Lie group methods

Part 2, the Methods

Brynjulf Owren

NTNU/CAS – Norway

From Euler to Lie-Euler

The Explicit Euler Method for the problem

$$\dot{y} = F(y), \quad y \in \mathbb{R}^m, \ F : \mathbb{R}^m \to \mathbb{R}^m$$

is given as

$$y_{n+1} = y_n + hF(y_n)$$

From Euler to Lie-Euler

The Explicit Euler Method for the problem

$$\dot{y} = F(y), \quad y \in \mathbb{R}^m, \; F : \mathbb{R}^m \to \mathbb{R}^m$$

is given as

$$y_{n+1} = y_n + hF(y_n)$$

Alternative interpretation of y_{n+1} is the exact solution of

$$\dot{y} = F(y_n) = \sum_{i=1}^{m} f_i(y_n)\mathbf{e}_i = F_{y_n}, \quad y(t_n) = y_n$$

From Euler to Lie-Euler

The Explicit Euler Method for the problem

$$\dot{y} = F(y), \quad y \in \mathbb{R}^m,\ F : \mathbb{R}^m \to \mathbb{R}^m$$

is given as

$$y_{n+1} = y_n + hF(y_n)$$

Alternative interpretation of y_{n+1} is the exact solution of

$$\dot{y} = F(y_n) = \sum_{i=1}^{m} f_i(y_n)\mathbf{e}_i = F_{y_n}, \quad y(t_n) = y_n$$

In the language of flows, this is just

$$y_{n+1} = \exp(hF_{y_n})\, y_n$$

Improved Lie-Euler

Has the form

$$y_{n+1} = y_n + \frac{h}{2}\big(F(y_n) + F(y_n + hF(y_n))\big)$$

Improved Lie-Euler

In Runge-Kutta format, we write

$$
\begin{aligned}
K_1 &= F(y_n) \\
K_2 &= F(y_n + hK_1) := F(Y_2) \\
y_{n+1} &= y_n + \tfrac{h}{2}(K_1 + K_2)
\end{aligned}
$$

Improved Lie-Euler

In Runge-Kutta format, we write

$$\begin{aligned} K_1 &= F(y_n) \\ K_2 &= F(y_n + hK_1) := F(Y_2) \\ y_{n+1} &= y_n + \tfrac{h}{2}(K_1 + K_2) \end{aligned}$$

In terms of flows, we get

$$\begin{aligned} K_1 &= F(y_n) := F_{y_n} \\ K_2 &= F(\exp(hF_{y_n})y_n = F(Y_2) := F_{Y_2} \end{aligned}$$

Improved Lie-Euler

In Runge-Kutta format, we write

$$\begin{aligned} K_1 &= F(y_n) \\ K_2 &= F(y_n + hK_1) := F(Y_2) \\ y_{n+1} &= y_n + \tfrac{h}{2}(K_1 + K_2) \end{aligned}$$

In terms of flows, we get

$$\begin{aligned} K_1 &= F(y_n) := F_{y_n} \\ K_2 &= F(\exp(hF_{y_n})y_n = F(Y_2) := F_{Y_2} \end{aligned}$$

But for y_{n+1} we could write either

$$y_{n+1} = \exp\big(\frac{1}{2}h(K_1 + K_2)\big)y_n$$

or (for instance)

$$y_{n+1} = \exp\big(\frac{1}{2}hK_2\big)\exp\big(\frac{1}{2}hK_1\big)\,y_n$$

Review of ODE representation on manifold

Given a formulation of the ODEs on the manifold $\mathcal{M}$ with either

1. Frames

$$\dot{y} = F(y) = \sum_i f_i(y) E_i(y)$$

2. Lie group actions; $G \times \mathcal{M} \rightarrow \mathcal{M}, \quad (g, m) \mapsto g.m$ induces a map $\mathfrak{g} \times \mathcal{M} \rightarrow T\mathcal{M}$

$$v.m = \frac{d}{dt}\Big|_{t=0} g(t).m, \quad g'(0) = v \in \mathfrak{g}$$

ODE is written

$$\dot{y} = f(y).y, \quad f : \mathcal{M} \rightarrow \mathfrak{g}$$

Examples

Manifold $\mathcal{M}$ could be some submanifold of $\mathbb{R}^{n\times k}$, Lie group $G \subseteq GL(n)$ and action is left multiplication.

$$\dot{y} = f(y) \cdot y, \quad f : \mathcal{M} \to \mathfrak{g}$$

where $\mathfrak{g}$ is the Lie algebra of G.

