N-body Integrators with Individual Time Steps from Hierarchical Splitting

Federico I. Pelupessy\textsuperscript{a}, Jürgen Jänes\textsuperscript{b,c}, Simon Portegies Zwart\textsuperscript{a}

\textsuperscript{a} Leiden Observatory, Leiden University, PO Box 9513, 2300 RA, Leiden, The Netherlands
\textsuperscript{b} Faculty of Science, University of Amsterdam, PO Box 94216, 1090GE, Amsterdam, The Netherlands
\textsuperscript{c} Cambridge Computational Biology Institute, Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, Wilberforce Road, Cambridge CB3 0WA, United Kingdom

Abstract

We review the implementation of individual particle time-stepping for N-body dynamics. We present a class of integrators derived from second order Hamiltonian splitting. In contrast to the usual implementation of individual time-stepping, these integrators are momentum conserving and show excellent energy conservation in conjunction with a symmetrized time step criterion. We use an explicit but approximate formula for the time symmetrization that is compatible with the use of individual time steps. No iterative scheme is necessary. We implement these ideas in the HUAYNO\textsuperscript{1} code and present tests of the integrators and show that the presented integration schemes shows good energy conservation, with little or no systematic drift, while conserving momentum and angular momentum to machine precision for long term integrations.

Keywords: Stellar dynamics; Methods: numerical, N-body

1. Introduction

Astrophysical N-body problems often show a large dynamic range of timescales within their component systems. Instead of a fixed or varying global time step most current astrophysical codes update the force and advance particles with a time step that is determined for each particle separately (for a recent review see [Dehnen and Read (2011)]. Such individual particle time step schemes (IPTS) allow efficient simulations by concentrating the computational resources on the parts of the system that experience the strongest evolution. The most popular IPTS is a block time step scheme

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Email address: pelupes@strw.leidenuniv.nl (Federico I. Pelupessy)

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where the particles are organized in a power of two hierarchy of time step bins \cite{McMillan1986, Hernquist1989, Makino1991}. The bin in which a particle resides determines the frequency of force evaluations and each successively higher bin has a factor 2 smaller interval between updates. This block time step scheme has been adopted in a wide range of codes, in for example codes for galactic simulations \cite{Dubinski1996, Magorrian2007}, cosmological simulations \cite{Stadel2001}, Smooth Particle Hydrodynamics codes \cite{Springel2005, Wadsley2004} and also modern Hermite integrators for collisional stellar systems \cite{Makino1991, Aarseth1999, PortegiesZwart2001, Harfst2008, Konstantinidis2010}. The popularity of this scheme stems from the fact that it allows for individual tailored time steps while still grouping particles with similar time steps together - which means that the cost of synchronizing the rest of the system is shared by all the particles in a given bin and parallelization of the force calculation is possible.

A notable exception where the simple block time step scheme is not used is when long term integration requires conservation of the integrals of motion to high precision. A prototype of a problem where this is required is the integration of planetary systems over billions of years. In this case care must be taken because IPTS typically do not conserve momentum and show drifts of the total energy. For these problems symplectic integrators based on Hamiltonian splitting \cite{Wisdom1991} are used, using the fact that the dynamics is dominated by a central object. For close encounters between objects orbiting the central body, additional splitting methods have been developed involving the interaction terms between orbiters \cite{Chambers1999, Duncan1998, Moore2011}.

Here we will derive a class of IPTS integrators applying these ideas for general N-body problems by splitting the N-body Hamiltonian starting from an initial pivot time step. We subdivide particles in two groups, according to whether their time step is shorter or longer than the pivot. The time evolution of the slow particles is evaluated using the current time step, where the terms involving particles with a shorter time step are grouped into a new Hamiltonian to which we apply the same procedure twice with a halved pivot time step. This procedure is repeated recursively until the time evolution of all particles is evaluated. In this way different integrators can be derived (depending on the details of the split) that retain a close resemblance to the block time step scheme, but which will conserve integrals of motion, in particular the total (angular) momentum, to machine precision. We will show that, when used in conjunction with an approximately symmetric time step criterion, they show good energy conservation and do not show energy drift. In section 2 we present our derivation and our symmetrization scheme. In section 3 we present various tests of these integrators, while we summarize and discuss the results in section 4.
2. Method

2.1. Derivation

The problem at hand is to evolve a set of particles $X$ for a time $dt$ under the dynamics generated by the Hamiltonian:

$$H = \sum_{i \in X} \frac{p_i^2}{2m_i} - \sum_{i,j \in X, i < j} \frac{Gm_im_j}{|r_i - r_j|}$$  \hspace{1cm} (1)

