Time Symmetrization Meta-Algorithms

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Abstract. We present two types of meta-algorithm that can greatly improve the accuracy of existing algorithms for integrating the equations of motion of dynamical systems. The first meta-algorithm takes an integrator that is time-symmetric only for constant time steps, and ensures time-symmetry even in the case of varying time steps. The second meta-algorithm can be applied to any self-starting integration scheme to create time-symmetry, both for constant and for variable time steps, even if the original scheme was not time-symmetric. Our meta-algorithms are most effective for Hamilton systems or systems with periodic solutions. If the system is not Hamiltonian (for example, if some dissipative force exists), our methods are still useful so long as the dissipation is small.

1. Introduction

Many problems in computational physics are governed by underlying equations that are intrinsically time-symmetric. In particular, for any simulation in Hamiltonian dynamics, we can run the movie of our computation equally well forwards as backwards, and in both cases obtain a physically allowable solution. Clearly, it is desirable to use an integration algorithm that reflects this time-symmetry as a built-in property. In that case, intuitively speaking, particles can no longer fly ‘off the tracks’, so to speak, when moving through a curve. An example of particular interest to this conference is astrophysical particle simulations, in which particles may correspond directly to physical units, such as molecules or stars, or may form tracers used to approximate the solution of a set of underlying equations with continuous variables.

The basic idea is this: if an algorithm would make a particle spiral out systematically in a given situation, it would have to do so equally in the forward and backward direction. Time reversal, however, would force an inward motion, and the conclusion is that the net spiral out (or spiral in) has to be zero, at

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least when averaged over a full period in a periodic system. The error in energy thus has to be periodic as well, and cannot build up from orbit to orbit. Of course, errors are still made for finite integration step size, but they show up as errors in phase. In many applications, phase errors are preferable over errors in quantities such as the total energy, that should be conserved.

Most algorithms that are in common use for orbit integration in simulations are not time-symmetric. Even those that are, typically lose their symmetry property as soon as one allows variable time steps. In the remainder of this paper, we offer two types of meta-algorithm for constructing a larger class of time-symmetric algorithms. In §§2,3 we show how to restore time symmetry for algorithms that were symmetric, but lose that property when one uses variable time steps. In §§4,5 we show how to create time symmetry even for those algorithms that were never time symmetric to begin with, not even in the constant time step case.

2. Building A Better Leapfrog

A celebrated example of an integration scheme with built-in time symmetry is the leapfrog scheme, also known as the Verlet method. It is widely used in many applications of particle simulations, such as in molecular dynamics, plasma physics, fluid dynamics and stellar dynamics(Hockney & Eastwood 1988; Barnes & Hut 1986). The time symmetry is manifest in the interleaved representation, which gave rise to the ‘leapfrog’ name:

\[ r_1 = r_0 + v_\frac{1}{2} \delta t \]
\[ v_\frac{3}{2} = v_\frac{1}{2} + a_1 \delta t, \]

where \( r \) can stand for the position vector of a single particle or the combined vector \( r_1, r_2, \ldots, r_N \) representing a system of \( N \) particles. The quantity \( v = dr/dt \) is the velocity and \( a(t) = a(r(t)) = dv/dt \) the acceleration. The subscripts after the various quantities indicate the time at which they apply, in units of the time step, i.e. \( v_\frac{1}{2} = v(t + \frac{1}{2} \delta t) \).

It is convenient to map the standard interleaved description into a form in which all variables are defined at the same instant in time:

\[ r_1 = r_0 + v_0 \delta t + \frac{1}{2} a_0 (\delta t)^2, \]
\[ v_1 = v_0 + \frac{1}{4} (a_0 + a_1) \delta t. \]

Starting from \( \{r_0, v_0, a_0\} \), one first computes \( r_1 \), then \( a_1(r_1) \), by evaluating the appropriate expression dictated by the system under consideration, and finally \( v_1 \). While Eq.(2) looks as though it has lost its explicit time symmetry, it is still equivalent to the original Eq.(1), as can be verified by direct substitution (Barnes & Hut 1989). However, if the time step \( \delta t \) is allowed to vary, through a functional dependence \( \delta t = h(r, v) \) for example, time symmetry is lost.