Lie-Euler. Obtained as the exact flow of the frozen ODE field

$$\dot{y} = F_{y_n}(y) = f(y_n) \cdot y \quad \Rightarrow \quad y_{n+1} = \mathtt{expm}(hf(y_n)) \cdot y_n$$

Examples (2)

Improved Lie-Euler

$$K_1 = F_{y_n} \quad \text{represented as } f(y_n)$$

$$Y_2 = \mathtt{expm}(hK_1) \cdot y_n$$

$$K_2 = F_{Y_2} \quad \text{represented as } f(Y_2)$$

$$y_{n+1} = \mathtt{expm}(\frac{h}{2}(K_1 + K_2)) \cdot y_n$$ RKMK

$$y_{n+1} = \mathtt{expm}(\frac{h}{2}K_2) \cdot \mathtt{expm}(\frac{h}{2}K_1) \cdot y_n$$ Crouch-Grossman

Outline

For Lie group methods in general, we have to be concerned about

- Classification of the various types of methods

Outline

For Lie group methods in general, we have to be concerned about

- Classification of the various types of methods
- Considering conditions for order of consistency

Outline

For Lie group methods in general, we have to be concerned about

- Classification of the various types of methods
- Considering conditions for order of consistency
- Optimize methods with respect to complexity

Outline

For Lie group methods in general, we have to be concerned about

- Classification of the various types of methods
- Considering conditions for order of consistency
- Optimize methods with respect to complexity

Classification. We distinguish methods based on. . .

- local coordinates for the Lie group (RKMK+generalisations)
- local coordinates in terms of tangent space parametrisations (Retractions)
- composition of (approximate) flows (Commutator-free methods)
- other approaches (e.g. Zanna's methods)

RKMK methods and their generalisations

Suppose we have a transitive Lie group action by G on the manifold $\mathcal{M}$.

Idea. Consider $g(t) \in G$ such that $y(t) = g(t).p := \Lambda_p(g(t))$ where $g(0) = e$.

Use some local diffeomorphism $\phi : \mathfrak{g} \supset U \to G,\ \phi(0) = e$ (e.g. $\phi = \exp$) such that $g(t) = \phi(\sigma(t))$ with $\sigma(t) \in \mathfrak{g}$

$$y(t) = \phi(\sigma(t)).p, \quad \text{near } p$$

Derive differential equation for $\sigma(t)$.

$$\begin{tikzcd}
T\mathcal{M} & TG \arrow[l, "T\Lambda_p"'] & T\mathfrak{g} \arrow[l, "T\phi"'] \\
\mathcal{M} \arrow[u, "F"] & G \arrow[l, "\Lambda_p"] \arrow[u] & \mathfrak{g} \arrow[l, "\phi"] \arrow[u, "\tilde{f}"']
\end{tikzcd}$$

Trivialisation of $T\phi$

Clearly $T\mathfrak{g} \cong \mathfrak{g} \times \mathfrak{g}$.

Every Lie group is trivial, i.e. $TG \cong G \times \mathfrak{g}$.

Set $\mathfrak{g} \sim T_eG$ and identify $v \in T_gG$ with $\xi = v \cdot g^{-1} \in \mathfrak{g}$ (right trivialisation).

Thus, we can think of

$$\begin{aligned} T\phi : \quad & (\mathfrak{g} \times \mathfrak{g}) \to (G \times \mathfrak{g}) \\ & (u, \xi) \mapsto (\phi(u), (T_u\phi)(\xi) \cdot \phi(u)^{-1}) \end{aligned}$$

Following tradition (Varadarajan (84), Munthe-Kaas, Engø, O. and others) we define the map in the second factor to be

$$\begin{aligned} d\phi_u : \quad & \mathfrak{g} \to \mathfrak{g} \\ & \xi \mapsto (T_u\phi)(\xi) \cdot \phi(u)^{-1} \end{aligned}$$

Example ($SO(2)$)

$G = SO(2)$ Orthogonal 2×2 matrices.

