A MOMENTUM CONSERVING N-BODY SCHEME WITH INDIVIDUAL TIMESTEPS

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ABSTRACT

N-body simulations study the dynamics of N particles under the influence of mutual long-distant forces such as gravity. In practice, N-body codes will violate Newton’s third law if they use either an approximate Poisson solver or individual timesteps. In this study, we construct a novel N-body scheme by combining a fast multipole method (FMM) based Poisson solver and a time integrator using a hierarchical Hamiltonian splitting (HHS) technique. We test our implementation for collision-less systems using several problems in galactic dynamics. As a result of the momentum conserving nature of these two key components, the new N-body scheme is also momentum conserving. Moreover, we can fully utilize the $O(N)$ complexity of FMM with the integrator. With the restored force symmetry, we can improve both angular momentum conservation and energy conservation substantially. The new scheme will be suitable for many applications in galactic dynamics and structure formation. Our implementation, in the code Taichi\textsuperscript{a)}, is publicly available.

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\textsuperscript{a)} \url{https://bitbucket.org/qirong_zhu/taichi_public/}. The name “Taichi(太极)” is inspired by the symmetries in the force computation and the time integration. The name also refers to the recursive relations and the hierarchical nature of FMM and the time integrator.
1. INTRODUCTION

The conservation of momentum is a manifestation of Newton’s third law. However, current N-body codes do not conserve momentum by introducing spurious net velocities, a direct consequence that most of the Poisson solvers are not momentum conserving and individual timesteps are not momentum conserving either. To some extent, momentum conserving error reveals the overall accuracy of N-body simulations.

As an approximate Poisson solver, the most famous BH tree method \( \text{(Barnes & Hut 1986)} \) dramatically speeds up force evaluations by organizing particles into oct-trees. To any sink particles, source particles within a distance cell can be efficiently approximated by a single particle. However, there is no guarantee that the approximation is symmetric when the role of sink and source reversed. Therefore, Newton’s third law is violated in the force evaluation phase.

For the time integration, adaptive individual timesteps play a crucial role in N-body codes by reducing the total number of force evaluations. However, force symmetry is broken between two particles with different timesteps. For the popular kick-drift-kick (KDK) integrator, particles with smaller timesteps receive kicks at a higher frequency than particles with larger timesteps while the positions of particles are not synchronized. While many modern codes use synchronized positions for inactive particles based on the velocities, this extrapolated position is slightly offset from the positions to perfectly respect the force symmetries with the active particles. As a result, the exact momentum conservation is also broken since the total kicks on all the particles do not cancel out. Again, we violate the force symmetry in Newton’s third law.

In this study, we propose a new momentum-conserving N-body scheme by combining two momentum-conserving components: a Poisson solver based on the fast multipole method \( \text{(FMM hereafter)} \) and a timestep integrator based on a hierarchical Hamiltonian splitting \( \text{(HHS hereafter)} \) proposed by Pelupessy et al. \( \text{(2012)} \). We note that neither of the two components is completely new to the community. Examples of FMM codes include HOT \( \text{(Warren & Salmon 1995)} \), FALCON \( \text{(Dehnen 2000, 2002)} \), and PKDGRAV3 \( \text{(Potter et al. 2017)} \). FMM is also implemented as a short-range force solver in SWIFT \( \text{(Schaller et al. 2016)} \), an ongoing project. The use of momentum conserving integrator can be traced back to the studies of planetary dynamics in the 90s \( \text{\text{(e.g., Wisdom & Holman 1991; Duncan et al. 1998)}} \). The HUAYNO code by Pelupessy et al. \( \text{(2012)} \) includes the implementation of the HHS integrator. Recently, a TreePM code AREPO \( \text{(Springel 2010)} \) with an implementation of the HHS integrator has been used in large scale cosmological production simulations \( \text{(see Springel et al. 2017)} \).

As we show later, the proposed new N-body scheme has some attractive features which might interest the community. In particular, this scheme offers substantial improvements in its accuracy over the existing practices. In § 2, we briefly review the Poisson solver and time integrator and outline our implementations. In § 3, we show the performance of the new scheme using a cold collapse test, an isolated disk galaxy, and the growth of a Milky Way-sized halo in a cosmological setup. We further discuss the prospects of this new scheme in § 4. We conclude with a summary in § 5.

2. METHOD

2.1. A FMM based Poisson solver

The tree method by Barnes & Hut \( \text{(1986)} \) approximates the gravitational force at a given sink particle for a group of source particles. In contrast, FMM starts with the expansion of gravitational potential at a group of sink particles in cell A with the cell centered at \( \mathbf{z}_A \) and a group of source particles in cell B centered at \( \mathbf{z}_B \). The key component of FMM maps the potential landscape generated by sources onto the sinks via a cell-cell interaction. This cell-cell interaction is performed for all the cell pairs if they are well-separated according some geometric or dynamic criteria. For example, we can use

\[ |\mathbf{z}_A - \mathbf{z}_B| > (R_A + R_B)/\theta, \tag{1} \]

where \( R_{A,B} \) is the cell size and the multipole-acceptance criterion \( \text{(MAC)} \) is denoted by a cell opening angle \( \theta \). While other criteria could offer advantages in terms of speed or force accuracy \( \text{(e.g., Dehnen 2002, 2014)} \), the simple geometric condition in Eq. (1) is easy to implement.

