Exponential Integrators and Lie group methods

Workshop on Exponential Integrators

October 20-23, 2004, Innsbruck.

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Outline

- The framework
- The choice of action
- LGI for semilinear problems
- Implementation issues
- Numerical experiments
- Conclusions
- Future work

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Lie group methods

- Designed to preserve certain qualitatively properties of the exact flow

Exp. int. and Lie group methods

Lie group methods

- Designed to preserve certain qualitatively properties of the exact flow
- The freedom in the choice of the action allows to define the basic motions on the manifold in such a way that they provide a good approximation to the flow of the original vector field.

Background theory

Lie group - $(\mathcal{G}, e, \star)$
Lie algebra $\mathfrak{g} = T_e\mathcal{G}$ - linear space with bracket

$$[\Theta_1, \Theta_2] = \left.\frac{\partial^2}{\partial s \partial t}\right|_{t=s=0} \gamma_1(s) \star \gamma_2(t) \star \gamma_1(s)^{-1},$$

where $\gamma_1(s)$ and $\gamma_2(t)$ are smooth curves in $\mathcal{G}$ such that $\gamma_1(0) = \gamma_2(0) = e$ and $\gamma_1'(0) = \Theta_1,\ \gamma_2'(0) = \Theta_2$.

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Define the product $\odot : \mathfrak{g} \times \mathcal{G} \to T\mathcal{G}$ by

$$\Theta \odot g = \left.\frac{d}{dt}\right|_{t=0} \gamma(t) \star g,$$

where $\gamma(t)$ is a smooth curve in $\mathcal{G}$ such that $\gamma(0) = e$ and $\gamma'(0) = \Theta$.

The Exp map

The exponential map provides connection between $\mathcal{G}$ and $\mathfrak{g}$.
Exp : $\mathfrak{g} \to \mathcal{G}$ is defined as Exp$(\Theta) = \gamma(1)$, where $\gamma(t) \in \mathcal{G}$ satisfies the differential equation

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The differential of the exponential map dExp : $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ is defined as the right trivialized tangent

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$$\begin{aligned} \mathrm{dExp}_{\widehat{\Theta}}(\Theta) &= \left.\frac{\mathrm{e}^z - 1}{z}\right|_{z=\mathrm{ad}_{\widehat{\Theta}}(\Theta)} = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}^k_{\widehat{\Theta}}(\Theta), \\ \mathrm{dExp}^{-1}_{\widehat{\Theta}}(\Theta) &= \left.\frac{z}{\mathrm{e}^z - 1}\right|_{z=\mathrm{ad}_{\widehat{\Theta}}(\Theta)} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k_{\widehat{\Theta}}(\Theta), \end{aligned}$$

where the coefficients B_k are the Bernoulli numbers and

$$\mathrm{ad}^k_{\widehat{\Theta}}(\Theta) = \mathrm{ad}_{\widehat{\Theta}}(\mathrm{ad}^{k-1}_{\widehat{\Theta}}\Theta) = [\widehat{\Theta}, [\ldots, [\widehat{\Theta}, \Theta]]], \quad \text{for } k > 1.$$

Actions on the manifold

A group action on a manifold $\mathcal{M}$ is a smooth map $\cdot : \mathcal{G} \times \mathcal{M} \to \mathcal{M}$ satisfying

$$\begin{aligned} e \cdot p &= p \quad \forall\, p \in \mathcal{M}, \\ g \cdot (k \cdot p) &= (g \star k) \cdot p \quad \forall\, g, k \in \mathcal{G},\ p \in \mathcal{M}. \end{aligned}$$

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Note: The algebra action is not uniquely determined by the group action. Every diffeomorphism

$$\Psi : \mathfrak{g} \to \mathcal{G},$$

such that $\Psi(0) = e$ and $\Psi'(0) = I$, where I is the identity of the algebra, defines an algebra action by the formula $\Theta * p = \Psi(\Theta) \cdot p$.

Generic presentation of a diff. eq.

The product $\circledast : \mathfrak{g} \times \mathcal{M} \to T\mathcal{M}$ between $\mathfrak{g}$ and $\mathcal{M}$ is defined by

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For a fix $\Theta \in \mathfrak{g}$ the product $\Theta \circledast p$ gives a vector field on $\mathcal{M}$

$$\mathcal{F}_\Theta(p) = \Theta \circledast p = \left.\frac{d}{dt}\right|_{t=0} \mathrm{Exp}(t\Theta) \cdot p.$$

The vector field $\mathcal{F}_\Theta$ is called a frozen vector field.

