Exponential Time Differencing and Lie-Group Methods for Stiff Problems

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Introduction

Consider partial differential equation of the form

$$u_t = \mathcal{L}u + \mathcal{N}(u, t)$$

where $\mathcal{L}$ is a higher-order linear term and $\mathcal{N}$ is low-order nonlinear term.

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After discretization in space we obtain a systems of ODEs

$$\dot{u} = \mathbf{L}u + \mathbf{N}(u, t)$$

Basic methods

- $LI = Linearly\ Implicit$ Use an explicit multi-step formula to advance the nonlinear part and implicit scheme to advance the linear part (Ascher, Ruuth and Wetton '95).

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- $SS = Split\ Step$ Write the solution in the form

$$u(t) \approx exp(c_1 t\mathbf{L})F(d_1 t\mathbf{N})exp(c_2 t\mathbf{L})F(d_2 t\mathbf{N}) \cdots exp(c_k t\mathbf{L})F(d_1 k\mathbf{N})u(0),$$

where c_i and d_i are constants (Sanz-Serna and Calvo '94, Boyd '01).

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where c_i and d_i are constants (Sanz-Serna and Calvo '94, Boyd '01).

- $SL = Sliders$ Extent ion of LI, split the linear part into three regions (low, medium and high), (Fornberg and Driscoll '99)

Basic methods

- $IF = Integrating\ Factor$ Make a change of variable then solve exactly for the linear part and use the numerical scheme for the transformed nonlinear equation (Mayday, Patera, Rønquist '90, Milewski and Tabak '99, Trefethen '00, Krogstad '03).

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$$v = exp(-\mathbf{L}t)u$$

$$\underbrace{exp(-\mathbf{L}t)u_t - \mathbf{L}u}_{v_t} = exp(-\mathbf{L}t)\mathbf{N}(u)$$

$$v_t = exp(-\mathbf{L}t)\mathbf{N}(exp(\mathbf{L}t)v)$$

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$$v_t = exp(-\mathbf{L}t)\mathbf{N}(exp(\mathbf{L}t)v)$$

- $ETD = Exponential\ Time\ Differencing$

Exponential Time Differencing

$$
(1) \qquad \left|
\begin{aligned}
\dot{u} &= \mathbf{L}u + \mathbf{N}(u(t), t) \\
u(t_0) &= u_0
\end{aligned}
\right.
$$

Use the same integrating factor like in IF

$$
\frac{d}{dt}(exp(-\mathbf{L}t)u) = exp(-\mathbf{L}t)\mathbf{N}(u(t))
$$

Exponential Time Differencing

$$(1) \qquad \begin{vmatrix} \dot{u} & = & \mathbf{L}u + \mathbf{N}(u(t), t) \\ \\ u(t_0) & = & u_0 \end{vmatrix}$$

Use the same integrating factor like in IF

$$\frac{d}{dt}(exp(-\mathbf{L}t)u) = exp(-\mathbf{L}t)\mathbf{N}(u(t))$$

Integrate over a single time step of length h

$$u_{n+1} = exp(\mathbf{L}h)u_n + exp(\mathbf{L}h)\int_0^h exp(-\mathbf{L}\tau)\mathbf{N}(u(t_n + \tau), t_n + \tau)d\tau$$

ETD (1/2)

- $\mathbf{N}(u(t), t) = \text{constant}$

ETD1: $u_{n+1} = exp(\mathbf{L}h)u_n + \mathbf{L}^{-1}\mathbf{N}_n(exp(\mathbf{L}h) - \mathbf{I})$, where $\mathbf{N}_n = \mathbf{N}(u_n, t_n)$

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- $\mathbf{N}(u(\tau), \tau) = \mathbf{N}_n + \frac{\tau}{h}(\mathbf{N}_n - \mathbf{N}_{n-1})$

