Spatio-Temporal Discretizations

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

\[ w'(t) = F(t, w(t)) \]

But of course we now need a \textit{temporal discretization} to solve this large system of ODEs. This approach is called \textit{MOL} = method of lines = spatial + temporal
2 In the MOL approach (very common) space and time are decoupled. This means spatial and temporal errors add.

Assume spatial order of convergence = \( p_1 \):

\[
\| U_h(t) - u(t) \| \leq C_1 h^{p_1} \quad \cdots \quad (1)
\]

Assume temporal integrator for ODEs is convergent of order = \( p_2 \):

\[
\| W(t_n) - W_n \| \leq C_2 h^{p_2}
\]

where \( W_n \approx W(t_n) \), \( n = 1, 2, 3, \ldots \)

\[
t_n - t_{n-1} = \frac{\Delta t}{\uparrow} \quad \text{time step size}
\]

\[
\uparrow \text{time step size}
\]
Here it is crucial that $C_2$ and $p_2$ are independent of $h$.

$E = \| u_h(t_n) - w_n \| = \text{global error (spatio-temporal)}$

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

$\leq C_1 h^{p_1} + C_2 \bar{t}^{p_2}$

Spatial error \hspace{1cm} Temporal error.

Often we choose $\bar{t} = C h^p$, where $p = 1$ or $2$ (adv. or diff. dominated).

$\Rightarrow E = O(h^{\min (p_1, p_2)})$ \hspace{1cm} convergence as $h \to 0$
Let us consider stability now for several very common and basic temporal integrators other MOL approaches. We will come back to state-of-the-art later.

Focus on linear PDE's for stability:

\[ w' = F(t, w) = AW + g(t) \]

We all know forward Euler method:

\[ w^{n+1} = w^n + F(t^n, w^n) \]
Forward Euler is first-order accurate and explicit. An explicit but second-order accurate integrator is the explicit trapezoidal rule:

\[
\begin{align*}
\tilde{w}^{n+1} &= w^n + \frac{1}{2} F(t^n, w^n) \quad \text{Forward Euler predictor} \\
\w^{n+1} &= w^n + \frac{1}{2} \left[ F(t^n, w^n) + F(t^{n+1}, \tilde{w}^{*, n+1}) \right] \quad \text{trapezoidal rule corrector}
\end{align*}
\]

In implementation, write it as:

\[
\w^{n+1} = \frac{1}{2} \left[ w^n + \tilde{w}^{*, n+1} + 2F(t^{n+1}, \tilde{w}^{*, n+1}) \right]
\]
16) For a linear problem

\[ \dot{w} = Aw + g, \text{ set } g = 0 \text{ (homogeneous)} \]

for stability analysis

\[ w_{n+1} = w_n + \tau A w^n \]

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

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

\[ w^{n+1} = R(\tau A) w^n \]

where the stability function

\[ R(A) = I + A + \frac{A^2}{2} \]
For stability

\[ \| \omega^n \| \leq \| R(TA)^n \| \| \omega^0 \| \]

Assume \( A \) is a normal matrix

\[ A = U \Lambda U^{-1} \]

\[ \Lambda = \text{Diag} \{ \lambda_1, \ldots, \lambda_m \} \]

\[ \Rightarrow \| R(TA)^n \|_2 = \max_{1 \leq k \leq m} | R(Te^{i \lambda_k}) | \]

So for stability we want

\[ \overline{\lambda_k} \in S \text{ for all } k \]

where \( S \) is the domain of the complex plane:

\[ S : | R(z) | \leq 1 \]
For forward Euler

\[ R(t) = 1 + t \]

For trapezoidal

\[ R(t) = 1 + t + \frac{t^2}{2} \]

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

Neither stability region includes a non-trivial part of the imaginary axes \( \rightarrow \) you need at least a third-order Runge-Kutta for that.
We can do much better for stability if we use an implicit method:

\[ W^{n+1} = W^n + F(t^n, W^{n+1}) \]

\[ W^{n+1} = W^n + \tau A W^{n+1} \]

- For \( W^{n+1} \) in a non-linear system of equations, solve a linear system of equations.

\[ W^{n+1} = (I - \tau A)^{-1} W^n \]

\[ R(t) = (1 - t)^{-1} \]
So the backward Euler method is unconditionally stable (A-stable), but it is only first-order. A second-order implicit method is the implicit trapezoidal rule.

\[
W^{n+1} = W^n + \frac{\Delta t}{2} \left[ F(t^n, W^n) + F(t^{n+1}, W^{n+1}) \right]
\]

For \( F = Aw \)

\[
W^{n+1} = \left( I - \frac{A \Delta t}{2} \right)^{-1} \left( I + \frac{A \Delta t}{2} \right) W^n
\]

\[
R(\tau) = \left( I - \frac{\tau}{2} \right)^{-1} \left( I + \frac{\tau}{2} \right)
\]

Also unconditionally stable (A-stable)
Recall the stability criterion

$$\tau \lambda_k \in S + k$$

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

For pure advection eq. (a > 0)

$$\hat{\mathbf{f}}_{k} = \frac{\alpha}{\Delta x} \left[ \cos \left( \frac{2\pi k}{m} \right) - 1 \right] - i \sin \left( \frac{2\pi k}{m} \right)$$

$$1 \leq k \leq m \quad \text{upwind}$$

$$\lambda_k = -\frac{\alpha}{\Delta x} \sin \left( \frac{2\pi k}{m} \right)$$
For forward Euler, centered advection is never stable, i.e., unconditionally unstable, and the same goes for trapezoidal explicit.

