Lecture 7

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Numerical Methods for Time-Dependent PDEs, Spring 2024

Outline of Lecture 7

- Exact finite differences
- Nonstandard finite differences
- Splitting methods
- Implicit-explicit methods
- Exponential integrators (optional)

Nonstandard FDs [1]

First, exact FD's:

$$\begin{cases} \dot{u} = f(u, \lambda) \\ u(t_0) = u^0 \end{cases}$$

λ: parameter in model

has an exact FD-scheme: $u^{n+1} = \Phi(\lambda, u^n, t^n, t^{n+1})$

with Φ such that $u(t) = \Phi(\lambda, u^0, t^0, t)$ is the exact solution of the ODE (and: $u^0 = \Phi(\lambda, u^0, t^0, t^0)$)

Example 1)

$$\begin{cases} \frac{du}{dt} = -\lambda u \\ u(t_0) = u^0 \end{cases}$$

solve $\Longrightarrow$ $u(t) = u^0 e^{-\lambda(t-t_0)}$

exact scheme: $u^{n+1} = u^n e^{-\lambda \Delta t}$

$\Updownarrow$ re-arrange

$$\frac{u^{n+1} - u^n}{\left(\frac{1 - e^{-\lambda \Delta t}}{\lambda}\right)} = -\lambda u^n$$

compare with EF: $\frac{u^{n+1} - u^n}{\Delta t} = -\lambda u^n$

replace $\Delta t \rightarrow \frac{1 - e^{-\lambda \Delta t}}{\lambda}$

$= \frac{1 - (1 - \lambda \Delta t + \lambda^2 (\Delta t)^2/2 - \dots)}{\lambda}$

$= \Delta t + O(\Delta t^2)\lambda$

Nonstandard FDs [2]

Example 2)

$$\begin{cases} \frac{du}{dt} = \lambda_1 u - \lambda_2 u^2 \\ u(t^0) = u^0 \end{cases}$$

"logistic DE" (two parameters: λ_1 and λ_2)

$\Rightarrow$ exact solution: $u(t) = \dfrac{\lambda_1 u^0}{(\lambda_1 - u^0\lambda_2)\, e^{-\lambda_1(t-t_0)} + \lambda_2 u^0}$

exact FD-scheme:

note: $t^0 \to t^n$, $t \to t^{n+1}$, $u^0 \to u^n$, $u(t) \to u^{n+1}$

$$\frac{u^{n+1} - u^n}{\left(\frac{e^{-\lambda_1 \Delta t} - 1}{\lambda_1}\right)} = \lambda_1 u^n - \lambda_2 u^{n+1} u^n$$

! !

Compare with EF: $\dfrac{u^{n+1} - u^n}{\Delta t} = \lambda_1 u^n - \lambda_2 (u^n)^2$

"standard" "standard"

$\Delta t \to \dfrac{e^{-\lambda_1 \Delta t} - 1}{\lambda_1}$

$(u^n)^2 \to u^{n+1} u^n$ "nonlocal"

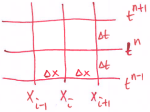
Nonstandard FDs [3]

Example 3) first order linear PDE: $u_t + u_x = 0$

exact solution: $u(x,t) = f(x-t)$ ← arbitrary function

n : time-index

i : space-index



exact "first order partial FD equation": $u_i^{n+1} = u_{i-1}^n$ with solution: $u_i^n = F(i-n)$ ← arbitrary

$\Delta t = \Delta x$ $\Rightarrow$ $\phi(\Delta t) = \phi(\Delta x)$

$$\frac{u_i^{n+1} - u_i^n}{\phi(\Delta t)} + \frac{u_i^n - u_{i-1}^n}{\phi(\Delta x)} = 0$$

with arbitrary $\phi(z) = z + O(z^2)$

forward in time, backward in space

Nonstandard FDs [4]

Example 4) first order nonlinear PDE: $\begin{cases} u_t + u_x = u(1-u) \\ u(x,0) = f(x) \end{cases}$

exact solution (via Method of Characteristics)

$$u(x,t) = \frac{f(x-t)}{e^{-t} + (1-e^{-t})f(x-t)}$$

exact finite differences:

$$\frac{u_i^{n+1} - u_i^n}{\phi(\Delta t)} + \frac{u_i^n - u_{i-1}^n}{\phi(\Delta x)} = u_{i-1}^n (1 - u_i^{n+1})$$

with $\phi(z) = e^z - 1$

$= 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 \dots - 1$

$= z + O(z^2)$

Solve for u_i^{n+1}, $h = \Delta t = \Delta x$

$$u_i^{n+1} = \frac{u_{i-1}^n}{1 + (e^h - 1)u_{i-1}^n}$$

explicit scheme!

