Topics on geometric integration

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Numerical integration

Numerical method

$$x_{k+1} = \Phi(x_k; h)$$

Relevant aspects

- precision of the solution
- computational effort
- preservation of the properties of the exact flow

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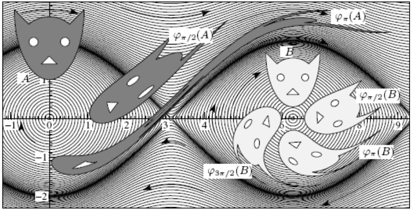
- precision of the solution
- computational effort
- **preservation of the properties of the exact flow**

...crucial for long time simulation!

Geometric integrators

Some properties of the continuous systems preserved by the flow are:

- energy
- symmetry
- momentum
- reversibility
- symplectic form
- configuration space



Area preservation of the flow of Hamiltonian systems.
Source: Hairer, Lubich, Wanner, *Geometric Numeric Integration*, Springer.

Geometric integrators are built in order to inherit exactly some properties of the continuous equation.

Outline

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Dynamics of a Hamiltonian system

Lagrangian $L(\mathbf{q},\dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}^T\mathbb{I}\dot{\mathbf{q}} - V(\mathbf{q})$.

$$\delta \int L(\mathbf{q},\dot{\mathbf{q}})dt = 0, \text{ null variations at the endpoints}$$

Equations of motion: $\dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{\mathbf{q}}} - \dfrac{\partial L}{\partial \mathbf{q}} = \dfrac{\partial V}{\partial \mathbf{q}}$.

Legendre transform $\mathbf{p} = \dfrac{\partial L}{\partial \dot{\mathbf{q}}}$.

Hamiltonian $H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbb{I}^{-1}\mathbf{p} + V(\mathbf{q})$.

Equations of motion: $\begin{cases} \dot{\mathbf{p}} = \dfrac{\partial H}{\partial \mathbf{q}}(\mathbf{q},\mathbf{p}) \\ \dot{\mathbf{q}} = -\dfrac{\partial H}{\partial \mathbf{p}}(\mathbf{q},\mathbf{p}) \end{cases}$

Symplecticity of Hamiltonian flow

A *symplectic form* is a non-degenerate skew-symmetric bilinear form on a manifold.
Canonical symplectic form Ω is a unique two-form defined on the cotangent bundle T^*Q:

$$\Omega = \sum_{i=1}^{n} d\mathbf{q}^i \wedge d\mathbf{p}_i$$

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The flow $\mathbf{y}(t) = \phi_t(\mathbf{y}_0)$ of every Hamiltonian system denotes a canonical transformation $\forall\, t > 0$, that is,

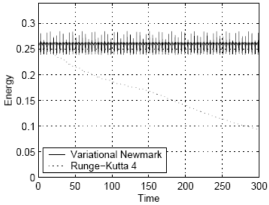
$$\phi_t^* \Omega = \Omega, \;\; \forall\, t > 0.$$

Symplectic integrator

Energy behavior

A symplectic integrator is
an exact integrator for
a modified Hamiltonian system.

Thus, a symplectic method of order p
nearly preserves the energy
of the original system
for exponentially long times
[Benettin and Giorgilli, 1994]:



Nearly energy conservation.
Source: Marsden and West, *Discrete Mechanics and Variational Integrators*, Acta Numerica, 2001.

$$H(\mathbf{y}_n) = H(\mathbf{y}_0) + \mathcal{O}(h^p), \text{ for } nh \le e^{\frac{h_0}{2h}}$$

Variational integrators

Discrete Lagrangian

$$L_d(\mathbf{q}_0, \mathbf{q}_1) \approx \int_{t_0}^{t_1} L(\mathbf{q}, \dot{\mathbf{q}})dt.$$

Discrete Euler-Lagrange equation (DEL)

$$\mathbf{D}_2\, L_d(\mathbf{q}_{k-1}, \mathbf{q}_k) + \mathbf{D}_1\, L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = 0$$

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Variational integrators yield to:

- symplecticity **(iff)**
- good energy behavior
- momentum conservation (in presence of symmetry)

Conjugate symplecticity

Conjugate method

$$\Phi_h = \chi_h^{-1} \circ \Psi_h \circ \chi_h,$$

where $\chi_h(x) = x + \mathcal{O}(h^s)$.

