda \Delta t)$:



$$\tilde{g} = e^{\lambda \Delta t}$$

$$g_{EF} = 1 + \lambda \Delta t$$

$$g_{EB} = \frac{1}{1 - \lambda \Delta t}$$

$$g_{CN} = \frac{1 + \frac{1}{2}\lambda \Delta t}{1 - \frac{1}{2}\lambda \Delta t}$$

- For CN, as $\lambda \Delta t \longrightarrow -\infty$, $g \longrightarrow -1$.

- *Slow decay* (and, alternating in sign). :(

- So, although it is unconditionally stable, CN is potentially unattractive because you cannot take a huge Δt.

Convergence

- So far we have focused on large $|\,\lambda\Delta t\,|$, which governs *stability*.

- The order of accuracy, on the other hand, is governed by the behavior of g as $\lambda\Delta t \longrightarrow 0$.

- Consider the following Taylor series:

$$\tilde{g} \;=\; e^{\lambda\Delta t} \;=\; 1 + \lambda\Delta t + \frac{(\lambda\Delta t)^2}{2!} + \frac{(\lambda\Delta t)^3}{3!} + \cdots \tag{33}$$

$$g_{EF} \;=\; 1 + \lambda\Delta t \;=\; \tilde{g} + \underbrace{O(\Delta t^2)}_{\text{LTE} \longrightarrow \text{GTE}=O(\Delta t)} \tag{34}$$

$$g_{EF} \;=\; \frac{1}{1 - \lambda\Delta t} \;=\; 1 + \lambda\Delta t + (\lambda\Delta t)^2 + O(\lambda\Delta t)^3, \quad \text{LTE}=O(\Delta t^2) \tag{35}$$

$$g_{CN} \;=\; \left(1 + \frac{1}{2}\lambda\Delta t\right)\left(1 + \frac{1}{2}\lambda\Delta t + \left(\frac{\lambda\Delta t}{2}\right)^2 + \left(\frac{\lambda\Delta t}{2}\right)^3 + \cdots\right) \tag{36}$$

$$=\; 1 + \lambda\Delta t + \frac{(\lambda\Delta t)^2}{2!} + \frac{(\lambda\Delta t)^3}{4} + \cdots \;=\; \tilde{g} + O(\lambda\Delta t)^3. \tag{37}$$

- We see that the difference between $\tilde{g}$ and g_{EF} is $O(\Delta t^2)$, which means that there is an $O(\Delta t^2)$ error on each step.

- To reach a final time, T (fixed, independent of Δt), we must take $n_{tot} = T/\Delta t$ steps.

- So, at time T we can expect a total error scaling like

$$C\, n_{tot}\, \Delta t^2 \;=\; C\,(n_{tot}\, \Delta t)\Delta t \;=\; C\, T \Delta t \;=\; O(\Delta t). \tag{38}$$

- We refer to the local, $O(\Delta t^2)$ error as the *local truncation error*, or LTE.

- We refer to the global, $O(\Delta t)$ error at time T as the *global truncation error*, or GTE.

- Invariably, GTE = LTE/Δt. That is, you lose one order in Δt as you time-march to the final time T.

BDFk/EXTk

- Consider the following splitting:

$$\frac{d\underline{u}}{dt} = L\underline{u} + N\underline{u} \tag{39}$$

$$\Longrightarrow \left.\frac{d\underline{u}}{dt}\right|_{t^n} = L\underline{u}|_{t^n} + N\underline{u}|_{t^n} \tag{40}$$

- Here, the idea is to evaluate each term in (40) using what is most effective.

- In the context of advection-diffusion, we can think of $L\underline{u}$ as the linear diffusion term, for which $|\lambda_{\max}| = O(\Delta x^{-2})$.

- We view $N\underline{u}$ as the (potentially nonlinear) advection term, for which $|\lambda_{\max}| = O(\Delta x^{-})$.
  The L term is thus more constraining and it would be sensible to evaluate implicitley at time t^n:

$$L\underline{u}|_{t^n} = L\underline{u}^n. \tag{41}$$

  Fortunately, for diffusion, $-L$ is SPD, so $I-\beta L$ will also be SPD, which is convenient from a solver standpoint.

- On the other hand, explicit treatment the advection term, $N\underline{u}$, would imply $\Delta t = O(\Delta x)$, which is generally also a requirement from an accuracy standpoint, so there is less need to treat this term implicitly.