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Every differential equation evolving on a homogeneous space $\mathcal{M}$ can always be written as

$$u'(t) = F(u) \circledast u, \qquad u(t_0) = u_0,$$

where $F : \mathcal{M} \to \mathfrak{g}$.

Lie group integrators

Algotithm. *(Crouch–Grossman'93)*

for $i = 1, \ldots, s$ **do**

$$U_i = \mathit{Exp}(h\alpha_{is}F_s)\cdots \mathit{Exp}(h\alpha_{i1}F_1)\cdot u_n$$
$$F_i = F(U_i)$$

end

$$u_{n+1} = \mathit{Exp}(h\beta_s F_s)\cdots \mathit{Exp}(h\beta_1 F_1)\cdot u_n$$

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Algotithm. *(Runge–Kutta Munthe-Kaas'99)*

for $i = 1, \dots, s$ **do**

$$\Theta_i = h \sum_{j=1}^{s} \alpha_{ij} K_j$$
$$F_i = F(\Psi(\Theta_i) \cdot u_n)$$
$$K_i = d\Psi^{-1}(F_i)$$

end

$$u_{n+1} = \Psi(h \sum_{i=1}^{s} \beta_i K_i) \cdot u_n$$

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The values on $\mathcal{M}$ can be computed via the formula $U_i = \Theta_i * u_n$.

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for $i = 1, \ldots, s$ **do**

$$U_i = \mathit{Exp}(h \sum_{k=1}^{s} \alpha_{iJ}^{k} F_k) \cdots \mathit{Exp}(h \sum_{k=1}^{s} \alpha_{i1}^{k} F_k) \cdot u_n$$
$$F_i = F(U_i)$$

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$$u_{n+1} = \mathit{Exp}(h \sum_{k=1}^{s} \beta_J^k F_k) \cdots \mathit{Exp}(h \sum_{k=1}^{s} \beta_1^k F_k) \cdot u_n$$

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An example of a fourth order method, based on the classical fourth order Runge–Kutta method

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

Basic motions on $\mathcal{M}$

Consider the following nonautonomous problem defined on $\mathbb{R}^d$

$$u' = f(u,t), \qquad u(t_0) = u_0.$$

By adding the trivial differential equation $t' = 1$, we can rewrite it in the form

$$y' = \mathsf{f}(y(t)), \qquad y(t_0) = y_0,$$

where

$$\mathsf{f} = \begin{bmatrix} f(u,t) \\ 1 \end{bmatrix}, \quad y = \begin{bmatrix} u \\ t \end{bmatrix}.$$

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Define:

- the basic movements on $\mathcal{M}$ to be given by the solution of a simpler diff. equation

$$y' = \mathcal{F}_\Theta(y), \qquad y(t_0) = y_0, \tag{2}$$

where $\mathcal{F}_\Theta(y)$ approximates $\mathsf{f}(y(t))$.

- the Lie algebra $\mathfrak{g}$ to be the set of all coefficients Θ of the *frozen* vector fields $\mathcal{F}_\Theta$.
- the algebra action $h\Theta * y_0$ to be the solution of (2) at time $t_0 + h$.

The choice of action

- The simplest case
  - $\mathfrak{g} = \{\mathrm{b} \in \mathbb{R}^{d+1}\} = \{(b^{[0]}, \lambda) : b^{[0]} \in \mathbb{R}^d, \lambda \in \mathbb{R}\}$.
  - The generic function is given by $F\left(\begin{bmatrix} u_0 \\ t_0 \end{bmatrix}\right) = (f(u_0, t_0), 1) = (b^{[0]}, 1)$.
  - The frozen vector field is $\mathcal{F}_{(b^{[0]},\lambda)}\left(\begin{bmatrix} u \\ t \end{bmatrix}\right) = \begin{bmatrix} b^{[0]} \\ \lambda \end{bmatrix}$.
  - The algebra action is $h(b^{[0]}, \lambda) * \begin{bmatrix} u_0 \\ t_0 \end{bmatrix} = \begin{bmatrix} u_0 + hb^{[0]} \\ t_0 + h\lambda \end{bmatrix}$ (translations).
  - The commutators are given by $[\Theta_1, \Theta_2] = (0, 0)$.

