GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK e.V.
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Novel geometric integrators for multibody systems

Motivation

Certain coordinate-choices for MBS can yield singular mass matrices, which complicate the direct transition from the Lagrangian framework with

$$L(\mathbf{q},\dot{\mathbf{q}}) = T(\mathbf{q},\dot{\mathbf{q}}) - V(\mathbf{q}) = \frac{1}{2}\dot{\mathbf{q}}^{\mathsf{T}}\mathbf{M}(\mathbf{q})\dot{\mathbf{q}} - V(\mathbf{q})$$

to Hamiltonian mechanics (Legendre transformation).

- **Problem:** Hamiltonian formulations, with $\mathbf{M}$ constant and invertible, are the standard choice for energy-momentum (EM) integrators.
- **Goal:** Provide a suitable dynamics framework and design EM scheme.

Livens principle with constraints

Mixed variational formulation with Lagrange multipliers $\boldsymbol{\lambda}, \mathbf{p}$

$$\delta \int_0^T \left[L(\mathbf{q},\mathbf{v}) + \mathbf{p}\cdot(\dot{\mathbf{q}} - \mathbf{v}) - \boldsymbol{\lambda}\cdot\mathbf{g}(\mathbf{q})\right] dt = 0$$

yields index-3 DAEs with independent $(\mathbf{q},\mathbf{v},\mathbf{p})$, see [1],

$$\begin{aligned}\dot{\mathbf{q}} &= \mathbf{v}\,,\\ \dot{\mathbf{p}} &= \partial_{\mathbf{q}}T(\mathbf{q},\mathbf{v}) - \nabla V(\mathbf{q}) - \nabla\mathbf{g}(\mathbf{q})^{\mathsf{T}}\boldsymbol{\lambda}\,,\\ \mathbf{p} &= \partial_{\mathbf{v}}T(\mathbf{q},\mathbf{v}) = \mathbf{M}(\mathbf{q})\mathbf{v}\,,\\ \mathbf{0} &= \mathbf{g}(\mathbf{q})\,.\end{aligned}$$

Conserved quantities:

- Generalized total energy $E(\mathbf{q},\mathbf{v},\mathbf{p}) = \mathbf{p}\cdot\mathbf{v} - L(\mathbf{q},\mathbf{v})$
- Momentum maps $L_\xi(\mathbf{q},\mathbf{p}) = \mathbf{p}\cdot\xi\mathbf{q}$ corresponding to symmetries

Application: Quaternion-based rigid body rotations, [1]

- Euler parameters $\mathbb{q} = (q_0,\mathbf{q}) \in S^3 \simeq \mathbb{R}^4$ satisfying $\mathbb{q}\cdot\mathbb{q} = 1$
- Convective angular velocity $\boldsymbol{\Omega}(\mathbb{q},\mathbb{v}) = 2\mathbf{G}(\mathbb{q})\mathbb{v}$, $\mathbf{G}\in\mathbb{R}^{3\times 4}$, yielding a singular mass matrix in

$$T = \frac{1}{2}\boldsymbol{\Omega}\cdot\mathbf{J}_0\boldsymbol{\Omega} = \frac{1}{2}\mathbb{v}\cdot\mathbf{M}_4(\mathbb{q})\mathbb{v} \quad \text{with} \quad \mathbf{M}_4(\mathbb{q}) = 4\mathbf{G}(\mathbb{q})^{\mathsf{T}}\mathbf{J}_0\mathbf{G}(\mathbb{q})$$

- Existing EM methods use rank augmentation techniques and artificial inertia parameters.
  $\Rightarrow$ **Here:** Singular matrix can be used as it is. ✓

Livens-based EM method

Making use of (partial) discrete derivatives by Gonzalez, one obtains the EM scheme with constant $h = t^{n+1} - t^n$ given by