$\mathfrak{g} = \mathfrak{so}(2)$ Skew-symmetric 2×2 matrices.

$$\exp : \mathbf{u} = \begin{pmatrix} 0 & u \\ -u & 0 \end{pmatrix} \mapsto \begin{pmatrix} \cos u & \sin u \\ -\sin u & \cos u \end{pmatrix}$$

Let $\gamma(t) \in \mathfrak{so}(2)$ such that $\gamma(0) = \mathbf{u}$ and $\dot{\gamma}(0) = \underline{\xi}$. Then

$$\begin{aligned} T_{\mathbf{u}} \exp(\underline{\xi}) &= \frac{d}{dt}\Big|_0 \exp(\gamma(t)) = \frac{d}{dt}\Big|_0 \begin{pmatrix} \cos u(t) & \sin u(t) \\ -\sin u(t) & \cos u(t) \end{pmatrix} \\ &= \begin{pmatrix} -\xi \sin u & \xi \cos u \\ -\xi \cos u & -\xi \sin u \end{pmatrix} = \begin{pmatrix} 0 & \xi \\ -\xi & 0 \end{pmatrix} \cdot \exp(\mathbf{u}) = \underline{\xi} \cdot \exp(\mathbf{u}) \end{aligned}$$

Thus, in this case, $d\exp_u = I$ (identity map on $\mathfrak{g}$).

Derivative of the exponential map

In general, $d\exp_u \neq I$. Recall matrix exponential

$$\exp(u(t)) = \sum_{k=0}^{\infty} \frac{u(t)^k}{k!}$$

But generally

$$\frac{d}{dt}u(t)^k = \dot{u}(t)\cdot u(t)^{k-1} + u(t)\cdot\dot{u}(t)\cdot u(t)^{k-2} + \cdots + u(t)^{k-1}\cdot\dot{u}(t) \neq k\,\dot{u}(t)\cdot u(t)^{k-1}$$

Notation. Let $\mathrm{ad}_v : \mathfrak{g} \to \mathfrak{g}$ be the linear map $\mathrm{ad}_v(w) = [v,w](= v\cdot w - w\cdot v)$. Similarly $\mathrm{ad}_v^2(w) = \mathrm{ad}_v(\mathrm{ad}_v(w)) = [v,[v,w]]$ and so on.

$$\exp(\mathrm{ad}_v) = \sum_{k=0}^{\infty} \frac{\mathrm{ad}_v^k}{k!}$$

Derivative of the exponential map (2)

Lemma A. For $v, w \in \mathfrak{g}$

$$\exp(v) \cdot w \cdot \exp(-v) = \exp(\mathrm{ad}_v)(w)$$

Lemma B. For $v, w \in \mathfrak{g}$

$$d\exp_v(w) = \int_0^1 \exp(r\ \mathrm{ad}_v)(w)dr$$

Proof. For $s, t \in \mathbb{R}$, let $y_s(t) = \exp(t(v + sw))$ so that

$$d\exp_v(w) = \frac{\partial}{\partial s}\bigg|_0 y_s(1)\exp(-v)$$

$y_s(t)$ satisfies the ODE

$$\dot{y}_s(t) = \frac{\partial}{\partial t} y_s(t) = (v + sw) \cdot y_s(t), \quad y_s(0) = e.$$

Derivative of the exponential map (3)

Clearly $y_s(t) = e^{tv} + \mathcal{O}(s)$ so

$$\dot{y}_s - v y_s = s w e^{tv} + \mathcal{O}(s^2)$$

Solving this linear ODE yields

$$y_s(t) = e^{tv} + s \int_0^t e^{rv} w e^{-rv} dr \, e^{tv} + \mathcal{O}(s^2)$$

and so

$$\left.\frac{\partial}{\partial s}\right|_0 y_s(1) e^{-v} = \int_0^1 e^{rv} w e^{-rv} dr$$

and the result follows by Lemma A.