Besides the opening angle, the approximation errors are also controlled by the expansion order \( p \). Unlike other Poisson solvers, FMM does not suffer the errors associated with the mass assignment, potential interpolation or aliasing. One distinct feature of FMM is that there is no distinction between the source and sink cells by construction. Therefore, this gravity solver is manifestly momentum conserving because the mutual forces are symmetric \( \text{(Dehnen 2000, 2002)} \) between cell A and B. Moreover, the force symmetry holds true for any pair consisting of particle \( i \) from cell A and particle \( j \) from cell B:

\[ \mathbf{F}_{ij} = -\mathbf{F}_{ji}, \tag{2} \]

Naturally, the total force between all the particles in cell A and cell B also cancels out as \( \mathbf{F}_{AB} = -\mathbf{F}_{BA} \). In
addition, when a desired magnitude of error is specified, FMM has an \(O(N)\) complexity because the higher order terms decay faster than the increase of total particle number \(N\).

The original FMM method proposed by Greengard & Rokhlin (1987) groups all the particles into a uniform grid. The data structure of a uniform grid is not optimal for highly irregular distributions. Alternatively, the same oct-tree structure used in BH method has been introduced to FMM (Warren & Salmon 1995; Dehnen 2000). An efficient dual tree walk is implemented by these two studies as well. Starting from the root cell, we test the cell from the source tree and the sink tree according to Eq. (1). If cell \(A\) and \(B\) are not well-separated, we split the cell with larger size and process its eight child cells. If neither \(A\) and \(B\) contain any more child cells, a direct summation is carried out for all the particles in cell \(A\) and \(B\).

The combination of oct-tree and dual tree walk forms the basis of a versatile and adaptive Poisson solver. For a detailed mathematical description of FMM and the tree walk procedure, we refer the readers to Dehnen (2000, 2002) and Dehnen & Read (2011).

2.2. A HHS time integrator with individual timesteps

As we explained in the introduction, adaptive individual timesteps introduce errors in momentum conservation by directly violating Newton’s third law. Pelupessy et al. (2012) proposed a time integrator with individual timesteps which is free from this error. With the notations from Pelupessy et al. (2012), the Hamiltonian of \(N\)-body system \(H\) consists of a momentum term \(T\) and a potential term \(V\) as

\[
H = T + V = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i\in N, j\in S} \frac{Gm_im_j}{|r_i - r_j|}.
\]

The fundamental idea is to split \(H\) into a slow system \(S\) with its own Hamiltonian \(H_S\) and a fast system \(F\) with \(H_F\) with a pivot timestep as

\[
H = H_S + H_F,
\]

where

\[
H_S = T_S + V_{SS} + V_{SF},
\]

and

\[
H_F = T_F + V_{FF}.
\]

To kick system \(F\) with kickS2F, we only need to include the terms \(V_{SS} + V_{SF}\). To kick system \(S\) with kickS2F, we need to sum the terms \(V_{SS} + V_{SF}\).

\[
V_{SF} = -\sum_{i\in S, j\in F} \frac{Gm_im_j}{|r_i - r_j|}.
\]

are only encountered at the timestep determined by system \(S\) (referring to the HOLD integrator, with \(V_{SF}\) ‘held’ on the slow timestep), as in Eq. (5). This Hamiltonian splitting is then applied to \(F\) with half of the original pivot timestep on \(F\), which leads to a new \(F+S\) splitting. The splitting then proceeds in a hierarchy of power of two till no further splitting can be found. The following pseudocode describes such iteration in the HOLD integrator constructed with a second-order accurate KDK’s integrator. After splitting the particles into a \(F\) and \(S\) system, we compute the forces between \(F\) and \(S\) on the same rung \(k\) while evolving the fast system \(F\) on rung \(k + 1\).

Algorithm 1

\[
\text{EVOLE\_HOLD(rung, system, time, dt, calc_timestep)}
\]

\[
\text{slow, fast = split\_slow\_fast(dt, system);}
\]

\[
\text{if(fast.size > 0)}
\]

\[
\text{EVOLE\_HOLD(rung+1, fast, time, dt/2, 0);}
\]

\[
\text{KDK(rung, slow, fast, time, dt);}
\]

\[
\text{if(fast.size > 0)}
\]

\[
\text{EVOLE\_HOLD(rung+1, fast, time+dt/2, dt/2, 1);}
\]

The splittings in Eq. (5) and (6) introduce two different kicks in each hierarchy: kickS2F (kick from slow to fast) due to the term \(V_{SF}\) and kickFS2S (kick from slow to fast) due to the terms \(V_{SS} + V_{SF}\). To kick system \(F\) with kickS2F, we only need to include the forces originated from \(S\). To kick system \(S\), gravity from both \(F\) and \(S\) systems are evaluated. Our implementation of HOLD integrator contains variations from Pelupessy et al. (2012). The following pseudocode describes the sequence of kicks and drifts operations in a KDK step within the HOLD integrator used in this study. The force/potential computation is part of each KICK operation.