Nonstandard FDs [5]

In general: $\boxed{\dfrac{du}{dt} = f(u,\lambda)}$

most general FD-model (on (t^n, t^{n+1})): $\boxed{\dfrac{u^{n+1}-u^n}{\phi(\Delta t,\lambda)} = F(u^n, u^{n+1}, \lambda, \Delta t)}$

which is a generalization of $\dfrac{du}{dt} \longrightarrow \dfrac{u^{n+1}-u^n}{\Delta t}$ and $f(u,\lambda) \longrightarrow f(u^{n+1},\lambda)$

Note: $\boxed{\phi(\Delta t,\lambda) = \Delta t + O((\Delta t)^2)}$, λ fixed and $\Delta t \to 0$

$$\boxed{\frac{du}{dt} = \lim_{\Delta t \to 0} \frac{u(t+\psi_1(\Delta t)) - u(t)}{\psi_2(\Delta t)}} \quad \text{with } \begin{cases} \psi_1(\Delta t) = \Delta t + O((\Delta t)^2) \\ \psi_2(\Delta t) = \Delta t + O((\Delta t)^2) \end{cases}$$

a generalization of $\displaystyle\lim_{\Delta t \to 0} \frac{u(t+\Delta t) - u(t)}{\Delta t}$

Nonstandard FDs [6]

Examples of $\phi_{1,2}$ functions:

$$\psi(\Delta t) = \begin{cases} \Delta t = \Delta t + 0 = \Delta t + O((\Delta t)^2) \\ \sin(\Delta t) = \Delta t - \frac{(\Delta t)^3}{3!} + \ldots = \Delta t + O((\Delta t)^3) = \Delta t + O((\Delta t)^2) \\ e^{\Delta t} - 1 = \Delta t + \frac{(\Delta t)^2}{2} + \frac{(\Delta t)^3}{6} + \ldots = \Delta t + O((\Delta t)^2) \\ 1 - e^{-\Delta t} = 1 - \left(1 - \Delta t + \frac{(\Delta t)^2}{2} - \ldots\right) = \Delta t + O((\Delta t)^2) \\ \frac{1 - e^{-\lambda \Delta t}}{\lambda} = \frac{1 - \left(1 - \lambda \Delta t + \frac{\lambda^2 (\Delta t)^2}{2} - \ldots\right)}{\lambda} = \Delta t + O((\Delta t)^2) \\ \text{---- etcetera} \end{cases}$$

in the limit $\Delta t \to 0$:

$$\lim_{\Delta t \to 0} \frac{u(t + \phi_1(\Delta t)) - u(t)}{\phi_2(\Delta t)} = \lim_{\Delta t \to 0} \frac{u(t + \Delta t) - u(t)}{\Delta t} = \frac{du}{dt}(t)$$

BUT: for finite values of Δt they differ greatly!

Nonstandard FDs [7]

Another way of writing:

replace EF $\frac{du}{dt} \rightarrow \frac{u^{n+1} - u^n}{\Delta t}$ by $\frac{u^{n+1} - (1 + O(\Delta t))u^n}{\Delta t + O((\Delta t)^2)}$

$$= \frac{u^{n+1} - \psi \cdot u^n}{\phi}$$

the functions ϕ and ψ vary from one equation to another (not clear how to choose in general)

ϕ is called denominator function ← determined by the requirement of having the correct stability properties

ψ is usually, not always, set $\equiv 1$

Nonstandard FDs [8]

A "justification": consider the scalar ODE $\boxed{\frac{du}{dt} = f(u)}$

set $\psi \equiv 1$: $\boxed{\frac{u^{n+1} - u^n}{\phi} = f(u^n)}$ with $\phi(\Delta t, R^*) = \frac{1 - e^{-R^* \Delta t}}{R^*} = \Delta t + O((\Delta t)^2)$ (see before with $\lambda = R^*$)