◇

Lemma B. For $v, w \in \mathfrak{g}$

$$d\exp_v(w) = \int_0^1 \exp(r \, \mathrm{ad}_v)(w) dr$$

Alternative expression for $d\exp_v(w)$

From Lemma B we get, by setting $z = \mathrm{ad}_v$

$$d\exp_v = \int_0^1 \exp(rz)dr\Big|_{z=\mathrm{ad}_v} = \frac{\exp(z)-1}{z}\Big|_{z=\mathrm{ad}_v}$$

or in terms of series expansion

$$d\exp_v = I + \frac{1}{2}\mathrm{ad}_v + \frac{1}{6}\mathrm{ad}_v^2 + \cdots + \frac{1}{(k+1)!}\mathrm{ad}_v^k + \cdots$$

In particular we see from this expression that

1. $d\exp_v = I$ if $\mathrm{ad}_v = 0$ ($[v,w] = 0 \forall w \in \mathfrak{g}$ – commutative Lie group/algebra).
2. $d\exp_0 = I$ for every Lie algebra $\mathfrak{g}$.

Deriving $\tilde{f}$

Differentiate $y(t) = \phi(\sigma(t)).p$ and compare to $\dot{y} = f(y).y$.

$$\dot{y} = T_\sigma \phi\,(\dot{\sigma}).p = d\phi_\sigma(\dot{\sigma}) \cdot \phi(\sigma).p = d\phi_\sigma(\dot{\sigma}).y = f(\phi(\sigma).p).y$$

A sufficient (but not always necessary) condition for this is

$$d\phi_\sigma(\dot{\sigma}) = f(\phi(\sigma).p)$$

Assumption: For σ 'small', $d\phi_\sigma : \mathfrak{g} \to \mathfrak{g}$ is invertible. In particular, we usually assume that $d\phi_0 = T_0\phi = I$. Check for $\exp$.

$$\dot{\sigma} = d\phi_\sigma^{-1} f(\phi(\sigma).p) = \tilde{f}(\sigma)$$

dexpinv

When g is an analytic function of a, say matrix, the (formal) inverse of $g(A)$ is given as $1/g(z)|_{z=A}$.
In particular, for the linear operator $d\exp_v = g(\mathrm{ad}_v)$ with $g(z) = (\exp(z) - 1)/z$, we get that

$$d\exp_v^{-1} = h(z)\big|_{z=\mathrm{ad}_v} = \frac{z}{\exp(z) - 1}\Big|_{z=\mathrm{ad}_v}$$

It is easily checked that $h(z) + z/2$ is even, in fact,

$$h(z) = 1 - \frac{z}{2} + \sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!}\, z^{2m}$$

convergent in the open disk $\{z : |z| < 2\pi\}$. B_{2m}: Bernoulli numbers. Concluding,

$$d\exp_v^{-1}(w) = w - \frac{1}{2}[v, w] + \frac{1}{12}[v, [v, w]] - \frac{1}{720}[v, [v, [v, [v, w]]]] + \cdots$$

The original RKMK algorithm

ODE given on the form $\dot{y} = f(y).y$. Explicit algorithm as follows

```
$p := y_n$
for $r = 1 : s$ do
    $u_r = h \sum_j a_r^j \tilde{k}_j$
    $k_r = f(\exp(u_r).p)$
    $\tilde{k}_r = d\exp_{u_r}^{-1}(k_r)$
end for
$v = h \sum_r b^r \tilde{k}_r$
$y_{n+1} = \exp(v).p$
```

The original RKMK algorithm

ODE given on the form $\dot{y} = f(y).y$. Explicit algorithm as follows

```
$p := y_n$
for $r = 1 : s$ do
    $u_r = h \sum_j a_r^j \tilde{k}_j$
    $k_r = f(\exp(u_r).p)$
    $\tilde{k}_r = d\exp_{u_r}^{-1}(k_r)$
end for
$v = h \sum_r b^r \tilde{k}_r$
$y_{n+1} = \exp(v).p$
```

- In practice, approximation is often used for $d\exp_{u_r}^{-1}$.
- Important observations: Every truncation of the infinite series for $d\exp_v^{-1}(w)$ belongs to $\mathfrak{g}$.
- In RKMK algorithm, $u_r = \mathcal{O}(h)$, thus $\mathrm{ad}_{u_r}^k = \mathcal{O}(h^k)$
- Some clever transformations on $\mathfrak{g}$ can lead to a reduced number of commutators to be calculated in the RKMK algorithm. Graded free Lie algebras.