- Thus, we approximate $N\underline{u}^n$ by kth-order extrapolation:

$$\text{EXT1:} \quad N\underline{u}|_{t^n} \;=\; N\underline{u}^{n-1} \;+\; O(\Delta t) \tag{42}$$

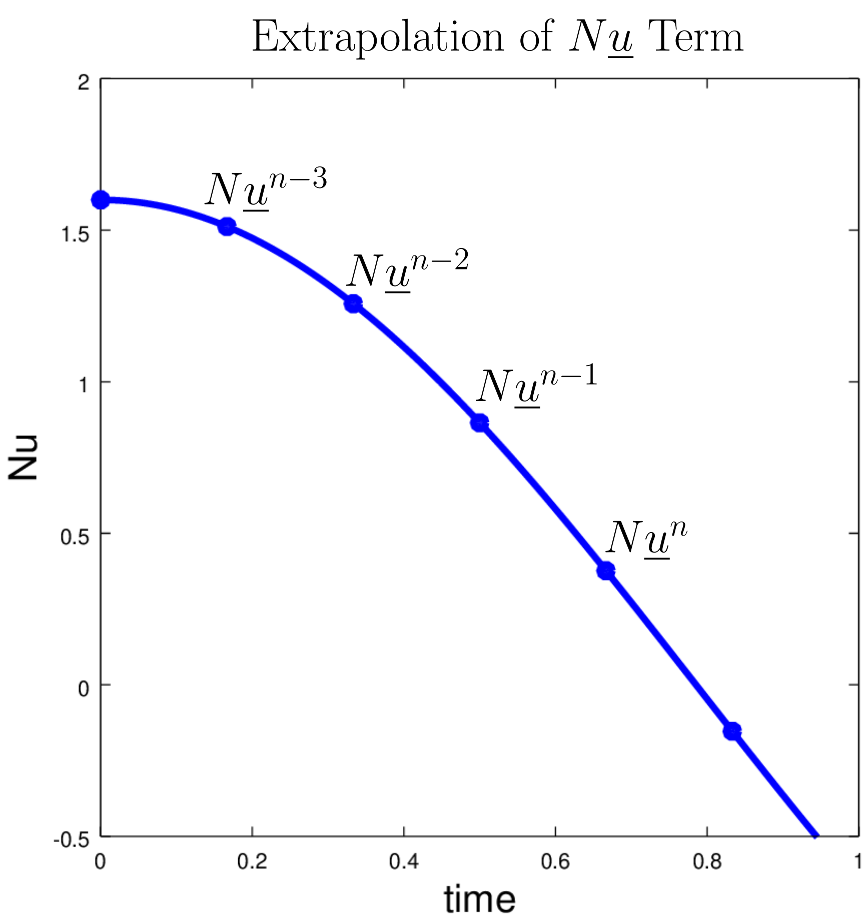
$$\text{EXT2:} \quad N\underline{u}|_{t^n} \;=\; 2N\underline{u}^{n-1} \;-\; N\underline{u}^{n-2} \;+\; O(\Delta t^2) \tag{43}$$

$$\text{EXT3:} \quad N\underline{u}|_{t^n} \;=\; 3N\underline{u}^{n-1} \;-\; 3N\underline{u}^{n-2} \;+\; N\underline{u}^{n-3} \;+\; O(\Delta t^3) \tag{44}$$

- The EXT1 formula amounts to piecewise-constant extrapolation (using a polynomial of degree 0).

- EXT2 passes a line through $N\underline{u}^{n-2}$ and $N\underline{u}^{n-1}$ to estimate $N\underline{u}^1$, which yields the desired $O(\Delta t^2)$ error.

- EXT3 fits a parabola through $N\underline{u}^{n-j}$, $j = 1, \ldots, 3$ to estimate $N\underline{u}^1$, which yields the desired $O(\Delta t^2)$ error.



- For general k, we can express the extrapolation as

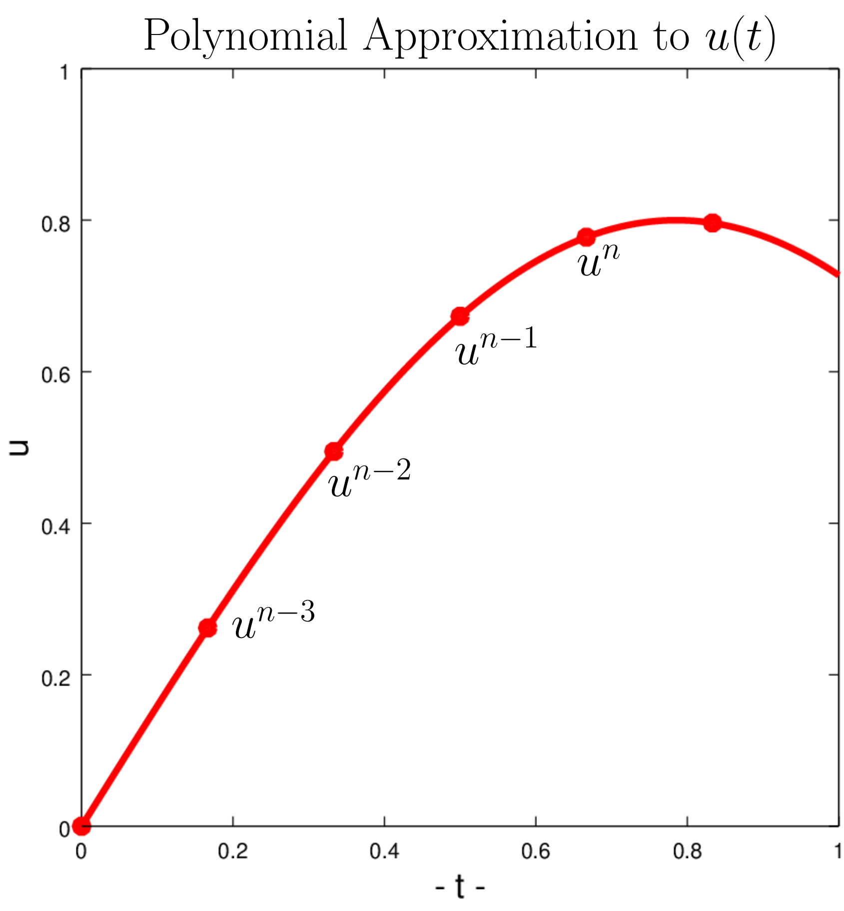
$$\text{EXTk:} \quad N\underline{u}|_{t^n} \;=\; \sum_{j=1}^{k} \alpha_j \, (N\underline{u})^{n-j} \;+\; O(\Delta t^k), \tag{45}$$