"parameter" R^* is determined as follows:

1) calculate fixed (stationary) points of ODE, i.e., find $\bar{u}$ such that $f(\bar{u}) = 0$
2) suppose there are M real solutions: $\bar{u}^{(1)}, \bar{u}^{(2)}, \ldots, \bar{u}^{(M)}$
3) define $R_i = \left.\frac{df}{du}\right|_{u=\bar{u}^{(i)}}$, $i = 1, \ldots, M$ (determines also the character of the fixed points: stable, unstable, ..)
4) define $R^* = \max_{i=1,\ldots,M} |R_i|$
5) note: $\phi \stackrel{d}{=} \frac{1 - e^{-R^* \Delta t}}{R^*} = \Delta t + O((\Delta t)^2)$; $t \sim$ seconds $\rightsquigarrow [R_i] \sim \frac{1}{\text{seconds}}$

time scales in ODE: $T_i = \frac{1}{R_i}$ (seconds), $i = 1, \ldots, M$

$T^* = \frac{1}{R^*}$ is smallest time scale $\leftrightarrow$ of importance for numerical stability ("stiffness" of ODE)

Nonstandard FDs [9]

6) ϕ can be interpreted as a "rescaled" timestep size !

(it is never larger than the smallest time scale of the system

Note: $0 < \phi(\Delta t, R^*) < T^*$

Remark from exact FD : $u^2 \not\to (u^n)^2$ but: $u^{n+1}u^n$ "nonlocal form"

example 2

and in example 4 : $u(1-u) = u - u^2 \not\to u_i^n - (u_i^n)^2$

but : $u_{i-1}^n \, u_i^{n+1}$ "nonlocal form"

$$\lim_{\substack{\Delta t \to 0 \\ n \to \infty \\ n\Delta t = t \text{ (fixed)}}} u^{n+1}u^n = \lim_{\substack{\Delta t \to 0 \\ n \to \infty \\ n\Delta t = t \text{ (fixed)}}} (u^n)^2 = (u(t))^2$$

ODE case

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0 \\ n \to \infty \\ i \to \infty \\ i\Delta x = x \text{ (fixed)} \\ n\Delta t = t \text{ (fixed)}}} u_{i-1}^n u_i^{n+1} = \lim (u_i^n)^2 = (u(x,t))^2$$

PDE case

BUT $u^{n+1}u^n \neq (u^n)^2$

and $u_{i-1}^n u_i^{n+1} \neq (u_i^n)^2$

for finite values of i and n (of course)

Nonstandard FDs [10]

general "rules" for nonstandard schemes:

- * non-trivial denominator function ϕ
- * non-local discrete formula for nonlinear terms
- * special conditions for DE must hold as well (for example $u \geq 0$)

nonstandard FD's $\neq$ exact FD's (but, in some sense, are related)

↳ they are constructed in such a way that elementary numerical instabilities can be prevented.

Example: $\begin{cases} \frac{du}{dt} = u^2(1-u) = u^2 - u^3 \\ u(0) = u^0 > 0 \end{cases}$

There are three fixed points $\bar{u}^{(1)} = \bar{u}^{(2)} = 0$ and $\bar{u}^{(3)} = 1$ (all solutions go monotonically to $\bar{u}^{(3)} = 1$)

We have: $R_1 = R_2 = 0$, $R_3 = 1 \Rightarrow R^* = 1$ $(T^* = 1)$

and $\phi(\Delta t) = 1 - e^{-\Delta t}$ (note: $0 < \phi(\Delta t) < 1 = T^*$)

Nonstandard FDs [11]

$\Rightarrow \quad \frac{du}{dt} \to \frac{u^{n+1} - u^n}{1 - e^{-\Delta t}}$ (instead of $\frac{u^{n+1} - u^n}{\Delta t}$)

note that: $u(t) > 0$ (for example, a chemical concentration, or a population density)

therefore, the discrete values **must** satisfy: $u^n \geq 0 \Rightarrow u^{n+1} \geq 0$

this can be enforced by taking: $\begin{cases} u^2 \longrightarrow 2(u^n)^2 - u^{n+1}u^n \\ u^3 \longrightarrow u^{n+1}(u^n)^2 \end{cases}$

$\Leftarrow$ substitute and solve

$$u^{n+1} = \frac{(1 + 2\phi . u^n) u^n}{1 + \phi . (u^n + (u^n)^2)}$$

an explicit scheme!

