Exponential Integrators
for ODEs

Aleks Donev, Courant

In our discussion of IMEX (implicit-explicit) schemes we considered ODEs of the form (these often arise when discretizing PDEs with the "method of lines"):

$$u'(t) = A\, u(t) + B(u(t))$$

stiff linear with A constant (e.g. diffusion)

non-stiff but non-linear (e.g. advection)

(1)

If $B \equiv 0$ then $u' = Au \Rightarrow$

$$u_A(t) = e^{At} u(0)$$

Requires action of matrix exponential

For small normal A, use eigenvalue or SVD decomposition:

$$A = U \Sigma V^* \Rightarrow$$

$$\exp(A) = U \exp(\Sigma) V^*$$

scalar exponential of singular values

Trivial for diagonal A !

②

If A is large but sparse, can use Krylov / Lanczos / Arnoldi to compute $\exp(At)u$.

An example

Pseudo spectral discretization m space for KdV (homeworks 2 & 4)

$$\frac{d\hat{\varphi}}{dt} = ik^3 \boxdot \hat{\varphi} - 3ik \boxdot \mathcal{F}\left(\left(\mathcal{F}^{-1}\hat{\varphi}\right)^2\right)$$

$$= A\hat{\varphi} + B(\hat{\varphi})$$

$$A = \text{Diag}(ik^3) \quad (\text{easy!})$$

③

For more general stiff ODES,
Rosenbroch methods simply
linearize the ODE around the
current solution. Take the
general autonomous ODE:

$$u' = f(u(t))$$

$$u' = \left(\frac{\partial f}{\partial u}\right)^n (u - u^n) + f^n \quad \Big\}\begin{array}{l}\text{linear}\\\text{part}\end{array}$$

$$+ f(u) - \left[\left(\frac{\partial f}{\partial u}\right)^n (u - u^n) + f^n\right]$$

$$(\text{add and subtract}) \qquad \textcircled{4}$$

$$\Rightarrow \quad u' = A^n u + B^n(u)$$

$$A^n = \frac{\partial f}{\partial u}\bigg|_{u=u^n}$$

$$\text{Jacobian}$$

$$B^n(u) = f(u) - \left(\frac{\partial f}{\partial u}\right)^n u$$

This is an exact splitting into stiff and (hopefully!) non-stiff terms. Note that

$$\frac{\partial B}{\partial u}(u^n) = \frac{\partial f}{\partial u}\bigg|_{u^n} - A^n = 0$$

⑤

which means $B(u)$ is _almost_ _constant_ during the time step!

$$u' = Au + B(u) = f(u)$$

Variation-of-constants / Duhamel's methods + Picard iteration give:

$$u^{n+1} = \left(e^{A\Delta t}\right)u^n + \int_{t^n}^{t^{n+1}} e^{A(t_{n+1}-\tau)} B(u(\tau)) d\tau$$

↑
Exact!

Approximate integral using a quadrature rule as for RK / multistep ⑥

If $A \equiv 0$, $\exp(A \Delta t) = $ Identity,
we want to get explicit RK.
If $B \equiv 0$, we want to get
exact solution $\exp(A \Delta t) \cdot u(t)$.

For example, for RK1 (forward
Euler), approximate/extrapolate:
$$B^n(u(\tau)) \simeq B^n(u^n)$$

and we
$$\int_{t_n}^{t_{n+1}} \exp(A^n(t_{n+1} - \tau)) \, d\tau = A_n^{-1}(e^{A_n \Delta t} - I)$$

⑦

$$u^{n+1} \overset{\text{to get}}{=} e^{A_n \Delta t} u^n + A_n^{-1} \left(e^{A_n \Delta t} - I \right) B_n(u^n)$$

$\Updownarrow$

Exponetial Euler scheme:

$$u^{n+1} = u^n + (A^n)^{-1} \left(e^{A_n \Delta t} - I \right) \underbrace{f(u^n)}_{\text{r.h.s.}}$$

If $\| A_n \|_2 \Delta t \ll 1$, then

$$u^{n+1} \approx u^n + \Delta t \, f(u^n)$$

which is the usual forward Euler, with <u>bad</u> stability properties.

⑧

Local truncation error (LTE):

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

from ODE

$$= \frac{\Delta t}{2} \left(\frac{\partial f}{\partial u}(u(t_n)) - A_n \right) u'(t_n) + O(\Delta t^2)$$

$$\Rightarrow \begin{cases} \text{second-order accurate if } A_n = \left(\frac{\partial f}{\partial u} \right)^n \\ \qquad\qquad\qquad (\text{Rosenbrock}) \\[2mm] \text{first-order in general} \\ (\text{but much better than} \\ \text{standard Euler for stiff ODEs}) \end{cases}$$

(9)

this method will be accurate
if $B(u)$ varies slowly over the
time step.
Note that if $u^{n+1} = u^n$ (fixed point)
then $f^n = 0$. This means
that this method <u>can</u> be used
to quickly find stable fixed
points of ODES/PDES.
This is <u>not</u> true for another class
of "Integrating Factor" Exponential
Integrators which are used in
some fields (10)

We can improve the order of
accuracy with the same ideas
we used for RK methods;

$$u^{n+1} = \left(e^{A^n \Delta t}\right) u^n + \int_{t^n}^{t^{n+1}} e^{A^n(t_{n+1} - \bar{\tau})} B^n(u(\bar{\tau}))\, d\bar{\tau}$$

$$B^n(u(\tau)) \simeq B^n + \frac{\bar{\tau}}{\Delta t}\left(B^n - B^{n-1}\right)$$

Now do the integral (assume
A is normal & diagonalize it)

$\textcircled{11}$

Exponential Time Differencing ETD2:

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

$$+ \underbrace{\frac{A_n^{-2}}{\Delta t}(e^{A_n \Delta t} - I - A_n \Delta t)(B^n - B^{n-1})}_{O(\Delta t^2) \; 2^{nd} \text{ order correction}}$$

This is an exponential multistep scheme (two step like AB2)

Excercise: Show that as $A \Delta t \rightarrow 0$ this becomes Adams-Bashforth 2

(12)

If we want an RK2 scheme instead, say explicit midpoint:

① Midpoint ETDRK1 (exponential Euler) predictor step:

$$u^{n+1/2,*} = \left(e^{A_n \Delta t/2}\right)u^n + A_n^{-1}\left(e^{A_n \Delta t/2} - I\right)B^n$$

② ETDRK2   corrector:

$$u^{n+1} = \left(e^{A_n \Delta t}\right)u_n + A_n^{-1}\left(e^{A_n \Delta t} - I\right)B^n$$

$$+ 2A_n^{-2}\left(\frac{e^{A_n \Delta t} - I - A_n \Delta t}{\Delta t}\right)\underbrace{}_{ETD2}\left(B^{n+1/2,*} - B^n\right)$$

⑬

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:

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

FROM PAPER BY $\mathbb{K}$ ASSAM & TREFETHEN (linked on course webpage)

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