  ETD2:
  $$\begin{aligned} u_{n+1} &= exp(\mathbf{L}h)u_n + h^{-1}\mathbf{L}^{-2}\mathbf{N}_n(exp(\mathbf{L}h)(I + \mathbf{L}h) - 2\mathbf{L}h - \mathbf{I}) \\ &+ h^{-1}\mathbf{L}^{-2}\mathbf{N}_{n-1}(-exp(\mathbf{L}h) + \mathbf{L}h + \mathbf{I}) \end{aligned}$$

ETD (1/2)

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- In general

  ETDs: $u_{n+1} = exp(\mathbf{L}h)u_n + h\sum_{m=0}^{s-1} g_m \sum_{k=0}^{m}(-1)^k \binom{m}{k}\mathbf{N}_{n-k}$, where g_m are given by

  $$\mathbf{L}hg_0 = exp(\mathbf{L}h) - \mathbf{I}$$
  $$\mathbf{L}hg_{m+1} + \mathbf{I} = g_m + \frac{1}{2}g_{m-1} + \frac{1}{3}g_{m-2} + \cdots + \frac{g_0}{m+1}, \quad m \geq 0.$$

ETD (2/2)

Another way of producing the same formulas (Krogstad '03)

Lemma 1 *Let* $\mathbf{N}_k = \left. \dfrac{d^k}{dt^k} \right|_{t=t_0} \mathbf{N}(u(t), t)$ *then the solution* $u(t)$ *of (1) is*

$$u(t_0 + h) = exp(\mathbf{L}h)u_0 + \sum_{k=0}^{\infty} t^{k+1}\phi_k(t\mathbf{L})\mathbf{N}_k,$$

where

$$\phi_0(z) = \frac{exp(z) - 1}{z}, \qquad \phi_{k+1}(z) = \frac{\phi_k(z) - \phi_k(0)}{z}, \qquad k = 1, 2, \ldots$$

Lie-group Methods

- *Crouch and Grossman Methods*

Lie-group Methods

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- *Munthe − Kaas Methods*

Lie-group Methods

- *Crouch and Grossman Methods*

- *Munthe − Kaas Methods*

- *Commutator − free Lie − Group Methods*

Algorithm (CF)

for $r = 1 : s$ do

$$Y_r = Exp(\textstyle\sum_k \alpha^k_{r,J} F_k) \cdots Exp(\textstyle\sum_k \alpha^k_{r,1} F_k)(p)$$

$$F_r = hF_{Y_r} = h \textstyle\sum_i f_i(Y_r) E_i$$

end

$$y_1 = Exp(\textstyle\sum_k \beta^k_J F_k) \cdots Exp(\textstyle\sum_k \beta^k_1 F_k) p$$

ETD1 and Lie-group Integrators

We can rewrite the equation (1) in the form

$$
\left|
\begin{array}{l}
\dot{u} \;=\; (\mathbf{L}, \mathbf{N}(u,t)).u \;=\; F_{u,t}(u) \\
u(0) = u_0
\end{array}
\right.
$$

where . represents the *Lie algebra action*

$$
(\mathbf{A}, a).u \;=\; \mathbf{A}u + a
$$

ETD1 and Lie-group Integrators

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where . represents the *Lie algebra action*

$$(\mathbf{A}, a).u \;=\; \mathbf{A}u + a$$

Let $F_{\hat{u},\hat{t}}(u)$ be the *Frozen Vector Field* at the point $(\hat{u}, \hat{t})$

$$F_{\hat{u},\hat{t}}(u) \;=\; (\mathbf{L}, \mathbf{N}(\hat{u}, \hat{t})).u \;=\; \mathbf{L}u + \mathbf{N}(\hat{u}, \hat{t})$$

ETD1 and Lie-group Integrators

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$$F_{\hat{u},\hat{t}}(u) \;=\; (\mathbf{L}, \mathbf{N}(\hat{u}, \hat{t})).u \;=\; \mathbf{L}u + \mathbf{N}(\hat{u}, \hat{t})$$

