HIGHER ORDER SYMPLECTIC INTEGRATION OF COLLECTIVE EFFECTS

Stephen D. Webb* and Dan T. Abell,
Tech-X Corporation, 5621 Arapahoe Ave., Boulder, CO 80303, USA

Abstract

Long time tracking simulations of intense beams requires a proper account for the collective effects. Many tracking codes allow the number of space charge kicks, for example, to be determined by the end user. This makes no guarantee that the integration is second order accurate in the step size. In this proceeding, we present results on the proper second- and fourth-order symplectic integration of the Hamiltonian dynamics of particles under collective interactions using a model Hamiltonian with collective space charge forces to illustrate the underlying principles.

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Symplectic integration [1, 2] places a strong constraint on any numerical scheme by assuring that the numerical results satisfy the symplectic condition to machine precision. This constraint guarantees that the phase space volume occupied by the numerical trajectories is constant, which prevents spurious "heating" of the particles. Single particle second-order symplectic integration has been a mainstay of tracking codes since before the TEAPOT library [3] implemented the symmetric drift-kick paradigm for high energy tracking, which assures second order accuracy.

As was shown by Forest and Ruth [4], symplectic integrators may be constructed using Lie algebraic splitting as an application of Dragt-Finn factorization [5, 6, 7]. In summary, the dynamics of a phase space variable z may be written in terms of Poisson brackets as

$$\dot{z} = -\{H, z\} \equiv -:H:z \tag{1}$$

where the Hamiltonian H has been promoted to the status of a Lie operator. For a time-independent Hamiltonian, the solution to the above operator differential equation is

$$z(t) = \exp\left(-:H:t\right) z(0) \tag{2}$$

For a Hamiltonian of the form $H = p^2/2 + V(q)$, the second order Ruth integrator would be written as a split operator of the form

$$\begin{aligned}\mathbf{M}_{\Delta t} = &\exp\left(-:p^2/2:\Delta t/2\right)\\ &\exp\left(-:V(q):\Delta t\right)\exp\left(-:p^2/2:\Delta t/2\right)\end{aligned} \tag{3}$$

where $\mathbf{M}$ is the transfer map forward in time by Δt. The Baker-Campbell-Hausdorff series from combining this symmetric splitting of the Hamiltonian yields the correct Hamiltonian up to second order in Δt. In the language of Talman's "exact solution of an approximate machine", this yields the correct machine up to second order in the step size.

Phrased another way, the solutions derived from a symplectic splitting are an *exact* solution to the Hamiltonian formed when the splitting is concatenated exactly to all orders in the time step. Thus, a second order symplectic integration scheme exactly solves a Hamiltonian which approximates the exact Hamiltonian at second order accuracy in the time step. This is a crucial property of symplectic integrators, and we will explore this in the context of grid spacing and approximate field solves later.

First order integrators are undesirable because there is no formal way to reduce the numerical error introduced by the splitting. To see this, consider a first order splitting on a time-indendent Hamiltonian H which yields the map

$$\mathbf{M}_{\Delta t} = \exp\left(-:H:\Delta t + :\tilde{H}^{(1)}:\Delta t^2 + \ldots\right) \tag{4}$$

To integrate to time $N\Delta t = T$ requires N applications of the above operator, which yields the net transfer map

$$\mathbf{M}_{T} = \exp\left(-:H:T + :\tilde{H}^{(1)}:N\Delta t^2 + \ldots\right) \tag{5}$$

where we have neglected higher order terms. The difficulty here is in reducing the error term. Since $N\Delta t$ must be fixed at T, the error term can only be reduced linearly by reducing the time step – doubling accuracy requires double the computing time. A higher order algorithm, one for which the error term is of the form $:H:^{(3)} N\Delta t^3$ can achieve much more rapid convergence. This is the point of second- and higher-order symplectic integrators.

