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MULTISYMPLECTIC INTEGRATORS FOR ACCELERATOR TRACKING CODES*

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Abstract

It has been long understood that long time single particle tracking requires symplectic integrators to keep the simulations stable. In contrast, space charge has been added to tracking codes without much regard for this. Indeed, multisymplectic integrators are a promising new field which may lead to more stable and accurate simulations of intense beams. We present here the basic concept, through a spectral electrostatic field solve which is suitable for adapting into existing tracking codes. We also discuss the limitations of current algorithms, and suggest directions for future development for the next generations of high intensity accelerators.

INTRODUCTION

Integrating single-particle orbits in storage rings using symplectic integration has been a staple of the accelerator field for decades[1]. The fundamental idea of symplectic integrators is: if the continuous equations of motion derive from an action principle, then so too should their discretization.

Keeping in this idea, recent work in the plasma-based accelerator field [2, 3] has expanded on early work [4, 5, 6] generalizing the idea of symplectic integration to field theories such as Maxwell's equations. Conventional particle-in-cell algorithms have discretized the particle motion and field solvers individually, then used charge deposition and force interpolation to enforce energy or momentum conservation. The difficulty with this approach is that conservation laws are encoded in the action principle, and arise from Noether's Theorem. Thus, momentum or energy conservation should be a natural result of the discretization of the continuum Lagrangian, not an *ad hoc* addition to impose certain physical constraints.

These ideas have a clear application to studying beam physics with intense space charge, or other dynamical effects over the long term. One can roughly understand non-symplectic versus symplectic integrators as being similar to secular versus canonical perturbation theory. In the secular theory, the expansion over a parameter ε is only valid for small times, so that $|\varepsilon t| \ll 1$. Canonical perturbation theory is valid for all time, so long as ε is small. As applied to accelerators, this means that a non-symplectic integrator will only give reliable results over time scales short compared to the space-charge tune shift (for example). Thus, a non-symplectic space charge simulation is likely only reliable for $n \propto (\Delta Q_{\mathrm{SC}})^{-1}$ turns, with additional scaling for the step size such that $n \to \infty$ as $h \to 0$.

We here present the basic concepts of multisymplectic integration using a Lagrangian approach. We discuss this first schematically, then using a specific example – a spectral electrostatic particle-in-cell algorithm. We conclude with a discussion of future work required to implement these ideas in accelerator tracking codes.

MULTISYMPLECTIC INTEGRATION

The current literature in the field deals primarily with Lagrangians, as the plasma physics community generally thinks in terms of the tangent space (position and velocity) rather than the cotangent space (coördinates and momenta). However, the geometric structures (symplectic 2-form, conserved momenta, etc.) have a clear translation between Lagrangian and Hamiltonian treatments, so the basic principles will be the same.

The so-called Low Lagrangian [7] can be written generally as

$$\begin{aligned} L = \int d\mathbf{x}_0 d\mathbf{v}_0 \Bigg[T\left(\frac{\partial \mathbf{x}}{\partial t}(\mathbf{x}_0, \mathbf{v}_0)\right) + \dots \\ \cdots - q\varphi + \frac{q}{c}\frac{\partial \mathbf{x}}{\partial t} \cdot \mathbf{A} \Bigg] f(\mathbf{x}_0, \mathbf{v}_0) + \dots \\ \cdots + \frac{1}{16\pi} \int d\mathbf{x} F_{\mu\nu} F^{\mu\nu} \end{aligned} \tag{1}$$

where T is the kinetic energy term and $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the antisymmetric electromagnetic tensor. We note that the conservation of phase space density implies that $f(\mathbf{x}_0, \mathbf{v}_0) = f(\mathbf{x}, \mathbf{v}, t)$. Variation with respect to the individual vector potential components A, and the position $\mathbf{x}$, lead to the familiar Lorentz force law and Maxwell's equations, assuming we are using the conventional coördinate systems (Cartesian, cylindrical, spherical...). The specific application for accelerator coördinates will diverge from these familiar forms.

The first step in discretizing this Lagrangian is to discretize the spatial components of the fields. Thus, each component of the 4-vector potential

$$A = \sum_\sigma \Psi_\sigma(\mathbf{x}) a_\sigma(t) \tag{2}$$

over some set of indices σ. These could be finite elements, structured finite elements (which lead to finite difference equations), Fourier decompositions, eigenmodes formulations, or a variety of other possibilities. Similarly, we dis-

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[1] see, e.g., [1] for an overview of the history and literature of this topic.