The flow of such vector field is the solution of $\dot{u} \;=\; F_{\hat{u},\hat{t}}(u), \quad u(0) = u_0$

$$Exp(tF_{\hat{u},\hat{t}}).u_0 \;=\; exp(t\mathbf{L})u_0 + t\phi_0(t\mathbf{L})\mathbf{N}(\hat{u}, \hat{t})$$

ETD2 and Lie-group Integrators (1/3)

We can rewrite the equation (1) in the form

$$
\dot{y} = (\mathbf{A}_{u,t}, a).y = \tilde{F}_{u,t}(y)
$$
$$
y(0) = y_0
$$

where

$$
\mathbf{A}_{u,t} = \begin{pmatrix} \mathbf{L} & \frac{\mathbf{N}(u,t)-\mathbf{N}_0}{t} \\ & \\ 0 & 0 \end{pmatrix}, \quad a = \begin{pmatrix} \mathbf{N}_0 \\ \\ 1 \end{pmatrix},
$$

$$
y = \begin{pmatrix} u \\ \\ v \end{pmatrix}, \quad y_0 = \begin{pmatrix} u_0 \\ \\ 0 \end{pmatrix}, \quad \mathbf{N}_0 = \mathbf{N}(u_0, 0)
$$

ETD2 and Lie-group Integrators (2/3)

Let $\tilde{F}_{\hat{u},\hat{t}}(y)$ be the *Frozen Vector Field* at the point $(\hat{u}, \hat{t})$

$$\tilde{F}_{\hat{u},\hat{t}}(u) \;=\; (\mathbf{A}_{\hat{u},\hat{t}}, a).y \;=\; \mathbf{A}_{\hat{u},\hat{t}}\, y + a,$$

where

$$\mathbf{A}_{\hat{u},\hat{t}} \;=\; \begin{pmatrix} \mathbf{L} & \dfrac{\hat{\mathbf{N}} - \mathbf{N}_0}{\hat{t}} \\[2em] 0 & 0 \end{pmatrix}, \quad \hat{\mathbf{N}} \;=\; \mathbf{N}(\hat{u}, \hat{t})$$

ETD2 and Lie-group Integrators (2/3)

Let $\tilde{F}_{\hat{u},\hat{t}}(y)$ be the *Frozen Vector Field* at the point $(\hat{u}, \hat{t})$

$$\tilde{F}_{\hat{u},\hat{t}}(u) = (\mathbf{A}_{\hat{u},\hat{t}}, a).y = \mathbf{A}_{\hat{u},\hat{t}} \, y + a,$$

where

$$\mathbf{A}_{\hat{u},\hat{t}} = \begin{pmatrix} \mathbf{L} & \frac{\hat{\mathbf{N}} - \mathbf{N}_0}{\hat{t}} \\ & \\ 0 & 0 \end{pmatrix}, \quad \hat{\mathbf{N}} = \mathbf{N}(\hat{u}, \hat{t})$$

The flow of such vector field is the solution of $\dot{y} = \tilde{F}_{\hat{u},\hat{t}}(y), \quad y(0) = y_0$

$$Exp(t\tilde{F}_{\hat{u},\hat{t}}).y_0 = \begin{pmatrix} exp(t\mathbf{L})u_0 + t\phi_0(t\mathbf{L})\mathbf{N}_0 + t^2\phi_1(t\mathbf{L})\frac{\hat{\mathbf{N}} - \mathbf{N}_0}{\hat{t}} \\ t \end{pmatrix}$$

ETD2 and Lie-group Integrators (3/3)

The commutator between two vector fields is

$$[(A, a).u \, , \, (B, b).u] \; = \; (C, c).u,$$

where $\; C = [A, B], \quad c = (Ab - Ba)$

3th order RK schemes

- Classical third-order RK method:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2} & & \\
1 & -1 & 2 & \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

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\hline
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\end{array}
$$

- ETDRK3: (Cox & Matthews)

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0 & & \\
1 & -\phi_0 & 2\phi_0 & \\
\hline
 & 4\phi_2 - 3\phi_1 + \phi_0 & -8\phi_2 + 4\phi_1 & 4\phi_2 - \phi_1
\end{array}
$$

