Geometric modelling, integration and optimal control of flexible multibody dynamics

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EXTENDED ABSTRACT

1 Introduction

Studying nonlinear mechanical systems from a geometric point of view, one finds that symmetries and invariants contain valuable information on their behaviour. These structural properties play a fundamental role when designing numerical methods leading to so called geometric or structure preserving simulation tools. For example, variational integrators yield symplectic-momentum conserving approximate trajectories. The benefits of structure preserving algorithms are widely accepted. On the one hand, the fidelity of the approximate solution is improved compared to standard methods by representing symmetries and invariants correctly. On the other hand, their preservation stabilises the numerical integration, which is beneficial for the computational costs with regard to the required grid resolution and longterm simulation.

First, this talk addresses the development of structure preserving variational numerical methods for the simulation of ordinary differential equations (ODEs) describing for example the dynamics of rigid multibody systems. Then, the focus is on the derivation of the nonlinear dynamic equations of geometrically exact beams in a variational setting and their integration in flexible multibody system dynamics, e.g. using redundant coordinate or LIE group formulations. In addition to the standard ODE case in time, variational integrators will be presented for static beam equilibria as well as for the partial differential equation (PDE) case of flexible multibody dynamics. After that, optimal control problems are considered and the role of structure perservation for their approximate solution is discussed.

2 Variational integrators – structure preservation

An overview on the derivation of the continuous and discrete EULER–LAGRANGE equations derived via variational principles as well as their structural properties is given in Figure 2. In general, the LAGRANGIAN of a dynamical ODE system consists of the difference between kinetic and potential energy. Then HAMILTON's principle of stationary action leads to the EULER–LAGRANGE equations. Thereby, the whole curve except for the end points is varied and the variational principle must hold for all possible varied curves. Classical mechanics tells us, that the solution of the EULER–LAGRANGE equations – the LAGRANGIAN flow – is symplectic and energy conserving. Furthermore, according to NOETHER's theorem, invariance of the Lagrangian leads to the conservation of a momentum map (for example linear or angular momentum) along the LAGRANGIAN flow.

Standard numerical schemes aim at a discretisation of the EULER–LAGRANGE equations. The key idea of variational integrators is to start the discretisation already at the level of the variational principle [10]. The curve is replaced by a discrete path of configurations and the LAGRANGIAN is replaced by a discrete LAGRANGIAN, which is an approximation of the action integral over the continuous one. In the shown case, it depends on two subsequent discrete configurations. The kinetic energy involves a finite difference approximation of the velocity and the potential energy is evaluated e.g. at the midpoint leading to a second order accurate scheme. In general, one can choose a polynomial to approximate the trajectory and a quadrature rule to approximate the action integral to derive higher order schemes.

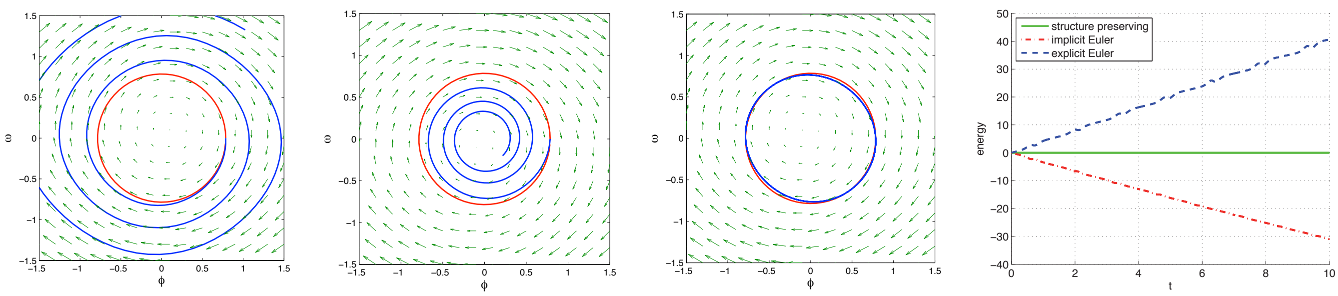

Figure 1: Phase portrait of a circular pendulum (red circle) in it's vector field (green arrows) and approximation of the phase portrait (blue line) using the explicit Euler method (left, spiraling outward), the implicit Euler method (second left, spiraling inward) and the structure preserving symplectic Euler method (second right, almost circular) and the corresponding evolution of the total energy of the simulations.