Algorithm 2

\[
\text{KDK(rung, slow, fast, time, dt)}
\]

\[
\text{if(fast.size > 0)}
\]

\[
\text{KICK(rung, fast, slow, dt/2, 1, 0); //kickS2F}
\]

\[
\text{KICK(rung, slow, fast, dt/2, 0, 0); //kickFS2S}
\]

\[
\text{drift(rung, slow, time, dt);}
\]

\[
\text{KICK(rung, slow, fast, dt/2, 0, 1); //kickFS2S}
\]

\[
\text{if(fast.size > 0)}
\]

\[
\text{KICK(rung, fast, slow, dt/2, 1, 1); //kickS2F}
\]

Figure 1 illustrates the sequence of drifts and kicks in the HOLD integrator. For particles on rung \(k\), we
Figure 1. A schematic of the HHS HOLD integrator. Here, particles on rung \( k \) march forward in time with a step size of \( \Delta t \). In a normal KDK step, a drift operation advances the particle positions from the starting to the end points and two kick operations update their velocities at the start and in the middle of the timestep. The HOLD integrator injects two kickS2F, as indicated by large arrows, right before \( t = \Delta t \). The frequency of kickS2F is determined by the step size of rung \( k - 1 \). Before each drift operation, the step size is adjusted by \( \Delta t_i = \sqrt{\eta/|\mathbf{a}|} \) by combining most recent kickS2F and kickFS2S.

A system which contains only two rungs, \( 0 \) and \( k \), we need to call Poisson solver \( (2 + 2 + 2^{k+1}) \) times for each step of rung 0. On the other hand, we can simply use a shared timestep based on rung \( k \) thus reduce the total number calls to Poisson solver to \( 2^k \). As a result, the new scheme can be quite inefficient for those systems (due to the fact that shared timestep can benefit from a leapfrog integrator), in particular, when \( k \) is small.

The following pseudocode of KICK operation illustrates our treatment of kickS2F and kickFS2S as well as timesteps. Similarly, as HUAYNO, we treat sink and source particles separately. When forces on \( F \) system are needed, we mask the masses of all particles in \( F \) to be zero. Their positions and masses are passed to a Poisson solver together with all particles from \( S \). As a result, only forces generated by \( S \) on \( F \) are computed. For kickFS2S, we use all the particles in both \( S \) and \( F \) systems such that the all the accelerations from particles with finer timesteps than \( S \) are included.

**Algorithm 3**

\[
\text{KICK}(\text{rung}, \text{system1}, \text{system2}, dt, \text{kickFS}, \text{secondkick})
\]

1. \( \text{joint_pos_mass} = \text{get_pos_mass}(\text{system1}, \text{system2}); \)
2. if (kickFS)
   1. \( \text{mask_mass_to_zero(\text{system1});} \)
3. \( \text{get_force_potential_from_exaFMM} \)
4. \( \text{(joint_pos_mass, force, potential);} \)
5. if (secondkick)
   1. \( \text{update_acceleration_old(\text{system1});} \)

2.3. Combining the two momentum conserving components

To implement the above ideas, we use ExaFMM\(^1\), a C++ FMM code, as our Poisson solver. ExaFMM builds an oct-tree structure using a top-down approach based on recursion, with each cell in the oct-tree containing a particle number no less than \( n_{\text{crit}} \), which is set to be 64 in this study. ExaFMM only includes an unsoftened Poisson solver, therefore we introduce force softening with a Wendland \( C^2 \) function (Wendland 1995) by modifying the \( 1/r \) potential to

\[
\phi(r) = \frac{1}{\epsilon} (uu((u(u(3u - 15) + 28) - 21)uu + 7) - 3),
\]

\(^1\) https://github.com/exafmm/minimal. This is a minimal version of ExaFMM with only spherical harmonics implemented for a Laplacian potential.
A momentum conserving $N$-body scheme

\[ u = \frac{r}{\epsilon} \quad \text{for} \quad r < \epsilon. \]

Since the spherical expansion does not apply to the softened potential, we additionally require the two cells can only enter cell-cell interaction when their distance is larger than the softening length $\epsilon$.

The way Huayno\(^2\) handles these two different kicks is straightforward, where a mass array consisting of both source and sink particles is passed into its direct summation solver. To ensure the momentum conservation with our new scheme, we set up two different mass configurations for kickSF and kickFS2S separately. The upper panel of Figure 2 shows the masking of the mass of particles in $F$ (in open circles) such that we only evaluate the accelerations from $S$ to $F$. Force symmetry is present for any pair of particles drawn from cell A and B. Therefore, the HHS integrator with adaptive individual timesteps retains the force symmetry.

Because ExaFMM uses the geometric size (cell side length) of each cell to test the well-separateness condition in Eq. (1), we will encounter a situation where we can split either cell A or B if they have equal size. This degeneracy is quite a subtle point that ruined the perfect force symmetry during tree traversal in our earlier attempts. To remove this asymmetry, we further require both cells to be opened if they are not well separated. Note this approach is suboptimal, a radius based on the smallest enclosing sphere (Dehnen 2014) do not lead to this degeneracy in the first place. The following code is our dual tree walk procedure. ExaFMM generates an interaction list for cell-cell interactions and a list for direct summation first. Then ExaFMM evaluates the potentials and forces altogether looping through the interaction lists for each cell in its evaluations phase.