3th **order CF schemes**

- CF3: (Celledoni, Martinsen, Owren)

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{3} & \frac{1}{3} & & \\
\frac{2}{3} & 0 & \frac{2}{3} & \\
\hline
& \frac{1}{3} & & \\
& -\frac{1}{12} & \frac{3}{4} &
\end{array}
$$

3th **order CF schemes**

- CF3: (Celledoni, Martinsen, Owren)

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\begin{array}{c|ccc}
0 & & & \\
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\hline
 & \frac{1}{3} & & \\
 & -\frac{1}{12} & \frac{3}{4} &
\end{array}
$$

- ETDCF3:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{3} & \frac{1}{3}\phi_0 & & \\
\frac{2}{3} & 0 & \frac{2}{3}\phi_0 & \\
\hline
 & \frac{1}{3}\phi_0 & & \\
 & -\frac{1}{12}\phi_0 & \frac{3}{4}\phi_0 &
\end{array}
$$

3th **order schemes and ETD2**

- ETD2RK3:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0 & & \\
1 & \phi_0 - 4\phi_1 & 4\phi_1 & \\
\hline
& 4\phi_2 - 3\phi_1 + \phi_0 & -8\phi_2 + 4\phi_1 & 4\phi_2 - \phi_1
\end{array}
$$

3th order schemes and ETD2

- ETD2RK3:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0 & & \\
1 & \phi_0 - 4\phi_1 & 4\phi_1 & \\
\hline
 & 4\phi_2 - 3\phi_1 + \phi_0 & -8\phi_2 + 4\phi_1 & 4\phi_2 - \phi_1
\end{array}
$$

- ETD2CF3:

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{3} & \frac{1}{3}\phi_0 & & \\
\frac{2}{3} & \frac{2}{3}\phi_0 - \frac{4}{3}\phi_1 & \frac{4}{3}\phi_1 & \\
\hline
 & 9\phi_2 - \frac{9}{2}\phi_1 + \phi_0 & -18\phi_2 + 6\phi_1 & 9\phi_2 - \frac{3}{2}\phi_1
\end{array}
$$

4th order schemes (1/4)

CF4:

(Celledoni, Martinsen, Owren)

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & \\
\frac{1}{2} & -\frac{1}{2} & 0 & 1 & \\
\hline
 & \frac{1}{4} & \frac{1}{6} & \frac{1}{6} & -\frac{1}{12} \\
 & -\frac{1}{12} & \frac{1}{6} & \frac{1}{6} & \frac{1}{4}
\end{array}
$$

4th order schemes (2/4)

ETDRK4:

(Krogstad)

$$
\begin{array}{c|cccc}
0 & & & & \\[4pt]
\frac{1}{2} & \frac{1}{2}\phi_0 & & & \\[4pt]
\frac{1}{2} & 0 & \frac{1}{2}\phi_0 & & \\[4pt]
\frac{1}{2} & \frac{1}{2}\phi_0 & 0 & 0 & \\[4pt]
\frac{1}{2} & -\frac{1}{2}\phi_0 & 0 & \phi_0 & \\[4pt]
\hline
& 4\phi_2 - 3\phi_1 + \phi_0 & -4\phi_2 + 2\phi_1 & -4\phi_2 + 2\phi_1 & 4\phi_2 - \phi_1
\end{array}
$$

4th order schemes (3/4)

ETDRK4B:

(Krogstad)

$$
\begin{array}{c|cccc}
0 & & & & \\[2mm]
\frac{1}{2} & \frac{1}{2}\phi_0 & & & \\[2mm]
\frac{1}{2} & \frac{1}{2}\phi_0 - \phi_1 & \phi_0 & & \\[2mm]
1 & \phi_0 - 2\phi_1 & 0 & 2\phi_1 & \\[2mm]
\hline
& 4\phi_2 - 3\phi_1 + \phi_0 & -4\phi_2 + 2\phi_1 & -4\phi_2 + 2\phi_1 & 4\phi_2 - \phi_1
\end{array}
$$