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cretize the phase space density

$$f(\mathbf{x},\mathbf{v},t) = \sum_i w_i \Lambda(\mathbf{x}-\mathbf{x}_i(t))\delta(\mathbf{v}-\mathbf{v}_i(t)) \tag{3}$$

where Λ is the spatial shape function and we assume every macroparticle has a single velocity. w is the macroparticle weight. Thus, we can view macroparticles as a finite element Lagrangian flow picture of the phase space "fluid".

These definitions create overlap integrals between the individual Ψ and products of Ψ and Λ. The former dictates the discretized form of the differential operators on the fields, while the later determines charge deposition and force interpolation. Discretization in time is an approximation of the action integral, described in greater detail in [8]. The discretization in time should be taken to be higher than first order accurate, and can be easily done by considering $S = \int dtL$ in terms of Riemann sums over L. This gives the discrete action which must be minimized with respect to the individual coördinates and field components to give the equations of motion.

To see these ideas in context, let us now consider a specific example.

SPECTRAL ELECTROSTATIC ALGORITHM

Let us restrict ourselves to a nonrelativistic electrostatic example, as this is the simplest nontrivial possibility. In this case, the Low Lagrangian simplifies greatly to

$$L = \int d\mathbf{x}_0 d\mathbf{v}_0 \left\{ \left[\frac{1}{2} m \left(\frac{\partial \mathbf{x}}{\partial t} \right)^2 - q\varphi(\mathbf{x}) \right] f(\mathbf{x}_0,\mathbf{v}_0) + \dots \right.$$
$$\left. \dots + \frac{1}{8\pi} \int d\mathbf{x} \, (\nabla\varphi)\cdot(\nabla\varphi) \right\}. \tag{4}$$

We choose to discretize the fields using a spectral decomposition

$$\varphi(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^D} \sum_\sigma e^{i\mathbf{k}_\sigma\cdot\mathbf{x}} \tilde{\varphi}_\sigma \tag{5}$$

This is the standard discrete Fourier transform, with indexing value(s) σ. We denote $-\sigma$ in terms of the k-vectors $\mathbf{k}_{-\sigma} = -\mathbf{k}_\sigma$ and furthermore, from the reality of the scalar potential, that $\varphi_{-\sigma} = \varphi_\sigma^*$.

We can similarly decompose the phase space density as

$$f(\mathbf{x},\mathbf{v},t) = \sum_i w_i \Lambda(\mathbf{x}-\mathbf{x}_i(t))\delta(\mathbf{v}-\mathbf{v}_i(t)) \tag{6}$$

to obtain a spatially discretized Lagrangian:

$$L_D = \sum_i \left\{ \underbrace{\frac{1}{2} w_i m \left(\frac{\partial \mathbf{x}_i}{\partial t} \right)^2}_{\text{kinetic energy}} - \dots \right.$$
$$\left. \dots - \underbrace{w_i q \sum_\sigma \tilde{\Lambda}(\mathbf{k}_\sigma)\tilde{\varphi}_\sigma e^{-i\mathbf{k}_\sigma\cdot\mathbf{x}_i}}_{\text{deposition/interpolation}} \right\} - \underbrace{\frac{1}{8\pi} \sum_\sigma |\tilde{\varphi}_\sigma|^2 |\mathbf{k}_\sigma|^2}_{\text{Poisson equation}} \tag{7}$$

where here $\tilde{\Lambda}(\mathbf{k})$ is the Fourier transform of the particle spatial shape function. We now discretize the action integral in time, by approximating $S = \int dtL_D$ as a Riemann sum. As noted in [8], we can use multi-step integrators and self-adjoint discretizations of the action integral to get second-order integrators in time.

For the sake of brevity, we simply that the *adjoint* of a discrete action $\mathcal{S}_D^*(q_{k+l}, q_k) = -\mathcal{S}_D(q_k, q_{k+1})$, and that a self-adjoint action must be even order accruate – thus by constructing a self-adjoint approximation to the action integral in time, we are guaranteed at least a second order accurate integrator. The details may be found in §2.4 of [8]. Doing this gives a discrete action for a single step by mapping $\mathbf{x} \mapsto \mathbf{x}^{(n+1/2)}$ and $\partial_t \mathbf{x} \mapsto (\mathbf{x}^{(n+1/2)} - \mathbf{x}^{(n)})/h/2$ to get the self-adjoint action:

$$\mathcal{S}_D = \sum_i \left\{ \frac{1}{2} w_i m \left(\frac{(\mathbf{x}_i^{(n+1)} - \mathbf{x}_i^{(n+1/2)})^2}{h/2} + \dots \right.\right.$$
$$\left.\left. \dots + \frac{(\mathbf{x}_i^{(n+1/2)} - \mathbf{x}_i^{(n)})^2}{h/2} \right) - \dots \right.$$
$$\left. \dots - w_i h \sum_\sigma \tilde{\Lambda}(\mathbf{k}_\sigma)\tilde{\varphi}_\sigma e^{-i\mathbf{k}_\sigma\cdot\mathbf{x}_i^{(n+1/2)}} \right\} - \frac{h}{8\pi} \sum_\sigma |\tilde{\varphi}_\sigma|^2 |\mathbf{k}_\sigma|^2 \tag{8}$$

Varying this using the discrete Euler-Lagrange equations for each of the electrostatic Fourier modes and the coördinates[2] to get the update sequence:

$$\underbrace{\frac{\mathbf{x}_i^{(n+1)} - 2\mathbf{x}_i^{(n+1/2)} + \mathbf{x}_i^{(n)}}{h}}_{\mathbf{v}_i^{(n+1)} - \mathbf{v}_i^{(n)}} = \dots$$
$$\dots \frac{q}{m} h \sum_\sigma -i\mathbf{k}_\sigma \Lambda(\mathbf{k}_\sigma) e^{-i\mathbf{k}_\sigma\cdot\mathbf{x}_i^{(n+1/2)}} \tilde{\varphi}_\sigma \tag{9a}$$

$$\tilde{\varphi}_\sigma = -\frac{4\pi q}{|\mathbf{k}_\sigma|^2} \sum_i w_i \tilde{\Lambda}(\mathbf{k}_\sigma) e^{-i\mathbf{k}_\sigma\cdot\mathbf{x}_i^{(n+1/2)}} \tag{9b}$$

Using those definitions for the velocity intermediate variable leads to a fairly standard leapfrog algorithm familiar from traditional macroparticle methods. We can see almost directly that eqn. (9a) is $\mathbf{a} = -q\nabla\varphi$ and eqn. (9b) is $\nabla^2\varphi = 4\pi\rho$ – Newton's Second Law and the Poisson equation.

We have thus constructed this algorithm using approximations at the level of the action, guaranteeing that the resulting integrator will satisfy a symplectic condition on both the particles and the fields. Because we have used a Fourier representation of the system, and because there are

[2] The paper by Marsden & West [8] is a more or less complete dictionary for how to get from continuous to discrete Lagrangian mechanics. There are analogous concepts to the Euler-Lagrange equations, a canonical momentum, etc. Notably, there is no discrete analog of the velocity – there are only the discrete coördinates. Thus, discrete Lagrangians lack a tangent space, but a Hamiltonian can be derived which implies a cotangent space. The "velocity" such as it is appears purely as a computational convenience and plays no role in the symplectic structure of discrete Lagrangian mechanics.

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no external forces to break the symmetry, this algorithm will also be "momentum conserving", to use the parlance of the computational plasma physics community.

CONCLUSION & OUTLOOK

We have thus presented a general picture of multisymplectic integration, and provided a first example of its derivation for an electrostatic system. The algorithm presented is not completely suitable for accelerator applications, but the basic concept is applicable. The result is a geometric integrator which preserves the symplectic structure of both the particles and the fields.

The path to extremely high intensity bunches, with space charge dominated dynamics, in storage rings will require reliable simulations over many turns with a self-consistent treatment of the fields. Multisymplectic integrators are the logical path forward for these simulations, as they extend the now-commonplace practice of symplectic integration of single particle orbits.

As noted above, non-symplectic space charge algorithms have a limited range of validity before non-Hamiltonian dynamics becomes apparent. For space charge dominated beams, or other applications with long term tracking of collective effects, the field solves will have to satisfy some form of symplectic condition to obtain reliable results.

There are a number of key developments to mature these ideas and make them suitable for storage ring tracking code applications:

1. Adapt the Lagrangian treatment to a Hamiltonian formulation compatible with a transfer map treatment of the problem
2. Determine how wake functions and other Green's function type forces can appear alongside the self-consistent fields
3. Develop a path to higher order algorithms similar to the method in [9]

Substantial intellectual effort will be required to fully adapt these algorithms in a suitable way for computational accelerator physics.

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