Time symmetry can be restored if we force the time step to be a symmetric function of the begin point and end point of each time step, as was first shown by Hut et al. (1995). For example, we can use

\[ \delta t = \frac{1}{2} [h(r_0, v_0) + h(r_1, v_1)], \]

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With this choice of time step, the combined set of equations (2,3) has become implicit: in order to determine \( \{r_1, v_1\} \) from \( \{r_0, v_0\} \), we need to know the time step size \( \delta t \), which in turn is dependent on \( \{r_1, v_1\} \). We can solve this problem by starting with \( \delta t = h(r_0, v_0) \) as a first approximation. This will give us approximate values for \( \{r_1, v_1\} \), from which we can determine a more accurate value for \( \delta t \) using equation (3). If necessary, this iteration process can be repeated several times, but in practice one or two iterations are generally sufficient to reach time symmetry to machine accuracy.

3. Restoring Time Symmetry

The notion of time symmetry restoration for variable time steps, given above for the particular case of the leapfrog scheme, carries over to any class of integration schemes that is explicitly time symmetric for constant time steps, as shown by Hut et al. (1995). Another example, given in the same paper, concerns the following natural fourth-order generalization of the leapfrog scheme:

\[
\begin{align*}
  r_1 &= r_0 + \frac{1}{2}(v_1 + v_0)\delta t - \frac{1}{12}(a_1 - a_0)(\delta t)^2, \\
  v_1 &= v_0 + \frac{1}{2}(a_1 + a_0)\delta t - \frac{1}{12}(j_1 - j_0)(\delta t)^2,
\end{align*}
\]

which is a truncated form of the Hermite scheme (Makino 1991a). Here the jerk \( j = da/dt \) is calculated directly by differentiation of the expression for the force (thereby introducing a dependency on velocity as well as position in the case of Newtonian gravitational forces). This set of equations is manifestly time symmetric for constant time steps. Unlike the original second-order leapfrog, given in eq. (2), the scheme in eq. (4) is implicit, already for constant time steps. Applying the same symmetrization procedure given in equation (3) leads, after iteration, to a fully time-symmetric fourth-order generalization of the leapfrog. In practice, iteration can give a quick convergence, leading to substantially improved accuracy for a fixed amount of computer time (Hut et al. 1995).

4. Creating Time Symmetry

Even if no time symmetry is present in a given algorithm, it is possible to construct an implicit version that is manifestly time symmetric, for the general class of self-starting (i.e. one-step) integration schemes. The meta-algorithm that performs this feat is described in detail by Funato et al. (1997), as a generalization of the prescription offered by Hut et al. (1995). Here we give a brief outline of the main idea behind the treatment.

Let us start with the ordinary differential equation

\[
\frac{dy}{dx} = f(x, y),
\]

and a given self-starting integration scheme, expressed as

\[
y_{i+1} = y_i + F(x_i, y_i; h_i),
\]

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where \( x_i \) and \( y_i \) are the values of the variables \( x \) and \( y \) after the \( i \)-th step, and \( h_i \) is the step size at \( x_i \).

Our meta-algorithm can be expressed as follows:

\[
y_{i+1} = y_i + \tilde{F}(x_i, y_i; \tilde{h}_i) = y_i + \frac{1}{2} \left[ F(x_i, y_i; \tilde{h}_i) - F(x_{i+1}, y_{i+1}; -\tilde{h}_i) \right],
\]

(3)

where \( \tilde{h}_i \) can be constructed in the form of a function \( \tilde{h}_i = f(h_i, h_{i+1}) \) that is symmetric in its arguments: \( f(x, y) = f(y, x) \). For example, we could take simply

\[
\tilde{h}_i = \frac{1}{2} [h(x_i, y_i) + h(x_{i+1}, y_{i+1})],
\]

(4)

or a root mean square, or any other symmetric combination. Equation (3) gives an implicit formula for \( y_{i+1} \). As before, we can solve this equation by iteration, starting with the original non-symmetric scheme as the initial trial function.