It can be shown for the discrete scheme/values: $\forall \Delta t > 0$

1) it also has three fixed points $\bar{u}^{(1)} = \bar{u}^{(2)} = 0$, $\bar{u}^{(3)} = 1$

2) first two are unstable, third is stable (as in ODE itself)

3) $u^0 > 0 \Rightarrow u^n \to \bar{u}^{(3)} = 1$ monotonically, $0 \leq u^0 \leq u^1 \leq u^2 \leq \ldots$

Nonstandard FDs [12]

Fisher PDE $u_t = u_{xx} + u(1-u)$

$u(x,t)$ satisfies: $0 \le u(x,0) \le 1 \Rightarrow 0 \le u(x,t) \le 1 \quad \forall t \ge 0$ "boundedness"

Nonstandard FD:

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + 2\bar{u}_i^n - u_i^{n+1} - \bar{u}_i^n u_i^{n+1}$$

FT (standard) — CS (standard) — nonstandard (nonlocal)

with $\bar{u}_i^n \stackrel{d}{=} \frac{u_{i+1}^n + u_i^n + u_{i-1}^n}{3}$

instead of: $u_i^n - (u_i^n)^2$

note: $u = 2u - u \to 2\bar{u}_i^n - u_i^{n+1}$

$u^2 \to \bar{u}_i^n u_i^{n+1}$

substitute and solve with $R = \frac{\Delta t}{(\Delta x)^2} = \frac{1}{2}$

$$u_i^{n+1} = \frac{\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t\, \bar{u}_i^n}{1 + \Delta t + \Delta t\, \bar{u}_i^n}$$

explicit expression!

Nonstandard FDs [13]

for <u>positivity</u> of the discrete solution values we need $R = \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$

<u>Boundedness</u> with this non-standard FD-scheme: ($= \frac{1}{2}$ ok, see previous page)

suppose $0 \leq u_i^n \leq 1$ (*) $\forall i$, certain n "induction"

$\Rightarrow \frac{1}{2}(u_{i+1}^n + u_{i-1}^n) \leq 1$ and $2\,\Delta t\,\bar{u}_i^n = \Delta t\,\bar{u}_i^n + \Delta t\,\bar{u}_i^n \leq \Delta t + \Delta t\,\bar{u}_i^n$

$\bar{u}_i^n = \frac{u_{i+1}^n + u_i^n + u_{i-1}^n}{3} \overset{(*)}{\leq} \frac{1+1+1}{3} = 1$

Adding these two: $\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t\,\bar{u}_i^n \leq 1 + \Delta t + \Delta t\,\bar{u}_i^n$

Dividing by $1 + \Delta t + \Delta t\,\bar{u}_i^n$: $\underbrace{\frac{\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t\,\bar{u}_i^n}{1 + \Delta t + \Delta t\,\bar{u}_i^n}}_{= u_i^{n+1}} \leq 1$

$\Rightarrow$ it holds for $n+1$

By induction: $0 \leq u_i^0 \leq 1 \Rightarrow 0 \leq u_i^n \leq 1$ for all $n \geq 1$, for all i ☒

(many other examples can be found in the extra files)

Splitting methods [1]

First order splitting:

Consider the linear homogeneous ODE system:

$$\begin{cases} \vec{w}'(t) = A\,\vec{w}(t), \quad t>0 \\ \vec{w}(0) = \vec{w}_0 \end{cases}$$

(for example, after semi-discretization of a linear PDE)

Assume: $A = A_1 + A_2$ (two-term splitting)

"Lie-Trotter splitting" (or "sequential splitting")

The exact solution on $t^n < t < t^{n+1}$ satisfies: $\vec{w}(t^{n+1}) = e^{\tau A} \cdot \vec{w}(t^n)$ with $\tau \stackrel{d}{=} \Delta t$ (the time step)

Approximation: not applying A, but A_1 and A_2 separately: $\vec{w}^{n+1} = e^{\tau A_2} \cdot e^{\tau A_1} \vec{w}^n$ with $\vec{w}^n \approx \vec{w}(t^n)$

