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A Mixed Variational Framework for the Structure-preserving Integration of Dynamical Systems with Primary and Secondary Constraints

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Constrained Dynamics

Systems with Scleronomic, Holonomic Constraints

- primary constraints on configuration level

$$\mathbf{g}(\mathbf{q}) = \mathbf{0}$$

- consistency condition induces secondary constraints

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{g}(\mathbf{q}) = \mathrm{D}\mathbf{g}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0}$$

- exhibit same conservation properties as unconstrained systems
- emerging index-3 DAEs are prone to numerical ill-conditioning

Classical Gear-Gupta-Leimkuhler Stabilization [1]

$$\begin{aligned}\dot{\mathbf{q}} &= \mathbf{M}^{-1}\mathbf{p} + \mathrm{D}\mathbf{g}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\\ \dot{\mathbf{p}} &= -\mathrm{D}V(\mathbf{q}) - \mathrm{D}\mathbf{g}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda}\\ \mathbf{0} &= \mathbf{g}(\mathbf{q})\\ \mathbf{0} &= \mathrm{D}\mathbf{g}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\end{aligned}$$

- minimal extension couples secondary constraints into equations
- equivalent to standard DAEs ($\gamma = \mathbf{0}$), lost Hamiltonian structure
- index reduced to 2, numerically more reliable

Novel GGL Variational Principle

Augmented Action Integral

$$S(\mathbf{q},\mathbf{v},\mathbf{p},\boldsymbol{\lambda},\boldsymbol{\gamma}) = \int_0^T \Big[L(\mathbf{q},\mathbf{v}) - \boldsymbol{\lambda}\cdot\mathbf{g}(\mathbf{q}) + \mathbf{p}\cdot\big(\dot{\mathbf{q}} - \mathbf{v} - \mathbf{M}^{-1}\mathrm{D}\mathbf{g}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\big)\Big]\,\mathrm{d}t$$

- enhances Livens principle [2] with multipliers $\boldsymbol{\lambda},\boldsymbol{\gamma}$ to account for primary and secondary constraints
- conjugate momenta $\mathbf{p}$ enforce kinematic relation $\dot{\mathbf{q}} = \mathbf{f}^{\gamma}(\mathbf{q},\mathbf{v})$
- unifies Lagrangian and Hamiltonian formalisms

Euler-Lagrange Equations: $\delta S = 0$

$$\begin{aligned}\dot{\mathbf{q}} &= \mathbf{v} + \mathbf{M}^{-1}\mathrm{D}\mathbf{g}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\gamma}\\ \dot{\mathbf{p}} &= \mathrm{D}_1 L(\mathbf{q},\mathbf{v}) - \mathbf{M}^{-1}\mathrm{D}\mathbf{g}(\mathbf{q})^{\mathrm{T}}\boldsymbol{\lambda} - \sum_{k=1}^{m}\gamma_k \mathrm{D}^2 g_k(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\\ \mathbf{p} &= \mathrm{D}_2 L(\mathbf{q},\mathbf{v})\\ \mathbf{0} &= \mathbf{g}(\mathbf{q})\\ \mathbf{0} &= \mathrm{D}\mathbf{g}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\end{aligned}$$

- Hamiltonian structure with augmented Hamiltonian

$$\mathcal{H}_{\lambda\gamma}(\mathbf{q},\mathbf{p}) = H(\mathbf{q},\mathbf{p}) + \boldsymbol{\lambda}\cdot\mathbf{g}(\mathbf{q}) + \boldsymbol{\gamma}\cdot\mathrm{D}\mathbf{g}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}$$

- equivalent to standard DAEs ($\gamma = \mathbf{0}$)
- conservation properties hold independent of value of γ

One-stage Variational Integrator

Discrete Action Integral

$$\mathcal{S}_{\mathrm{d}} = \sum_{n=0}^{N-1}\Big[L_{\mathrm{d}}^{\lambda}(\mathbf{q}^n,\mathbf{Q}^n,\mathbf{v}^{n+1}) + \mathbf{p}^{n+1}\cdot\big(\mathbf{q}^{n+1} - \mathbf{q}^n - \mathbf{f}_{\mathrm{d}}^{\gamma}(\mathbf{q}^n,\mathbf{Q}^n,\mathbf{v}^{n+1})\big) + \mathbf{P}^n\cdot\big(\mathbf{Q}^n - \mathbf{q}^n - \mathbf{f}_{\mathrm{d}}^{\gamma}(\mathbf{q}^n,\mathbf{Q}^n,\mathbf{v}^{n+1})\big)\Big]$$

