

A Supplementary Information for Fourth-Order Symplectic Integrator

Any numerical integration scheme that preserves the symplectic two-form $d\mathbf{p} \wedge d\mathbf{q}$ is said to be a symplectic integrator. These integrators are highly accurate and commonly employed for computing the time evolution of Hamiltonian systems. For a separable Hamiltonian $\mathcal{H} = T(\mathbf{p}) + V(\mathbf{q})$ with states $(\mathbf{q}_i, \mathbf{p}_i)$ at time t_i , a fourth order symplectic integrator may be implemented as shown in Algorithm 1. When implemented in PyTorch with tensor operations, we may use automatic differentiation to readily back-propagate through the integrator and accumulate losses.

Algorithm 1: Fourth-order Symplectic Integrator

Input : $\mathbf{q}_i, \mathbf{p}_i, t_i, t_{i+1}, \frac{\partial T}{\partial \mathbf{p}}, \frac{\partial V}{\partial \mathbf{q}}, \text{eps}$
Output : $\mathbf{q}_{i+1}, \mathbf{p}_{i+1}$

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1 steps  $\leftarrow (t_{i+1} - t_i) / (4 * \text{eps})$ ;
2 h  $\leftarrow (t_{i+1} - t_i) / \text{steps}$ ;
3 kq  $\leftarrow \mathbf{q}_i$ ;
4 kp  $\leftarrow \mathbf{p}_i$ ;
5 for i  $\leftarrow 1$  to steps do
6   | for j  $\leftarrow 1$  to 4 do
7   |   | tp  $\leftarrow \mathbf{kp}$ ;
8   |   | tq  $\leftarrow \mathbf{kq} + c_j * h * \frac{\partial T}{\partial \mathbf{p}}(\mathbf{kp})$ ;
9   |   | kp  $\leftarrow \mathbf{tp} - d_j * h * \frac{\partial V}{\partial \mathbf{q}}(\mathbf{kq})$ ;
10  |   | kq  $\leftarrow \mathbf{tq}$ ;
11  |   end
12 end
13 return kq, kp

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Note that $c = [c_1, c_2, c_3, c_4]$ and $d = [d_1, d_2, d_3, d_4]$ are constants defined as follows:

$$c_1 = c_4 = \frac{1}{2(2 - 2^{1/3})} \quad (1)$$

$$c_2 = c_3 = \frac{1 - 2^{1/3}}{2(2 - 2^{1/3})} \quad (2)$$

$$d_1 = d_3 = \frac{1}{2 - 2^{1/3}} \quad (3)$$

$$d_2 = \frac{2^{1/3}}{2 - 2^{1/3}} \quad (4)$$

$$d_4 = 0 \quad (5)$$