**Algorithm 4**

\[
\text{GET\_INTERACTION\_LIST(\text{Cell } Ci, \text{ Cell } Cj)}
\]

1. if\( (\text{well\_seperated}(Ci, Ci)) \)
   \( Ci.\text{M2L\_list\_add}(Cj); \)

2. else if\( (Ci == \text{leaf} \text{ and } Cj == \text{leaf}) \)
   \( \text{Ci.P2P\_list\_add}(Cj); \)

3. else if\( (Ci == \text{leaf} \text{ and } Cj != \text{leaf}) \)
   for (all child cells cj of Cj)
   \( \text{GET\_INTERACTION\_LIST}(Ci, cj); \)

4. else if\( (Ci != \text{leaf} \text{ and } Cj == \text{leaf}) \)
   for (all child cells ci of Ci)
   \( \text{GET\_INTERACTION\_LIST}(ci, Cj); \)

5. else
   for (all child cell pairs \( \{ci, cj\} \) of \( \{Ci, Cj\} \))
   \( \text{GET\_INTERACTION\_LIST}(ci, cj); \)

In each kick, we pass the position and mass arrays to ExaFMM to complete a complete FMM evaluation step. The gravitational potentials and forces computed by FMM are then passed to the integrator to advance the system to the next step. The expense of each tree building is non-negligible. However, the hierarchical splitting of the total system dramatically reduces the cost of the average FMM computation. In each hierarchy, only a subset of particles participates in FMM as all the other particles in its lower hierarchies do not. As a result, the problem size of FMM is progressively reduced for the more dynamic part of the system. This feature is attractive for a system with a small fraction of very active particles. Even though we only need to evaluate the forces on the active particles, we still have to build the tree and evaluate the moments for all the particles, which can pose a significant overhead thus slows down the entire simulation. In a simplified case where

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\(^2\) Huayno is available at [www.amusecode.org](http://www.amusecode.org).
each hierarchy is occupied with a smaller particles numbers (say half of the previous hierarchy), only an additional factor \( \sim \sum_{l=1}^{n} 1/2^l \) is introduced in a total of \( n \sim \ln(N) \) steps. As a result, the HHS time integrator can maintain the \( \mathcal{O}(N) \) complexity of FMM using individual timesteps. Therefore, the combination of these two key components offers two highly attractive features into a new \( N \)-body scheme: momentum conserving and an \( \mathcal{O}(N) \) complexity.

Our implementation is in the code Taichi, which is largely built upon huayno using its routines for Hamiltonian splitting and ExaFMM for force calculations. The momentum conserving nature of our new scheme is demonstrated in our tests, as we show in the next sections. The fiducial values are \( \{\theta = 0.45, p = 5\} \) if not stated otherwise. Since we have used two momentum conserving components in Taichi, we also implement a traditional integrator with individual timesteps with FMM as the Poisson solver. For each active step, we evaluate gravitational forces on all the active particles due to all the mass in the system. For the inactive particles, we only use their positions without synchronization to the current timestep.

3. RESULTS

3.1. Run-time efficiency of the new scheme

![Figure 3](image_url)

Figure 3. Wall-clock time of a series of cold collapse simulation of particles from an initial cubic configuration with Taichi code. The image shows the distribution of \( 3 \times 10^6 \) particles at \( t = 1 \) within the unit box. The system undergoes collapse at \( t \approx 0.5 \) and forms a core-envelope structure. The measured wall-time scales as \( N^{1.22} \), slightly above the rate of \( N^{7/6} \).

We first test the performance of the new scheme using a cold collapse of particles released from a cubic configuration. We place random points at rest with a total mass of unity within a cube of unit size with the total number varied from 100 to \( 3 \times 10^6 \). We use Hénon units with \( G = M = R = 1 \) and evolve the system from \( t = 0 \) to 1. Besides, we vary the softening length \( \epsilon \) according to \( \epsilon = 0.01(N/10^4)^{-1/3} \) to mimic the usual practice in the community (Power et al. 2003; Springel et al. 2008). This simple setup is non-trivial for \( N \)-body codes as the system will undergo a quick collapse at \( t \sim 0.5 \). As a result, a dense core forms in the center while a diffuse envelope due to ejected particles develops in the vicinity as shown in the image in Figure 3. Throughout the simulation, the gravitational force varies strongly both in space and in time. Each simulation is performed in parallel using OpenMP with 16 cores on a quad 2.80GHz Xeon E5-2680 server node.

Figure 3 also shows the measured wall-clock time as a function of \( N \) compared with two guiding lines of \( N^{7/6} \) and \( N^{3/2} \) trends. With the timestep function \( \Delta t = \sqrt{\eta \epsilon / |\mathbf{r}|} \), one would expect the running time scale up between \( N^{1/6} \) and \( N^{1/2} \) due to the decreasing \( \epsilon \) alone. The former bound is obtained assuming the typical acceleration does not change. The latter is obtained by considering the typical acceleration changes as \( \epsilon^{-2} \) hence \((\Delta t)^{-1} \propto \epsilon^{-1.5} \propto N^{0.5}\). Both trends are assuming the \( \mathcal{O}(N) \) complexity for FMM force computation. Our test demonstrates that the performance of the scheme agrees better with the \( N^{7/6} \) trend than the other. Only with \( N(<10^4) \), we see some collisional behavior described by \( N^{3/2} \) due to the very small particle number. In addition, we compare the particle distribution in the dense core, which is indeed better resolved with higher resolutions. This result means the acceleration of a subset of particles is much stronger in higher resolutions. Therefore, the complexity of FMM perhaps is close to \( \mathcal{O}(N) \) (see also Dehnen 2002, 2014). Nevertheless, we can retain the excellent efficiency of FMM in the new scheme even we invoke a full FMM procedure, including tree building, at every individual timestep.

