Simulating the *N*-body problem with variational integrators

Xavier Gràcia, Ángel Martínez*, Xavier Rivas

(*) Universitat Politècnica de Catalunya, Facultat de Matemàtiques i Estadística

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ABSTRACT Lagrangian and Hamiltonian formalisms offer powerful frameworks for analysing the dynamics of mechanical systems. A deeper insight into them is achieved by the usage of the tools of differential geometry. These tools can also be applied to improve the classical numerical methods by preserving the underlying geometric structures of the system. These methods, referred to as geometric integrators, are usually more robust and demonstrate better long-term stability.
We compare symplectic integrators with the well-known Runge–Kutta methods by applying them to several cases of the *n*-body problem. Through the simulations, we observe that variational integrators exhibit excellent preservation of the energy and angular momentum, whereas classical integrators do not conserve these quantities as well.

DISCRETE MECHANICS AND VARIATIONAL INTEGRATORS

The so-called variational integrators are obtained by discretising the variational principles, the action is approximated rather than the equations of motion. They constitute a modern approach towards the creation of numerical methods with structure-preserving qualities for Lagrangian and Hamiltonian systems. The main reference on this topic is the article [1] by J.E. Marsden and M. West.

Some of the most remarkable properties of variational integrators are:

- There exists a discrete version of Noether's theorem. This means that there is a conservation of the dynamic invariants corresponding to the symmetries of the original mechanical system if the discrete action sum is designed to preserve the same symmetries.
- There exists a discrete version of the Legendre transform. This allows for an equivalent construction of the variational integrator, which defines a discrete symplectic flow, i.e. a symplectic integrator.
- Provided a sufficiently small time-step there is a good conservation of the system's energy over long time periods.

DISCRETE LAGRANGIAN MECHANICS Take a configuration manifold Q. Instead of its tangent bundle $\mathrm{T}Q$, we consider $Q \times Q$, *the discrete state space* (which is locally diffeomorphic to $\mathrm{T}Q$). If we do this, the description of motion changes, as we do not consider paths on Q now, but rather sequences of points.

Definition

A *discrete Lagrangian* is a function $L_d \colon Q \times Q \times \mathbb{R} \to \mathbb{R}$. If we fix $h \in \mathbb{R}$, the *time-step*, we denote it by $L_d^h \colon Q \times Q \to \mathbb{R}$.

In discrete Lagrangian mechanics, the discrete Lagrangian at a point (q_0, q_1) serves as an approximation of the continuous action integrated over a solution path with fixed end-points q_0 and q_1, for a fixed time-step $h \in \mathbb{R}$. This means that

$$L_d^h(q_0, q_1) \approx \int_0^h L(q_{0,1}(t), \dot{q}_{0,1}(t))\,\mathrm{d}t\,,$$

where $q_{0,1}(t)$ is the unique solution of the Euler–Lagrange equations which connects points q_0 and $q_1 \in Q$.

Definition

Given $h \in \mathbb{R}$ and $N \in \mathbb{N}$, we can construct an increasing sequence of times $\{t_k = kh \mid k = 0, \dots, N\}$ and define the *discrete path space* to be

$$C_d^N(Q) = \{\gamma_d \colon \{t_k\}_{k=0}^N \to Q\}\,.$$

Consider a discrete Lagrangian $L_d^h \colon Q \times Q \to \mathbb{R}$. The *discrete action map* $S_d \colon C_d^N(Q) \to \mathbb{R}$ is given by

$$S_d(\gamma_d) = \sum_{k=0}^{N-1} L_d^h(q_k, q_{k+1})\,,$$

where $\gamma_d \in C_d(Q)$, with $\gamma_d(t_k) = q_k$, is a discrete path in Q.

Theorem

A sequence $\{q_k\}_{k=0}^N \subset Q$ is a critical value of the discrete action map among all sequences of points with fixed end-points if and only if it is a solution of the discrete Euler–Lagrange equations

$$\mathrm{D}_2 L_d^h(q_{k-1}, q_k) + \mathrm{D}_1 L_d^h(q_k, q_{k+1}) = 0\,, \tag{1}$$

for all $k = 1, \dots, N-1$.