The Hamiltonian consists of momentum terms

$$P_X = \sum_{i \in X} \frac{p_i^2}{2m_i}$$ \hspace{1cm} (2)

and potential terms

$$V_{XX} \equiv -\sum_{i,j \in X, i < j} \frac{Gm_im_j}{|r_i - r_j|}$$ \hspace{1cm} (3)

The evolution of the state of the system is given by the flow operator $\exp(dtH)$ where $H$ is the Hamiltonian vector field corresponding to $H$. In cases the Hamiltonian can be split in two parts $H = H_A + H_B$, where $\exp dtH_A$ and $\exp dtH_B$ can be calculated, the flow of $H$ can be approximated by composing $\exp dtH_A$ and $\exp dtH_B$, e.g.

$$\exp(dtH) \approx \exp(dt/2H_B) \exp(dtH_A) \exp(dt/2H_B)$$ \hspace{1cm} (4)

in this case the approximation holds to second order in $dt$ (Hairer et al., 2006). An example of this is the division in $H_A = V_{XX}$ and $H_B = P_X$ which generates the familiar second order Drift-Kick-Drift (DKD) verlet integrator.

The derivation of approximate solvers by the division of the Hamiltonian into simpler, solveable, subsystems is a general method not limited to the above division in momentum and potential terms. For example, efficient planetary integrators may be constructed by splitting the Hamiltonian in a part that describes the Keplerian motion around the central star and a part that describes the perturbation of the planetary bodies on each other (Wisdom and Holman, 1991). Additionally, splitting can be used as a strategy for focusing the computational effort on the parts of the system that are evolving most strongly, either by decomposing the potential in two (Springel, 2005, for a split into long range and short range forces in cosmological simulations) or more components (Duncan et al., 1998, employing a series of successive shells), or by grouping particles according to their dynamical evolution timescale (e.g. Fujii et al., 2007; Saha and Tremaine, 1994).

Here we derive multiple time step methods by choosing the division of the
Hamiltonian adaptively and recursively based on the current time step assigned to the particles such that one system \( S \) contains the interaction terms of all the particles with a time step larger than \( dt \), and the other system \( F \) contains all the interaction terms of the particles with a time step smaller than \( dt \). This method of subdividing the system according to the timestep is very close to splitting in Saha and Tremaine (1994) (the “PASS” method we present below employs the same split as their method), apart from the fact that we allow the partitioning of the system to change continuously. This last property means that we have to be careful choosing the timesteps (discussion of which we defer to section 2.2).

For example, we may choose the split

\[
H_S = P_S + V_{SS} + V_{SF}
\]
\[
H_F = P_F + V_{FF}
\]  

(Note that indeed \( H = H_S + H_F \)) and approximate

\[
\exp(dtH) \approx \exp(dt/2H_F) \exp(dtH_S) \exp(dt/2H_F)
\]

The evolution operator \( \exp dtH_S \) is then approximated by the DKD (or any other second order scheme). This consists of drifts of the particles in \( S \) (from \( P_S \)) and kicks on the particles in \( S \) and \( F \) (from \( V_{SS} + V_{SF} \)). These kicks consists of updates of the particle positions where every \(-Gm_i m_j/|r_i - r_j|\) term in the potential part generates kicks

\[
dp_i = dt \frac{Gm_i m_j}{|r_i - r_j|^3} (r_i - r_j)
\]
\[
dp_j = dt \frac{Gm_i m_j}{|r_i - r_j|^3} (r_j - r_i)
\]

For the two \( \exp dt/2H_F \) operators of the \( F \) system we apply the same procedure as for the \( \exp dtH_S \) operator (with halved time step). The splitting can thus be applied recursively to the evolution operators with time step \( dt/2^k \). The recursion ends when a time step sufficiently small is reached such that no particles end up in the \( F \) system (of that level). Note that we made a choice in subdividing the system: Eq. 5 is certainly not the only possible split. For example, the potential cross terms \( V_{SF} \) could also be put in \( H_F \), resulting in a different method. The difference between the two is that in the former case (eq. 5) the interactions between particles in \( S \) and \( F \) systems are done on the slowest of the time steps of the \( i \) and \( j \) particle pair. In the latter case the interactions propagate to the fast system, and will in the end be updated on the minimum of the time steps of each \( (i,j) \) particle pair, thus the split in eq. 5 can be expected to be computationally faster. Note that the integration scheme that results is similar to conventional individual block time step schemes, where the time step is subdivided in powers of