3.2. Momentum conservation, angular momentum conservation, and energy conservation of the new scheme

3.2.1. Exact momentum conservation

Next, we examine the momentum conversation using the same collapse test. We set up the initial condition with a total number of \( 10^4 \) and evolve it with Taichi. We monitor the total momentum, angular momentum, and total energy during the simulation. At \( t = 1 \), the r.m.s velocity is close to unity. Therefore, we simply
take the magnitude of the net momentum of the entire system $|\mathbf{P}|$ as a proxy for momentum conservation error.

Figure 4 shows the momentum conservation error as a function of $\theta$ (left panel) and $p$ (right panel). The values of $\log(|\mathbf{P}|)$ confirm that our implantation is indeed momentum conserving, which validates our proposal in the previous section. There are some residual errors due to round-offs in FMM, which slowly increases with a larger opening angle $\theta$. The accumulation of the round-off errors depends on the inhomogeneity of the particle distribution and the parameter $n_{\text{crit}}$. In practice, this tiny error should not be of any concern.

![Figure 4](https://wwwmpa.mpa-garching.mpg.de/gadget/)

**Figure 4.** Momentum conservation error at $t = 1$, as a function of $\theta$ and $p$, in the cold collapse test. We vary $\theta$ from 0.7 to 0.05 while keeping $p = 5$ fixed and $p$ from 3 to 20 with $\theta = 0.45$. The combination of FMM and HHS is momentum conserving while the error is at $\log(|\mathbf{P}|) \sim -3.2$ for the traditional integrator with individual timesteps.

In Figure 4, we also include the momentum conservation error with FMM but with the traditional integrator with individual timesteps in the open circles. $\log(|\mathbf{P}|)$ stays rather flat at -3.2 with varying $\theta$ or $p$, which originates from the force asymmetries in the integration with individual timesteps.

For tree codes, only in the joint limits of $\theta \to 0$ and $p$ with the traditional integrator: a standard geometric opening angle in BH tree codes and a relative criterion based on particle acceleration. With $\theta$ changes from 0.8 to 0.05, we find $\log(|\mathbf{P}|)$ reduced from -2.2 to -3.5. If we use the relative criterion with force tolerance parameter $\alpha$ from $0.02$ to $1 \times 10^{-4}$, $\log(|\mathbf{P}|)$ changes from -1.2 to -3.5$^3$.

Because the monopoles in GADGET can be updated with a half-step (Springel et al. 2001; Springel 2005) using the velocity of the node, the error in momentum conservation is 0.5 dexes better than FMM with individual timesteps in Figure 4. Nevertheless, the remaining error which does not converge away with smaller $\theta$, originated from individual timesteps.

3.2.2. Angular momentum conservation

![Figure 5](https://wwwmpa.mpa-garching.mpg.de/gadget/)

**Figure 5.** Angular momentum conservation error at $t = 1$ vs. $\theta$ and $p$. The error decreases as a strong function with $\theta^p$. When $\theta \to 0$, the error is reaching machine zero. Meanwhile, increasing the expansion order $p$ also reduces the angular momentum conservation error albeit at a slightly slower rate than with lowering $\theta$. With the traditional integration with individual timesteps, we cannot further reduce the error once $\theta < 0.25$ or $p > 7$ when the force asymmetry in the time integrator start to dominate over force asymmetry in space.

While FMM conserves linear momentum by construction, it is well-known angular momentum is not conserved exactly due to the fact $|\mathbf{F}_{ij} \times \mathbf{r}_{ij}| \neq 0$. Recently, Marcello (2017) has proposed a corrective torque term that restores angular momentum conservations on the cell level. (However, $|\mathbf{F}_{ij} \times \mathbf{r}_{ij}| \neq 0$ still holds true among particle pairs.) Since the force approximation error in FMM scales as $\theta^p$ (Dehnen 2002, 2014), the angular momentum conservations error also follows a similar trend.

We use the net angular momentum $|\mathbf{L}|$ as a proxy for angular momentum conservation error. Figure 5 shows $\log(|\mathbf{L}|)$ changes from -2.2 to -3.5.

$^3$ We find that the relative criterion, although more efficient in tree walking given the same relative force error, introduced more momentum conserving error in this test. The net acceleration of the system is comparable between $\theta = 0.6-0.7$ using the standard geometrical criterion of BH and $\alpha = 1 \times 10^{-3}$ with the relative criterion.
the angular momentum conservation error vs. $\theta$ and $p$. Reassuringly enough, we can also reduce angular momentum conservation error with either a smaller $\theta$ or a larger $p$. In particular, a small $\theta$ can drastically reduce the error close to machine zero as in $\theta = 0.05$ case.