  In this case we recover the traditional integration schemes.

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- When $f(u,t) = L(u,t)u + N(u,t)$ (such a representation is always possible)
  - $\mathfrak{g} = \{(\mathsf{A}, \mathsf{b}) \in \mathbb{R}^{d+1 \times d+1} \rtimes \mathbb{R}^{d+1}\}$, with

$$\mathsf{A} = \begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathsf{b} = \begin{bmatrix} b^{[0]} \\ \lambda \end{bmatrix},$$

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  - The frozen vector field is $\mathcal{F}_{(A,b^{[0]},\lambda)}\left(\begin{bmatrix} u \\ t \end{bmatrix}\right) = \begin{bmatrix} Au + b^{[0]} \\ \lambda \end{bmatrix}$.
  - The algebra action is given by $h(A, b^{[0]}, \lambda) * \begin{bmatrix} u_0 \\ t_0 \end{bmatrix} = \begin{bmatrix} e^{hA} u_0 + hb^{[0]} \phi^{[1]}(hA) \\ t_0 + h\lambda \end{bmatrix}$,
    where e^{hA} denotes the matrix exponential and $\phi^{[1]}$ is the first ETD $\phi^{[i]}$ function.
  - The commutators are given by $[\Theta_1, \Theta_2] = (A_1A_2 - A_2A_1, A_1b_2^{[0]} - A_2b_1^{[0]}, 0)$.

  In this case we recover the affine algebra action proposed by Munthe-Kaas'99.

Nonautonomous frozen vector fields

- Similarly, when $f(u,t) = L(u,t)u + N^{[0]}(u,t) + tN^{[1]}(u,t)$.
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    where $c_0 = b^{[0]} + t_0(1-\lambda)b^{[1]}$ and $c_1 = \lambda b^{[1]}$.
  - The algebra action is given by
    $h(A, b^{[1]}, b^{[0]}, \lambda) * \begin{bmatrix} u_0 \\ t_0 \end{bmatrix} = \begin{bmatrix} e^{hA}u_0 + h(b^{[0]} + t_0 b^{[1]})\phi^{[1]}(hA) + h^2\lambda b^{[1]}\phi^{[2]}(hA) \\ t_0 + h\lambda \end{bmatrix}$.
  - The commutators are given by
    $[\Theta_1, \Theta_2] = \left([A_1, A_2], A_1 b_2^{[1]} - A_2 b_1^{[1]}, A_1 b_2^{[0]} - A_2 b_1^{[0]} + \lambda_2 b_1^{[1]} - \lambda_1 b_2^{[1]}, 0\right)$.

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  - The commutators are given by
    $[\Theta_1, \Theta_2] = \left([A_1, A_2], A_1 b_2^{[1]} - A_2 b_1^{[1]}, A_1 b_2^{[0]} - A_2 b_1^{[0]} + \lambda_2 b_1^{[1]} - \lambda_1 b_2^{[1]}, 0\right)$.
- Can generalize this approach to the case $f(u,t) = L(u,t)u + \sum_{k=0}^{p} t^k N^{[k]}(u,t)$.
  - append p trivial differential equations corresponding to $t, t^2, \ldots, t^p$.

LGI for semilinear problems

Consider the semilinear problem

$$u' \; = \; Lu + N(u,t), \; u(t_0) = u_0, \tag{1}$$

- Natural choice for $*$ is the affine action.

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A third order Crouch–Grossman method

$$\left[\begin{array}{ccc|c} 0 & 0 & 0 & I \\ \frac{3}{4}\phi^{[1]} & 0 & 0 & e^{\frac{3}{4}hL} \\ \frac{119}{216}e^{\frac{17}{108}hL}\phi^{[1]}(\frac{119}{216}hL) & \frac{17}{108}\phi^{[1]}(\frac{17}{108}hL) & 0 & e^{\frac{17}{24}hL} \\ \hline \frac{13}{51}e^{\frac{38}{51}hL}\phi^{[1]}(\frac{13}{51}hL) & -\frac{2}{3}e^{\frac{24}{17}hL}\phi^{[1]}(-\frac{2}{3}hL) & \frac{24}{17}\phi^{[1]}(\frac{24}{17}hL) & e^{hL} \end{array}\right]$$

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Consider the semilinear problem