4
two. However, existing direct N-body codes with block time step schemes (e.g. McMillan, 1986; Makino, 1991, and modern variants) put particles in a hierarchy of time step bins to dictate the frequency in which the total forces for the particles in that bin are updated. A particle in a fast time step bin is evolved using a force calculated from all other particles - the particles that need less updates (higher in the time step hierarchy) are extrapolated to the time of the fast particle if necessary. In the scheme presented here the total force is never (or only incidentally) calculated: all the velocity changes are effected by momentum kicks (which need only originate from a subset of the particles) - and always pairwise: every $i \leftarrow j$ interaction kick is accompanied by its corresponding $i \rightarrow j$ interaction kick. The scheme is therefore manifestly momentum conserving. The extrapolating schemes, including their Hermite generalizations, are not momentum conserving.

By putting the $V_{SF}$ in the slow system in Eq. 5 we made the choice of calculating the interactions between ‘slow’ and ‘fast’ system on the time step of the slow particles - hence we refer to this integrator as the HOLD integrator (the $V_{SF}$ are ‘held’ on the slow time step). Alternatively, when we put the $V_{SF}$ terms in the fast system:

$$
H_S = P_S + V_{SS} + V_{SE} \\
H_F = P_F + V_{FF} + V_{FS} + V_{FE}
$$

(8)

Note that we have included the $V_{SE}$ and $V_{FE}$, these denote any interactions that are inherited from the higher levels. As we will see below this integrator does not conserve the position of the center of mass, the corresponding integrator that does is

$$
H_S = V_{SS} + V_{SE} \\
H_F = P_S + P_F + V_{FF} + V_{FS} + V_{FE}
$$

(9)

We refer to this scheme as PASS (and to eq. 8 as PASS1).

We will compare the HOLD and PASS integrators with the conventional integrator without individual time steps but with shared adaptive time steps (SHARED) and the conventional block time step integrator which extrapolates particle positions (BLOCK). A cartoon representation and overview of the differences between the different integrators is given in Figure 1.

2.2. Symmetric time-stepping

The above integrators are symplectic only as long as the particles do not change their timestep. For general N-body simulation codes, where particles experience very different dynamical timescales during their evolution, we need to relax this condition and let the particles move between timestep sets. Using adaptive timesteps dependent on the phase space coordinates will in general destroy the symplecticity (and hence the conservation properties) of the integrator (Skeel and Gear, 1992; Preto and Tremaine, 1999).
Figure 1: Schematic overview of the different integrators. Panel A shows the interactions that are calculated between two particles (1 and 2) by the SHARED integrator for a fiducial trajectory of these two particles, where particle 1 has a time step 4× larger than particle 2, which is also globally in the smallest time step bin (with the rest of the system is represented by the greyed out trajectory). All the interactions between the particle are calculated on the smallest time step. Panel B shows the case of the conventional block time step scheme (BLOCK integrator). In this case the total force on each particle is calculated determined by the individual time step of that particle. Panel C shows the HOLD integrator (Eq. 5). In this case particle 2 only feels the interaction of particle 1 with a frequency determined by the time step of particle 1. In between the particle may be kicked by interactions with other particles. Panel D shows the PASS integrator (Eq. 9). For this integrator the mutual interactions between 1 and 2 are calculated on a time step determined by the fast particle 2 (note that in this figure the same number of interactions is calculated for the SHARED and PASS integrators - in general this is not the case). The difference with panel B is the fact that each kick of the velocity of particle 2 is matched by the corresponding kick on particle 1.
Mikkola and Tanikawa, 1999), although with some restrictions it is possible to construct adaptive timestep symplectic integrators by considering the Hamiltonian in an extended phase space (Preto and Tremaine, 1999; Mikkola and Tanikawa, 1999) or using a variational approach (Farr and Bertschinger, 2007). For the integrators we present here it is however possible to recover long term energy conservation by ensuring time reversibility of the integrator. This can be done by using a time-symmetrized time step criterion for the particles (Hut et al., 1995; Preto and Tremaine, 1999).