Summing up RKMK

So far we have derived the original RKMK methods in detail and hinted on generalisations. Some issues to remember

- The RKMK methods can be thought of in terms of a change of variable which locally transforms the manifold problem to a linear space, the Lie algebra $\mathfrak{g}$ of the acting group. A classical integrator is applied to the corresponding problem on $\mathfrak{g}$ and the result is mapped back to the manifold.

Summing up RKMK

So far we have derived the original RKMK methods in detail and hinted on generalisations. Some issues to remember

- The RKMK methods can be thought of in terms of a change of variable which locally transforms the manifold problem to a linear space, the Lie algebra $\mathfrak{g}$ of the acting group. A classical integrator is applied to the corresponding problem on $\mathfrak{g}$ and the result is mapped back to the manifold.
- Since the transformation is smooth, the RKMK method has (at least) the same order of convergence as the classical method applied on the Lie algebra problem.

Summing up RKMK

So far we have derived the original RKMK methods in detail and hinted on generalisations. Some issues to remember

- The RKMK methods can be thought of in terms of a change of variable which locally transforms the manifold problem to a linear space, the Lie algebra $\mathfrak{g}$ of the acting group. A classical integrator is applied to the corresponding problem on $\mathfrak{g}$ and the result is mapped back to the manifold.
- Since the transformation is smooth, the RKMK method has (at least) the same order of convergence as the classical method applied on the Lie algebra problem.
- If the acting Lie group is of much higher dimension than the manifold, the RKMK method transforms the ODE to a space of high dimension, this poses computational challenges and issues we need to address.

Summing up RKMK

So far we have derived the original RKMK methods in detail and hinted on generalisations. Some issues to remember

- The RKMK methods can be thought of in terms of a change of variable which locally transforms the manifold problem to a linear space, the Lie algebra $\mathfrak{g}$ of the acting group. A classical integrator is applied to the corresponding problem on $\mathfrak{g}$ and the result is mapped back to the manifold.
- Since the transformation is smooth, the RKMK method has (at least) the same order of convergence as the classical method applied on the Lie algebra problem.
- If the acting Lie group is of much higher dimension than the manifold, the RKMK method transforms the ODE to a space of high dimension, this poses computational challenges and issues we need to address.
- The exponential mapping is often expressed in terms of the matrix exponential.

  General software is very expensive, $25 - 30\,n^3$ arithmetic complexity.

Other choices of $\phi : \mathfrak{g} \to G$

The exponential map $\exp : \mathfrak{g} \to G$ can be thought of as a coordinate map.

Suppose $\mathbf{e}_1, \ldots, \mathbf{e}_d$ is a basis for $\mathfrak{g}$. Then $v = (v_1, \ldots, v_d)$ are coordinates on G expressed through

$$(v_1, \ldots, v_d) \mapsto \exp(v_1\mathbf{e}_1 + \cdots + v_d\mathbf{e}_d) \in G$$

Such coordinates are called: Canonical coordinates of the first kind, they work for any Lie group G.

Other choices of ϕ include

1. Canonical coordinates of the second kind.
2. Coordinates for special groups, e.g. Cayley coordinates.

Second kind coordinates

Let $\phi : \mathfrak{g} \to G$ be the map

$$\phi(v_1\mathbf{e}_1 + \cdots + v_d\mathbf{e}_d) = \exp(v_1\mathbf{e}_1) \cdot \exp(v_2\mathbf{e}_2) \cdots \exp(v_d\mathbf{e}_d)$$

where $\mathbf{e}_1, \ldots, \mathbf{e}_d$ is some fixed basis for $\mathfrak{g}$.