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A fourth order RKMK method with exact Exp

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\phi^{[1]} & 0 & 0 & 0 & e^{\frac{1}{2}hL} \\ \frac{1}{2}\phi^{[1]} - \frac{1}{2}I & \frac{1}{2}I & 0 & 0 & e^{\frac{1}{2}hL} \\ \widehat{\phi}^{[3]^2}(\frac{hL}{2}) & -\widehat{\phi}^{[2]}\widehat{\phi}^{[3]}(\frac{hL}{2}) & \widehat{\phi}^{[2]} & 0 & e^{hL} \\ \hline b_1(hL) & b_2(hL) & b_3(hL) & \frac{1}{6}I & e^{hL} \end{array}\right],$$

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where

$$\begin{aligned}
\widehat{\phi}^{[2]}(z) &= \phi^{[1]}(z)\phi^{[1]^{-1}}\left(\frac{z}{2}\right) = \frac{e^{\frac{z}{2}} + I}{2}, \\
\widehat{\phi}^{[3]}(z) &= \phi^{[1]^{-1}}(z) - I = \frac{e^z - z - I}{I - e^z}, \\
b_1(hL) &= \frac{1}{6}\phi^{[1]} - \frac{1}{3}\phi^{[1]}\widehat{\phi}^{[3]}\left(\frac{hL}{2}\right) - \frac{1}{6}\phi^{[1]}\left(\widehat{\phi}^{[3]} - 2I\right)\widehat{\phi}^{[3]^2}\left(\frac{hL}{2}\right), \\
b_2(hL) &= \frac{1}{3}\widehat{\phi}^{[2]} + \frac{1}{6}\widehat{\phi}^{[2]}\left(\widehat{\phi}^{[3]} - 2I\right)\widehat{\phi}^{[3]}\left(\frac{hL}{2}\right), \\
b_3(hL) &= \frac{1}{3}\widehat{\phi}^{[2]} - \frac{1}{6}\widehat{\phi}^{[2]}\widehat{\phi}^{[3]}.
\end{aligned}$$

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RKMK methods with approximations to the Exp map

With appropriate choices for the diffeomorphism Ψ it is possibel to show that:
- IF RK methods are RKMK methods (Krogstad'03);
- GIF/RK methods are also RKMK methods.

LGI for semilinear problems

Consider the semilinear problem

$$(1) \qquad u' = Lu + N(u,t), \; u(t_0) = u_0,$$

- Natural choice for $*$ is the affine action.

A fourth order CF method

$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & I \\
\frac{1}{2}\phi^{[1]} & 0 & 0 & 0 & e^{\frac{hL}{2}} \\
0 & \frac{1}{2}\phi^{[1]} & 0 & 0 & e^{\frac{hL}{2}} \\
\frac{1}{2}\phi^{[1]} & 0 & 0 & 0 & \left.\begin{array}{c} e^{\frac{hL}{2}} \\ e^{\frac{hL}{2}} \end{array}\right\} \\
-\frac{1}{2}\phi^{[1]} & 0 & \phi^{[1]} & 0 & \\
\hline
\frac{1}{4}\phi^{[1]} & \frac{1}{6}\phi^{[1]} & \frac{1}{6}\phi^{[1]} & -\frac{1}{12}\phi^{[1]} & \left.\begin{array}{c} e^{\frac{hL}{2}} \\ e^{\frac{hL}{2}} \end{array}\right\} \\
-\frac{1}{12}\phi^{[1]} & \frac{1}{6}\phi^{[1]} & \frac{1}{6}\phi^{[1]} & \frac{1}{4}\phi^{[1]} &
\end{array}\right],$$

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$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & I \\
\frac{1}{2}\phi^{[1]} & 0 & 0 & 0 & e^{\frac{1}{2}hL} \\
0 & \frac{1}{2}\phi^{[1]} & 0 & 0 & e^{\frac{1}{2}hL} \\
\frac{1}{2}\phi^{[1]}\left(\frac{hL}{2}\right)\left(e^{\frac{hL}{2}} - I\right) & 0 & \phi^{[1]}\left(\frac{hL}{2}\right) & 0 & e^{hL} \\
\hline
\frac{1}{2}\phi^{[1]} - \frac{1}{3}\phi^{[1]}\left(\frac{hL}{2}\right) & \frac{1}{3}\phi^{[1]} & \frac{1}{3}\phi^{[1]} & -\frac{1}{6}\phi^{[1]} + \frac{1}{3}\phi^{[1]}\left(\frac{hL}{2}\right) & e^{hL}
\end{array}\right]$$