In contrast, a traditional integrator with individual timesteps gives a very different trend of $\log(|L|)$ vs. $\theta$ and $p$. When the opening angle $\theta > 0.25$ or the expansion order $p < 7$, $\log(|L|)$ shows a very similar trend as TAICHI. On the other hand, we cannot further reduce $\log(|L|)$ below -5.3 when the force asymmetry in the time integrator takes over the torque error in FMM in the total error budget.

For comparison, $\log(|L|)$ with GADGET can be reduced to $-5.4$ in its BH mode with $\theta = 0.05$ or $-6.0$ with $\alpha = 1 \times 10^{-4}$ with its relative criterion. These errors are slightly better than that obtained with FMM with individual timesteps but significantly worse than TAICHI.

3.2.3. Energy conservation

![Figure 6](image)

**Figure 6.** Energy conservation error at $t = 1$, as a function of $\theta$ and $p$, in the cold collapse test. We also present TAICHI integrations with smaller timesteps using $\epsilon = 0.005$. It is clear that force asymmetry in the traditional integration with individual timesteps is also a source of error in energy conservation.

The source of energy conservation error in N-body codes is a more complicated issue when compared with momentum and angular momentum. In a fixed potential, energy conservation error can be reduced with smaller step size or with a time-symmetric formulation of timestep choice (Dehnen & Read 2011; Pelupessy et al. 2012; Dehnen 2017). Energy conservation errors due to time integration are extensively studied for test particles in a fixed potential (e.g., Springel 2005; Dehnen 2017).

Nevertheless, there are other sources of error in a time-varying potential, including the force asymmetry when integrated using the traditional individual timesteps. In Figure 6, we compare the energy errors in terms of $\log(E/E_0 - 1)$ at $t = 1$, where $E$ is the total energy, with results obtained by TAICHI and the traditional individual timesteps. The energy error obtained with traditional individual timesteps is very close the errors obtained with TAICHI. Additionally, we use a smaller timestep with $\epsilon = 0.005$ instead of 0.02 for TAICHI. As expected, the energy error can be reduced from $-2.5$ to $-3.2$ with finer step sizes. Besides, the energy error does not show substantial systematic variation with $\theta$ or $p$. The energy conservation error flattens out with $\theta \to 0$ or $p \to 20$.

3.3. The cost towards higher accuracy

![Figure 7](image)

**Figure 7.** The computational cost in terms of wall time vs. the error of total angular momentum $\log(|L|)$ at $t = 1$. The errors decrease with $\theta \to 0$ or with an increasing $p$, although the former strategy is more efficient given the same cost. On the other hand, angular momentum conservation error with individual timesteps can only be lowered to $\log(|L|) \sim -6$ without any further improvement.

With the momentum conserving nature of TAICHI by construction, and the energy conservation error from multiple sources, we use angular momentum $\log(|L|)$ as a proxy for the overall accuracy of our code. In Figure 7, we plot the computational cost in terms of wall time vs. the $\log(|L|)$. Higher accuracies can be achieved in FMM with $\theta \to 0$ or with an increasing expansion order. It is more cost effective to use a smaller opening angle than a larger expansion order when higher accuracy is desired. On the other hand, the traditional integrator with in-
individual timesteps cannot further improve once below 
\[ \log(|L|) = -6. \]

3.4. Applications in galactic dynamics

It is quite common to observe isolated galaxy disks drift away from their starting point over a long integration time in the literature. This drifting velocity is a manifestation of momentum conservation violation in the N-body codes. Using the method outlined in Springel et al. (2005), we set up an exponential stellar disk (800,000 particles) with a central bulge (160,000 particles) within a dark matter halo (1,000,000 particles) of a Hernquist profile (Hernquist 1990) with \( V_{200} = 160 \) km/s. We then evolve it with GADGET and the new scheme. We use \( a = 2.5 \times 10^{-3} \) together with its relative opening criterion with GADGET. The force softening length is set to be 15 pc. By \( t = 2 \) (1.94 Gyr in physical units), the stellar disk drifts upwards along the \( z \)-axis with a net velocity of 1.4 km/s. If we use the geometric opening angle in BH mode with GADGET with \( \theta = 0.45 \) instead, the net drifting velocity is much smaller, \( \sim 0.1 \) km/s. As a result, we do not observe any apparent drift of the galaxy disk. For the traditional individual timesteps with FMM, the net drifting velocity is \( \sim 0.02 \) km/s. For comparison, momentum is conserved with the new scheme and we do not have any residual drifting velocity at all.

It turns out our default timestep function is inadequate for an accurate long term energy conservation. We find that the fractional error in total energy conservation from our isolated disk galaxy simulation is 2.3% by the end of an integration of 4.9 Gyr with TAICH. This error is unexpectedly large. To fix this problem, we have experimented a scheme by imposing a minimum timestep, determined by the total acceleration due to all particles \( |a|_{\text{tot}} \) in

\[ \Delta t_i = \frac{\eta_i \epsilon_i}{|a|_i}. \tag{9} \]

During the simulation, \( |a|_{\text{tot}} \) can be obtained in a kickSF2S step when all particles are passed to the Poisson solver, i.e., when the bottom rung is evaluated. With this additional timestep constraint, the total energy conservation with TAICH performs very well when compared to GADGET. The fractional energy conservation error is about \( 3 \times 10^{-4} \), slightly better than the result obtained with GADGET in its relative opening criterion mode. Interestingly, while momentum conservation error is quite small with GADGET in its BH tree mode, the energy conservation error is quite large, reaching to \( 10^{-3} \) by \( t = 2 \). Therefore, it appears tricky to achieve good momentum conservation and energy conservation simultaneously with GADGET.