Definition

Given a discrete Lagrangian $L_d^h \colon Q \times Q \to \mathbb{R}$, we can define two *discrete Legendre transformations* $\mathcal{F}^{\pm} L_d^h \colon Q \times Q \to \mathrm{T}^*Q$ as

$$\mathcal{F}^+ L_d^h(q_{k-1}, q_k) = (q_k, \mathrm{D}_2 L_d^h(q_{k-1}, q_k))\,, \quad \mathcal{F}^- L_d^h(q_{k-1}, q_k) = (q_{k-1}, -\mathrm{D}_1 L_d^h(q_{k-1}, q_k))\,.$$

We say that L_d^h is *regular* if at least one of the discrete Legendre transformations is a local diffeomorphism, which is equivalent to the matrix $\mathrm{D}_1\mathrm{D}_2 L_d^h$ being regular.

If L_d^h is regular then the discrete Euler–Lagrange equations (1) may be rewritten as

$$\mathcal{F}^+ L_d^h(q_{k-1}, q_k) = \mathcal{F}^- L_d^h(q_k, q_{k+1})\,.$$

This equation allows us to calculate q_{k+1} in terms of q_{k-1} and q_k, as the unique solution of the equation. Thus, we have a well-defined *discrete Lagrangian flow* $F_{L_d^h} \colon Q \times Q \to Q \times Q$ defined by

$$F_{L_d^h}(q_{k-1}, q_k) = (q_k, q_{k+1})\,.$$

DISCRETE SYMPLECTIC STRUCTURE The *discrete Lagrangian 1-forms* are defined by $\theta^{\pm}_{L_d^h} = (\mathcal{F}^{\pm} L_d^h)^* \theta_Q$, where θ_Q is the canonical 1-form. Their local expression is

$$\theta^+_{L_d^h}(q_0, q_1) = \mathrm{D}_2 L_d^h(q_0, q_1)\,\mathrm{d}q_1 = \frac{\partial L_d^h}{\partial q_1^i}\mathrm{d}q_1^i\,, \quad \theta^-_{L_d^h}(q_0, q_1) = -\mathrm{D}_1 L_d^h(q_0, q_1)\,\mathrm{d}q_0 = -\frac{\partial L_d^h}{\partial q_0^i}\mathrm{d}q_0^i\,.$$

If L_d^h is regular, then we can define the *discrete Lagrangian 2-form* as $\Omega_{L_d^h} = -\mathrm{d}\theta^+_{L_d^h} = -\mathrm{d}\theta^-_{L_d^h}$, its local expression is

$$\Omega_{L_d^h} = -\frac{\partial L_d^h}{\partial q_0^i \partial q_1^i}\mathrm{d}q_0^i \wedge \mathrm{d}q_1^i\,.$$

If the discrete Lagrangian L_d^h is regular, then $\Omega_{L_d^h}$ is a symplectic form. This symplectic form is preserved by the discrete Lagrangian flow $F_{L_d^h}$.

DISCRETE HAMILTONIAN MECHANICS Given a regular discrete Lagrangian L_d^h, the *discrete Hamiltonian flow* $\widetilde{F}_{L_d^h} \colon \mathrm{T}^*Q \to \mathrm{T}^*Q$ is defined as

$$\widetilde{F}_{L_d^h} = \mathcal{F}^+ L_d^h \circ (\mathcal{F}^- L_d^h)^{-1}\,, \qquad \widetilde{F}_{L_d^h} = \mathcal{F}^+ L_d^h \circ F_{L_d^h} \circ (\mathcal{F}^+ L_d^h)^{-1}\,, \qquad \widetilde{F}_{L_d^h} = \mathcal{F}^- L_d^h \circ F_{L_d^h} \circ (\mathcal{F}^- L_d^h)^{-1}\,,$$

where all equations are equivalent. The discrete Hamiltonian flow $\widetilde{F}_{L_d^h} \colon (q_0, p_0) \to (q_1, p_1)$ is defined locally by

$$p_0 = -\mathrm{D}_1 L_d^h(q_0, q_1)\,, \quad p_1 = \mathrm{D}_2 L_d^h(q_0, q_1)\,.$$

The discrete Hamiltonian flow $\widetilde{F}_{L_d^h}$ is symplectic with respect to the canonical 2-form ω_Q.