LGI for semilinear problems

Consider the semilinear problem

$$u' = Lu + N(u,t),\ u(t_0) = u_0, \tag{1}$$

- Natural choice for $*$ is the affine action.
- Other possible choice is to use nonautonomous frozen vctor fields

$$N(u,t) = N_n + t\,\frac{N(u,t)-N_n}{t} = N^{[0]} + t\,N^{[1]}$$

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$$N(u,t) = N_n + t\,\frac{N(u,t)-N_n}{t} = N^{[0]} + t\,N^{[1]}$$

or

$$N(u,t) = N_n + t\,\frac{N_n - N_{n-1}}{t} + t^2\,\frac{N(u,t) - 2N_n + N_{n-1}}{t^2},$$

where N_n and N_{n-1} are the values of N at the end of step number n and $n-1$.

Note: In this way we again obtain GLMs.

Implementation issues

Consider the ETD $\phi^{[i]}$ functions

$$\phi^{[1]}(z) = \frac{e^z - 1}{z}, \qquad \phi^{[i+1]}(z) = \frac{\phi^{[i]}(z) - \frac{1}{i!}}{z}, \quad \text{for} \quad i = 2, 3, \ldots.$$

A straightforward implementation suffers from cancellation errors (Kassam and Trefethen).

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Numerical techniques

- Decomposition methods
- Krylov subspace approximations
- Cauchy integral approach

Cauchy integral approach

Based on the Cauchy integral formula

$$\phi^{[i]}(A) = \frac{1}{2\pi i} \int_{\Gamma_A} \phi^{[i]}(\lambda)(\lambda I - A)^{-1} d\lambda,$$

where Γ_A is a contour in the complex plane that encloses the eigenvalue of A, and it is also well separated from 0. It is practical to choose the contour Γ_A to be a circle centered on the real axis.
Using the trapezoid rule, we obtain the following approximation

$$\phi^{[i]}(A) \approx \frac{1}{k} \sum_{j=1}^{k} \lambda_j \phi^{[i]}(\lambda_j)(\lambda_j I - A)^{-1},$$

where k is the number of the equally spaced points λ_j along the contour Γ_A.

Cauchy integral approach

To achieve computational savings we can use the formula

$$\phi^{[i]}(A) = \phi^{[i]}(\gamma hL) = \frac{1}{2\pi i}\int_\Gamma \phi^{[i]}(\gamma\lambda)(\lambda I - hL)^{-1} d\lambda,$$

where the contour Γ encloses the eigenvalues of γhL and $\gamma\Gamma$ is well separated from 0 for all γ in the integration process.
As before

$$\phi^{[i]}(A) \approx \frac{1}{k}\sum_{j=1}^{k} \lambda_j \phi^{[i]}(\gamma\lambda_j)(\lambda_j I - hL)^{-1},$$

where now λ_j are the equally spaced points along the contour Γ.

Note: The inverse matrices no longer depend of γ.

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where now λ_j are the equally spaced points along the contour Γ.

When L arises from a finite difference approximation, we can benefit from its sparse block structure and find the action of the inverse martices to a given vector by:

- iterative methods - *preconditioned conjugate gradient* and *multigrid methods*.

- direct methods - CR, FFT, $FACR$, LU factorization.

Numerical experiments

The methods

- **ETD RK4(Kr)** The fourth order method of Krogstad;
- **IF RK4** The fourth order Integrating Factor Runge–Kutta methd (classical RK);
- **CF4** The fourth order Commutator Free Lie group method with affine action;
- **CF4A1** A fourth order CF method with action corresponding to nonautonomous FVF.

