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
Numerical integration

Numerical method

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Relevant aspects

- 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

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

1. Long-time stability of rigid body integrators

2. Numerical integration on homogeneous spaces
Outline

1. Long-time stability of rigid body integrators
Dynamics of a Hamiltonian system

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

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

Equations of motion: \[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = \frac{\partial V}{\partial q}. \]

**Legendre transform** \( p = \frac{\partial L}{\partial \dot{q}}. \)

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

\[ \dot{p} = \frac{\partial H}{\partial q}(q, p) \]

Equations of motion: \[ \dot{q} = -\frac{\partial H}{\partial p}(q, p) \]
A *symplectic form* is a non-degenerate skew-symmetric bilinear form on a manifold.
Canonical symplectic form $\Omega$ is a unique two-form defined on the cotangent bundle $T^*Q$:

$$
\Omega = \sum_{i=1}^{n} dq^i \wedge dp_i
$$
Symplecticity of Hamiltonian flow

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$$

The flow $y(t) = \phi_t(y_0)$ 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]:

$$H(y_n) = H(y_0) + O(h^p), \text{ for } nh \leq e^{h_0/2h}$$

Nearly energy conservation.
Variational integrators

**Discrete Lagrangian**

\[ L_d(q_0, q_1) \approx \int_{t_0}^{t_1} L(q, \dot{q}) dt. \]

**Discrete Euler-Lagrange equation (DEL)**

\[ D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0 \]
Variational integrators

Discrete Lagrangian

\[ L_d(q_0, q_1) \approx \int_{t_0}^{t_1} L(q, \dot{q}) \, dt. \]

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Variational integrators yield to:

- symplecticity \((\text{iff})\)
- 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 \( \chi_h(x) = x + O(h^s) \).

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:

\[ H(y_n) = H(y_0) + O(h^{\min\{s,p\}}) \text{ for } nh \leq e^{\frac{h_0}{2h}}. \]
Rigid body dynamics of rotation (trivialized)

Lagrangian formulation

The configuration is described by a couple

$$(\mathbf{R}, \mathbf{\omega}) \in T\text{SO}(3) \cong \text{SO}(3) \times \mathfrak{so}(3),$$

where

- $\mathbf{R} \in \text{SO}(3)$ is the attitude;
- $\mathbf{\omega} \in \mathbb{R}^3$ is the body angular velocity.
Rigid body dynamics of rotation (trivialized)

**Lagrangian formulation** Configuration space $SO(3) \times \mathfrak{s}o(3)$

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

$\mathbb{I}$ is the inertia matrix (symmetric positive definite).
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$$\mathcal{L}(\mathbf{R}, \mathbf{\omega}) = \frac{1}{2} \mathbf{\omega}^T \mathbb{I} \mathbf{\omega} - V(\mathbf{R})$$

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Equations of motion:

$$\begin{align*}
\dot{R} &= R \hat{\omega} \\
\mathbb{I} \dot{\omega} + \omega \times \mathbb{I} \omega &= \tau(R).
\end{align*}$$
**Lagrangian formulation** Configuration space \( \text{SO}(3) \times \mathfrak{so}(3) \)

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\]

Equations of motion:

\[
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\dot{R} &= R \hat{\omega} & \text{← reconstruction equation} \\
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\end{align*}
\]
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$$\begin{cases} \dot{R} = R \hat{\omega} \\ \mathbb{I} \dot{\omega} + \omega \times \mathbb{I} \omega = \tau(R). \end{cases} \leftarrow \text{Euler-Lagrange equation}$$
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**Legendre transform** \( \mu = \frac{\partial \ell}{\partial \omega} \in \mathfrak{so}^*(3) \).
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Rigid body dynamics of rotation (trivialized)

**Lagrangian formulation** Configuration space $\text{SO}(3) \times \mathfrak{s}\mathfrak{o}(3)$

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

Equations of motion:

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**Hamiltonian formulation** Phase space $\text{SO}(3) \times \mathfrak{s}\mathfrak{o}^*(3)$.

Equations of motion:

$$\begin{cases} \dot{R} = R \hat{\omega} \\ \dot{\mu} = \text{ad}^* \omega \mu + R \frac{\partial \ell}{\partial R}. \end{cases}$$
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\dot{R} = R \hat{\omega} \\
\mu = \frac{\partial \ell}{\partial \omega} \\
\dot{\mu} = \text{ad}^*_{\omega} \mu + R \frac{\partial \ell}{\partial R}. \quad \leftarrow \text{Lie-Poisson equation}
\end{cases}$$
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\end{cases}$$

Energy: $H(R, \mu) = \frac{1}{2} \mu^T \mathbb{I}^{-1} \mu + V(R)$. 
Survey: rigid body integrators