- structure with auxiliary variables $\mathbf{Q}^n$,$\mathbf{P}^n$ inspired by [3]
- discrete augmented Lagrangian L_{d}^{λ} and discrete kinematic relation $\mathbf{f}_{\mathrm{d}}^{\gamma}$ yield various integrators
- yields symplectic methods: $\mathrm{d}\mathbf{q}^{n+1}\wedge\mathrm{d}\mathbf{p}^{n+1} = \mathrm{d}\mathbf{q}^{n}\wedge\mathrm{d}\mathbf{p}^{n}$

One-parameter VI

$$\begin{aligned}L_{\mathrm{d}}^{\lambda}(\mathbf{q}^n,\mathbf{Q}^n,\mathbf{v}^{n+1}) &= L(\mathbf{q}^{n+\theta},\mathbf{v}^{n+1}) - \boldsymbol{\lambda}^n\cdot\mathbf{g}_{\mathrm{d}}(\mathbf{q}^n,\mathbf{Q}^n)\\ \mathbf{q}^{n+\theta} &= (1-\theta)\,\mathbf{q}^n + \theta\,\mathbf{q}^{n+1}\end{aligned}$$

- discrete capture of conserved angular momentum: $L_i^{n+1} = L_i^n$
- $\mathbf{g}_d = \mathbf{g}(\mathbf{q}^{n+\theta})$: second-order for $\theta = 0.5$, violates constraints
- $\mathbf{g}_{\mathrm{d}} = \frac{h}{2}\left[\mathbf{g}(\mathbf{q}^n) + \mathbf{g}(\mathbf{q}^{n+1})\right]$: first-order accurate, fulfills both constraints for $\theta = 1$

Energy-Momentum Scheme for GGL

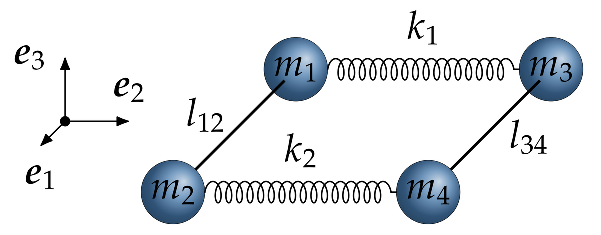
- application of discrete derivatives to equations of motion in abstract Hamiltonian form, extension of [4]