Kuramoto-Sivashinsky equation

$$u_t = -uu_x - u_{xx} - u_{xxxx}, \quad x \in [0, 32\pi]$$

with periodic boundary conditions and with the initial condition

$$u(x,0) = \cos(\frac{x}{16})(1 + \sin(\frac{x}{16})).$$

Kuramoto-Sivashinsky equation

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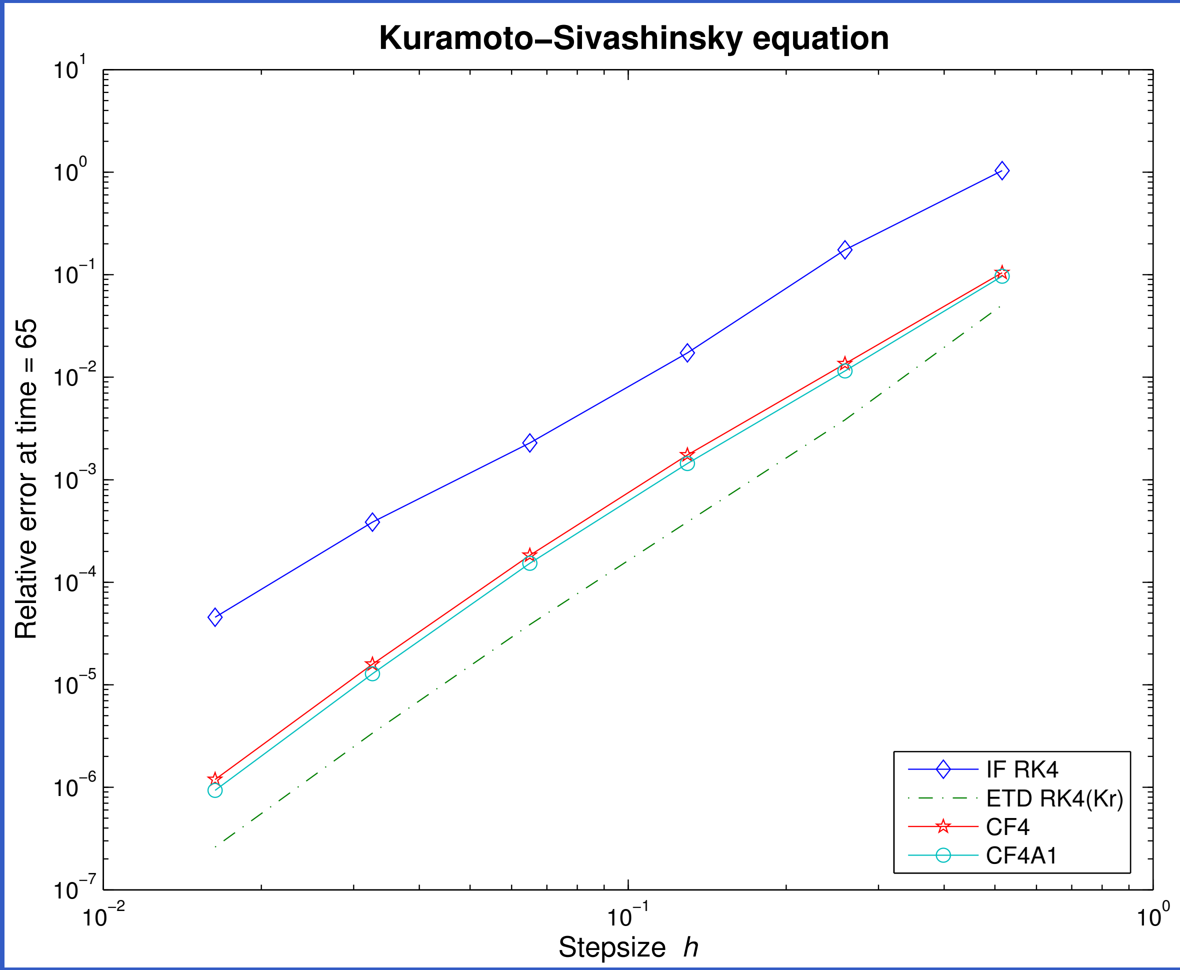
$$u(x,0) = \cos(\frac{x}{16})(1 + \sin(\frac{x}{16})).$$