Example. Let $\mathfrak{g} = \mathfrak{so}(3)$ and consider the basis

$$\mathbf{e}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \; \mathbf{e}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \; \mathbf{e}_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$\phi(\cdot) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \cos v_1 & -\sin v_1 \\ 0 & \sin v_1 & \cos v_1 \end{pmatrix} \cdot \begin{pmatrix} \cos v_2 & 0 & \sin v_2 \\ 0 & 0 & 0 \\ -\sin v_2 & 0 & \cos v_2 \end{pmatrix} \cdot \begin{pmatrix} \cos v_3 & -\sin v_3 & 0 \\ \sin v_3 & \cos v_3 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The derivative

Letting $v(t)$ be a curve in $\mathfrak{g}$ such that $v(0) = v,\ \dot{v}(0) = w$, we calculate

$$\begin{aligned}
\left.\frac{d}{dt}\right|_0 \phi(v(t)) &= w_1\mathbf{e}_1 e^{v_1\mathbf{e}_1}\cdots e^{v_d\mathbf{e}_d} + e^{v_1\mathbf{e}_1} w_2\mathbf{e}_2 e^{v_2\mathbf{e}_2}\cdots e^{v_d\mathbf{e}_d} \\
&\quad + \cdots + \\
&\quad e^{v_1\mathbf{e}_1}\cdots e^{v_{d-1}\mathbf{e}_{d-1}} w_d\mathbf{e}_d e^{v_d\mathbf{e}_d} \\
&= w_1\mathbf{e}_1\cdot\phi(v) + e^{v_1\mathbf{e}_1} w_2\mathbf{e}_2 e^{-v_1\mathbf{e}_1}\cdot\phi(v) + \cdots + \\
&\quad e^{v_1 e_1}\cdots e^{v_{d-1}\mathbf{e}_{d-1}} w_d\mathbf{e}_d e^{-v_{d-1}\mathbf{e}_{d-1}}\cdots e^{-v_1\mathbf{e}_1}\cdot\phi(v)
\end{aligned}$$

Introduce the operator $\mathrm{Ad}_i(w) := \mathrm{Ad}_{e^{v_i\mathbf{e}_i}}(w) = e^{v_i\mathbf{e}_i} w e^{-v_i\mathbf{e}_i}$, so

$$d\phi_v(w) = \sum_{k=1}^{d} w_k \mathrm{Ad}_1\cdots\mathrm{Ad}_{k-1}(e_k)$$

What about $d\phi_v^{-1}$?

Cayley transform

An important family of Lie matrix groups are those described as

$$G_J = \{A \in GL(n) : A^T \cdot J \cdot A = J\}$$

Its Lie algebra is readily shown to be

$$\mathfrak{g}_J = \{a \in \mathfrak{gl}(n) : a^T J + Ja = 0\}$$

Examples $SO(n)$, $SP(n)$, $SO(p,q)$.

Let ϕ be any analytic function satisfying $\phi(z) \cdot \phi(-z) = 1$. Then

$$a \in \mathfrak{g}_J \quad \Rightarrow \quad \phi(a) \in G_J$$

Most popular ϕ is the Cayley transform which we define to be

$$\phi(z) = \frac{1 + \frac{1}{2} z}{1 - \frac{1}{2} z}$$

Retraction methods

Retractions can be thought of as a generalization of the exponential (flow) map. Suppose $\mathcal{M}$ is a manifold and consider $\mathcal{R} : T\mathcal{M} \to \mathcal{M}$ whose restriction $\mathcal{R}_p$ to $T_p\mathcal{M}$ satisfies

- $\mathcal{R}_p$ is defined on some neighborhood of $0 \in T_p\mathcal{M}$
- $\mathcal{R}_p(v) = 0 \;\Leftrightarrow\; v = 0$
- $T_0\mathcal{R}_p(v) = v$ for all $v \in T_p\mathcal{M}$

Generalize local coordinate idea by setting (locally)

$$y(t) = \mathcal{R}_p(\sigma(t)), \quad \text{where } y(0) = p \text{ and } \sigma(0) = 0.$$

Similar to the RKMK idea we would now obtain, (for $\dot{y} = F(y)$)

$$\dot{\sigma}(t) = T_\sigma^{-1} F(\mathcal{R}_p(\sigma))$$

Example – Retractions

$\mathcal{M}$ Stiefel manifold: $\{Q \in \mathbb{R}^{n\times k} : Q^T Q = I_k\}$.

Tangent space: $\{v \in \mathbb{R}^{n\times k} : Q^T v \in \mathbb{R}^{k\times k}$ is skew-symmetric$\}$.

Define $\mathcal{R}_p(v)$ through: $p + v = Q \cdot R$ (reduced QR-factorisation).