Even if a method is not symplectic, it can still be conjugate symplectic, and sharing the same long-time excellent behavior.

In particular, the error on the Hamiltonian again remains bounded over exponentially long times:

$$H(\mathbf{y}_n) = H(\mathbf{y}_0) + \mathcal{O}(h^{\min\{s,p\}}) \text{ for } nh \leq e^{\frac{h_0}{2h}}.$$

Rigid body dynamics of rotation (trivialized)

Lagrangian formulation

The configuration is described by a couple

$$(\mathbf{R}, \boldsymbol{\omega}) \in T\mathrm{SO}(3) \simeq \mathrm{SO}(3) \times \mathfrak{so}(3),$$

where

- $\mathbf{R} \in \mathrm{SO}(3)$ is the attitude;
- $\boldsymbol{\omega} \in \mathbb{R}^3$ is the body angular velocity.

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Lagrangian formulation Configuration space $SO(3) \times \mathfrak{so}(3)$

$$\ell(\mathbf{R}, \boldsymbol{\omega}) = \frac{1}{2}\boldsymbol{\omega}^T \mathbb{I}\, \boldsymbol{\omega} \;-\; V(\mathbf{R})$$

$\mathbb{I}$ is the inertia matrix (symmetric positive definite).

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$$\begin{cases} \dot{\mathbf{R}} = \mathbf{R}\,\widehat{\boldsymbol{\omega}} & \leftarrow \text{reconstruction equation} \\ \mathbb{I}\,\dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \times \mathbb{I}\,\boldsymbol{\omega} = \tau(\mathbf{R}). \end{cases}$$

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Equations of motion:
$$\begin{cases} \dot{\mathbf{R}} = \mathbf{R}\,\hat{\boldsymbol{\omega}} \\ \boldsymbol{\mu} = \dfrac{\partial \ell}{\partial \boldsymbol{\omega}} \\ \dot{\boldsymbol{\mu}} = \mathrm{ad}^*_{\boldsymbol{\omega}}\boldsymbol{\mu} + \mathbf{R}\dfrac{\partial \ell}{\partial \mathbf{R}}. \end{cases}$$

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Energy: $H(\mathbf{R}, \boldsymbol{\mu}) = \dfrac{1}{2}\boldsymbol{\mu}^T \mathbb{I}^{-1} \boldsymbol{\mu} + V(\mathbf{R}).$

Survey: rigid body integrators

Algorithm	Year	*Free rigid body*			*Rigid body with generic potential*		
		Symplectic	Energy	Momentum	Symplectic	Energy	Momentum
Lie-Newmark	1988	?			?		
Algo_1	1991		✓			?	
Algo_C1	1991		✓	✓		?	?
Austin et al.	1993		✓	✓		?	?
Lewis & Simo	1994	✓	✓	✓			
RATTLE	1994	✓	✓	✓	✓	nearly	✓
Variational	1998	✓	nearly	✓	✓	nearly	✓
LIEMID(EA)	2005	?			?		
PRK	2007	?	✓	✓	?	?	?
MCG	2007	?	✓		?	?	
NEW3	2010	?		✓	?		

Synoptic table of the most relevant rigid body integrators. Their geometric properties are highlighted.