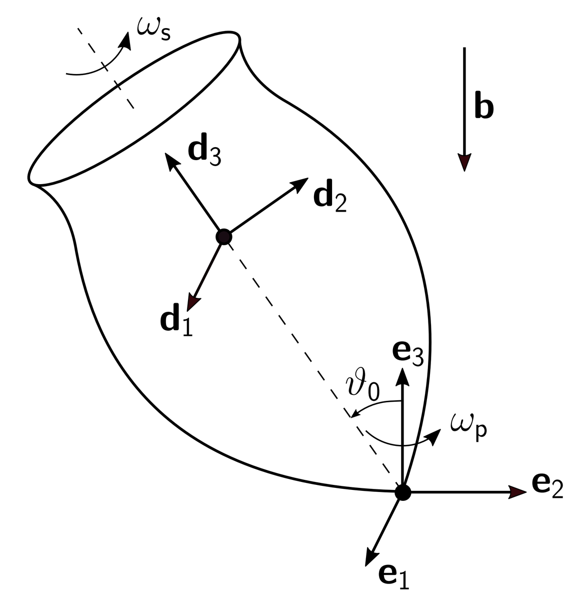
$$\begin{aligned}\mathbf{q}^{n+1} - \mathbf{q}^n &= h\,\mathbf{v}^{n+1/2}\,,\\ \mathbf{p}^{n+1} - \mathbf{p}^n &= h\overline{\partial}_{\mathbf{q}}T(\mathbf{q},\mathbf{v}) - h\overline{\nabla}V(\mathbf{q}) - h\sum_{k=1}^m \lambda_k\overline{\nabla}g_k(\mathbf{q})\,,\\ \mathbf{p}^{n+1/2} &= \overline{\partial}_{\mathbf{v}}T(\mathbf{q},\mathbf{v}) = \frac{1}{2}\left(\mathbf{M}(\mathbf{q}^n) + \mathbf{M}(\mathbf{q}^{n+1})\right)\mathbf{v}^{n+1/2}\,,\\ \mathbf{g}(\mathbf{q}^{n+1}) &= \mathbf{0}\,.\end{aligned}$$

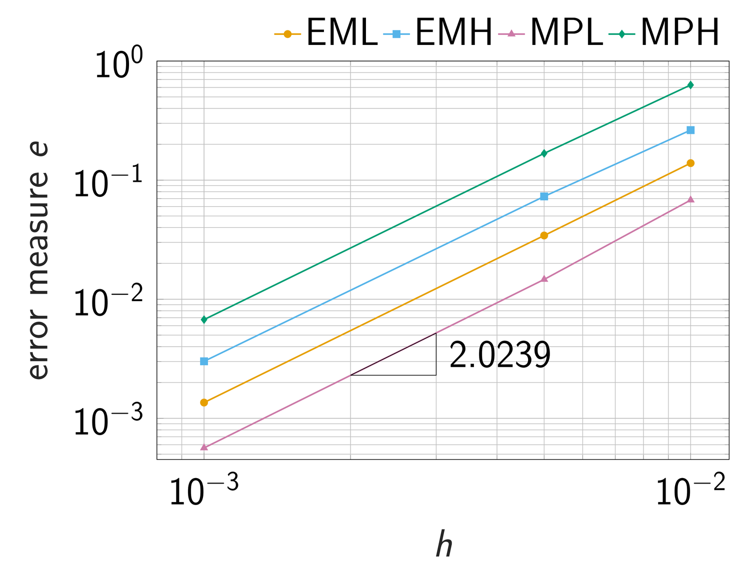
- Discrete conservation properties $\forall n \in \{0,\dots,N-1\}$

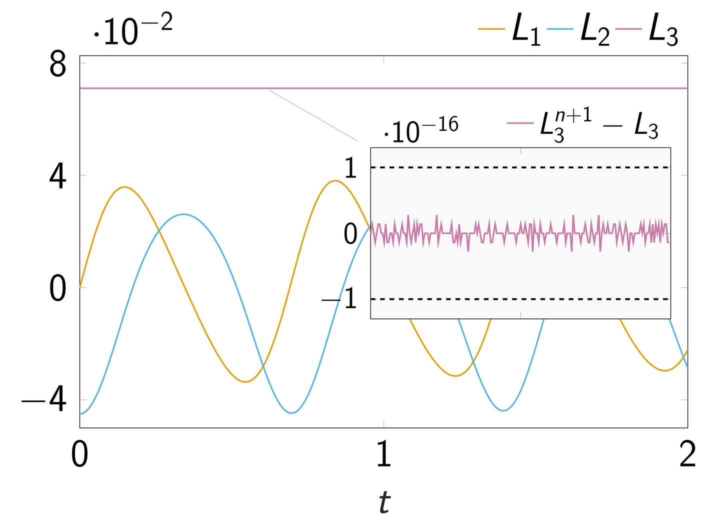
$$E^{n+1} - E^n = 0\,,\quad L_\xi^{n+1} - L_\xi^n = 0\,,\quad \mathbf{g}^{n+1} = \mathbf{0}\,.$$