Solve two subproblems: first $\begin{cases} \frac{d\vec{w}^*}{dt}(t) = A_1 \vec{w}^*(t) \\ \vec{w}^*(t^n) = \vec{w}^n \end{cases}$ on $t^n < t < t^{n+1}$

and then $\begin{cases} \frac{d\vec{w}^{**}}{dt}(t) = A_2 \vec{w}^{**}(t) \\ \vec{w}^{**}(t^n) = \vec{w}^*(t^{n+1}) \end{cases}$ and finally set: $\vec{w}^{n+1} = \vec{w}^{**}(t^{n+1})$

Splitting methods [2]

Replacing $\vec{w}(t^{n+1}) = e^{\tau A} \cdot \vec{w}(t^n)$ (exact) by $\vec{w}^{n+1} = \underbrace{e^{\tau A_2}}_{\text{second}} \underbrace{e^{\tau A_1}}_{\text{first}} \vec{w}^n$ $\odot$

introduces an error: the splitting error

Inserting the exact solution w into $\odot$ gives: $\vec{w}(t^{n+1}) = e^{\tau A_2} e^{\tau A_1} \vec{w}(t^n) + \tau \rho^n$

with $\tau \rho^n$ the local splitting error

We have: $e^{\tau A} = e^{\tau(A_1+A_2)} = I + \tau(A_1+A_2) + \frac{1}{2}\tau^2 (A_1+A_2)^2 + \cdots$

$$(A_1+A_2)^2 = A_1^2 + A_1A_2 + A_2A_1 + A_2^2$$

and: $e^{\tau A_2} \cdot e^{\tau A_1} = (I + \tau A_2 + \cdots)(I + \tau A_1 + \cdots)$

$$= I + \tau(A_1+A_2) + \frac{1}{2}\tau^2 (A_1^2 + 2A_2A_1 + A_2^2) + \cdots$$

$$\Rightarrow \rho^n = \frac{1}{\tau}\left[e^{\tau A} - e^{\tau A_2} \cdot e^{\tau A_1} \right] w(t^n) + \mathcal{O}(\tau^2)$$

Splitting methods [3]

$$e^{\tau A_2} e^{\tau A_1} = \left(I + \tau A_2 + \frac{\tau^2}{2}A_2^2 + \cdots\right)\left(I + \tau A_1 + \frac{\tau^2}{2}A_1^2 + \cdots\right)$$

$$= I + \tau A_2 + \frac{\tau^2}{2}A_2^2 + \tau A_1 + \tau^2 A_2 A_1 + \frac{\tau^2}{2}A_1^2 + \cdots$$

$$= I + \tau(A_1 + A_2) + \frac{\tau^2}{2}\left(A_1^2 + 2A_2A_1 + A_2^2\right) + \cdots$$

$$e^{\tau(A_2+A_1)} = I + \tau(A_2 + A_1) + \frac{\tau^2}{2}(A_2 + A_1)^2 + \cdots$$

$$\parallel$$

$$e^{\tau A} = I + \tau(A_2 + A_1) + \frac{\tau^2}{2}\left(A_2^2 + A_2A_1 + A_1A_2 + A_1^2\right) + \cdots$$

---

difference: $A_2A_1 + A_1A_2 - 2A_2A_1 = A_1A_2 - A_2A_1 \stackrel{\text{def}}{=} [A_1, A_2]$

the commutator of A_1 and A_2

("Lie-bracket")

Splitting methods [4]

Baker – Campbell – Hausdorff formula: (solution Z of equation $e^X e^Y = e^Z$)

$$
\begin{aligned}
Z(X,Y) &= \log(\exp X \exp Y) \\
&= X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}\left([X,[X,Y]] + [Y,[Y,X]]\right) \\
&\quad - \frac{1}{24}[Y,[X,[X,Y]]] \\
&\quad - \frac{1}{720}\left([Y,[Y,[Y,[Y,X]]]] + [X,[X,[X,[X,Y]]]]\right) \\
&\quad + \frac{1}{360}\left([X,[Y,[Y,[Y,X]]]] + [Y,[X,[X,[X,Y]]]]\right) \\
&\quad + \frac{1}{120}\left([Y,[X,[Y,[X,Y]]]] + [X,[Y,[X,[Y,X]]]]\right) \\
&\quad + \frac{1}{240}\left([X,[Y,[X,[Y,[X,Y]]]]]\right) \\
&\quad + \frac{1}{720}\left([X,[Y,[X,[X,[X,Y]]]]] - [X,[X,[Y,[Y,[X,Y]]]]]\right) \\
&\quad + \frac{1}{1440}\left([X,[Y,[Y,[Y,[X,Y]]]]] - [X,[X,[Y,[X,[X,Y]]]]]\right) + \cdots
\end{aligned}
$$