Numerical experiment

Distance function Define $\mathrm{dist} : \mathrm{SO}(3) \times \mathrm{SO}(3) \to \mathbb{R}$

$$\mathrm{dist}(\mathbf{R}_1, \mathbf{R}_2) = \sqrt{2\,\mathrm{tr}(I - \mathbf{R}_2^T \mathbf{R}_1)}$$

Potential energy

$$V_\alpha(\mathbf{R}) = (\mathrm{dist}(\mathbf{R}, I) - 1)^2 - \frac{\alpha}{\mathrm{dist}(\mathbf{R}, \mathbf{R}_m)}.$$

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Potential energy

$$V_\alpha(\mathbf{R}) = \underbrace{(\mathrm{dist}(\mathbf{R}, I) - 1)^2}_{\text{bounded potential}} - \frac{\alpha}{\mathrm{dist}(\mathbf{R}, \mathbf{R}_m)}.$$

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Potential energy

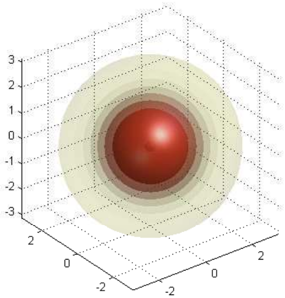
$$V_\alpha(\mathbf{R}) = (\mathrm{dist}(\mathbf{R}, I) - 1)^2 - \underbrace{\frac{\alpha}{\mathrm{dist}(\mathbf{R}, \mathbf{R}_m)}}_{\text{Coulomb potential}}.$$

$\alpha = 0$

Minimum values for the potential attained in

$$S \stackrel{\text{def}}{=} \{\mathbf{R} \in SO(3) : \mathrm{dist}(\mathbf{R}, I) = 1\}.$$

$S \times \{0\}$ is stable in the sense of Lyapunov.

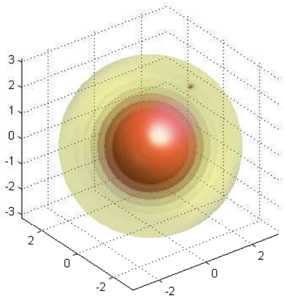


Potential field with $\alpha = 0$ in the angle/axis representation.

$\alpha \neq 0$

If α is sufficiently small and $\mathbf{R}_m$ is sufficiently far, S gets sligthly perturbated into S_α, a set of local minima.

$S_\alpha \times \{0\}$ inherits the same stability properties.



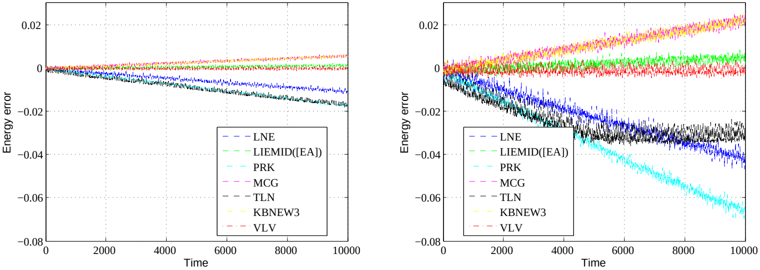
Potential field with $\alpha \neq 0$ in the angle/axis representation.

Tested algorithms

- Explicit Lie-Newmark method (ELN)
- Trapezoidal Lie-Newmark method (TLN)
- Krysl's explicit Lie-Midpoint algorithm (LIEMID[EA])
- Partitioned Runge-Kutta Munthe-Kaas method (PRK)
- Modified Crouch-Grossman method (MCG)
- Koziara-Bicanic algorithm (NEW3)
- Variational Lie-Verlet algorithm (VLV)

Energy behaviour

We choose the initial rotation near S_α, with small body angular velocity.



Energy behavior with the two algorithms, for different timesteps: $h = 0.125$ [s] and $h = 0.25$ [s].