In this test, TAICH finishes with a speed comparable to GADGET using the same CPU cores. However, given the similar computational cost, TAICH offers much higher accuracies. TAICH is also 40% faster than FMM code using the traditional individual timesteps.

3.5. Applications in cosmological simulations

The new N-body scheme can be readily extended to cosmological simulations. The high accuracy of FMM can also be beneficial where the mass distribution is nearly uniform at high redshift. Periodic boundary conditions can be treated either with Ewald summation (Hernquist et al. 1991) as in Potter et al. (2017) or with a renormalization procedure using the same cell–cell interactions within FMM (Berman & Greengard 1994), which EXA FMM has already implemented.

The cosmological integration is straightforward following the GADGET code paper by Springel (2005). We use the comoving coordinate \( x \) and its canonical momentum \( p(= a^2 m x^2) \) with the scale factor \( a \). The cosmological factors in the drift operator

\[ x \rightarrow x + \frac{p}{m} \int_t^{t+\Delta t} \frac{dt}{a^2}, \tag{10} \]

and in the kick operator

\[ p \rightarrow p + (-\nabla \Phi) \int_t^{t+\Delta t} \frac{dt}{a}, \tag{11} \]

are stored in lookup tables as a function of \( a \).

We integrate the initial condition of a Milky Way-sized halo in its a dark matter only version\(^5\). This halo is Aq-C5 in the Aquarius project (Springel et al. 2008) and its hydrodynamic version is used for the Aquila comparison project (Scannapieco et al. 2012). Figure 10 shows the dark matter distribution in its projected mass density at redshift \( z = 4, 2, 1, \) and 0. The top panels show the formation of the dark matter halo with GADGET (in its TreePM mode) and the lower with TAICH. Qualitatively, dark matter filaments, halos, and halo substructures are very similar between GADGET and TAICH. The raw speed of TAICH is much slower than GADGET due to the fact GADGET only uses the tree method to calculate the short range force. We note that the speed comparison between the two codes in this case is unfair because the force accuracies are not on the same level. If we run GADGET with only the tree method, it is much slower than TAICH, as expected. In principle, particle mesh method could also be integrated with

\(^5\) ICs are available at http://www.aip.de/People/cscannapieco/aquila/ICs/Gadget/Aq-C5/.
Figure 8. A sequence of images of an isolated disk galaxy simulated with GADGET and TAICHI. We run GADGET with the relative opening criterion (RC) in this test with $\alpha = 2.5 \times 10^{-3}$. For BH tree method with GADGET, we use $\theta = 0.45$. By $t = 2$, the galaxy has gained a net velocity of 1.4 km/s using GADGET with the relative opening criterion. This error is visible in the top panels as the galaxy disk gradually drift upwards along the z-axis. This momentum conservation error is much smaller with GADGET using its BH tree mode with a velocity of 0.1 km/s by $t = 2$. In contrast, momentum is conserved with the new scheme. An animation of the isolated disk galaxy, can be found at https://youtu.be/1aE5OpBhXXk.
FMM as a long-range force solver as in TreePM codes. However, it is not clear whether FFT is necessary after all because FFT complicates the error analysis (see also Ishiyama et al. 2009; Schneider et al. 2016). The benefits with a hybrid FFT+FMM solver are unwarranted. The performance of FFT has become a major bottleneck in many large scale applications. On the other hand, Yokota et al. (2014) have argued FMM has very attractive communication complexities. Also, a more efficient tree walk and further optimizations in the FMM solver can considerably speed up Taichi.

4. DISCUSSIONS

4.1. Major shortcomings of the new N-body scheme

As shown in the isolated galaxy disk test, it is also necessary to impose an additional constraint to get excellent energy conservation. This highlights one primary shortcomings of this new scheme: the full acceleration on each particle can only be computed when all the particles are passed in the Poisson solver, which can be inadequate for the highly dynamical regions in some cases.

One possible remediation to this shortcoming is to use a higher order integrator, such as a forward step-C4N12-only fourth-order integrator proposed by Chin & Chen (2005). This integrator is a promising alternative to the traditional second-order KDK integrator. Although the approximation of the force gradient $\nabla a_i$ is lower than the acceleration itself, FMM should give a reasonably accurate measure of $\nabla a_i$ with a high expansion order. Our preliminary tests show that the fourth order integrator by Chin & Chen (2005) gives at least two orders of magnitude smaller energy error even with variable timesteps than the second order KDK integrator given the same cost.

In the absence of a totally satisfactory treatment of timestep function, we would recommend to use some monitoring of total energy, momentum, and angular momentum during the course of a simulation as suggested by Dehnen & Read (2011). As demonstrated by the isolated disk galaxy, Taichi can deliver excellent momentum and total energy conservation in its current form.