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Year</th>
<th>Free rigid body</th>
<th>Rigid body with generic potential</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>Symplectic</td>
<td>Energy</td>
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<td>Austin et al.</td>
<td>1993</td>
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<td>✓</td>
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<tr>
<td>Lewis &amp; Simo</td>
<td>1994</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>RATTLE</td>
<td>1994</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Variational</td>
<td>1998</td>
<td>✓</td>
<td>nearly</td>
</tr>
</tbody>
</table>

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

**Distance function** Define \( \text{dist} : \text{SO}(3) \times \text{SO}(3) \rightarrow \mathbb{R} \)

\[
\text{dist}(R_1, R_2) = \sqrt{2 \text{tr}(I - R_2^T R_1)}
\]

**Potential energy**

\[
V_\alpha(R) = (\text{dist}(R, I) - 1)^2 - \frac{\alpha}{\text{dist}(R, R_m)}.
\]
**Numerical experiment**

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bounded potential
Numerical experiment

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$$\text{dist}(R_1, R_2) = \sqrt{2 \text{tr}(I - R_2^T R_1)}$$

**Potential energy**

$$V_\alpha(R) = (\text{dist}(R, I) - 1)^2 - \frac{\alpha}{\text{dist}(R, R_m)}. \quad \text{Coulomb potential}$$
Minimum values for the potential attained in

\[ S \overset{\text{def}}{=} \{ \mathbf{R} \in SO(3) : \text{dist}(\mathbf{R}, I) = 1 \}. \]

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

Potential field with \( \alpha = 0 \) in the angle/axis representation.
If $\alpha$ is sufficiently small and $\mathbf{R}_m$ is sufficiently far, $S$ gets slightly perturbated into $S_{\alpha}$, a set of local minima.

$S_{\alpha} \times \{0\}$ inherits the same stability properties.
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 $S_\alpha$, with small body angular velocity.

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

- (conjugate-)symplecticity as a key property for the long-time behavior of numerical integrators
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- 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
Numerical integration on homogeneous spaces
Introduction

Unitary sphere $\mathbb{S}^2$

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

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

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

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

$$q(t) = R(t)q(0)$$
Problems arising

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

**Isotropy group**

$$\mathcal{H}_q = \{ R \in \text{SO}(3) | Rq = q \}$$

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

To our knowledge, in literature there exist no methods to describe in a unique way the flow on the quotient space $\text{SO}(3)/\mathcal{H}_q$. 
**Variational approach**

**Lagrangian**

The configuration is described by \((q_i, \dot{q}_i), \ i = 1, \ldots, n\), where

- \(q_i \in S^2;\)
- \(\dot{q}_i \in T_{q_i}S^2, \ \dot{q}_i \perp q_i.\)

The unit sphere \(S^2\) with the tangent space \(T_qS^2\).
Variational approach

**Lagrangian** Configuration space $T(S^2)^n$.

$$L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) = \sum_{i=1}^{n} \frac{1}{2} \dot{q}_i^T \mathbb{I} \dot{q}_i - V(q_1, \ldots, q_n)$$
Variational approach

**Lagrangian** Configuration space $T(S^2)^n$.

$$L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) = \sum_{i=1}^{n} \frac{1}{2} \dot{q}_i^T \mathbb{I}_i \dot{q}_i - V(q_1, \ldots, q_n)$$

Equations of motion (Lee et al., 2009) on $T(S^2)^n$:

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

where

$$0 = q_i \cdot \omega_i$$
$$0 = q_i \cdot \dot{\omega}_i$$
Adapting Lie methods

Basic idea:

\[ \dot{q}_i(t) = \dot{R}_i(t)q_i(0) \]
\[ = \omega_i \times q_i(t) \]
\[ = \omega_i \times R_i(t)q_i(0) \]

Dynamics on SO(3):

\[ \dot{R}_i = \omega_i \times R_i \]

\[ \mathbb{I}_{ij} \omega_i = \sum_{j=1 \atop j \neq i}^n \left( \mathbb{I}_{ij} R_iq_i(0) \times (R_j q_j(0) \times \dot{\omega}_j) + \right. \]
\[ \left. + \mathbb{I}_{ij} \|\omega_j\|^2 R_iq_i(0) \times R_j q_j(0) \right) - R_iq_i(0) \times \frac{\partial V}{\partial q_i} \]
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Dynamics on SO(3):

\[ \dot{R}_i = \omega_i \times R_i \]

\[ \sum_{j=1}^{n} (\mathbb{I}_{ij} R_i q_i(0) \times (R_j q_j(0) \times \omega_j) + \mathbb{I}_{ij} \| \omega_j \|^2 R_i q_i(0) \times R_j q_j(0)) - R_i q_i(0) \times \frac{\partial V}{\partial q_i} \]

\( \omega_i \) is the spatial angular velocity!
Numerical example

Double spherical pendulum

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

- geometric method which preserves the configuration space of the system
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- off-the-shelf Lie methods can be used for the integration of Hamiltonian systems on unitary spheres, obtaining arbitrarily high order methods
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Future work

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