Exponential time integration ①

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When dealing with PDEs, we often arrive at ODE systems of the following form:

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

A: Stiff but linear part

B: (hopefully) non-stiff but non-linear part

If $B \equiv 0$ then

$$u'(t) = Au(t)$$

with constant A can be solved exactly

$$\boxed{\underset{A}{u}(t) = e^{At}\, u(0)}$$

Matrix exponential

We need a matrix-vector product between matrix exponential and a vector of initial conditions.

For sparse A, this can be computed using iterative Krylov methods.

If <u>A is diagonal</u>, then

$$e^{At} = \mathrm{Diag}\{e^{a_{ii}t}\}$$

is trivial to evaluate.

If A is diagonalizable (normal)

$$A = X \Lambda X^{-1}$$

then

$$e^{At} = X \,\mathrm{Diag}\{e^{\lambda_{ii}t}\}\, X^{-1}$$

$$\boxed{e^{At} = X e^{\Lambda t} X^{-1}}$$

As an example, consider the pseudospectral discretization of the KdV equation we discussed earlier (HW2) (4)

$$\frac{d\hat{\varphi}}{dt} = \underbrace{i k^3 \boxed{\cdot}\, \hat{\varphi}} - \underbrace{3 i \vec{k} \boxed{\cdot}\, \mathcal{F}\left(\left(\mathcal{F}^{-1} \hat{\varphi} \right)^{\boxed{2}}\right)}$$

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

where $A = \mathrm{Diag}\{ i k^3 \}$

so the linear part can be integrated exactly <u>trivially</u> using an <u>exponential method</u>.

In other cases, we can linearize the ODE around the current solution to get: (5)

Timestep between t and $t+\Delta t$:

$$u' = f(u(t)) \quad \text{(autonomous)}$$

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

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

(just add and subtract linear part)

This leads to

$$u' = A^n u + B^n(u)$$

where $A^n = \frac{\partial f}{\partial u}(u = u^n)$ (Jacobian)

This approach goes under the name of <u>Rosenbrock methods</u>

(can be used with RK, exponential, etc.)

These are often simpler <u>or</u> more accurate than methods that fix A to be constant, as we will see soon.

$$\boxed{u' = Au + B(u) = f(u)}$$ 7

Duhamel's principle

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

Once we somehow approximate the integral we get an <u>exponential method</u>

We do this by using some <u>quadrature</u> rule for the integral similar to what we do for Runge-Kutta.

This way if $A=0$ we get an RK scheme we know and like

Approximate $B^n(u(\tau)) \simeq B^n(u^n)$ (8)

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

Elliptic solve if
A_n 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

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

$$= \frac{\Delta t}{2} \underbrace{\left(f'(u(t_n)) - A_n \right)} u'(t_n)$$

If A_n is Jacobian
then this is ___zero___!
(but must be invertible)

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

$$u^{n+1} = u^n + (A^n)^{-1}\left[e^{A^n \Delta t} - I\right] f^n \qquad (10)$$

is the <u>exponential Euler method</u>

<u>Observations</u>

1. If $B=0$ this is an <u>exact</u> integrator: Δt can be as large as you want without stability issues

2. First order in general but Second order as Rosenbrock

3. Accurate if $B(u)$ <u>varies slowly</u>

4. Fixed point $u^{n+1} = u^n$ is <u>same as ODE</u>: $f^n = 0$

One can derive higher order multistep or RK schemes. (11)

For example, if we extrapolate $B(u)$ from the past linearly

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

and we perform the integral we get a second-order ETD2:

$$\boxed{\begin{aligned} u^{n+1} &= e^{A^n \Delta t} u^n + A_n^{-1}\left(e^{A_n \Delta t} - I\right) B^n \\ &\quad + \frac{A_n^{-2}}{\Delta t}\left(e^{A_n \Delta t} - I - A_n \Delta t\right)\left(B^n - B^{n-1}\right) \end{aligned}}$$

One can also construct RK schemes, for example, an explicit midpoint based scheme (ETDRK2): (12)

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

(step to midpoint)

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

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

ETDRK is usually better than multistep

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: 13

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

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

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

$|z| \ll 1$