To be specific, we start by reviewing in more detail why the numerical integration of a particle trajectory loses its time symmetry (and hence its energy conserving properties) when a variable time step is adopted. Given a particle trajectory \((r(t), v(t))\) one tries numerically to integrate this using a time step function \(\tau(t)\) (which is a function of time through its dependence on the state variables \(r\) and \(v\)). If we advance a state \(r(t) \rightarrow r(t+\tau_1), v(t) \rightarrow v(t+\tau_1)\) we reach a new state with a new time step \(\tau_2\). If we would run the integration backwards in time, in general \(\tau_1 \neq \tau_2\), so we would not arrive at the original state, and due to the numerical errors we would not follow the same numerical approximation to the trajectory. This situation would not arise if the time step function had the property that \(\tau(t+\tau(t)) = \tau(t)\). Note that \(\tau(t)\) refers to a time step in positive direction while \(\tau(t+\tau(t))\) refers to a time step in the negative direction, so the requirement should be read as \(\tau^-(t+\tau(t)) = \tau^+(t)\). In fact we can introduce such a symmetric time step function \(\tau_{\text{sym}}\):

\[
\begin{align*}
\tau^-_{\text{sym}}(t) &= \tau(t)/2 + \tau(t - \tau^-_{\text{sym}})/2 \\
\tau^+_{\text{sym}}(t) &= \tau(t)/2 + \tau(t + \tau^+_{\text{sym}})/2
\end{align*}
\]

(10)

this becomes a workable ansatz if we approximate

\[
\tau^+_{\text{sym}}(t) \approx \tau(t) + \frac{1}{2} \frac{d\tau}{dt} \tau^+_{\text{sym}}
\]

(11)

so we can write:

\[
\tau_{\text{sym}} = \frac{\tau(t)}{(1 - \frac{1}{2} \frac{d\tau}{dt})}
\]

(12)

which is the approximation we will use below. For a time step proportional to the inter-particle free-fall times

\[
\tau_{ij} = \eta_1 \sqrt{\frac{r_{ij}}{a_{ij}}} = \eta_1 \sqrt{\frac{r_{ij}^3}{\mu_{ij}}}
\]

(13)

with \(\mu_{ij} = m_i + m_j\), the derivative is

\[
\frac{d\tau_{ij}}{dt} = \frac{3\pi_{ij} \cdot \pi_{ij}}{2r_{ij}^2} \tau_{ij}
\]

(14)
hence the symmetrized version of the free-fall time step criterion becomes

$$\tau_i = \min_j \left( \frac{\tau_{ij}}{(1 - \frac{1}{2} \frac{d\tau_{ij}}{dt})} \right)$$

(15)

A time step proportional to the interparticle flyby times

$$\tau_{ij} = \eta_2 \frac{\tau_{ij}}{v_{ij}}$$

(16)

with

$$\frac{d\tau_{ij}}{dt} = \frac{\nabla v_{ij} \cdot \nabla \tau_{ij}}{v_{ij}^2} \tau_{ij} (1 + \frac{\mu_{ij}}{v_{ij}^2 r_{ij}})$$

(17)

can be similarly made symmetric (note that eq. 17 simplifies the expression by only considering the \(i\) and \(j\) particle for the time derivative of \(v_{ij}\)). We will take the particle time step to be equal to the minimum of the symmetrized free-fall (defined by eqs. 13, 14, and 15) and symmetrized flyby time step (eq. 16, 17 and 15).

There are various other ways in the literature to symmetrize the time step. Hut et al. (1995) advocated an iterative procedure to symmetrize Eq. 10. In this case an trial step is taken, after which the average of the new and old time step is taken. This can be repeated to converge to the solution of Eq. 10. This has the drawback that the iteration is an expensive operation which needs multiple force evaluations for the system. Alternatively, a time step determined by

$$\tau_{old} \tau_{new} = \tau(t)^2$$

(18)

provides an explicit symmetrized time step (Dehnen and Read, 2011). Both of these do not work when used with a block time step scheme (Makino et al., 2006; Dehnen and Read, 2011). For the former iterative solution this is because of a “flip-flop” problem where convergence is not reached because of the restriction of the time step to powers of two of a base time step. A solution in case is available (Makino et al., 2006), but entails saving the whole system state over a time interval and multiple iterations.

To test whether the expressions given here (which due to the truncation after first order in \(\tau\) in Eq. 12 are only approximately time-symmetric) yield a conservative variable time step method when using a power of two hierarchy of time steps, we integrate a Kepler orbit with eccentricity \(e = 0.9\) for 1000 orbits and a \(\eta = 0.01\) (this is the same test as fig. 1 and 2 of Hut et al., 1995). The test uses the symmetrized free-fall time step (eq. 13). The time steps are chosen to be block time steps as in the integrators presented in section 2.1 (for the two body problem the integrators of section 2.1 and the usual block time-stepping are equivalent). The orbital elements for the orbit are plotted in Fig. 2. As can be seen there is no systematic drift in energy (the orbit does precess with a constant speed). The performance of the
integrator is similar to the iterative scheme of (Hut et al., 1995), and does not show the systematic drift in \( a \) and \( e \) of a non-symmetrized integrator.

