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CFD Spring 2013 — A. Donev

Spatio-Temporal Discretizations

So far we discussed spatial discretization only, leading to a system of ODEs for the discrete $w \in \mathbb{R}^m$

$$w'(t) = F_h(t, w(t))$$

But of course we now need a temporal discretization to solve this large system of ODEs. This approach is called

$$\boxed{\text{MOL} = \text{method of lines} = \text{spatial} + \text{temporal}}$$

(2) In the MOL approach (very common) space and time are decoupled. This means spatial and temporal errors <u>add</u>:

Assume spatial order of convergence $= p_1$:

$$\| u_h(t) - w(t) \| \leq C_1 h^{p_1} \quad \ldots \quad (1)$$

Assume temporal integrator for ODEs is convergent of order $= p_2$:

$$\| w(t_n) - w_n \| \leq C_2 \tau^{p_2}$$

where $w_n \approx w(t_n)$, $\underset{\uparrow\ \text{time step (index)}}{n} = 1, 2, 3, \ldots$

$$t_n - t_{n-1} = \underset{\uparrow\ \text{time step size}}{\tau}$$

(3) Here it is crucial that C_2 and p_2 are <u>independent of</u> h.

$\varepsilon = \| u_h(t_n) - w_n \|$ = global error (spatio-temporal)

$$\leq \| u_h(t_n) - w(t_n) \| + \| w(t_n) - w_n \|$$

$$\leq \underbrace{C_1 h^{p_1}}_{\text{spatial error}} + \underbrace{C_2 \tau^{p_2}}_{\text{temporal error.}}$$

Often we choose $\tau = c h^p$, where $p = 1$ or 2 (adv.- or diff.-dominated)

$$\Rightarrow \varepsilon = O\left(h^{\min(p_1, p p_2)}\right)$$

$\rightarrow$ convergence as $h \to 0$

(14) <u>MOL stability</u>

Let us consider stability now for several very common and basic temporal integrators for MOL approaches. We will come back to state-of-the-art later.

Focus on <u>linear</u> PDE's for stability:

$$w' = F(t,w) = Aw + g(t)$$

We all know <u>forward Euler</u> method:

$$w^{n+1} = w^n + F(t^n, w^n)\,\tau$$

(15) Forward Euler is first-order accurate and explicit. An explicit but second-order accurate integrator is the explicit trapezoidal rule:

$$\begin{cases} \tilde{w}^{*,n+1} = w^n + \tau F(t^n, w^n) \leftarrow \text{Forward Euler } \underline{\text{predictor}} \\ w^{n+1} = w^n + \frac{\tau}{2}\left[F(t^n, w^n) + F(t^{n+1}, \tilde{w}^{*,n+1})\right] \end{cases}$$

$\uparrow$ trapezoidal rule corrector

In implementation, write it as:

$$w^{n+1} = \frac{1}{2}\left[w^n + \tilde{w}^{*,n+1} + \tau F(t^{n+1}, \tilde{w}^{*,n+1})\right]$$

(16) For a linear problem

$$w' = Aw + g, \quad \text{set } g=0 \text{ (homogeneous)}$$

for stability analysis

$$w^{*,n+1} = w^n + \tau A w^n$$

$$w^{n+1} = w^n + \frac{\tau}{2}\left[A w^n + A w^n + \tau A^2 w^n \right]$$

$$w^{n+1} = \left[I + (\tau A) + \frac{(\tau A)^2}{2} \right] w^n$$

$$w^{n+1} = R(\tau A)\, w^n$$

where the <u>stability function</u>

$$R(A) = I + A + \frac{A^2}{2}$$

(17) For stability

$$\| w^n \| \leq \| R(\tau A)^n \| \, \| w^0 \|$$

Assume A is a normal matrix

$$A = U \Lambda U^{-1}, \quad \Lambda = \mathrm{Diag}\{\lambda_1, \dots, \lambda_m\}$$

$$\Rightarrow \| R^n(\tau A) \|_2 = \max_{1 \leq k \leq m} | R^n(\tau \lambda_k) |$$

