CFD FALL 2018, A. DONEV

EXPONENTIAL INTEGRATORS

This is a brief interlude before Nick Trefethen's lecture, not a complete lecture on the topic.

MANY (O/P)DEs have the form

$$u'(t) = \underset{\uparrow}{A}\, u(t) + \underbrace{B\big(u(t)\big)}_{\text{Non-Stiff / Nonlinear part}}$$

Stiff Linear part (e.g. diffusion, u_{xxx})

MOL discretization of PDE

The matrix A could be constant

or it can change with time / u

e.g. $$A(u) \Longleftrightarrow \partial_x\left(d(u)\,u_x\right)$$

$$A\,u \Longleftrightarrow \partial_x\left(d(\underset{\substack{\uparrow \\ \text{value at } n^{th} \\ \text{time step.}}}{u^n})\,u_x\right)$$

Or, for $u' = f(u)$

$$A \Longleftrightarrow \underbrace{f'(u^n)}_{\text{Jacobian}}$$

or approximate Jacobian

The key is that A captures the stiff part of dynamics

Duhamel's principle gives ③

$$u^{n+1} = \underbrace{e^{A^n \Delta t} u^n}_{\text{Linear}} + \int_{t^n}^{t^{n+1}} e^{A^n(t^{n+1}-\tau)} B^n(u(\tau))\,d\tau$$

Questions:

(1) HARDEST: HOW TO COMPUTE THE ACTION OF $\exp(A^n \Delta t)$?

ANSWER: Krylov methods

(2) How to approximate the NONLINEAR INTEGRAL

NOTE: If A diagonal (FFT) $\Rightarrow \exp(A\Delta t) = \mathrm{Diag}(\exp(A_{ii}\Delta t))$

Approximate $B^n(u(\tau)) \simeq B^n(u^n)$

$$\int_{t_n}^{t_{n+1}} \exp(A^n(t_{n+1}-\tau))\, d\tau = \underset{\uparrow}{A_n^{-1}}(e^{A_n k} - I)$$

Elliptic solve if
An is diffusion
(harder than implicit-explicit)

$$u^{n+1} = e^{A^n \Delta t} u^n + A_n^{-1}(e^{A_n \Delta t} - I) B_n(u^n)$$

$$\boxed{u^{n+1} = u^n + (A^n)^{-1}(e^{A^n \Delta t} - I)\underbrace{f(u^n)}_{\text{rhs}}}$$

Truncation error analysis

$$\sigma^n = \left(\frac{u(t_{n+1}) - u(t_n)}{\Delta t}\right) - \frac{1}{\Delta t}(A^n)^{-1}\left(e^{A^n \Delta t} - I\right)u'(t_n)$$

$$= \frac{\Delta t}{2}\underbrace{\left(f'(u(t_n)) - A_n\right)}_{\substack{\text{If } A_n \text{ is Jacobian} \\ \text{then this is } \underline{\text{zero}}\text{!} \\ \text{(but must be invertible)}}} u'(t_n)$$

So first-order accurate if $A_n \neq f'(u_n)$,
second-order if $A_n = f'(u_n)$

Cox and Matthews also derive a set of ETD methods based on Runge–Kutta time-stepping, which they call ETDRK schemes. In this report we consider only the fourth-order scheme of this type, known as ETDRK4. According to Cox and Matthews, the derivation of this scheme is not at all obvious and requires a symbolic manipulation system. The Cox and Matthews ETDRK4 formulae are:

$$\boxed{\begin{aligned}
a_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(u_n, t_n),\\
b_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{N}(a_n, t_n + h/2),\\
c_n &= e^{\mathbf{L}h/2}a_n + \mathbf{L}^{-1}(e^{\mathbf{L}h/2} - \mathbf{I})(2\mathbf{N}(b_n, t_n + h/2) - \mathbf{N}(u_n, t_n)),\\
u_{n+1} &= e^{\mathbf{L}h}u_n + h^{-2}\mathbf{L}^{-3}\{[-4 - \mathbf{L}h + e^{\mathbf{L}h}(4 - 3\mathbf{L}h + (\mathbf{L}h)^2)]\mathbf{N}(u_n, t_n)\\
&\quad + 2[2 + \mathbf{L}h + e^{\mathbf{L}h}(-2 + \mathbf{L}h)](\mathbf{N}(a_n, t_n + h/2) + \mathbf{N}(b_n, t_n + h/2))\\
&\quad + [-4 - 3\mathbf{L}h - (\mathbf{L}h)^2 + e^{\mathbf{L}h}(4 - \mathbf{L}h)]\mathbf{N}(c_n, t_n + h)\}.
\end{aligned}}$$

FROM PAPER BY KASSAM & TREFETHEN (linked on course webpage)

PROBLEM: Roundoff in $\dfrac{e^z - 1}{z}$ (use complex contour integration)

$|z| \ll 1$