Conclusions

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- (conjugate-)symplecticity as a key property for the long-time behavior of numerical integrators

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- (conjugate-)symplecticity as a key property for the long-time behavior of numerical integrators
- easy-to-implement numerical experiment that has proven effective in detecting the possible energy drift of a rigid body integrator
- necessity test for (conjugate-)symplecticity

Outline

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Unitary sphere $\mathbb{S}^2$

$$\mathbb{S}^2 = \{\mathbf{q} \in \mathbb{R}^3 | \|\mathbf{q}\| = 1\}.$$

Many classical and interesting mechanical systems evolve on the 2-sphere or on a product of 2-spheres.
Examples Double spherical pendulum, interconnection of spherical pendulums, elastic rod.

The configuration of the system on $\left(\mathbb{S}^2\right)^n$ is usually described using $2n$ angles or n unitary constraints; these representations should be however avoided, since they yield additional complexity in the computation.

Geometric approach

Homogeneous space Be G a group.
A *homogeneous space* for G is a non-empty topological space X on which G acts in a transitive way.

$\mathbb{S}^2$ is a homogeneous space under the action of SO(3).

Since SO(3) acts transitively on $\mathbb{S}^2$, we can lift the problem from the configuration space to the action space, that is, we can solve for a trajectory $\mathbf{R}(t) \subset \mathrm{SO}(3)$ which generates the actual flow:

$$\mathbf{q}(t) = \mathbf{R}(t)\mathbf{q}(0)$$

Problems arising

The action of SO(3) on $\mathbb{S}^2$ is **not free**.

Isotropy group

$$\mathcal{H}_{\mathbf{q}} = \{\mathbf{R} \in \mathrm{SO}(3) | \mathbf{R}\mathbf{q} = \mathbf{q}\}$$

$\mathcal{H}_{\mathbf{q}}$ depends on the current configuration $\mathbf{q} \in \mathbb{S}^2$. Therefore a given flow on $\mathbb{S}^2$ corresponds to continuous families of flows on SO(3).

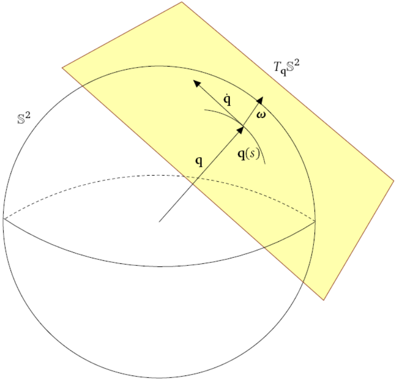
To our knowledge, in literature there exist no methods to describe in a unique way the flow on the quotient space $\mathrm{SO}(3)/\mathcal{H}_{\mathbf{q}}$.

Variational approach

Lagrangian

The configuration is described by $(\mathbf{q}_i, \dot{\mathbf{q}}_i)$, $i = 1, \dots, n$, where

- $\mathbf{q}_i \in \mathbb{S}^2$;
- $\dot{\mathbf{q}}_i \in T_{\mathbf{q}_i}\mathbb{S}^2$, $\dot{\mathbf{q}}_i \perp \mathbf{q}_i$.



The unit sphere $\mathbb{S}^2$ with the tangent space $T_{\mathbf{q}}\mathbb{S}^2$.

Variational approach

Lagrangian Configuration space $T\left(\mathbb{S}^2\right)^n$.

$$L(\mathbf{q}_1, \dots, \mathbf{q}_n, \dot{\mathbf{q}}_1, \dots, \dot{\mathbf{q}}_n) = \sum_{i=1}^{n} \frac{1}{2} \dot{\mathbf{q}}_i^T \mathbb{I} \dot{\mathbf{q}}_i - V(\mathbf{q}_1, \dots, \mathbf{q}_n)$$