The symmetric splitting in the drift-kick or other schemes used in single particle tracking achieves this second-order accuracy, but the implementation of collective effects such as space charge or wake fields frequently violates this. A common example is a user-defined number of space charge kicks, which will frequently violate the second order requirements unless the user is particularly careful. The frequent net result is a first-order splitting of the collective component of the Hamiltonian $\mathcal{V}$ with second-order accuracy on the remaining components $H_0 + H_1$, where we have assumed the total Hamiltonian

$$H = H_0 + H_1 + \mathcal{V} \tag{6}$$

As an example problem for the proper higher-order integration, consider the one-dimensional harmonic oscillator

* swebb@txcorp.com

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Hamiltonian with 1D Coulomb interaction

$$H = \sum_j \frac{1}{2}\left(p_j^2 + \omega^2 q_j^2\right) + \frac{q^2}{2}\sum_{i\neq j}|q_i - q_j| \qquad (7)$$

where q is the particle charge. Because this Hamiltonian is autonomous, the total energy is time-independent and makes an excellent metric for the order of accuracy in the numerical schemes presented.

To properly bookkeep when to compute the force, we introduce the extended phase space formalism described in [8] for example. In this, we introduce a new Hamiltonian K which depends upon an independent variable σ and is given by

$$K(p, q, p_t, t; \sigma) = H(p, q, t) + p_t \qquad (8)$$

where p_t is the canonically conjugate momentum to the t dependent variable, and gives $t' = 1$ with σ as the independent variable.

A pure first order integration scheme would take the splitting

$$\mathbf{M}^{(1)}_{\Delta t} = \exp\left(-:H_0:\Delta t\right)\exp\left(-:H_1:\Delta t\right)\exp\left(-:\mathcal{V}:\Delta t\right) \qquad (9)$$

while a hybrid $3/2$ integration scheme would be split as

$$\mathbf{M}^{(3/2)}_{\Delta t} = \exp\left(-:H_0:\Delta t/2\right) \exp\left(-:H_1:\Delta t\right)\exp\left(-:H_0:\Delta t/2\right)\exp\left(-:\mathcal{V}:\Delta t\right) \qquad (10)$$

The hybrid $3/2$ scheme will be second-order accurate in $H_0 + H_1$, but only first-order accurate in $\mathcal{V}$. This scheme seems to typify most accelerator tracking codes. A fully second-order scheme would take the form

$$\mathbf{M}^{(2)}_{\Delta t} = \exp\left(-:H_0:\Delta t/2\right)\exp\left(-:H_1:\Delta t\right) \exp\left(-:\mathcal{V}:\Delta t\right)\exp\left(-:H_1:\Delta t/2\right)\exp\left(-:H_0:\Delta t\right) \qquad (11)$$

Here the selection to place the $\mathcal{V}$ map in the symmetric middle is based on the idea that the calculation of the collective forces is much slower than the single-particle components, and thus reducing the number of collective force calculations leads to much faster simulations compared to other splitting schemes. As was shown by Yoshida [2], a fourth-order integrator may be obtained by three second-order integrators as

$$\mathbf{M}^{(4)}_{\Delta t} = \mathbf{M}^{(2)}_{\Delta t/(2-2^{1/3})}\mathbf{M}^{(2)}_{-2^{1/3}\Delta t/(2-2^{1/3})}\mathbf{M}^{(2)}_{\Delta t/(2-2^{1/3})} \qquad (12)$$

What this negative time-stepping means is made clear by the extended phase space formalism discussed above: it is obtained by moving σ back in time, but because all the associated particle σ also move back in time, it is simply taken by performing all maps to the right of the $\mathcal{V}$ mapping, computing $\mathcal{V}$ with these intermediate coordinates, and then applying the appropriate map.