In this way, the action integral transforms into an action sum. Stationarity of this action sum requires to take variations of the discrete configurations and the variational principle must hold for all paths of varied configurations. This procedure results in the discrete EULER–LAGRANGE equations which constitute a time-stepping scheme. Due to its derivation via a discrete variational principle, the solution is guaranteed to be structure preserving, which means it is symplectic, and there exists a discrete NOETHER's theorem guaranteeing that it conserves (maximally quadratic) momentum maps exactly in the presence of symmetry. Furthermore, backward error analysis [13] tells us, that the energy error stays bounded also for longterm simulations. Finally, there is a tool called variational error analysis [10, 12] relating the order of accuracy of a variational integrator to the accuracy of the approximation of the action integral.

Since symplecticity and also NOETHER's theorem are geometric properties (often called the geometric structure related to the differential geometry background of the formulation), integrators which are able to inherit this are named geometric or structure preserving integrators. Even though they approximate the trajectory, they are able to represent the unique fingerprint of a dynamical system correctly [10, 12, 5, 6, 13].

Figure 1 shows the approximation of the phase portrait of a circular pendulum using standard methods and symplectic integration. It can be observed that the standard methods exhibit an artificial gain or dissipation of energy. In contrast to that, the structure preserving symplectic method yields a phase portrait enclosing the correct area corresponding to a very good approximation of the system's energy conservation.

- LAGRANGIAN $L : T\mathscr{Q} \to \mathbb{R}$
- stationary action

$$\delta S = \delta \int_0^{t_N} L(q, \dot{q})\, dt = 0$$

- EULER–LAGRANGE equations

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = 0$$

- LAGRANGIAN flow

$$F_L^t : T\mathscr{Q} \to T\mathscr{Q}$$

- symplecticity
- NOETHER theorem
- energy conservation

- discrete LAGRANGIAN $L_d : \mathscr{Q} \times \mathscr{Q} \to \mathbb{R}$
- stationary discrete action

$$\delta S_d = \delta \sum_{i=0}^{N-1} L_d(q_i, q_{i+1}) = 0$$

- discrete EULER–LAGRANGE equations

$$D_1 L_d(q_i, q_{i+1}) + D_2 L_d(q_{i-1}, q_i) = 0$$

- discrete LAGRANGIAN flow

$$F_{L_d}^{\Delta t} : \mathscr{Q} \times \mathscr{Q} \to \mathscr{Q} \times \mathscr{Q}$$

- symplecticity
- discrete NOETHER theorem
- good longterm energy behaviour
- variational error analysis

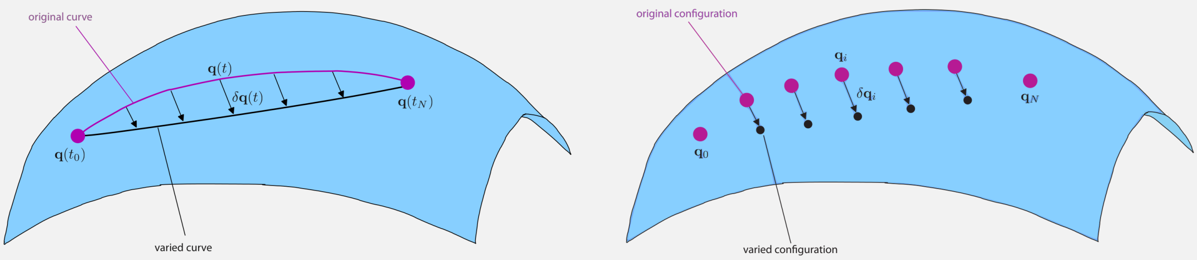

Figure 2: Derivation and structural properties of the continuous (left) and discrete (right) EULER–LAGRANGE equations. Here $\mathscr{Q}$ denotes the configuration manifold and $T\mathscr{Q}$ its tangent bundle containing the time dependent configuration and velocity $(q(t), \dot{q}(t))$ with time $t \in [0, t_N]$. In the discrete setting, q_i approximated the configuration at time node t_i and Δt denotes the time step.