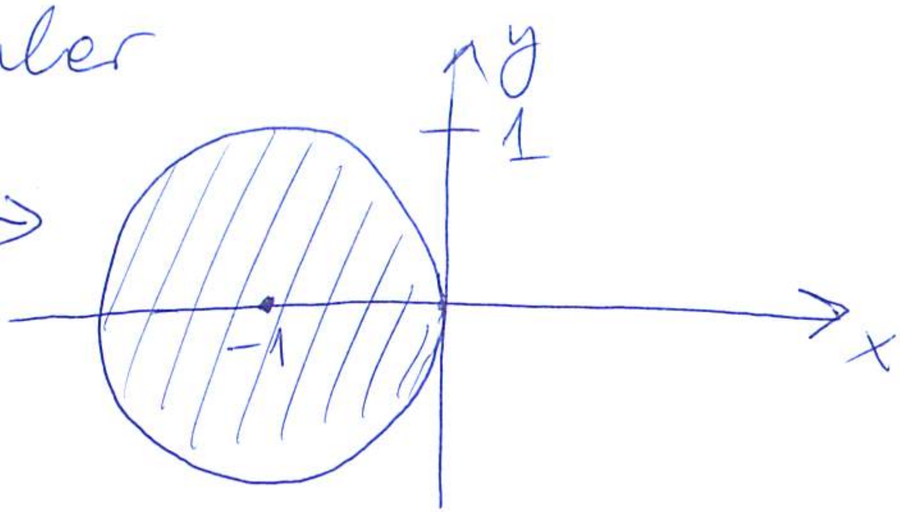
So for stability we want

$$\boxed{\tau \lambda_k \in S \text{ for all } k}$$

where S is the domain of the complex plane $z \in \mathbb{C}$: $\boxed{S : |R(z)| \leq 1}$

(18) For forward Euler

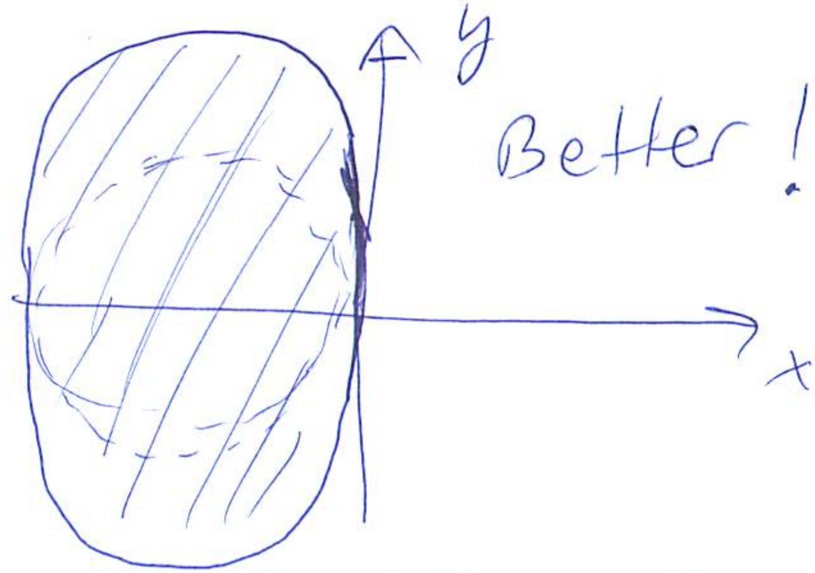
$R(z) = 1 + z$ →



For trapezoidal

$R(z) = 1 + z + \frac{z^2}{2}$

which is much better because it gets much closer to imaginary axes →



Better!

<u>Neither</u> stability region includes a non-trivial part of the imaginary axes → you need at least a <u>third-order</u> Runge-Kutta for that

(19) We can do much better for stability if we use an *implicit* method:

Backward Euler:

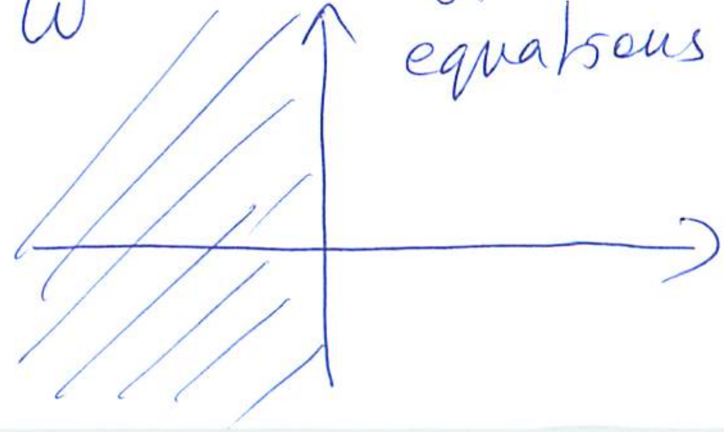
$$w^{n+1} = w^n + F(t^n, w^{n+1})\tau$$

generally a non-linear system of equations for w^{n+1}, but for linear:

$$w^{n+1} = w^n + \tau A w^{n+1}$$ ← SOLVE LINEAR SYSTEM of equations

$$w^{n+1} = (I - \tau A)^{-1} w^n$$

$$R(z) = (1-z)^{-1}$$



(20) So the backward Euler method is <u>unconditionally stable</u> (<u>A-stable</u>)
but it is only first-order.
A second-order implicit method is the <u>implicit trapezoidal rule</u>

$$w^{n+1} = w^n + \frac{\tau}{2}\left[F(t^n, w^n) + F(t^{n+1}, w^{n+1})\right]$$

For $F = Aw$

$$w^{n+1} = \left(I - \frac{A\tau}{2}\right)^{-1}\left(I + \frac{A\tau}{2}\right)w^n$$

$$R(z) = (1 - z/2)^{-1}(1 + z/2)$$

<u>Also</u> unconditionally stable (A-stable)

(21) Recall the stability criterion

$$\tau \lambda_k \in S \quad \forall k$$

For linear schemes with periodic BCs, we can find the eigenvalues easily in Fourier space, in fact, we already did in Lecture 1!

For <u>pure advection</u> eq. $(a > 0)$

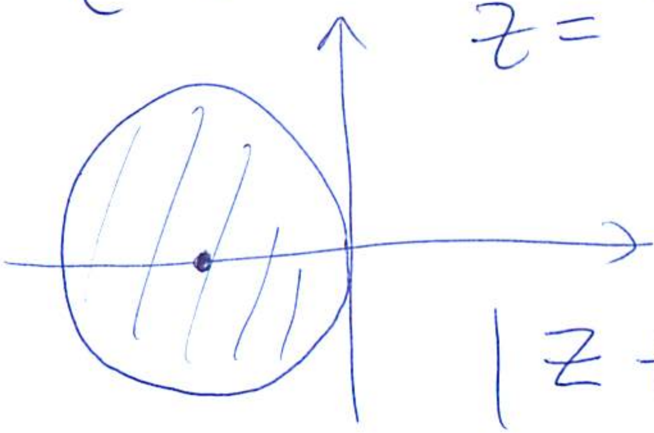
$$\begin{cases} \lambda_k = \dfrac{a}{h}\left[\left(\cos\left(2\pi \dfrac{k}{m}\right) - 1\right) - i \sin\left(2\pi \dfrac{k}{m}\right)\right] \\ \qquad 1 \leq k \leq m \qquad \text{upwind} \\ \\ \lambda_k = -\dfrac{ia}{h} \sin\left(\dfrac{2\pi k}{m}\right) \end{cases}$$

(22) For forward Euler, centered advection is never stable, i.e., unconditionally unstable, and the same goes for trapezoidal explicit.

For upwinding and forward Euler (same for explicit trapezoidal)

$$z = \tau \lambda_k = \underset{\text{CFL}}{\nu} \left[(\cos x - 1) - i \sin x \right]$$

$$0 \le x \le 2\pi$$



$$|z + 1| \le 1$$

$$\Rightarrow \quad 2\nu \underbrace{(\nu - 1)}_{\le 0} \underbrace{[\cos x - 1]}_{\le 0} \ge 0$$

$$\Rightarrow \quad \boxed{\nu \le 1} \quad \text{classic CFL}$$

(23) What we just performed is a variant on the classical <u>von Neumann stability analysis</u> (which you should have seen already)

For <u>third-order upwind-biased</u>,

$$\begin{cases} z = \tau\lambda = -\frac{4}{3}\nu \sin^4(x) - \frac{1}{3} i \nu \sin(2x)(4-\cos 2x) \\ x \in [0, \pi] \end{cases}$$

Forward Euler is an <u>unstable</u> scheme!