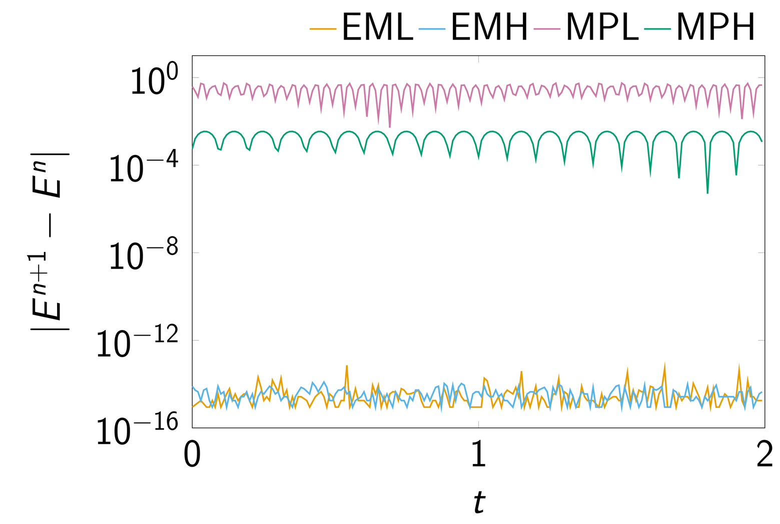
- If $\mathbf{M} = \mathbf{M}(\mathbf{q})$: No direct transition to Lagrange/Hamilton is feasible in discrete time. Livens-based equations largely facilitate the EM design.

Numerical results: Heavy top









Previous work: GGL principle

Variational principle with explicit velocity constraints, see [2],

$$\delta \int_0^T \left[L(\mathbf{q},\mathbf{v}) - \boldsymbol{\lambda}\cdot\mathbf{g}(\mathbf{q}) + \mathbf{p}\cdot(\dot{\mathbf{q}} - \mathbf{v} - \mathbf{M}^{-1}\nabla\mathbf{g}(\mathbf{q})^{\mathsf{T}}\boldsymbol{\gamma})\right] dt = 0$$

mimics the well-known GGL stabilization, yielding index-2 DAEs with Hamiltonian structure

$$\begin{aligned}\dot{\mathbf{q}} &= \mathbf{v} + \mathbf{M}^{-1}\nabla\mathbf{g}(\mathbf{q})^{\mathsf{T}}\boldsymbol{\gamma}\,,\\ \mathbf{M}\dot{\mathbf{v}} &= \partial_{\mathbf{q}}L(\mathbf{q},\mathbf{v}) - \nabla\mathbf{g}(\mathbf{q})^{\mathsf{T}}\boldsymbol{\lambda} - \sum_{k=1}^m \gamma_k\nabla^2 g_k(\mathbf{q})\mathbf{v}\,,\\ \mathbf{0} &= \mathbf{g}(\mathbf{q})\,,\\ \mathbf{0} &= \nabla\mathbf{g}(\mathbf{q})\mathbf{v}\,.\end{aligned}$$

- Derivation of novel variational integrators and EM method, see [3]
- **Outlook:** Overcome restriction in [2],[3] to constant and invertible mass matrices with newly gained insights

References

[1] P. L. Kinon and P. Betsch. "Conserving integration of multibody systems with singular and non-constant mass matrix including quaternion-based rigid body dynamics". In: *Multibody Syst. Dyn. (under revision)* (2024). (pre-print). DOI: https://doi.org/10.21203/rs.3.rs-3999974/v1

[2] P. L. Kinon, P. Betsch, and S. Schneider. "The GGL variational principle for constrained mechanical systems". In: *Multibody Syst. Dyn.* 57 (2023), pp. 211–236

[3] P. L. Kinon, P. Betsch, and S. Schneider. "Structure-preserving integrators based on a new variational principle for constrained mechanical systems". In: *Nonlinear Dyn.* 111 (2023), pp. 14231–14261

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