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

$$\hat{u}_t \;=\; -\frac{ik}{2}\hat{u^2} + (k^2 - k^4)\hat{u},$$

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

Kuramoto-Sivashinsky equation



Allen-Cahn equation

$$u_t \;=\; \varepsilon u_{xx} + u - u^3, \quad x \in [-1, 1]$$

with $\varepsilon = 0.01$ and with boundary and initial conditions

$$u(-1,t) = -1, \;\; u(1,t) = 1, \quad u(x,0) = .53x + .47\sin(-1.5\pi x)$$

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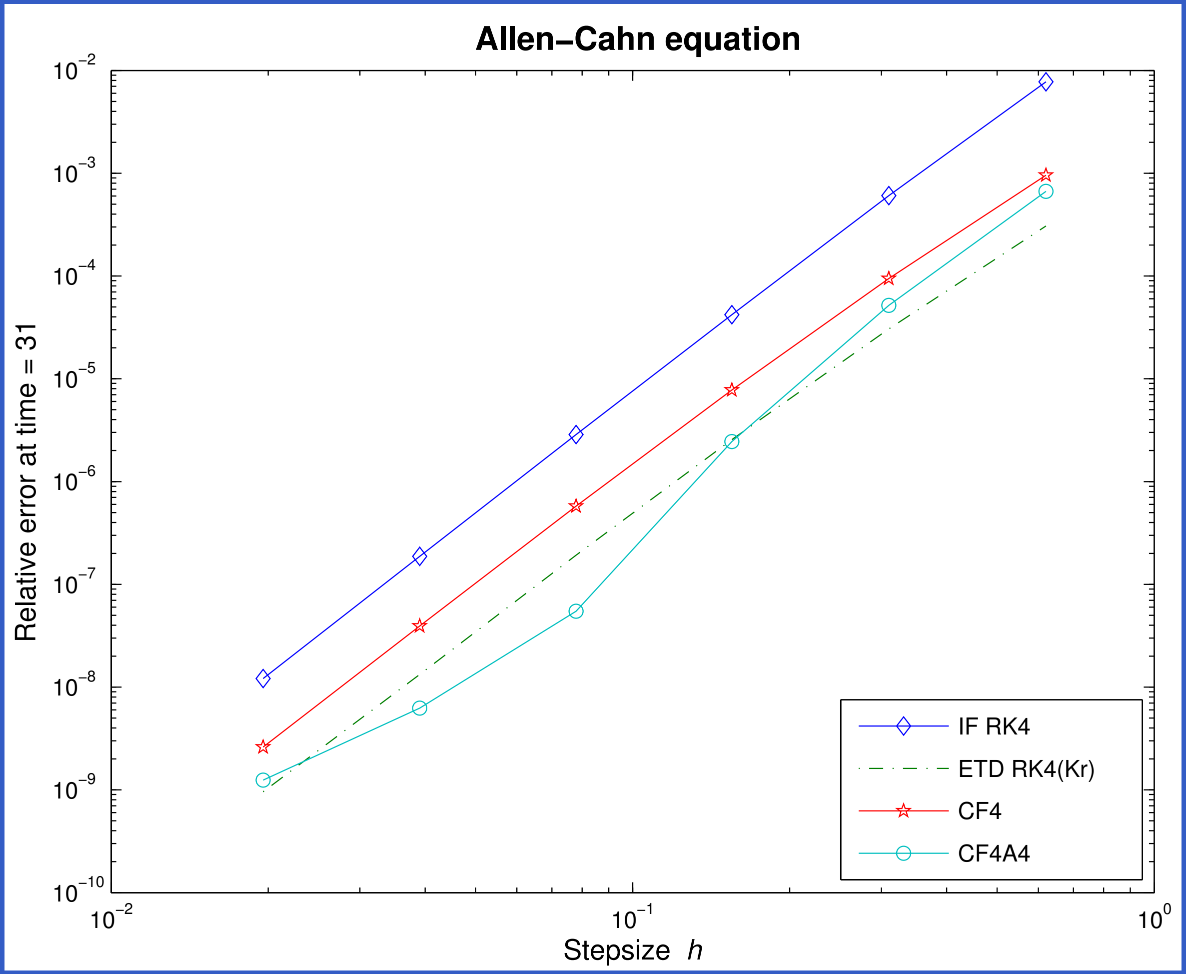
After discretisation in space.

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

where $\mathbf{L} = \varepsilon D^2$, $\mathbf{N}(u(t)) = u - u^3$ and D is the Chebyshev differentiation matrix.

Allen-Cahn equation



Conclusions

- Studied the connection between exponential integrators and Lie group methods.
- Proposed how to construct exponential integrators with algebra action arising from the solutions of differential equations with nonautonomous frozen vector fields.
- The proposed approach is promising for non-diagonal examples

Future work

- Study the connections between the order of the action and the order of the methods.
- How to find a good algebra action?
- Stability analysis.
- Extensive numerical experiments.

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