4th order schemes (3/4)

ETDCF4:

$$
\begin{array}{c|cccc}
0 & & & & \\[4pt]
\frac{1}{2} & \frac{1}{2}\phi_0 & & & \\[4pt]
\frac{1}{2} & 0 & \frac{1}{2}\phi_0 & & \\[4pt]
\frac{1}{2} & \frac{1}{2}\phi_0 & 0 & 0 & \\[4pt]
\frac{1}{2} & -\frac{1}{2}\phi_0 & 0 & \phi_0 & \\[6pt]
\hline
& \frac{1}{4}\phi_0 & \frac{1}{6}\phi_0 & \frac{1}{6}\phi_0 & -\frac{1}{12}\phi_0 \\[6pt]
& -\frac{1}{12}\phi_0 & \frac{1}{6}\phi_0 & \frac{1}{6}\phi_0 & \frac{1}{4}\phi_0
\end{array}
$$

Stability

We consider the model equation

$$\left|\begin{array}{rcl} \dot{u} &=& cu + \lambda u \\ u(0) &=& 1 \end{array}\right.$$

where c and λ are scalars

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$$\begin{aligned} \dot{u} &= cu + \lambda u \\ u(0) &= 1 \end{aligned}$$

where c and λ are scalars

For computing the ϕ_i functions we use the approach suggested by Kassam and Trefethen

$$\phi_i(\mathbf{L}) \;=\; \frac{1}{2\pi i} \int_\Gamma \phi_i(t)(t\mathbf{I} - \mathbf{L})^{-1}\, dt,$$

where Γ is a contour well separated from 0

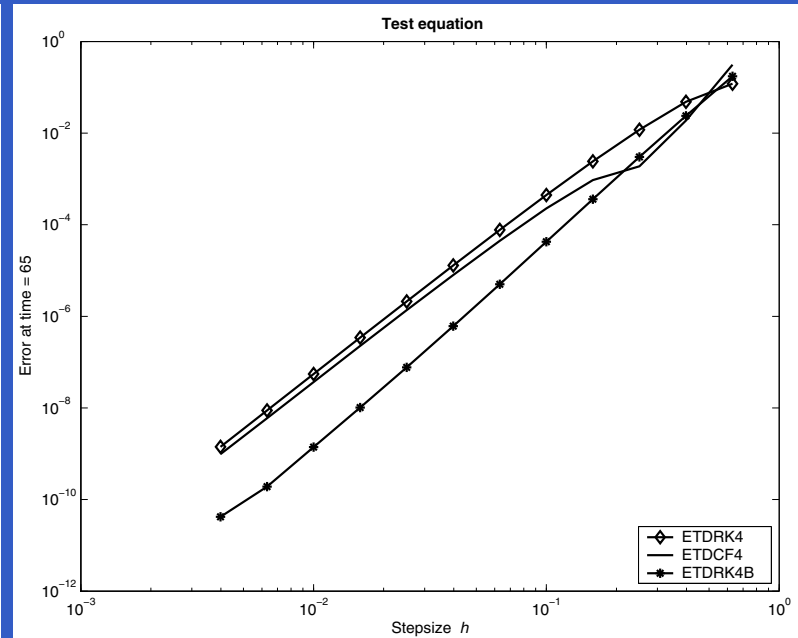# Stability regions for 3th order schemes