We should also point out another potential shortcoming with the new N-body scheme. In the collision-less system, particles should follow the trajectories determined by the smooth potential. However, the hierarchical splitting introduces additional perturbations on top of the existing potential fluctuations (e.g., Hernquist et al. 1993). We can use the vertical thickening of the initially thin disks as a useful diagnose of collisional heating (Sellwood 2013). In Figure 11, we show the evolution of vertical velocity dispersion of the stellar disk in our previous test. The vertical velocity dispersion gradually but slowly increases as a function of time. And the time evolution of velocity dispersion profiles obtained with our four simulations is also consistent with each other.

We have also compared the evolution of a Hernquist halo using Taichi and GADGET and found the evolution of the central density cusp are very similar to each other. It indicates that shot noise (Hernquist et al. 1993) is likely to dominate over the additional perturbations from the hierarchical splitting. It is safe to conclude the new scheme is as good as the existing ones treating collision-less dynamics.

4.2. Roads towards fast and accurate N-body schemes for collision-less and collisional dynamics

As an approximate Poisson solver, FMM is suitable for a rigorous error analysis following the classic text of Kellogg (1929) and the error analysis in the seminal work of Greengard & Rokhlin (1987). When coupled with the HHS time integrator, we have demonstrated that it is possible to construct a practical N-body scheme with individual timesteps that (1) retains the $O(N)$ algebraic complexity of FMM, (2) conserves linear momentum accurate to the round-off errors. Both properties are highly desired in a broad range of astrophysical ap-
Figure 10. Dark matter distributions of Aq-C-5 halo simulated with Gadget (in its TreePM mode) and Taichi at redshift $z = 4, 2, 1$ and 0.

Figure 11. Time evolution of the vertical velocity dispersion profiles of the stellar disk in our isolated galaxy test. Each profile is normalized by the vertical velocity dispersion at $t = 0$.

Currently, our understandings of dark matter distributions have almost exclusively relied on numerical simulations. It has been shown recently that halo density profiles and shapes are affected by the dynamics of baryons as well (e.g., Pontzen & Governato 2014; Chan et al. 2015). The distribution of dark matter essentially reflects the shape of individual orbit (More et al. 2015; Zhu et al. 2017). It is therefore sensible to invest in a more accurate $N$-body scheme to compare with the current codes before any complex baryonic dynamics are included. Force accuracies in the current $N$–body codes are already hinted in a recent study of matter clustering by Schneider et al. (2016) where three different codes show discrepancies bigger than one per cent level in matter power spectra.

We could also improve the accuracy of the proposed new scheme with some time-symmetric stepping formulation Dehnen (2017). The improvements are within a single and consistent framework. After finishing the first draft, we learned that a combination of FMM and HHS has also already been incorporated into the latest version of GADGET for a while (Volker Springel, private communication; Springel et. al, in prep). FMM with HHS integrator has a potential to be a highly accurate code for computational cosmology.

On the computational side, the $O(N)$ algebraic complexity and the low communication complexity makes
FMM petascale friendly (e.g., Lashuk et al. 2012; Yokota 2013). The expensive direct summation part of FMM can be accelerated with either GPU or AVX instructions. Also, multipole expansion in the Cartesian coordinates runs much faster than in spherical coordinates when \( p \) is small (Dehnen 2000; Yokota et al. 2013). We can then customize this scheme with a low order expansion for collision-less simulations accordingly due to their Monte Carlo nature.

This study focuses on collision-less systems such as galaxies and dark matter halos. The HHS time integrator by Pelupessy et al. (2012) is proposed in the context of collisional dynamics, though a more efficient splitting has been proposed by Jänes et al. (2014). Another possible follow-up development of this study is to incorporate an error-controlling MAC (Dehnen 2014) to make the Poisson solver accurate enough for collisional systems. It is quite reasonable to expect that many currently prohibiting problems in collisional dynamics can benefit from the proposed new \( N \)-body scheme.

5. SUMMARY

In this paper, we discuss the origins of momentum conserving error in the previous \( N \)-body codes and propose an exact momentum-conserving scheme with a Poisson solver based on FMM and a time integrator based on HHS. We implement the new \( N \)-body scheme in the Taichi code. Using cold collapse test, we show the combination of these two momentum conserving components also improves both angular momentum and energy conservations. We then test Taichi in an isolated disk galaxy evolution and a cosmological structure formation simulation. Our main findings are

- Traditional \( N \)-body codes violate Newton’s third law due to force asymmetries in space from approximate Poisson solvers and asymmetries in time when individual timesteps are employed.

- The new \( N \)-code scheme, on the other hand, is momentum conserving by construction. The momentum-conserving nature of the new scheme is verified with our implementation in the Taichi code.

- The \( O(N) \) complexity of FMM can be retained in the new scheme as the Hamiltonian splitting continuously reduces the problem size for more dynamic part of the system.

- The new \( N \)-code scheme can be readily extended to cosmological simulations, as we have shown with a zoom-in simulation of a Milky-Way sized halo.

The main shortcoming of the new \( N \)-code scheme is the lack of an accurate and reliable timestep function. Future work also include a higher order integrator, multipole expansions in the Cartesian coordinates, and an efficient tree walk with error controls. There is also large room to improve the code efficiency of with various optimizations. Lastly, we would like to emphasize this work does not in any way imply the simulations done by the current codes are inaccurate/incorrect. In many applications of collision-less systems, a modest accuracy is already sufficient. When high accuracies are required, new schemes such as the one proposed in this study can have advantages over the traditional schemes.

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