3 LIE group formulation of flexible multibody dynamics

Over the history of modelling multibody systems [15, 1], a multitude of descriptions has evolved for the kinematics of interconnected masspoints, rigid and flexible bodies. Dealing with finite rotations and the interconnecting constraints imposes major challenges on the modelling as well as on numerical simulation procedures. In contrast to displacements/translations living in linear spaces, finite rotations live in nonlinear spaces, specifically in the special orthogonal LIE group $SO(3)$. As the latter is a manifold, the modelling of multibody systems is naturally and inextricably related to differential geometry and we may speak of geometric modelling.

A commonly used element in flexible multibody dynamics are geometrically exact COSSERAT beams. The COSSERAT beam model can undergo shear, elongation, bending and torsion. At every point $s \in [0, L]$ of the central line and at every time $t \in [0, t_N]$, the beam configuration variable can be chosen to represent the placement and a director triad representing the orientation of the cross-section. The assumption of rigidity of the cross-section requires orthonormality of the directors giving rise to holonomic constraints. Other structural elements like geometrically exact shells and rigid bodies can be modelled similarly by redundant configuration variables consisting of placements and directors subject to constraints. In this constrained description, the coupling of structural elements into flexible multibody systems via further constraints is straightforward – one arrives at a system of differential algebraic equations (DAEs). A simple model for the deformation energy of a COSSERAT beam is e.g. of ST. VENANT-KIRCHHOFF type. It is part of the potential energy involving derivatives with respect to the spatial parameter. The LAGRANGIAN density of beam dynamics also includes the kinetic energy with temporal derivatives such that the EULER–LAGRANGE equations of motion are PDEs on a domain with one temporal and one spatial dimension, see Figure 3.

However, the choice of coordinates representing the finite rotations is challenging, in particular spatial interpolations are necessary for the spatial discretisation. When the interpolation is done independently for the translational and the rotational degrees of freedom, this might lead to shear locking, meaning that the beam reacts overly stiff regarding shear. A standard workaround known from the field of finite element methods is under-integration. In contrast to that, shear locking can also be avoided when translational and rotational degrees of freedom are treated in a coupled way, which has to do with the geometric structure of the chosen configuration manifold. The special Euclidian group $SE(3)$ is a LIE group with a group operation that acts in a coupled way on the translational and rotational degrees of freedom [16, 7]. Of course, there are other ways to represent the translational and rotational degrees of freedom like EULER or CARDAN angles, or different LIE group formulations like unit quaternions, which all have advantages and and disadvantages for the representation of finite rotations.

For flexible multibody systems consisting of masspoints, rigid bodies and geometrically exact beams, the equations of motion can be derived as constrained PDEs from a variational principle, as summarised in Figure 3. Here, the action is a space-time integral. The solution is multisymplectic, energy-conserving and also a NOETHER theorem holds. We can derive structure preserving approximations to the flow via a discrete variational principle by approximating this action integral and requiring stationarity.

- LAGRANGIAN density $\quad L : SE(3) \times \mathfrak{se}(3)^2 \to \mathbb{R}$

$$L(q(s,t)\,\dot{q}(s,t)\,q'(s,t)) = T(q(s,t)\,\dot{q}(s,t)) - V(q(s,t)\,q'(s,t))$$

- constrained variational principle

$$\delta S = \delta \int_0^{t_N}\int_0^L \left[L\left(q(s,t),\dot{q}(s,t),q'(s,t)\right) + \langle \lambda(s,t), c(q(s,t))\rangle\right] \mathrm{d}s\,\mathrm{d}t = 0$$