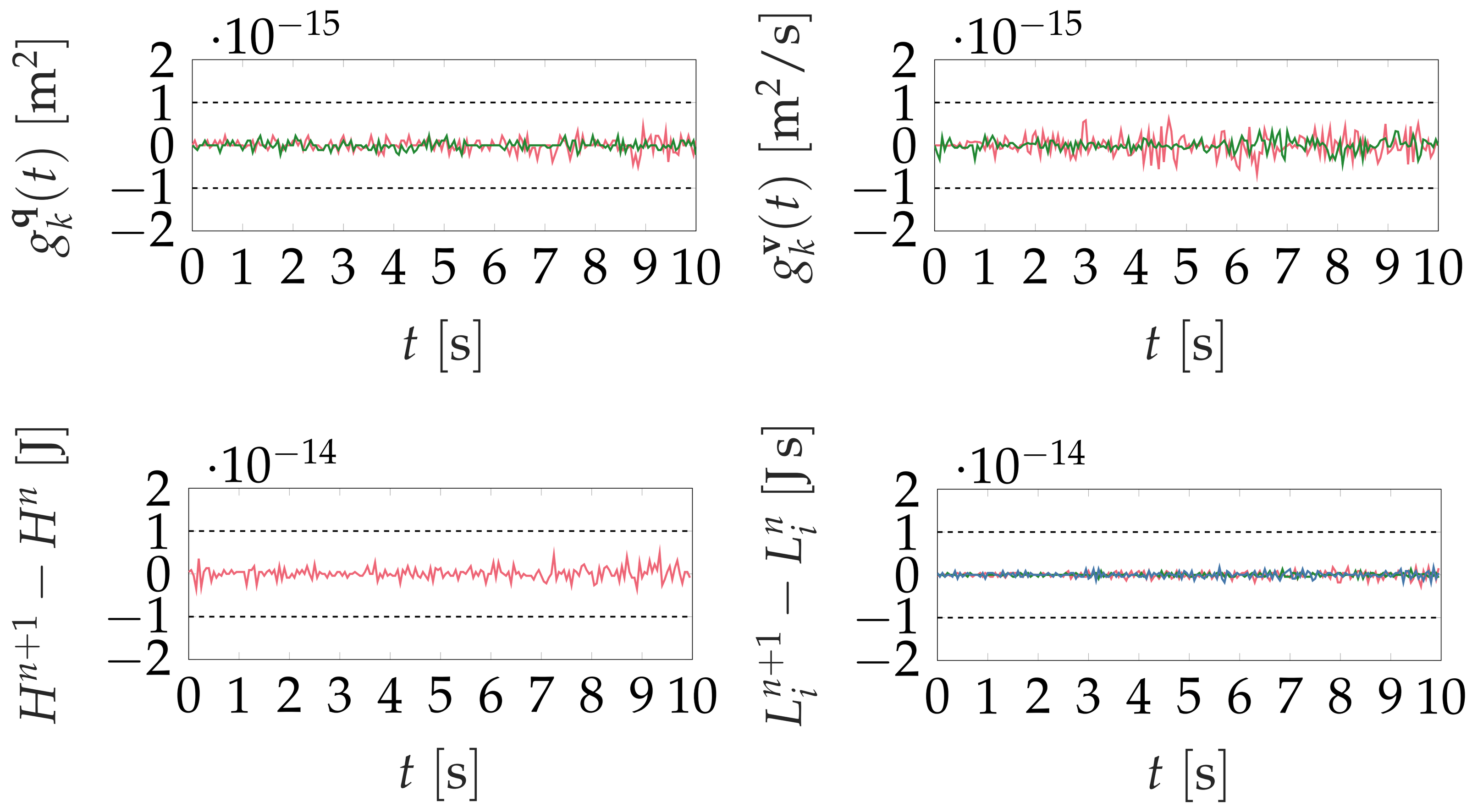
$$\begin{aligned}\dot{\mathbf{z}} &= \mathbb{J}\mathrm{D}\mathcal{H}_{\lambda\gamma}(\mathbf{z}) & \mathbf{z}^{n+1} - \mathbf{z}^n &= h\,\mathbb{J}\,\mathrm{D}^{\mathrm{G}}\mathcal{H}_{\lambda\gamma}(\mathbf{z}^n,\mathbf{z}^{n+1})\\ \mathbf{0} &= \mathbf{g}(\mathbf{q}) & \mathbf{0} &= \mathbf{g}(\mathbf{q}^{n+1})\\ \mathbf{0} &= \mathrm{D}\mathbf{g}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p} & \mathbf{0} &= \mathrm{D}\mathbf{g}(\mathbf{q}^{n+1})\mathbf{M}^{-1}\mathbf{p}^{n+1}\end{aligned}$$

- phase space vector and canonical symplectic structure matrix

$$\mathbf{z} = \begin{bmatrix}\mathbf{q}\\ \mathbf{p}\end{bmatrix}, \quad \mathbb{J} = \begin{bmatrix}\mathbf{0} & +\mathbf{I}\\ -\mathbf{I} & \mathbf{0}\end{bmatrix}$$

- G-equivariant discrete derivative fulfills directionality condition
- conserves momentum maps, primary and secondary constraints and Hamiltonian, not symplectic
- numerical example: 4-particle-system





References

[1] Gear, C., Leimkuhler, B., and Gupta, G. Automatic integration of Euler-Lagrange equations with constraints. In: *Journal of Computational and Applied Mathematics*, 12-13: 77–90, 1985.

[2] Livens, G. On Hamilton's principle and the modified function in analytical dynamics. In: *Proceedings of the Royal Society Edinburgh*, 39(IX): 113–119, 1919.

[3] Betsch, P. and Becker, C. Conservation of generalized momentum maps in mechanical optimal control problems with symmetry. In: *International Journal for Numerical Methods in Engineering*, 111(2): 144–175, 2017.

[4] Gonzalez, O. Mechanical systems subject to holonomic constraints: Differential–algebraic formulations and conservative integration. In: *Physica D: Nonlinear Phenomena*, 132(1-2): 165–174, 1999.