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Symplectic integration of magnetic systems

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ABSTRACT

Simulation of the long time behavior of systems requires more than just numerical stability to return dependable results – it must preserve the underlying geometric structure of the continuous equations. Symplectic integrators are the most common form of geometric integrator, and are therefore of interest in simulating plasmas for many plasma periods, for example. We present here results on generating symplectic integrators for magnetic systems, and in particular show that the algorithms due to Boris and Vay are symplectic.

1. Introduction

Symplectic integration [1–5] has become a staple of accelerator physics and astrophysics simulations, as it provides unconditional stability, if not the short term accuracy of Runge–Kutta type schemes. While numerical solutions for systems such as magnetized plasmas are not derived directly from Hamiltonian systems, the canonical method due to Boris [6–8] shows many of the properties of a symplectic integrator.

The primary difficulty in developing symplectic integrators for magnetic systems, as was pointed out by Ruth [1], is the $\vec{p} \cdot \vec{A}$ term that leads to implicit forms and which is not separable into an exactly integrable Hamiltonian. Even worse is for relativistic systems, where no clear expansion parameter for the radical in the Hamiltonian exists. In this case, the kinetic energy is not even close to separable. This problem does not appear in Lagrangian mechanics, where the vector potential appears in a $\dot{q} \cdot \vec{A}$ form outside the radical. However, Lagrangian mechanics lacks the canonical transformation formalism used in deriving symplectic integrators.

To obtain geometric integrators from a Lagrangian formalism, it is best to approach the problem using a discretized action integral. This method, described in [9] and the citations therein, obtains recursion relations for the q_k in configuration space that conserve the symplectic two-form.

In this paper, we present the formalism necessary to show that the Boris method is a symplectic integrator. An overview of discrete Lagrangian mechanics based on the work of Marsden and West [9] is first presented. This method is then applied to Lagrangians with vector potentials, first the nonrelativistic limit, where this is shown to be the Boris update. For the relativistic dynamics of particles in magnetic fields, we find that the generalization of the Boris update developed by Vay is symplectic.

2. Discretized Lagrangian mechanics

As discussed by Marsden and West ([9], and citations therein), the Lagrangian action integral may be approximated by some discretization scheme by

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$$\int_0^t L(q, \dot{q}, t')\, dt' \approx \sum_{k=0}^{N-1} L_D(q_{k+1}, q_k, t_k) \tag{1}$$

where $t_k = t_0 + kh$ for a time step h. Thus, under this derivation, each L_D has the units of action, or $[L] \times [dt]$. Minimizing this action against variations δq_k of the physical trajectory, with $\delta q_0 = \delta q_N = 0$ to fix the endpoints, gives a variation of the discrete action

$$\begin{aligned}\delta S_D = \sum_{k=1}^{N-1} \left(\frac{\partial}{\partial q_{k+1}} L_D(q_{k+1}, q_k, t_k)\delta q_{k+1} + \frac{\partial}{\partial q_k} L_D(q_{k+1}, q_k, t_k)\delta q_k \right) \\ + \partial_{q_0} L_D(q_0, q_1)\delta q_0 + \partial_{q_N} L_D(q_N, q_{N-1})\delta q_N = 0\end{aligned} \tag{2}$$

By shifting the summations to match the indices of the variations, this gives the discrete Euler–Lagrange (DEL) equations

$$D_2 L_D(q_{k+1}, q_k) + D_1 L_D(q_k, q_{k-1}) = 0 \tag{3}$$

where D_n is the derivative with respect to the nth variable.

In the continuous Lagrangian limit, the symplectic two-form

$$\Omega_L(q, \dot{q}) = \frac{\partial^2 L}{\partial q_i \partial \dot{q}_j} \mathbf{d}q^i \wedge \mathbf{d}q^j + \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \mathbf{d}\dot{q}^i \wedge \mathbf{d}q^j \tag{4}$$

is conserved under the Euler–Lagrange equations. For the discretized Lagrangian, the tangent bundle $T\mathbb{Q}$ does not include $\dot{q}$, as the time derivatives do not appear in the Lagrangian. The discretized symplectic two-form that is conserved is given by

$$\Omega_{L_D}(q_0, q_1) = \frac{\partial^2 L}{\partial q_0^i \partial q_1^j} \mathbf{d}q_0^i \wedge \mathbf{d}q_1^j \tag{5}$$

Because $\Omega_{L_D} = \mathbf{d}\Theta_L$ is an exterior derivative, and $\mathbf{d}^2 = 0$, this symplectic two-form is conserved for all solutions of the DEL equations. This proof is provided in detail in Marsden and West.

Because $\dot{q}$ is replaced by a finite difference in the discrete Lagrangian, it is important to note that any velocity-like variables are auxiliary and do not play a role in the underlying geometric structure. This is an important distinction with Hamiltonian symplectic integrators, where the p and q both play a role in the geometry – the Hamiltonian symplectic two form explicitly involves the momentum.

As an example of how this yields a symplectic integrator, consider the Lagrangian for a one dimensional particle in a potential

$$L(q, \dot{q}, t) = \frac{1}{2}\dot{q}^2 - V(q, t) \tag{6}$$

The discretization is non-unique – indeed choosing $q \mapsto (q_k + q_{k+1})/2$ yields an implicit integration scheme for general V, while choosing $q \mapsto q_{k+1}$ will yield the explicit integrator below. Because we are interested in explicit integrators, we will consider the discrete Lagrangian

$$L_D(q_{k+1}, q_k) = \frac{1}{2}\frac{(q_{k+1} - q_k)^2}{h} - V\big(q_{k+1}, (k+1)h\big)h \tag{7}$$

for a discrete time step t. Applying the DEL equations to this discrete Lagrangian yields

$$q_{k+1} - 2q_k + q_{k-1} = -\frac{\partial V}{\partial q_k}(q_k, kh)h \tag{8}$$

which we recognize immediately as $F = m\ddot{q}$ in the form of a central differencing. If we define the velocity vector to be

$$v_{k+1} = \frac{q_{k+1} - q_k}{h} \tag{9}$$

then this yields the first order symplectic integrator

$$v_{k+1} = v_k - \frac{\partial V}{\partial q_k}(q_k, kt)h \tag{10}$$

$$q_{k+1} = q_k + v_{k+1}h \tag{11}$$

which has the usual first order leapfrog scheme.

Unlike in Hamiltonian symplectic integration schemes, where the generating function defines the p and q update sequences explicitly, we were forced here to introduce the velocity as an auxiliary variable, turning our N second order