Stability region for ETDRK3

Stability region for ETD2RK3
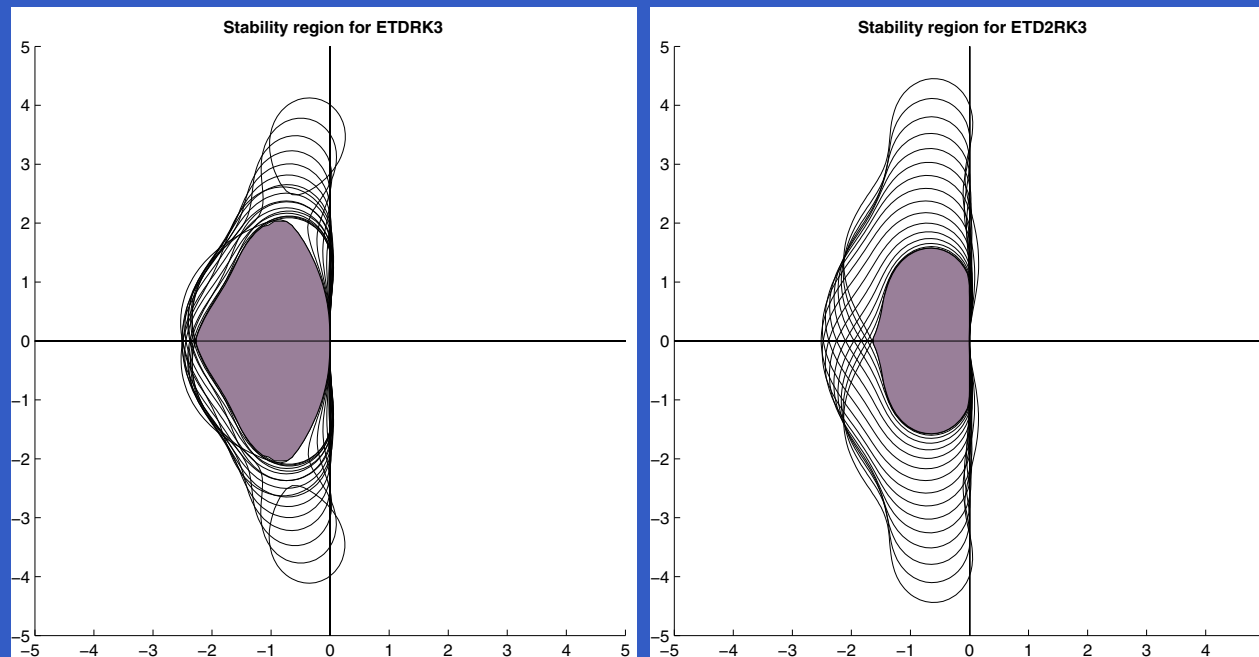
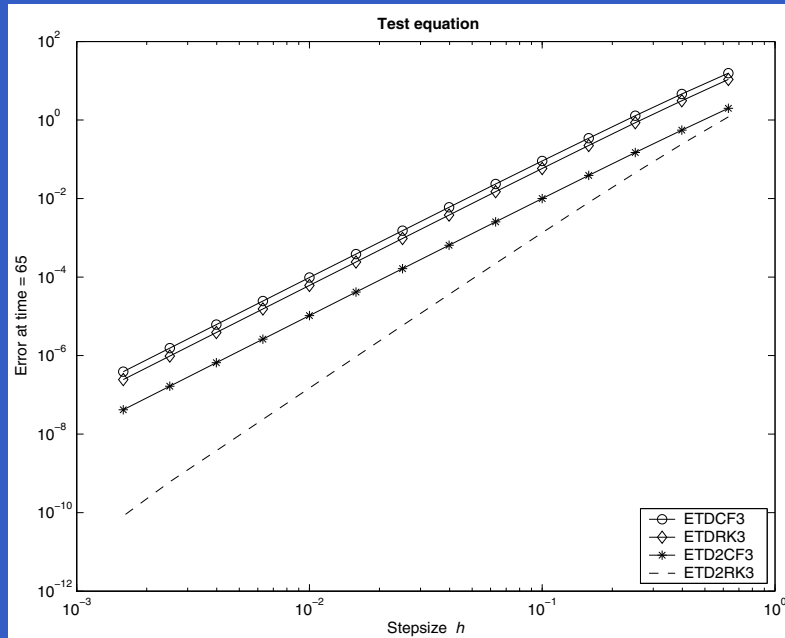# Stability regions for 4th order schemes
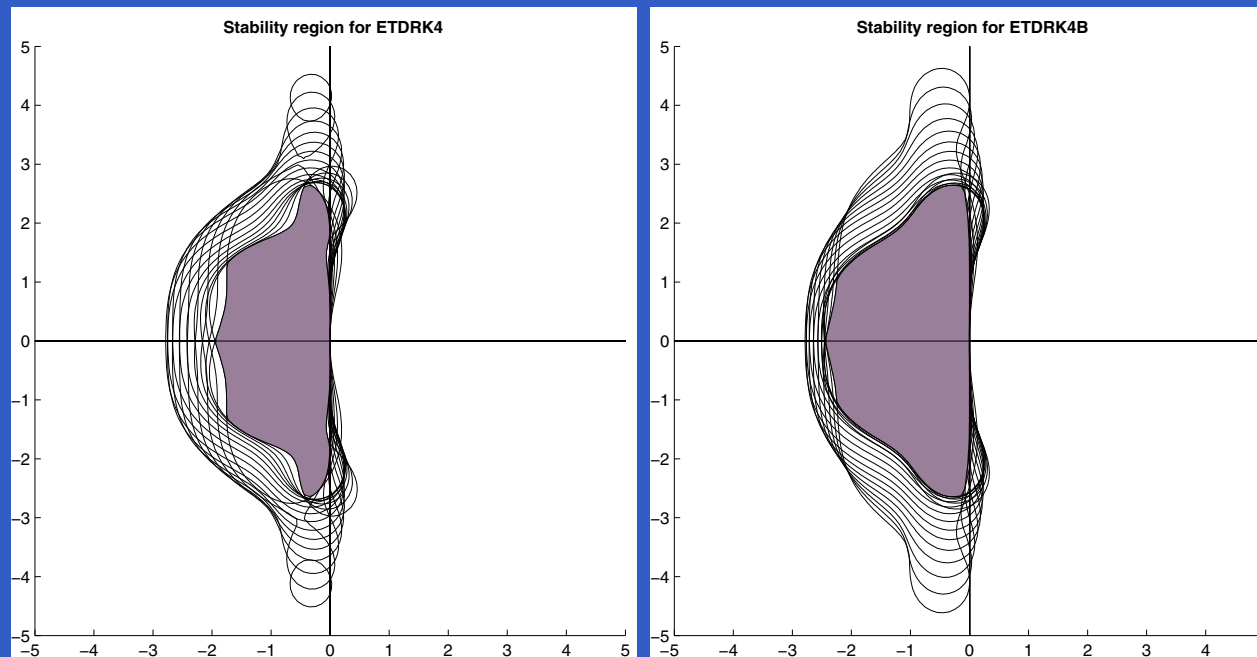
Numerical experiments