While this recipe is surprisingly simple, we can do even better. Instead of taking a given estimate for the step size, we can use the difference

\[
\Delta F_i \equiv \tilde{F}(x_i, y_i, \tilde{h}_i) - F(x_i, y_i, \tilde{h}_i),
\]

(5)

to estimate the local truncation error. This information can be used to implement a form of adaptive step size control. See Funato et al. (1997) for further details.

5. Building A Better Runge-Kutta

As an example application of our more general meta-algorithm, we have constructed a time-symmetric version of the popular fourth-order Runge-Kutta integration scheme. Figure 1 shows the behavior of the errors in the relative energy and angular momentum for a binary orbit with initial eccentricity \( e = 0.9 \) (the values plotted are determined at apocenter). The dashed and solid curves show the time evolution of the errors for the standard Runge-Kutta scheme and for the symmetrized Runge-Kutta scheme, respectively. In both cases, variable step sizes have been used. The number of time steps is comparable in both cases (around 600 per orbit).

Figure 1 shows that no discernible secular error is produced, even after 1000 orbital periods, for the run integrated by the time-symmetric fourth-order Runge-Kutta Method. In contrast, the error increases linearly for the run integrated by the standard fourth-order Runge Kutta Method. Further quantitative details will be provided in the cost/performance analysis by Funato et al. (1997).

6. Discussion

We have reviewed two types of meta-algorithm, based upon a time-symmetrization procedure. The first meta-algorithm preserves time symmetry that would otherwise be lost when integration step sizes are allowed to change during integration. The second meta-algorithm creates time symmetry, even for those algorithms where no symmetry was present in the equal-step-size case.
Figure 1. Effects of our meta-algorithm applied to a fourth-order Runge-Kutta scheme. Plotted is the growth of the relative error in energy (left) and angular momentum (right) for a Kepler orbit with eccentricity 0.9. Dashed and full lines correspond to the standard Runge-Kutta scheme and the time-symmetrized Runge-Kutta version, respectively.

We mention here briefly a few recent applications of these ideas. McMillan & Hut (1996) have constructed a fully automated package for performing gravitational three-body scattering experiments, where the central orbit integrator is built along the principles outlined by Hut et al. (1995). They found that the symmetrization meta-algorithm gave a significant speed-up to the fourth-order Hermite scheme used. Most importantly, they found that the fraction of rejected experiments was diminished greatly, compared to the standard integration scheme. The problem here is that some resonant scattering experiments can stay in an intermediate state for a very long time, before finally decaying into a final state. No matter how accurate an initial time step criterion has been chosen, there will always been a small fraction of such lingering states that will ultimately lead to an unacceptable build-up of errors (both integration errors and round-off errors). Time symmetrization, while not circumventing this problem, can greatly alleviate the situation.

Another application has been discussed by Funato et al. (1996a,b). They have applied time symmetrization to the Kustaanheimo-Stiefel regularization method, a sophisticated way to ‘unfold’ the singularity of the three-dimensional Kepler problem by mapping each point in three dimensional space to a unit circle in an auxiliary four dimensional space. The combination of these two powerful techniques has resulted in the most accurate way yet designed to integrate orbits near collision singularities.

For some applications, specific adaptations of our general meta-algorithm can make good use of the known constraints inherent in the underlying problem. One example that we have recently explored is that large-scale simulations of planetary formation. The problem is that close encounters and physical collisions of planetesimals make it absolutely necessary to use individually variable
time steps (Aarseth 1985). All standard choices for highly accurate integration schemes, such as the symplectic schemes, lose their desirable properties once we allow individual particles to change their integration time step length at will. In contrast, our meta-algorithm shows a way out, as demonstrated by Kokubo & Makino (1997). They made use of the fact that most planetesimals have nearly circular orbits \( (e << 0.01) \), which means that their time step is practically constant when block time step (McMillan 1986, Makino 1991b) are used, even if we allow the use of variable time steps. Even though the time step size of a particle shrinks significantly during a close encounter, leading to a break-down of time-symmetry, this occurs only for a very small fraction of time, for a typical particle. Since most of the integration error actually comes from the integration of nearly unperturbed orbits around the sun, reserving strict time symmetry for unperturbed orbits turns out to be a good compromise, leading to high overall accuracy. Details will be provided by Kokubo & Makino (1997).

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