VARIATIONAL INTEGRATORS We can use discrete Lagrangian systems to approximate a given continuous Lagrangian system. This means that, if we consider a regular discrete Lagrangian L_d^h approximating a Lagrangian L, the discrete Lagrangian flow $F_{L_d^h} \colon (q_{k-1}, q_k) \to (q_k, q_{k+1})$ and its corresponding discrete Hamiltonian flow $\widetilde{F}_{L_d^h} \colon (q_k, p_k) \to (q_{k+1}, p_{k+1})$ are integrators for the respective continuous systems.

SIMULATING THE *N*-BODY PROBLEM

Let us simulate two cases of the *N*-body problem using different numerical methods. We study how symplectic integrators preserve the energy and the angular momentum and how this reflects on the trajectories of the system. We see the different behaviours that symplectic integrators exhibit in comparison to well-known Runge–Kutta integration schemes. The simulations were performed with MATLAB, and the codes are available at [3].

The *N*-body problem deals with predicting the motion of *n* point masses interacting through gravitational forces. In general, there is no closed-form solution for the *N*-body problem, and therefore we often require the use of numerical methods to solve it.
The Hamiltonian of the general *n*-body problem is

$$H = T(\mathbf{p}_1, \dots, \mathbf{p}_n) + U(\mathbf{r}_1, \dots, \mathbf{r}_n) = \sum_{i=1}^n \frac{|\mathbf{p}_i|^2}{2m_i} - \sum_{i<j}^n \frac{Gm_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}\,,$$

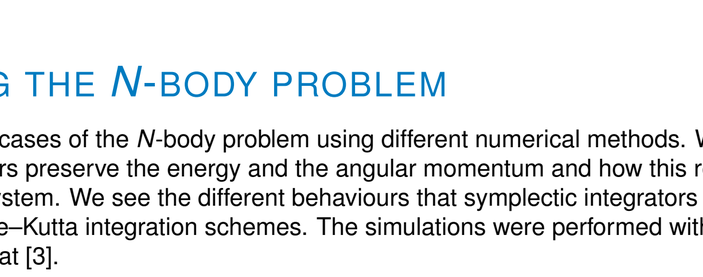
where G represents the gravitational constant and m_i, $\mathbf{r}_i = (x_i, y_i, z_i)$, $\mathbf{p}_i = (p_{x_i}, p_{y_i}, p_{z_i})$ represent respectively the mass, positions and momenta of the i-th body. From this, Hamilton's equations are

$$\dot{\mathbf{r}}_i = \frac{\partial H}{\partial \mathbf{p}_i} = \frac{\mathbf{p}_i}{m_i}\,, \quad \dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{r}_i} = -\sum_{j \neq i}^n \frac{Gm_i m_j(\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^3}\,.$$

The angular momentum L is also a constant of motion of this problem. It is given by

$$L = \sum_{i=1}^n m_i(\mathbf{r}_i \times \mathbf{p}_i)\,,$$

2-BODY PROBLEM We begin with an example of a case with $N = 2$. It is a well-known result that in this case all the trajectories are always confined to a plane.



(a) Explicit Euler (b) Symplectic Euler

Figure: Two-body problem total trajectories for explicit and symplectic Euler integrators with conditions $t = [0, 1000]$, $h = 0.01$, $m1 = 1$, $m2 = 5$, $G = 1$, $\mathbf{r}_{1,0} = (5, 0)$, $\mathbf{r}_{2,0} = (0, 0)$, $\mathbf{p}_{1,0} = (0, -1)$, $\mathbf{p}_{2,0} = (0, 1)$.

