

Variational integrators

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Discrete variational mechanics provides a geometric foundation for understanding symplectic and multisymplectic integrators for mechanical ODEs and PDEs. In this talk we will show how variational integrators are derived, including examples from existing methods, and discuss new methods which have been derived using the variational framework.

Variational integrators are constructed from a discrete version of Lagrangian mechanics, based on a discrete variational principle. This has the advantage that much of the structure of Lagrangian mechanical systems can be replicated on a discrete level, with variational proofs extending from the continuous to the discrete setting. In particular, variational integrators are naturally symplectic (for ODEs) or multisymplectic (for PDEs), and have conserved discrete momenta arising from symmetries of the system. In addition, the standard backward error analysis method can be applied to show that they typically have excellent long-time energy behavior.

Many standard methods have elegant variational derivations, including the conservative Newmark method in structural dynamics, the Verlet method in molecular dynamics, all symplectic and collocation Runge-Kutta methods, and some special methods such as the Moser-Veselov rigid body integrator. Variational integrators can be extended to include many additional features of mechanical systems. In particular, the discrete Lagrange-d'Alembert principle allows variational integrators to be constructed for systems with dissipation or external forcing, and constrained variational principles generate integrators for systems with holonomic or nonholonomic constraints. The detailed understanding of the discrete geometry also permits the construction of a discrete symmetry reduction theory, as well as the extension of variational methods to time-adaptive integrators and to the discretization of nonsmooth mechanical systems, such as those involving collisions and impact.

Aside from ODE problems, variational integrators provide a means of discretizing mechanical PDEs while preserving the geometric structure. Two particular examples of this are the construction of conservative asynchronous methods for structural mechanics problems and the development of circulation preserving integrators for fluid systems.