- constrained EULER–LAGRANGE equations

$$P^T(q)\cdot\left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{d}{ds}\left(\frac{\partial L}{\partial q'}\right)\right] = 0$$
$$c(q) = 0$$

- multisymplecticity
- NOETHER theorem
- energy conservation

Figure 3: Fully variational derivation of the equations of motion for flexible multibody systems consisting of masspoints, rigid bodies and geometrically exact beams. Here, the Lagrangian density (kinetic T minus potential V energy density) depends on the space-time dependent configuration variable $q(s,t)$ as well as on its temporal and spatial derivatives $\dot{q}(s,t), q'(s,t)$, respectively. The constraints $c(q) = 0$ represent the coupling of the interconnected bodies as well as internal constraints depending on the representation of the finite rotations. They are enforced via LAGRANGE multipliers λ, which are then eliminated by a null-space matrix $P(q)$, that project the dynamics to the correct tangent space.

In Figure 7 (left), an example of a forward dynamics simulation of a flexible slider crank system is shown, where the colours represent the stress in the flexible parts. Figure 4 shows snapshots of the motion of a beam with concentrated masses. This beam's LAGRANGIAN is invariant with respect to translation and rotation. Thus according to NOETHER's theorem, linear and angular momentum are conserved after the loading phase, as is the total energy.

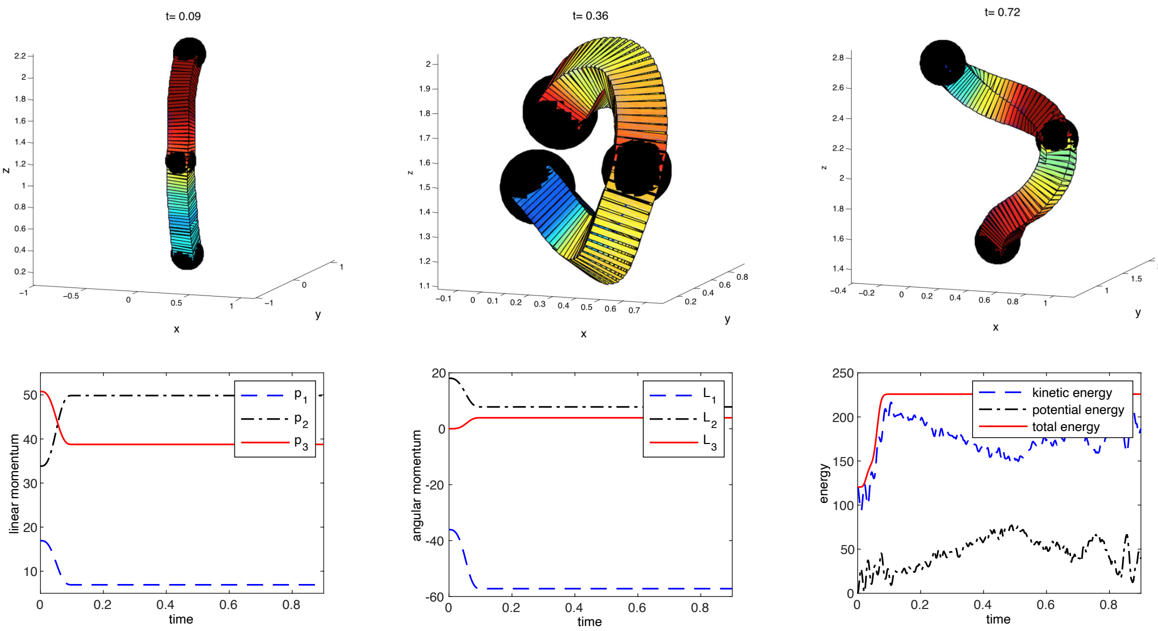

Figure 4: Geometrically exact beam with concentrated masses; snapshots of motion and deformation (top) and preservation of linear and angular momentum and energy after the loading phase (bottom) [3].