Splitting methods [5]

The first, second, third, and fourth order terms are:

$$z_1 = X + Y$$

$$z_2 = \frac{1}{2}\underbrace{(XY - YX)}_{=[X,Y]}$$

$$z_3 = \frac{1}{12}\underbrace{\left(X^2Y + XY^2 - 2XYX + Y^2X + YX^2 - 2YXY\right)}_{=[X,[X,Y]]+[Y,[Y,X]]}$$

$$z_4 = \frac{1}{24}\underbrace{\left(X^2Y^2 - 2XYXY - Y^2X^2 + 2YXYX\right)}_{=-[Y,[X,[X,Y]]]}.$$

etcetera !

Splitting methods [6]

Sequential splitting: $e^{\tau A_2} e^{\tau A_1}$

(Marchuk-)Strang splitting: $e^{\frac{\tau}{2} A_1} e^{\tau A_2} e^{\frac{\tau}{2} A_1}$ (*) (Marchuk 1971, Strang 1968)

Lie-splitting: $(I - \tau A_2)^{-1} (I - \tau A_1)^{-1}$

Peaceman-Rachford splitting: $(I - \frac{\tau}{2} A_1)^{-1} (I + \frac{\tau}{2} A_2)(I - \frac{\tau}{2} A_2)^{-1} (I + \frac{\tau}{2} A_1)$

parallel splitting: $\frac{1}{2} (e^{\tau A_2} e^{\tau A_1} + e^{\tau A_1} e^{\tau A_2})$

etcetera ...

(*) $$\rho_n = \frac{1}{24} \tau^2 \left([A_1, [A_1, A_2]] + 2 [A_2, [A_1, A_2]] \right) w(t^{n+\frac{1}{2}}) + O(\tau^4)$$

↑ consistency order of 2

series expansion + tedious calculations (local error)

*Splitting methods [7]; nonlinear case

$$\begin{cases} w'(t) = F(t, w(t)), & t > 0 \\ w(0) = w_0 \end{cases}$$

with two-term splitting: $F(t, v) = F_1(t, v) + F_2(t, v)$

$$\begin{cases} \dfrac{dw^*}{dt}(t) = F_1(t, w^*(t)), & t_n < t < t_{n+1} \\ w^*(t_n) = w_n \end{cases}$$

and

$$\begin{cases} \dfrac{dw^{**}}{dt}(t) = F_2(t, w^{**}(t)), & t_n < t < t_{n+1} \\ w^{**}(t_n) = w^*(t_{n+1}) \end{cases} \Rightarrow w_{n+1}$$

*Splitting methods [8]; nonlinear case

$w^{**}(t_n) = w(t_{n+1})$

$w_{n+1} = w^{**}(t_{n+1}) \approx w(t_{n+1})$

for $w_n = w(t_n)$ "exact" $\Rightarrow$ $\rho_{(LTE)} = \frac{1}{2}\tau \left(\frac{\partial F_1}{\partial w} F_2 - \frac{\partial F_2}{\partial w} F_1\right)(t_n, w(t_n)) + O(\tau^2)$

consistency order of 1

[It can be derived from taylor expansions of $w^{*}(t_{n+1})$ and $w^{**}(t_{n+1})$ around $t = t_n$:]

if $\frac{\partial F_1}{\partial w} F_2 = \frac{\partial F_2}{\partial w} F_1$ then $LTE = O(\tau^2)$

*Splitting methods [9]; nonlinear case

Abstract Initial Value Problem

6

$$u_t(\vec{x},t) = f(\vec{x}, u(\vec{x},t))$$

$$= -\nabla\cdot(\vec{a}u) + \nabla\cdot(D\nabla u) + s(u)$$

convection diffusion reaction

spatial differential operator

Define "solution operator" S_τ such that: $u(t+\tau) = S_\tau(u(t))$

(this generalizes the exp-operator e^{tA} for the linear ODE system $w'(t) = Aw(t)$)