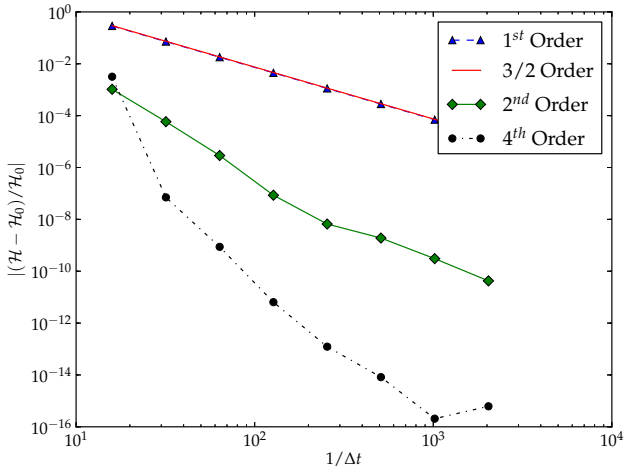

Figure 1: Polynomial convergence for 1^{st}, $3/2^{th}$, 2^{nd}, and 4^{th} order integration schemes.

Explicitly, if we start with $z(t)$, the fourth order update will follow the sequence:

$$\begin{aligned} z(t) &\mapsto \mathbf{M}^{(2)}_{\Delta t/(2-2^{1/3})} z(t) \mapsto \\ \mathbf{M}^{(2)}_{-2^{1/3}\Delta t/(2-2^{1/3})} z(t + \Delta t/(2-2^{1/3})) &\mapsto \\ \mathbf{M}^{(2)}_{\Delta t/(2-2^{1/3})} z(t + \Delta t(1-2^{1/3}/2-2^{1/3})) &\mapsto \\ z(t + \Delta t) & \end{aligned} \qquad (13)$$

While $t' < t$ in the middle of the time step, this is merely formalism. There is no physical meaning to any of the values of z between $z(t)$ and $z(t + \Delta t)$ during the time step – one cannot simply stop the time step half way and ask questions expecting sensible answers; the integrator does not resolve any smaller than Δt.

The resulting convergence of $|(E - E_0)/E_0|$ for the four schemes is shown in figure (1). In this integration, we have considered a direct N^2 computation of the collective forces of N harmonically confined particles in one dimension, which removes the effects of grid size. However, the integer-order splittings show a clear improvement with step size.

The N^2 computation is intractable for any realistic beam simulations. The role of grid spacing, however, does make an appearance for the approximate potential being computed. The grid spacing will give an exact Hamiltonian

$$\tilde{H} = H_0(p, q) + \mathcal{V}(q, \Delta x) \qquad (14)$$

where Δx represents the grid spacing. This Hamiltonian is approximately solved for through the splitting methods described above. For a second order accurate calculation

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of the potential, this yields a result of the form

$$\tilde{H} \approx \underbrace{H_0(p,q) + \mathcal{V}(q, \Delta x = 0)}_{H_{exact}(p,q)} + \ldots \\ \ldots \frac{1}{2} \frac{\partial^2 \mathcal{V}}{\partial \Delta x_i \partial \Delta x_j} \Delta x_i \Delta x_j + \mathcal{O}(\Delta x^3) \quad (15)$$

and thus the exact solution may be arrived upon at arbitrary accuracy by reducing the grid spacing. The goal is to exactly solve the dynamics of H_{exact}. There is an interplay between the convergence of $\tilde{H}$ to H, the exact Hamiltonian solved by the splitting, and the convergence of H to H_{exact}. Thus, the grid spacing affects our understanding of the exact solution for the approximate machine, and the time stepping affects how closely our approximate machine resembles the exact machine.

One requirement, a known issue within tracking codes, is the simultaneity of the independent variable in the field solves. We skirt this issue in these examples by using a constant focusing force, which does not apply to real accelerator systems. The issue of simultaneous in t for the Poisson equation and the use of s based tracking codes we propose to resolve elsewhere in these proceedings [9], which, in light of these results, may help guide future development in tracking codes for intense beam transport.

As beam intensity increases, it is important to obtain quantitative, and not merely qualitative, accuracy in numerical simulations of these future machines. Higher order accuracy is the most straightforward method of obtaining this convergence. We have thus presented a first-, second-, and fourth-order accurate symplectic integration scheme for systems with collective effects, which assures both rapid numerical convergence and preservation of the symplectic condition. We have furthermore illustrated, using the $^3/_2$-order scheme, that the convergence of a tracking code is only first order if the collective effects are not handled with care.

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