4 Optimal control problem simulation

A classical optimal control problem is e.g. the reorientation of a spacecraft from a given initial to a given final state while minimising a certain objective like the consumption of energy. The spacecraft in Figure 7 (right) can be represented as a rigid main body and flexible appendages.

· minimise objective functional

$$\min_{y,\tau} J(y,\tau) = \int_0^{t_N} C(y(t),\tau(t))dt + \Phi(y(t_N))$$

$$\text{subject to} \quad \dot{y}(t) = f(y(t),\tau(t)) \qquad y(t_0) = \bar{y}_0$$

· indirect methods: first optimise – then discretise

· direct methods: first discretise – then optimise

Figure 5: In an optimal control problem, an objective functional J (here e.g. consisting of the integral over a running cost C and a boundary term Φ) is minimised with respect to the state and control trajectories $y(t),\tau(t)$, while fulfilling the system's dynamics equations (e.g. with a right hand side function f) and boundary conditions (e.g. given initial state $\bar{y}_0$). For the numerical solution , one can classify direct and indirect methods, which differ in the order of optimisation and discretisation.

Why is structure preserving integration also interesting in the numerical solution of optimal control problems? One distinguishes two different approaches for the numerical solution of optimal control problems, as illustrated in Figure 5. First optimise then discretise yields an indirect method. PONTRYAGIN's maximum principle is applied to the HAMILTONIAN of the optimal control problem, yielding the necessary optimality conditions. This results in the state-adjoint system being a boundary value problem, which can be discretised and solved. On the other side, direct methods first discretise then optimise. The discretisation yields a finite dimensional constrained nonlinear optimisation problem. A cost function depending on the discrete path of state and control is minimised, while a discretisation of the system equations (together with boundary values) serves as constraints. The optimisation results in the KARUSH KUHN TUCKER (KKT) conditions.

Naturally, the question arises, under which conditions the discretisation and optimisation steps commute and what are the convergence orders for the state, control and adjoint variables. While in indirect methods, one actively chooses numerical methods of particular order for the state-adjoint system, in direct methods one only chooses an integrator for the system equations and the particular integration scheme (and its order) for the adjoint and control variables is determined in the procedure of deriving the KKT conditions.

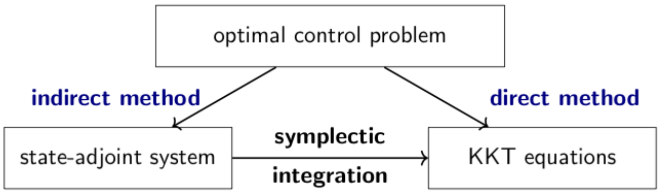

Figure 6: Symplectic methods provide a link between indirect and direct methods for the approximate solution of optimal control problems.

To answer these questions, symplectic methods play a major role. First of all, they provide a link between indirect and direct methods in the sense that direct methods can be interpreted as a symplectic integration of the necessary optimality conditions [14, 11], as illustrated in Figure 6. In particular, solving the constrained nonlinear optimisation problem in direct methods means to augment the objective function by the product of the discretised system equations and a LAGRANGE multiplier and the derivation of the necessary optimality conditions (i.e. the KKT equations) can be interpreted as a discrete variational integrator which is thus symplectic. Thus the same approximation can be obtained by solving the state-adjoint system from the indirect method by a symplectic method. However, in general for direct methods, the schemes (and order) of approximation differs for the state, adjoint and control variables. This is the second place, where symplectic integration shows its benefits. Using a symplectic integration for the approximation of the system equations in the direct method, automatically yields the same scheme for the approximation in all variables, and thus also the same order or approximation [4, 2, 11].