*Splitting methods [10]; nonlinear case

Assume two-term splitting: $f(u) = f_1(u) + f_2(u)$

and $\begin{cases} u_t = f_1(u) \leftrightarrow S_{1,\tau} & \text{(solution operator of 1st part)} \\ u_t = f_2(u) \leftrightarrow S_{2,\tau} & \text{(solution operator of 2nd part)} \end{cases}$

basic splitting method "$w_{n+1} = e^{\tau A_2} e^{\tau A_1} w_n$"

is now formulated as:

$$u_{n+1} = S_{2,\tau}\left(S_{1,\tau}(u_n)\right)$$

with $u_n \approx u(t_{n+1})$

*Splitting methods [11]; nonlinear case

insert exact solution: (a formal expression) (+

$$\Rightarrow u(t_{n+1}) = S_{2,\tau}(S_{1,\tau}(u(t_n))) + \tau \rho_n$$

Taylor expansion

$$\rho_n = \frac{1}{2}\tau \left(\frac{\partial f_1}{\partial u} f_2 - \frac{\partial f_2}{\partial u} f_1 \right)(u(t_n)) + O(\tau^2)$$

Compare with ODE system case:

$$\rho_n = \frac{1}{2}\tau \left(\frac{\partial F_1}{\partial w} F_2 - \frac{\partial F_2}{\partial w} F_1 \right)(t_n, w(t_n)) + O(\tau^2)$$

Implicit-explicit methods

IMEX – θ method (as a special case of IMEX Multistep Methods)

ODE (or semi-discrete ODE system ⟺ Method of Lines): $\dot{u}(t) = f(u(t),t)$

$= f_0(u(t),t) + f_1(u(t),t)$

advection part of PDE ⟷ non-stiff term (explicit?!) scheme

stiff term (implicit scheme?!) — reaction or diffusion part of PDE

$$u^{n+1} = u^n + \Delta t\, f_0(u^n,t^n) + (1-\theta)\,\Delta t\, f_1(u^n,t^n) + \theta\,\Delta t\, f_1(u^{n+1},t^{n+1})$$

"EF" — "implicit θ-method", $\theta \geq \frac{1}{2}$

$\Rightarrow$ local truncation error:

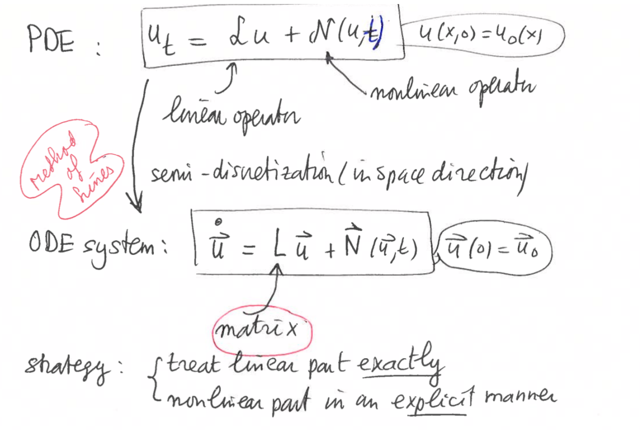
$$\delta_n = \left(\tfrac{1}{2} - \theta\right)\Delta t\, u''(t^n) + \theta\,\Delta t\, \varphi'(t^n) + O((\Delta t)^2)$$

with $\varphi(t) = f_0(u(t),t)$

stability function $R(z_0,z_1) = \dfrac{1 + z_0 + (1-\theta)z_1}{1-\theta z_1}$; stability: $|R(z_0,z_1)| \leq 1$

$z_0 = \lambda_0\Delta t,\ z_1 = \lambda_1 \Delta t$

*Exponential integration [1]



*Exponential integration [2]

properties:

1) if $L = 0$, then the scheme reduces to a "standard" method
2) if $\vec{N} = \vec{0}$, then the scheme reproduces the exact solution of $\dot{\vec{u}} = L\vec{u}$

example: $\dot{\vec{u}} = a\vec{u} + \vec{b}$ ← constants

the numerical integrator $\vec{u}_{n+1} = e^{\tau a}\vec{u}_n + \dfrac{e^{\tau a}-1}{\tau a}\tau\vec{b}$