In Figure 3 we show the resulting (maximum) energy error for a set of \( 10^4 \) orbit integrations for different values of the eccentricity and time step parameter \( \eta \), plotted vs the number of steps per orbit. Although the integration scheme is in general robust, this figure shows that for a given \( \eta \) it tends to keep the number of steps per orbit constant. This could be a disadvantage if such a time step is used in a run with multiple bodies where encounters with different \( e \) can occur. This can be remedied by choosing an error control time step \( \tau_{ec} \)

\[
\tau_{ec} = \tau \left( \frac{\tau}{\tau_0} \right)^\gamma
\]

with \( \gamma \) a small exponent such that the time steps become smaller as \( \tau \) decreases. Such an expression is also easily symmetrized. Figure 3 also shows the results for this time-stepping scheme (with \( \gamma = 1/3 \)). As can be seen, in this case runs with constant \( \eta \) show a much less marked increase in error, showing an almost flat profile for the orbits with extreme \( e \) (albeit at the price of a rapidly increasing number of steps per orbit). For the other tests below we do not use the \( \tau_{ec} \) as these tests are not especially sensitive to the high eccentricity behavior.

2.3. Implementation

The integrators are implemented in the HUAYNO (for Hierarchical split-Up Astrophysical N-body sOlver) N-body code, released as part of the Astrophysical Multi-purpose Software Environment (AMUSE, Portegies Zwart et al., 2009). HUAYNO is written in C as testbed for the N-body integrators described here. There is a very close correspondence of procedures in HUAYNO and the mathematical operators for the algorithm: evolve, drift and kick operators have their counterpart in the code (this is illustrated in the pseudocode for the HOLD integrator given in fig. 4). The particles themselves are stored in an array which is reshuffled to match the partitioning required by the integrator (this partitioning is very similar to the block time step implementation of McMillan and Aarseth, 1993). The subsystems are then contiguous memory blocks conveniently referred to by a pointer and size. This has the added benefit that the particles which end up accessed the most end up close to each other in memory. The shuffling itself is an \( O(N) \) operation with negligible impact on the performance.

The code implements an optional Plummer softening parameter \( \epsilon \) for the gravitational interactions. It allows to set separately \( \eta_1 \) and \( \eta_2 \), for the time step parameter of the free-fall (eq. 13) and flyby (eq. 16) time step criteria. If not explicitly mentioned they are taken to be the same (and referred to by

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Figure 2: Orbital elements for the variable time step leapfrog integrator with symmetrized time step criterion (eqs. 13, 14, and 15). Plotted are the changes in semi-major axis $a$, eccentricity $e$, longitude of apo-center $l$ and the time of apocenter passage as a function of orbit number (sampled at apocenter). The time steps are varied in the same way as in the blocktime step schemes.
Figure 3: Maximum relative energy error vs number of steps per orbit. For this a Kepler orbit is integrated for 10000 orbits. The lines in black use the standard symmetrized time step criterion (eqs. 13, 14, and 15) for different values of the eccentricity (from bottom to top $e = 0.6, 0.9, 0.99, 0.999, 0.9999, 0.99999$), dotted lines connect runs with the same $\eta$. Thin red lines show the same for runs with the error control time step Eq. 19.

Figure 4: Pseudo code of the HOLD integrator.

```python
function evolve_hold(system, dt)
    calculate_timestep(system)
    fast, slow=sort_in_fast_and_slow(system,dt)
    evolve_hold(fast, dt/2)
    drift(slow,dt/2)
    kick(slow, fast, dt)
    kick(fast, slow, dt)
    drift(slow,dt/2)
    evolve_hold(fast, dt/2)
```
\( \eta \) in the tests below. Unless explicitly given the tests below use unsoftened gravity, \( \epsilon = 0 \).

3. Tests

To examine the differences between the 5 integrators presented in section 2.1 we evolve an \( N = 100 \) Plummer sphere of particles with equal mass. Total mass is 1 and units are scaled such that \( G=1 \), total mass \( M=1 \) and \( E=-0.25 \) (Nbody units, Heggie and Mathieu, 1986). Figure 5 shows the evolution of the Energy \( E \), momentum \( P \), angular momentum \( L \) and the center of mass position \( X \) for each integrator, all evolved with the same \( \eta = 0.01 \).