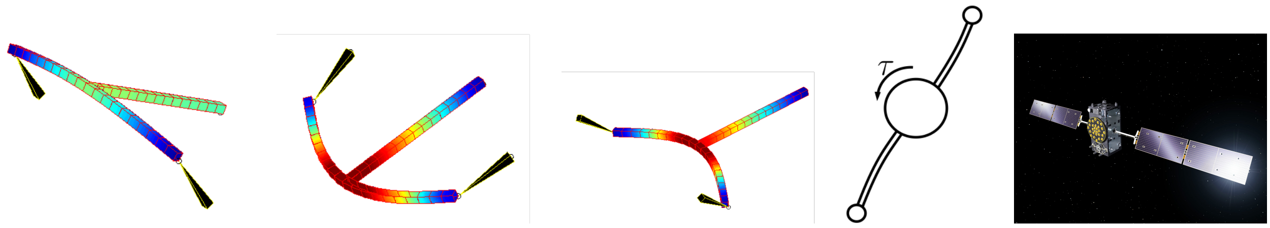

Figure 7: Slider crank mechanism consisting of geometrically exact beams and rigid bodies (left) [8] and spacecraft model consisting of rigid main body and flexible appendages (right) [9].

Acknowledgments

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References

[1] O. A. Bauchau. "Flexible multibody dynamics". Vol. 176. Springer (2011).

[2] J. F. Bonnans and J. Laurent-Varin. "Computation of order conditions for symplectic partitioned Runge-Kutta schemes with application to optimal control". In: *Numerische Mathematik* 103 (2006), pp. 1–10.

[3] F. Demoures, F. Gay-balmaz, S. Leyendecker, S. Ober-Blöbaum, T. Ratiu, and Y. Weinand. Discrete variational Lie group formulation of geometrically exact beam dynamics. In: *Numerische Mathematik* 130 (2014), pp. 73-123.

[4] W. W. Hager. "Runge-Kutta methods in optimal control and the transformed adjoint system". In: *Numerische Mathematik* 87 (2000), pp. 247– 282.

[5] E. Hairer, C. Lubich, and G. Wanner. "Geometric numerical integration illustrated by the Störmer–Verlet method". In: *Acta numerica* 12 (2003), pp. 399–450.

[6] E. Hairer, G. Wanner, and C. Lubich. Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. Springer (2006).

[7] T. Leitz, Rodrigo T. Sato Martin de Almagro, S. Leyendecker. Multisymplectic Galerkin Lie group variational integrators for geometrically exact beam dynamics based on unit dual quaternion interpolation – no shear locking. In: *Comput. Methods Appl. Mech. Engrg.* 374 (2021) 113475.

[8] S. Leyendecker, P. Betsch, and P. Steinmann. The discrete null space method for the energy-consistent integration of constrained mechanical systems. Part III: Flexible multibody dynamics. In: *Multibody Syst. Dyn.* 19 (2008), pp. 45-72.

[9] Y. Lishkova, S. Ober-Blöbaum, M. Cannon, and S. Leyendecker. A multirate variational approach to simulation and optimal control for flexible spacecraft. In: *Advances in the Astronautical Sciences* 175 (2021), pp. 395-410.

[10] J. E. Marsden and M. West. "Discrete mechanics and variational integrators". In: *Acta numerica* 10 (2001), pp. 357–514.

[11] S. Ober-Blöbaum, O. Junge, and J. E. Marsden. "Discrete mechanics and optimal control: an analysis". In: *ESAIM: Control, Optimisation and Calculus of Variations* 17.2 (2011), pp. 322–352.

[12] G. W. Patrick and C. Cuell. "Error analysis of variational integrators of unconstrained Lagrangian systems". In: *Numerische Mathematik* 113 (2009), pp. 243–264.

[13] S. Reich. "Backward error analysis for numerical integrators". In: *SIAM Journal on Numerical Analysis* 36.5 (1999), pp. 1549–1570

[14] J. Sanz-Serna. "Symplectic methods". In: *Encyclopedia of Applied and Computational Mathematics*, B Engquist, Springer (2015), pp. 1451– 1458.

[15] W. Schiehlen. "Multibody system dynamics: roots and perspectives". In: *Multibody system dynamics* 1 (1997), pp. 149–188.

[16] V. Sonneville, O. Brüls, and O. A. Bauchau. Interpolation schemes for geometrically exact beams: A motion approach. In: *Internat. J. Numer. Methods Engrg.*, (2017), pp. 1129-1153.