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Equations of motion (Lee *et al.*, 2009) on $T\left(\mathbb{S}^2\right)^n$:

$$\begin{cases} \mathbb{I}_{ii}\dot{\boldsymbol{\omega}}_i & = \sum_{\substack{j=1 \\ j\neq i}}^{n} \left(\mathbb{I}_{ij}\mathbf{q}_i \times (\mathbf{q}_j \times \dot{\boldsymbol{\omega}}_j) + \mathbb{I}_{ij}\|\boldsymbol{\omega}_j\|^2 \mathbf{q}_i \times \mathbf{q}_j\right) - \mathbf{q}_i \times \frac{\partial V}{\partial \mathbf{q}_i} \\ \dot{\mathbf{q}}_i & = \boldsymbol{\omega}_i \times \mathbf{q}_i \end{cases}$$

where

$$0 = \mathbf{q}_i \cdot \boldsymbol{\omega}_i$$
$$0 = \mathbf{q}_i \cdot \dot{\boldsymbol{\omega}}_i$$

Adapting Lie methods

Basic idea:

$$\begin{aligned}\dot{\mathbf{q}}_i(t) &= \dot{\mathbf{R}}_i(t)\mathbf{q}_i(0)\\ &= \boldsymbol{\omega}_i \times \mathbf{q}_i(t)\\ &= \boldsymbol{\omega}_i \times \mathbf{R}_i(t)\mathbf{q}_i(0)\end{aligned}$$

Dynamics on SO(3):

$$\dot{\mathbf{R}}_i = \omega_i \times \mathbf{R}_i$$

$$\mathbb{I}_{ii}\dot{\boldsymbol{\omega}}_i = \sum_{\substack{j=1\\ j\neq i}}^{n} \Big(\mathbb{I}_{ij}\mathbf{R}_i\mathbf{q}_i(0) \times (\mathbf{R}_j\mathbf{q}_j(0) \times \dot{\boldsymbol{\omega}}_j) + \mathbb{I}_{ij}\|\boldsymbol{\omega}_j\|^2\mathbf{R}_i\mathbf{q}_i(0) \times \mathbf{R}_j\mathbf{q}_j(0)\Big) - \mathbf{R}_i\mathbf{q}_i(0) \times \frac{\partial V}{\partial \mathbf{q}_i}$$

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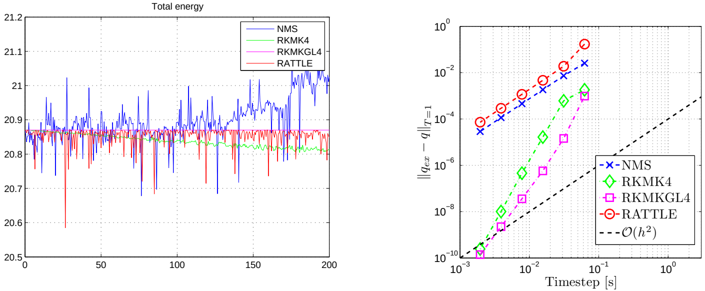
Dynamics on SO(3):

$$\dot{\mathbf{R}}_i = \boldsymbol{\omega}_i \times \mathbf{R}_i$$

$\boldsymbol{\omega}_i$ is the **spatial angular velocity**!

$$\mathbb{I}_{ii}\dot{\boldsymbol{\omega}}_i = \sum_{\substack{j=1\\ j\neq i}}^{n} \Big(\mathbb{I}_{ij}\mathbf{R}_i\mathbf{q}_i(0) \times (\mathbf{R}_j\mathbf{q}_j(0) \times \dot{\boldsymbol{\omega}}_j) + \\ + \mathbb{I}_{ij}\|\boldsymbol{\omega}_j\|^2 \mathbf{R}_i\mathbf{q}_i(0) \times \mathbf{R}_j\mathbf{q}_j(0)\Big) - \mathbf{R}_i\mathbf{q}_i(0) \times \frac{\partial V}{\partial \mathbf{q}_i}$$

Double spherical pendulum



Numerical results obtained for the double spherical pendulum: energy and the accuracy precision diagram.

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Future work

- under what conditions are the properties of the Lie methods preserved also by the flow on $\mathbb{S}^2$?