The first thing to notice in these plots is the different behavior of the BLOCK integrator with respect to momentum conservation. The error in center of mass and momenta (linear and angular) remain at machine precision for the conservative integrators, whereas the BLOCK integrator shows an error of \( \approx 10^{-7} \). Note also that the center of mass of the PASS1 integrator run is not conserved - this may be surprising: this integrator does...
Figure 6: Growth of relative energy error for 20 symmetrized (black lines) and 20 non-symmetrized time step (red lines) runs. This is the same test as in Makino et al. (2006). The same set of $N = 100$ Plummer sphere initial conditions were used for the two sets of simulations. Symmetrized runs took $\approx 20\%$ longer than unsymmetrized runs (26 vs 22 sec in total).

conserve linear momentum because of the pairwise force kicks (as can be seen in fig. 5). The reason for the shift in the center of mass is the fact that this integrator includes kicks between particles that are not synchronized in time: combining Eq. 6 with Eq. 8 we see that midway in the half step of the evolution of $\exp{dt/2H_F}$ the kicks between the S and F system are calculated. At that point the positions of the S system particles lag $dt/4$ with respect to the F system. After the kicks are applied the position of an S particles drifts an extra $\Delta v_1 dt/4$ from the first $\Delta v_1$ kick. In the second half step this is compensated by missing a $\Delta v_2 \Delta t/4$ drift, but these two will in general not cancel out exactly: hence the center of mass position is not conserved. This will happen irrespective of whether a DKD or KDK split is taken as the basis for PASS1. The proper formulation (PASS), which ensures time synchronized kicks, does show conservation of the center of mass position (fig. 5). Note also that applying the KDK method with the HOLD integrator (for $\exp{dtH_S}$ in eq. 5) will result in kicks between particles at different evolve times, and thus a deviation of the center of mass.

The energy errors are very similar for all the integrators. They remain all at a level of few $\times 10^{-7}$ and do not show any linear drift. The reason that the BLOCK integrator performs competitive with the other integrators is that the errors in momentum etc. remain small enough not to induce energy errors (Note that the Plummer sphere initial conditions represent a problem that is not especially sensitive to errors in momentum conservation).

As we mentioned above, our symmetrization scheme (eq. 12) of the time
Fig. 7: Energy error as versus time step parameter and run time. Each run evolves an $N = 1024$ plummer sphere for 1 N-body time unit (lines use the same legend as in fig. 5). Left panel shows relative energy error as a function of time step parameter $\eta$, right panel shows error versus the wallclock time elapsed for that run. Energy error is the maximum recorded over the run.

The Kepler test of the symmetrization scheme in section 2.2 suggests that it is adequate, however for larger $N$ simulations the additional terms in the timestep derivatives in Eq. (12) or the selection of minimum timesteps in Eq. (15) could cause the timestep symmetrization to fail. Hence, we conduct an additional test of our scheme by repeating the test of Makino et al. (2006) presented in their figure 4. This test consists of running $N = 100$ Plummer sphere models for symmetrized and non-symmetrized time steps. Makino et al. (2006) showed that the linear drifts of the non-symmetrized time step runs are suppressed when using the symmetrized version (they used a scheme for block time steps using 6 iterations to symmetrize the time step). Our result for this test is shown in figure 6. The integrator we use for both sets of runs is the HOLD integrator. The result is very similar to the Makino et al. (2006) figure. This shows that our symmetrization scheme works at least as well as the approach given there, and seems sufficient for the second order integrators employed here.

In figure 7 we show the behavior of the integrators as a function of the time step parameter $\eta$. All integrators show the second order dependence on $\eta$ as expected. The actual energy errors at the same $\eta$ also lie within a narrow band. If we look at the trend with run-time we see that the SHARED integrator is a factor 300-1000 slower than the other integrators. Within the integrators with individual time steps the HOLD integrator is most efficient, then the PASS1 and PASS integrators and lastly the BLOCK scheme. Looking at energy error dependence on $\eta$ we see that BLOCK and HOLD are actually very similar, so the difference (of a factor $\approx 3$) in efficiency as measured by wall-clock time is a result of the lower number of force evaluations of the HOLD method.
3.1. Core collapse