($\tau = \Delta t$) solves this equation exactly (check by substitution)

$$\lim_{a\to 0}\frac{e^{\tau a}-1}{\tau a} = \lim_{a\to 0}\frac{1+\tau a+\tau^2 a^2 \cdots -1}{\tau a} = \lim_{a\to 0}(1+\tau a+\cdots) = 1$$

and $\vec{u}_{n+1} = e^{\tau a}\vec{u}_n + \tau\vec{b} \Rightarrow \vec{u}_{n+1} = \vec{u}_n + \tau\vec{b}$ (EF)

*Exponential integration [3]

crucial to ETD-schemes is the evaluation of the φ-functions (*)

for small values of ℓ and $z>0$ there are:

$$\varphi_1(z) = \frac{e^z - 1}{z}$$

$$\varphi_2(z) = \frac{e^z - z - 1}{z^2}$$

$$\varphi_3(z) = \frac{e^z - \frac{1}{2}z^2 - z - 1}{z^3}$$

$$\varphi_\ell(0) = \frac{1}{\ell!}$$

$$\varphi_0(z) \stackrel{\text{def}}{=} e^z$$

recurrence

$$\varphi_{\ell+1}(z) = \frac{\varphi_\ell(z) - \frac{1}{\ell!}}{z}, \quad \ell = 0, 1, \ldots$$

evaluation of these φ-functions has numerical issues

*Exponential integration [4]

take $\sigma = t_n + \theta\tau$

$$\Rightarrow \quad \vec{u}(t_{n+1}) = e^{\tau L}\,\vec{u}(t_n) + \tau \int_0^1 e^{(1-\theta)\tau L}\,\vec{N}(\vec{u}(t_n+\theta\tau), t_n+\theta\tau)\,d\theta$$

this is still an exact representation of the solution!

exponential time differencing (ETD)-schemes arise from approximating $\vec{N}$ by a polynomial $p(\theta)$ (in fact $\vec{p}(\theta)$) and then integrating exactly

simplest choice: approximating by a constant at $\theta = 0$, leads to ETD-Euler:

$$\vec{u}_{n+1} = e^{\tau L}\vec{u}_n + \tau\,\varphi_1(\tau L)\,\vec{N}(\vec{u}_n, t_n)$$

$$\varphi_1(z) = \frac{e^z - 1}{z}$$

*Exponential integration [5]

Lemma: the exact solution of

$$\begin{cases} \dot{\vec{u}}(t) = L\vec{u}(t) + \vec{N}(\vec{u}(t)) \\ \vec{u}(0) = \vec{u}_0 \end{cases}$$

has the expansion $\vec{u}(t) = e^{tL}\vec{u}_0 + \sum_{\ell=1}^{\infty} t^{\ell}\varphi_{\ell}(tL)\vec{N}^{(\ell-1)}(\vec{u}_0)$

where $\varphi_{\ell}(z) = \frac{1}{(\ell-1)!}\int_0^1 e^{(1-\theta)z}\theta^{\ell-1}d\theta$ (*)

(alternative:)

Lawson-Euler scheme: $\vec{u}_{n+1} = e^{\tau L}\vec{u}_n + \tau e^{\tau L}\vec{N}(\vec{u}_n, t_n)$

(1967) $(\tau = \Delta t)$ "the integrating factor method"

*Exponential integration [6]

crucial to ETD-schemes is the evaluation of the φ-functions (*)

for small values of ℓ and $z>0$ these are:

$$\varphi_1(z) = \frac{e^z - 1}{z}$$

$$\varphi_2(z) = \frac{e^z - z - 1}{z^2}$$

$$\varphi_3(z) = \frac{e^z - \frac{1}{2}z^2 - z - 1}{z^3}$$

$$\varphi_\ell(0) = \frac{1}{\ell!}$$

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recurrence

$$\varphi_{\ell+1}(z) = \frac{\varphi_\ell(z) - \frac{1}{\ell!}}{z}, \quad \ell = 0, 1, \ldots$$

evaluation of these φ-functions has numerical issues

Outlook

- Exercises 7 (exponential integration: optional)
- Check hand-in exercise C1!!
- C2A (April) and C2B (May ⇔ two guest lectures)
- Next lecture: Hamiltonian ODEs and PDEs