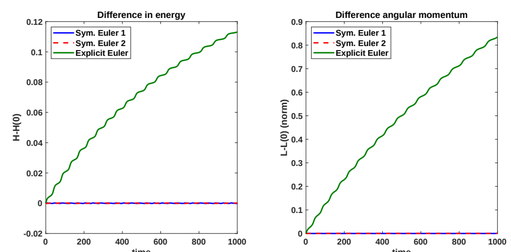
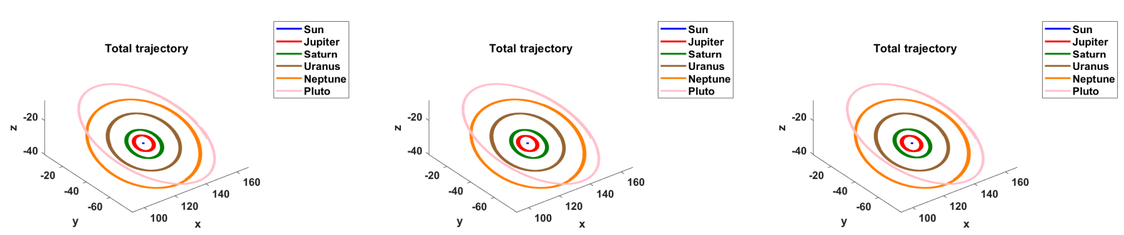


Figure: Comparison of energies and norms of angular momentum between explicit and symplectic Euler integrators, for a two-body problem with conditions $t = [0, 1000]$, $h = 0.01$, $m1 = 1$, $m2 = 5$, $G = 1$, $\mathbf{r}_{1,0} = (5, 0)$, $\mathbf{r}_{2,0} = (0, 0)$, $\mathbf{p}_{1,0} = (0, -1)$, $\mathbf{p}_{2,0} = (0, 1)$.

The explicit Euler method does not preserve the orbits of the bodies effectively, unlike the symplectic Euler method which demonstrates excellent performance. This is because the explicit Euler integrator steadily introduces energy into the system, the angular momentum is not preserved effectively either. Contrary to this, the symplectic Euler method demonstrates very good preservation of both the energy and the angular momentum.

THE OUTER SOLAR SYTEMS ($N = 6$) In this last example of the *n*-body problem, we simulate the outer solar system. The bodies considered are the Sun, Jupiter, Saturn, Uranus, Neptune and Pluto, and so $n = 6$. The initial data is from [2]. The masses are taken relative to the Sun, and the distances are in au (astronomical units). The time is in Earth days and the gravitational constant is $G = 2.95912208286 \cdot 10^{-4}$.



(a) Ralston (b) Runge–Kutta 3 (c) Störmer–Verlet

Figure: Simulation of the outer solar system with Störmer–Verlet 2 integrator. For $t = [0, 20000000]$, $h = 10$. The figures only show the last 20000 points.

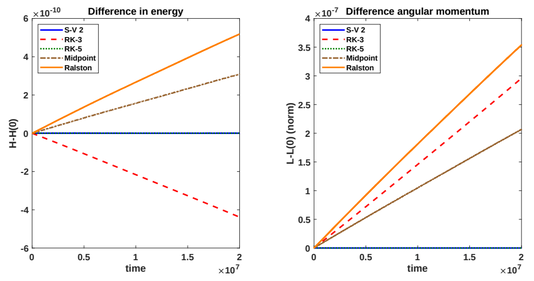


Figure: Simulation of the energies and norms of angular momentum from Störmer–Verlet 2 and Runge–Kutta methods for simulating the outer solar system. For $t = [0, 20000000]$ and $h = 10$. The Störmer–Verlet and Runge–Kutta 5 closely follow the $y = 0$ line in both figures.

The Störmer–Verlet method, which is symplectic and has order 2, is only comparable in its ability to preserve the two constants of motion to the Runge–Kutta 5 integrator. The other order 2 integrators exhibit a linear increase of energy and norm of angular momentum. Similarly, the Runge–Kutta 3 integrator exhibits a linear decrease of energy over time and an increase in the norm of angular momentum.

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