As a last test we evolve a $N = 1024$ Plummer sphere of equal mass particles to core collapse. First we employ smoothing with an $\epsilon = 1/256$ ($\eta = 0.01$). In this case we evolve to $t = 700$. The setup was chosen to match the test in Nitadori and Makino (2008). We plot the Lagrangian radii, energy and momentum error in figure 8 (The angular momentum and center of mass errors are omitted as they show the same pattern as the momentum error). We plot the results for the PASS, BLOCK and HOLD integrators. As can be seen in the plot of the Lagrangian radii all integrators show the expected evolution of the mass distribution. Differences within the runs fall within the expected statistical variation (see also Nitadori and Makino, 2008). Note that although the runs start with the exact same initial conditions these can be considered effectively different runs as they diverge exponentially on the crossing time timescale. The energy errors in Figure 8 show similar results for the integrators, the BLOCK integrator showing a consistently factor 2 to 3 larger error. Note the absence of energy drift also
Figure 9: Lagrangian radii, energy error and wallclock time for the N=1024 Plummer sphere core collapse test with $\epsilon = 0$ for the HOLD integrator. Upper panel shows Lagrangian radii, Middle panel shows the relative energy error, lower panel shows the wallclock time for the simulation.
in this long term integration (the energy errors do increase somewhat as the integration progresses, but they return to zero and change sign). In the plot of the momentum error we can see that the PASS and HOLD integrators conserve momentum to machine precision. A slight increase in error is visible at the end. This is due to the loss of precision in calculations involving escaping stars. If we compare the time needed to advance the simulation of the three integrators we notice a clear difference: at the beginning the HOLD integrator is a factor $\approx 3$ faster (which is consistent with the tests in fig. 5), as the simulation evolves the difference between HOLD and the other two integrators increases to a factor 12 at the end. The HOLD integrator becomes more efficient as the timescale differences within the system become larger.

As an additional test for the HOLD integrator we run the same problem for $\epsilon = 0$. This is a demanding test as in this case strongly bound binaries form during core collapse (Giersz and Heggie, 1994). This test calculation is shown in figure 9. In this case the core collapse occurs at $t \approx 350$, and the evolution of the Lagrangian radii and core radius shows a pattern consistent with Giersz and Heggie (1994). The energy errors increase during the core collapse (for reference this can be compared with current Hermite codes in Konstantinidis and Kokkotas, 2010, their fig. 21). Note that the error increases during very short episodes, after which the error remains bounded. These error jumps occur during strong interactions with the binary that forms in the center, and may be caused by failures of the timestep symmetrization, although similar error jumps occur also in codes using completely different timestepping criteria (see again Konstantinidis and Kokkotas, 2010, for an example) A more uniform error behavior may be obtained by decreasing the $\eta$ parameter during these ‘rough patches,’ for a modest increase in computation time (for very close encounters the loss of accuracy may be due to the numerical precision, in this case some form of regularization is necessary). Plotting the wall-clock time of the simulation we see that towards the end of the simulations slows down (for the BLOCK and PASS integrators this would mean an additional slowdown by a factor 100). This is due to the formation of hard binaries. The HOLD integrator therefore is able to integrate systems without smoothing, although a more efficient handling of binaries is desirable.

4. Discussion

We have presented a set of conservative individual time step integrators derived using recursive Hamiltonian splitting. These integrators are remarkably simple and closely follow previous work: specifically they can be seen as a generalization of the scheme used in the mesh-based integrator for collision-less systems GROMMET (Magorrian, 2007) and are closely related to the Hamiltonian splitting methods used in planetary dynamics
Duncan et al. (1998, Saha and Tremaine, 1994) or the force splitting methods used in molecular dynamics (e.g. Tuckerman et al., 1992). In contrast to the usual formulation of block time steps they conserve momentum and angular momentum to machine precision and in conjunction with the (approximately) symmetrized timestep criterion presented here they show good conservation of energy. Our tests show that the energy conservation is a consequence of the use of a symmetrized time step criterion (as the conventional BLOCK integrator shows similar error behavior with the symmetrized time step). Of the new integrators HOLD and PASS the former is more efficient because it calculates the interaction between two particles with different time steps at an interval determined by the slower of the two particles. The Hamiltonian splitting considered here can be applied more generally. For example, Smooth Particle Hydrodynamics (SPH) codes also use a similar time-stepping scheme, and the scheme presented here directly carries over to SPH codes.

One drawback of the subdivision in terms of the time steps assigned to the particles is that the interactions for a given particle in a time bin are calculated together with all other particles with the same time step. For example, if the system contains multiple binary stars (and assume all these binaries have the same orbital parameters) then the stars that form these binaries all have the same time step and will end up in the same bin, with all their mutual interactions calculated on the fastest time step. The worst case scenario (which is however physically significant) is that all the stars are in binaries. In this case the split time step scheme as presented here does not save computing time with respect to a shared time step simulation (this is also the case for conventional block time step integrators). To ameliorate this one would need a subdivision at each level of the system in multiple systems based on e.g. a spatial partitioning at each level, as opposed to a simple split in a fast and a slow system.