Set $\mathcal{R}_p(v) = Q$

Commutator-free methods

$$\begin{aligned}
Y_i &= \exp\Bigl(\sum_r \alpha_{i,J}^r K_r\Bigr) \cdots \exp\Bigl(\sum_r \alpha_{i,1}^r K_r\Bigr)\, p \\
K_i &= hF_{Y_i} = h\sum_\ell f_\ell(Y_i) E_\ell \\
y_1 &= \exp\Bigl(\sum_r \beta_J^r K_r\Bigr) \cdots \exp\Bigl(\sum_r \beta_1^r K_r\Bigr)\, p
\end{aligned}$$

Commutator-free methods

$$
\begin{aligned}
Y_i &= \exp\Big(\sum_r \alpha_{i,J}^r K_r\Big)\cdots\exp\Big(\sum_r \alpha_{i,1}^r K_r\Big)\,p \\
K_i &= hF_{Y_i} = h\sum_\ell f_\ell(Y_i)E_\ell \\
y_1 &= \exp\Big(\sum_r \beta_J^r K_r\Big)\cdots\exp\Big(\sum_r \beta_1^r K_r\Big)\,p
\end{aligned}
$$

Particularly well suited for

- Problems on manifolds with large isotropy groups
- Stiff problems

CF methods – reusing exponentials

Example. Third order explicit method

CF methods – reusing exponentials

Example. Third order explicit method

$$
\begin{aligned}
Y_1 &= p, & K_1 &= hF_{Y_1} \\
Y_2 &= \exp(\tfrac{1}{3}K_1)\,p, & K_2 &= hF_{Y_2} \\
Y_3 &= \exp(\tfrac{2}{3}K_2)\,p, & K_3 &= hF_{Y_3}
\end{aligned}
$$

$$
y_1 = \exp(-\tfrac{1}{12}K_1 + \tfrac{3}{4}K_3)\,\exp(\tfrac{1}{3}K_1)\,p
$$

CF methods – reusing exponentials

Example. Third order explicit method

$$
\begin{aligned}
Y_1 &= p, & K_1 &= hF_{Y_1} \\
Y_2 &= \exp(\tfrac{1}{3}K_1)\,p, & K_2 &= hF_{Y_2} \\
Y_3 &= \exp(\tfrac{2}{3}K_2)\,p, & K_3 &= hF_{Y_3}
\end{aligned}
$$

$$
y_1 = \exp(-\tfrac{1}{12}K_1 + \tfrac{3}{4}K_3)\,Y_2
$$

CF methods – reusing exponentials

Example. Third order explicit method

$$\begin{aligned} Y_1 &= p, & K_1 &= hF_{Y_1} \\ Y_2 &= \exp(\tfrac{1}{3}K_1)\,p, & K_2 &= hF_{Y_2} \\ Y_3 &= \exp(\tfrac{2}{3}K_2)\,p, & K_3 &= hF_{Y_3} \end{aligned}$$

$$y_1 = \exp(-\tfrac{1}{12}K_1 + \tfrac{3}{4}K_3)\,Y_2$$

Generally, we have derived CF methods of

- order 3 with 3 exponentials
- order 4 with 5 exponentials

Example – Heat conduction

Consider PDE (Munthe-Kaas 99, Lodden 00, Suslowicz 01)

$$u_t = \nabla \cdot (\mu(x)\nabla u)$$

Example – Heat conduction

Consider PDE (Munthe-Kaas 99, Lodden 00, Suslowicz 01)

$$u_t = \nabla \cdot (\mu(x)\nabla u) = \mu_c \nabla^2 u + \nabla \cdot (\mu(x) - \mu_c)\nabla u$$

Example – Heat conduction

Consider PDE (Munthe-Kaas 99, Lodden 00, Suslowicz 01)

$$u_t = \nabla \cdot (\mu(x)\nabla u) = \mu_c \nabla^2 u + \nabla \cdot (\mu(x) - \mu_c)\nabla u$$

Discretize in space to obtain system

$$\dot{U} = MU + b(U), \quad U \in \mathbb{R}^N$$

Example – Heat conduction

Consider PDE (Munthe-Kaas 99, Lodden 00, Suslowicz 01)

$$u_t = \nabla \cdot (\mu(x)\nabla u) = \mu_c \nabla^2 u + \nabla \cdot (\mu(x) - \mu_c)\nabla u$$

Discretize in space to obtain system

$$\dot{U} = MU + b(U), \quad U \in \mathbb{R}^N$$

$\mathbb{R}$-linear span of frames contains vector fields

$$F_{\alpha,b}(U) = \alpha MU + b, \quad \alpha \in \mathbb{R},\ b \in \mathbb{R}^N$$

Heat conduction – Num. ex.