Example 1: Test equation

$$
\left|
\begin{aligned}
\dot{u} &= -1.5u + 2t^2 - t + u \\
u(0) &= 2
\end{aligned}
\right.
$$

$L = -1.5$ and $N = 2t^2 - t + u$

Test equation

# Numerical experiments

Example 2:   Kuramoto-Sivashinsky equation

$$
\left|
\begin{aligned}
u_t &= -uu_x - u_{xx} - u_{xxxx} \quad x \in [0, 32\pi] \\
u(x,0) &= cos(\tfrac{x}{16})(1 + sin(\tfrac{x}{16}))
\end{aligned}
\right.
$$

Numerical experiments

Example 2:   Kuramoto-Sivashinsky equation

$$
\begin{vmatrix}
u_t & = & -uu_x - u_{xx} - u_{xxxx} & x \in [0, 32\pi] \\
u(x,0) & = & cos(\frac{x}{16})(1 + sin(\frac{x}{16}))
\end{vmatrix}
$$

We discretise the spatial part using Fourier spectral method. The transformed equation

in the Fourier space is

$$
\hat{u}_t = -\frac{ik}{a}\hat{u}^2 + (k^2 - k)\hat{u},
$$

$(\mathbf{L}\hat{u})(k) = (k^2 - k^4)\hat{u}(k)$ and $\mathbf{N}(\hat{u}, t) = -\frac{ik}{2}(F((F^{-1}(\hat{u}))^2))$