We have limited ourselves to second order integrators. The second order nature of the integrators is a consequence of Eq. 6: this is the second order leapfrog composition. There is no reason why we could not use a higher order composition scheme (McLachlan, 1993), as long as we take care selecting the same (or at least of the same order) composition schemes for the component integrators. A problem with using higher order integrators is that the compositions contain terms with negative time steps. While in principle this is not a problem, it does present a problem for the efficiency of the integrator as the time interval that the integrator follows is bigger than the integration time interval by a factor $\alpha > 1$. Note that within a recursive scheme every level in the time step hierarchy will increase the length of this interval by this factor, so that unless $\alpha$ is very close to 1, $\alpha^k$ can increase rapidly.

In addition to the algorithmic enhancements mentioned above, the numerical implementation of the integrators can be improved. For large scale
production work they would need to be parallelized and probably also be adapted to use Graphic Processor Units (GPUs). At the moment a partial implementation on GPUs is available, where only the kicks are implemented on the GPU. This implementation suffers from the inefficiencies of transferring data to and from the GPU. With these improvements we expect that the code will be competitive with modern Hermite codes.

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References

Aarseth, S. J.: 1999, PASP 111, 1333
Chambers, J. E.: 1999, MNRAS 304, 793
Dehnen, W. and Read, J. I.: 2011, European Physical Journal Plus 126, 55
Dubinski, J.: 1996, New A 1, 133
Duncan, M. J., Levison, H. F., and Lee, M. H.: 1998, AJ 116, 2067
Farr, W. M. and Bertschinger, E.: 2007, ApJ 663, 1420
Fujii, M., Iwasawa, M., Funato, Y., and Makino, J.: 2007, PASJ 59, 1095
Giersz, M. and Heggie, D. C.: 1994, MNRAS 268, 257
Hairer, E., C., L., and Wanner, G.: 2006, Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations, Springer Verlag
Harfst, S., Gualandris, A., Merritt, D., and Mikkola, S.: 2008, MNRAS 389, 2
Heggie, D. C. and Mathieu, R. D.: 1986, in P. Hut & S. L. W. McMillan (ed.), The Use of Supercomputers in Stellar Dynamics, Vol. 267 of Lecture Notes in Physics, Berlin Springer Verlag, pp 233–+
Hernquist, L. and Katz, N.: 1989, ApJS 70, 419
Hut, P., Makino, J., and McMillan, S.: 1995, ApJ 443, L93
Konstantinidis, S. and Kokkotas, K. D.: 2010, A&A 522, A70+
Magorrian, J.: 2007, MNRAS 381, 1663
Makino, J.: 1991, PASJ 43, 859
Makino, J., Hut, P., Kaplan, M., and Saygın, H.: 2006, *New A* **12**, 124

McLachlan, R.: 1995, *SIAM J. Sci. Comput* **16**, 151

McMillan, S. L. W.: 1986, in P. Hut & S. L. W. McMillan (ed.), *The Use of Supercomputers in Stellar Dynamics*, Vol. 267 of *Lecture Notes in Physics, Berlin Springer Verlag*, pp 156–+

McMillan, S. L. W. and Aarseth, S. J.: 1993, *ApJ* **414**, 200

Mikkola, S. and Tanikawa, K.: 1999, *Celestial Mechanics and Dynamical Astronomy* **74**, 287

Moore, A. and Quillen, A. C.: 2011, *New A* **16**, 445

Nitadori, K. and Makino, J.: 2008, *New A* **13**, 498

Portegies Zwart, S., McMillan, S., Harfst, S., Groen, D., Fujii, M., Nuallán, B. Ó., Glebbeek, E., Heggie, D., Lombardi, J., Hut, P., Angelou, V., Banerjee, S., Belkus, H., Fragos, T., Fregeau, J., Gaburov, E., Izzard, R., Jurić, M., Justham, S., Sototoriva, A., Teuben, P., van Bever, J., Yaron, O., and Zemp, M.: 2009, *New Astronomy* **14**, 369

Portegies Zwart, S. F., McMillan, S. L. W., Hut, P., and Makino, J.: 2001, *MNRAS* **321**, 199

Preto, M. and Tremaine, S.: 1999, *AJ* **118**, 2532

Saha, P. and Tremaine, S.: 1994, *AJ* **108**, 1962

Skeel, R. D. and Gear, C. W.: 1992, *Physica D Nonlinear Phenomena* **60**, 311

Springel, V.: 2005, *MNRA* **364**, 1105

Stadel, J. G.: 2001, *Ph.D. thesis*, UNIVERSITY OF WASHINGTON

Tuckerman, M., Berne, B. J., and Martyna, G. J.: 1992, *J. Chem. Phys.* **97**, 1990

Wadsley, J. W., Stadel, J., and Quinn, T.: 2004, *New A* **9**, 137

Wisdom, J. and Holman, M.: 1991, *AJ* **102**, 1528