  where the α_j's can be adjust to accommodate variable-sized timesteps if needed. (One can use the same Lagrange polynomial interpolation routines that we use for spatial discretization.)

- Note that we don't need k function evaluations at each step since we can simply save the k active vectors, $N\underline{u}^{n-j}$, $j = 1, \dots, k$ and resuse them on the next step.

- We then discard the oldest one and put the new one on the stack.

- The next term to approximate is the derivative, $\frac{du}{dt}$.
- The idea behind BDFk is to approximate $\frac{du}{dt}$ at time the current timestep, t^n, with a finite difference formula based on the unknown value, u^n, and known past values $u^{n-1}, u^{n-2}, \ldots, u^{n-k}$.
- One way to generate the finite difference formula is to fit an interpolating polynomial of degree k through the solution $u(t)$ at time points t^n, $t^{n-1}, \ldots, t^{n-k}$ and evaluate the derivative of this polynomial at the current timestep level, t^n.
- The situation is as pictured below



For *uniform* Δt, the formulas for $k = 1$, 2, and 3 are

$$\text{BDF1:} \quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{u^n - u^{n-1}}{\Delta t} + O(\Delta t) \tag{46}$$

$$\text{BDF2:} \quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{3u^n - 4u^{n-1} + u^{n-2}}{2\Delta t} + O(\Delta t^2) \tag{47}$$

$$\text{BDF3:} \quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{11u^n - 18u^{n-1} + 9u^{n-2} - 2u^{n-3}}{6\Delta t} + O(\Delta t^3). \tag{48}$$

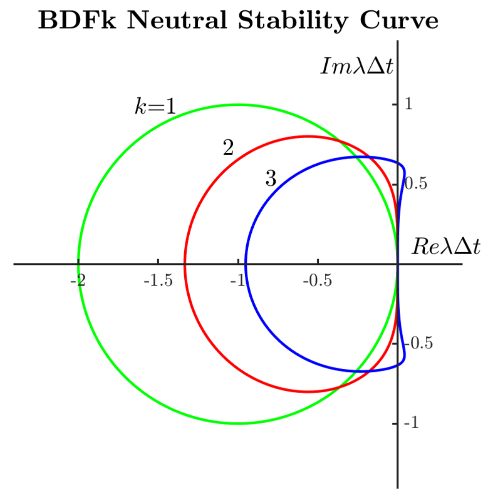
- With implicit treatment of the diffusion term, the general BDFk/EXTk formulation is

$$(\beta_0 I - \Delta t L)\,\underline{u}^n = -\sum_{j=1}^{k} \beta_j\,\underline{u}^{n-j} + \sum_{j=1}^{k} \alpha_j\,(N\underline{u})^{n-j}. \tag{49}$$

- It's clear that this formula simply requires assembly of a few vectors on the right and solution of a single (usually) SPD system.

- The coefficients are summarized in the accompanying figure below.

k	β_0	β_1	β_2	β_3	α_1	α_2	α_3
1	1	-1	0	0	1	0	0
2	$\frac{3}{2}$	$-\frac{4}{2}$	$\frac{1}{2}$	0	2	-1	0
3	$\frac{11}{6}$	$-\frac{18}{6}$	$\frac{9}{6}$	$-\frac{2}{6}$	3	-3	1



- At the right of the figure we plot the neutral stability for BDFk/EXTk with $L \equiv 0$, which implies that we have a purely explicit scheme.

- Note that for $k = 1$ we recover EF.

- Most importantly, for $k = 3$, the stability region encompasses part of the imaginary axis, which is what we need for stable advection.

- Generally, for other timesteppers such as Adams-Bashforth (ABk), Runge-Kutta (RKk) and the like, we need $k \geq 3$ in order to capture a segment of the imaginary axis in the stability region.

- Although we don't show it here, BDFk is L stable for the case $N \equiv 0$, for which it is a fully-implicit scheme.