\[ \frac{\Delta t}{\lambda} = \gamma \left[ (\cos x - 1) - i \sin x \right] \]

CFL  \[ 0 < \gamma \leq 2\pi \]

\[ |Z + 1| \leq 1 \]

\[ \Rightarrow \quad 2 \gamma (\gamma - 1) \left[ \cos x - 1 \right] \leq 0 \leq 0 \]

\[ \Rightarrow \quad \gamma \leq 1 \quad \text{classic CFL} \]
(23) What we just performed is a variant on the classical von Neumann stability analysis (which you should have seen already).

For third-order upwind-biased,

\[
\tau = \frac{\tau \lambda}{\tau} = -4 \gamma \sin^4(x) - \frac{1}{3} \nu \sin(2x)(4 - \cos(2x))
\]

\[
x \in [0, \pi]
\]

Forward Euler is an unstable scheme!

But explicit trapezoidal rule gives

\[
\gamma = \frac{1}{\lambda} \frac{a_1}{h} \leq 0.87 < \text{empirical, a typical result}
\]
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: \( U_t = d U_{xx} \)

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

For forward Euler, \(|1 + 2| \leq 1\)

\[ t = \frac{2\lambda_k}{2d} = -4M \sin^2(kx) \]

\[ M = \frac{2d}{h^2} \leq \text{CFL number} \]
\[ | 1 - 4 \mu \sin^2(x) | \leq 1 \] for \( 0.5 \leq x \leq 1 \)

When \( x = \pi/2 \) we get

\[ M = \frac{\varepsilon h}{h^2} \leq \frac{1}{2} \]

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

Since \( T_{\text{max}} \sim h^2 \) is required, reducing \( h \) to improve spatial resolution will rapidly reduce \( T_{\text{max}} \).

Because of this stiffness we often handle diffusion implicitly.

Implicit trapezoidal \( \Rightarrow \) Crank-Nicolson method
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:

In dimension $d$, explicit diffusion requires

\[ \mu = \frac{T d}{h^2} \leq \frac{1}{2d} \]

So it gets worse and worse,

DIY: Solve this yourself!
For advection-diffusion with second-order centered discretization in 1D:

Explicit Euler:
\[ \gamma^2 \leq 2\mu \leq 1 \]

- adv. CFL
- diffusive CFL

Explicit trapezoidal:
\[ \frac{\gamma^2}{3} \leq 2\mu \leq 1 \]

not necessary but sufficient

Of course, the implicit methods are unconditionally stable. In practice we often use mixed explicit-implicit (see future lectures)
Just because a scheme is unconditionally stable does not mean it is accurate!

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

In this respect, Backward Euler is much more robust 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)
Take $h \to 0$ to get a semi-discretization in time

$$U' = Au$$

where $A$ is some linear (differential) operator.

Consider the $\theta$-method:

$$u^{n+1} = u^n + (1-\theta) \frac{\Delta t}{2} Au^n + \theta \frac{\Delta t}{2} Au^{n+1}$$

$\theta = 0$: Forward Euler

$\theta = 1$: Backward Euler

$\theta = \frac{1}{2}$: Crank-Nicolson.

Temporal truncation error:

$$S_n = \frac{1}{2} [u(t_{n+1}) - u(t_n)] - \left( \frac{u^{n+1} - u^n}{2} \right)$$
By Taylor series of \( u' = A u \)

\[
S_n = \left( \frac{1}{2} - \theta \right) \frac{u''(t_n)}{A^2} + \left( \frac{1}{6} - \frac{1}{2} \theta \right) \frac{u'''(t_n)}{A^3}
\]

This means that our scheme is closer to solving the modified equation

\[
\hat{u}' = \hat{A} \hat{u}
\]

\[
\hat{A} = A + (\theta - \frac{1}{2}) \frac{\bar{r}}{A^2} + (\frac{\theta}{2} - \frac{1}{6}) \frac{\bar{r}^2}{A^3}
\]

\( \uparrow \) modified operator

\[
\begin{align*}
\hat{A} & = A \quad \text{for} \quad \theta = \frac{1}{12} \quad (CN) \\
\hat{A} & = A + \frac{\bar{r}}{12} A^2 \quad \text{for} \quad \theta = 1 \quad (BE)
\end{align*}
\]
For pure advection equation,

\[ A = -a \partial_x \Rightarrow A^2 = a^2 \partial_{xx} \Rightarrow A^3 = -a^3 \partial_{xxx} \]

So the modified equation is

\[
\begin{align*}
\text{BE} & \left[ \tilde{\mu}_t + a \tilde{\mu}_x = \frac{Ta^2}{2} \tilde{\mu}_{xx} \right. \\
\text{CN} & \left[ \tilde{\mu}_t + a \tilde{\mu}_x = -\frac{1}{12} \tau^2 a^3 \tilde{\mu}_{xxx} \right. \\
\text{for } \theta = 1/2 & \end{align*}
\]

Artificial diffusion!

See HW 3!