Kuramoto-Sivashinsky equation
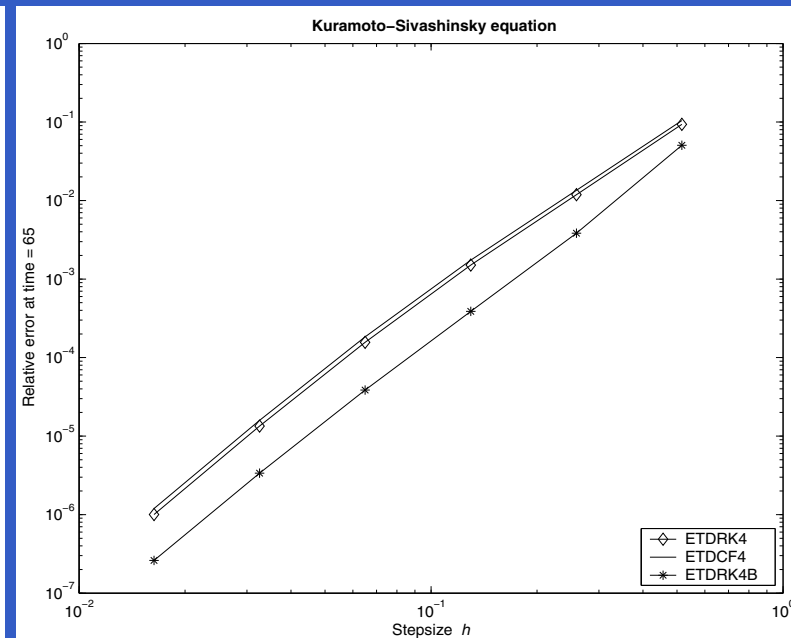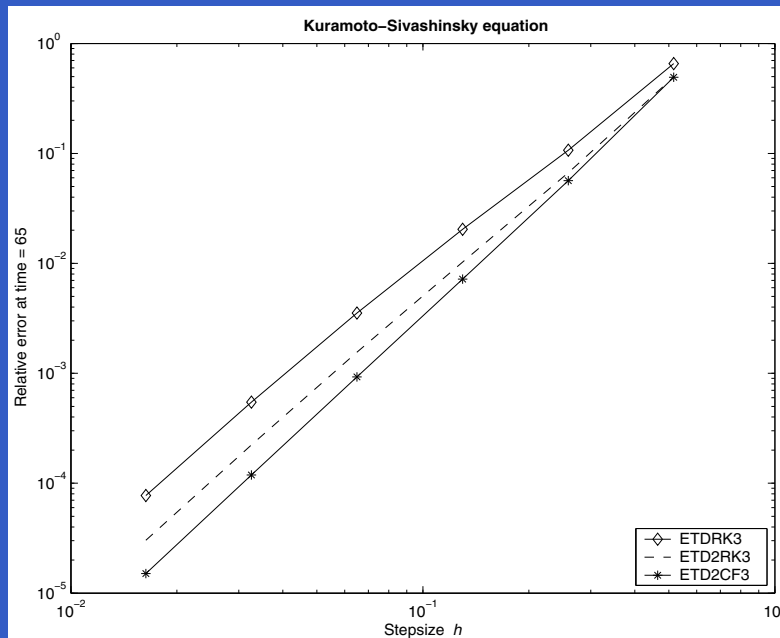
Conclusion

- We present a constructive way of generating exponential time differencing Runge-Kutta (ETDRK) methods from Lie group methods. In particular we show how to choose the algebra action in order to recover the classical ETD and ETDRK methods.

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- Better stability properties

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- We present a constructive way of generating exponential time differencing Runge-Kutta (ETDRK) methods from Lie group methods. In particular we show how to choose the algebra action in order to recover the classical ETD and ETDRK methods.

- We discuss how to choose the frozen vector field in order to receive better approximation of the nonlinear part.

- Better stability properties

- The above approach can be successfully applied when the nonlinear part of the system is periodic.

References

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