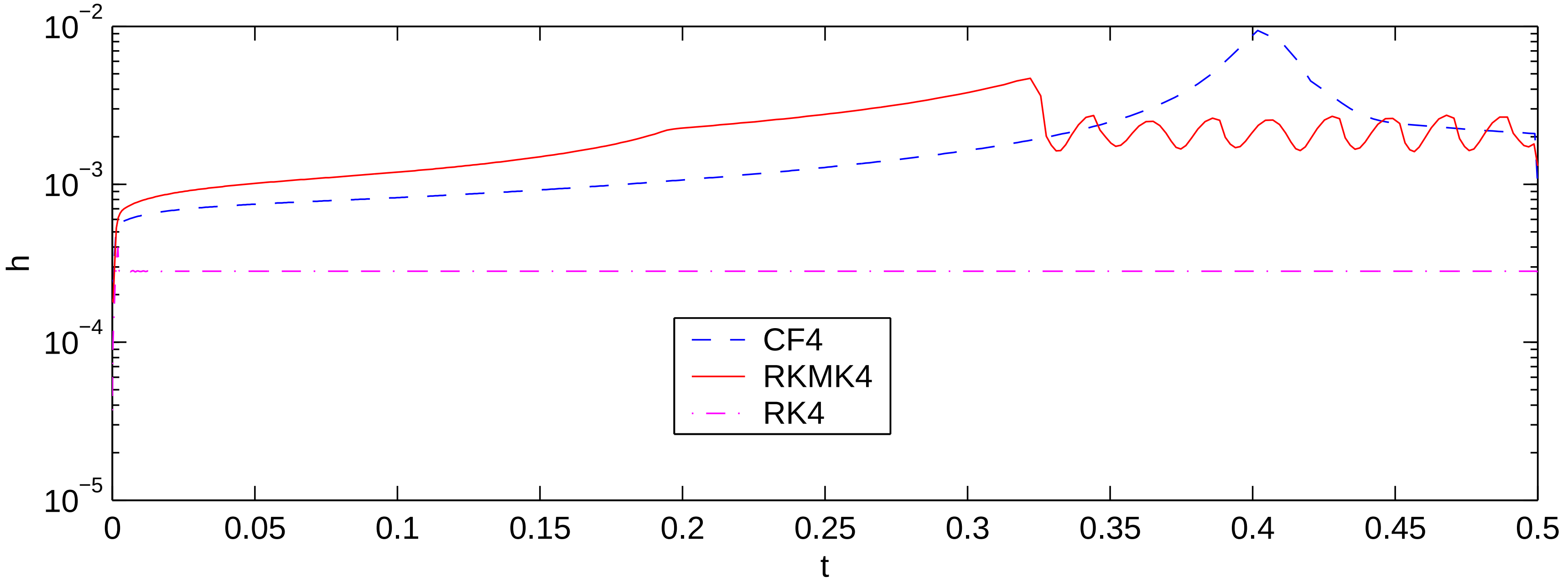
FD, $1D,\ t \in [0, \frac{1}{2}],\ x \in [-1, 1],\ \mu(x) = 1 - x^2,\ u_0(x) = 1 - |x|$.

RK4, RKMK4, CF4. Variable stepsize,

Heat conduction – Num. ex.

FD, $1D$, $t \in [0, \frac{1}{2}]$, $x \in [-1, 1]$, $\mu(x) = 1 - x^2$, $u_0(x) = 1 - |x|$.

RK4, RKMK4, CF4. Variable stepsize, `tol=1.0e-6`



Heat conduction – Num. ex.

FD, $1D$, $t \in [0, \frac{1}{2}]$, $x \in [-1, 1]$, $\mu(x) = 1 - x^2$, $u_0(x) = 1 - |x|$.

RK4, RKMK4, CF4. Variable stepsize, `tol=1.0e-3`