But explicit trapezoidal rule gives

$$\nu = \frac{\tau|a|}{h} \leq 0.87 \leftarrow \text{empirical, a } \underline{\text{typical result}}$$

24 We therefore see that the choice of time stepping scheme matters a lot not just for accuracy but also for stability.

Now let's consider pure diffusion and centered discretization: $u_t = d\,u_{xx}$

$$\lambda_k = -\frac{4d}{h^2}\sin^2(x), \quad x \in [0, \pi]$$

For forward Euler $|1+z| \le 1$

$$z = \tau\lambda_k = -4\mu\sin^2(x)$$

$$\boxed{\mu = \frac{\tau d}{h^2}} \leftarrow \text{viscous/diffusive CFL number}$$

(25)

$$\left| 1 - 4\mu \sin^2(x) \right| \le 1 \text{ for } 0 \le x \le \pi$$

When $x = \pi/2$ we get

$$\boxed{\mu = \frac{\tau d}{h^2} \le \frac{1}{2}}$$

which is the same for most (all?) explicit time stepping schemes.

Since $\tau_{max} \sim h^2$ is required, reducing h to improve spatial resolution will rapidly reduce τ_{max} = stiffness

Because of this stiffness we often handle diffusion implicitly

Implicit trapezoidal $\Rightarrow$ Crank-Nicolson method

(26) Performing complete stability analysis is often hard if not impossible in higher dimensions or when advection and diffusion are present. Here are some known (important) results:

(a) In dimension d, explicit diffusion requires $\boxed{\mu = \frac{\tau d}{h^2} \leq \frac{1}{2d}}$

so it gets worse and worse.

DIY: SHOW THIS YOURSELF!

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For advection-diffusion with second-order centered discretization in 1D:

Explicit Euler: $\boxed{\nu^2 \leq \underbrace{2\mu \leq 1}}$

adv CFL

diffusive CFL

Explicit trapezoidal: $\boxed{\frac{\nu^2}{3} \leq 2\mu \leq 1}$

not necessary but sufficient

Of course, the implicit methods are unconditionally stable. In practice we often use mixed explicit-implicit (see future lectures)

(28) <u>Just because a scheme is unconditionally stable does not mean it is accurate!</u>

That is, you cannot just take a huge time step and expect correct answers!

In this respect, <u>Backward Euler</u> is <u>much</u> more <u>robust</u> than Crank-Nicolson (implicit trapezoidal), but not more accurate necessarily.

We can see this by considering the case $h \to 0$! (only for unconditionally stable)

(29) Take $h \to 0$ to get a semi-discretization in time

$$u' = A u$$

where A is some <u>linear</u> (differential) operator.

Consider the θ-method:

$$\boxed{u^{n+1} = u^n + (1-\theta)\tau A u^n + \theta \tau A u^{n+1}}$$

$\theta = 0$: forward Euler

$\theta = 1$: backward Euler

$\theta = 1/2$: Crank-Nicolson.

<u>Temporal truncation error</u>:

$$\delta_n = \frac{1}{\tau}\left[u(t_{n+1}) - u(t_n)\right] - \left(\frac{u^{n+1} - u^n}{\tau}\right)$$

30 By Taylor series of $u' = Au$

$$\rho_n = \left(\frac{1}{2} - \theta\right)\tau \underbrace{\mathbf{u}''(t_n)}_{A^2} + \left(\frac{1}{6} - \frac{1}{2}\theta\right)\tau^2 \underbrace{\mathbf{u}'''(t_n)}_{A^3}$$

This means that our scheme is closer to solving the <u>modified equation</u>

$$\tilde{u}' = \tilde{A}\tilde{u}$$

$$\tilde{A} = A + \left(\theta - \frac{1}{2}\right)\tau A^2 + \left(\frac{\theta}{2} - \frac{1}{6}\right)\tau^2 A^3$$

↑ modified operator

$\tilde{A} \approx A$ [redacted] $\frac{\tau^2}{12} A^3$ for $\theta = 1/2$ (CN)

$\tilde{A} \approx A + \frac{\tau}{2} A^2$ for $\theta = \underline{1}$ (BE)

For pure advection equation,

$$A \equiv -a\,\partial_x \Rightarrow A^2 = a^2 \partial_{xx}$$
$$\Rightarrow A^3 = -a^3 \partial_{xxx}$$

So the modified equation is

BE $\left[\ \tilde{u}_t + a\tilde{u}_x = \dfrac{\tau a^2}{2}\,\tilde{u}_{xx} \quad \text{for } \theta = 1\right.$

Artificial diffusion!

CN $\left[\ \tilde{u}_t + a\tilde{u}_x = -\dfrac{1}{12}\,\tau^2 a^3\,\tilde{u}_{xxx} \quad \text{for } \theta = \dfrac{1}{2}\right.$

artificial dispersion

See HW 3!