ngravs: Distinct gravitational interactions in GADGET-2

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ABSTRACT

We discuss an extension of the massively parallel cosmological simulation code GADGET-2, which enables investigation of distinct gravitational force laws between particle species. In addition to simplifying investigations of a universally modified force law, the ngrav extension allows state-of-the-art collisionless cosmological simulations of quite exotic gravitational scenarios. We briefly review the algorithms used by GADGET-2, and present our extension to multiple gravities, highlighting additional features that facilitate consideration of exotic force laws. We discuss the accuracy and performance of the ngrav extension, both internally and with an unaltered GADGET-2, under all relevant operational modes. The ngrav extension is publicly released to the research community.

Key words: methods: numerical – gravitation – cosmology: dark matter

1 INTRODUCTION

At present, there is substantial evidence that most of the mass and energy within our universe is non-luminous. Big bang nucleosynthesis and baryon acoustic oscillations strongly constrain (e.g. Dodelson 2003) the fraction of non-luminous matter with respect to the luminous component from radiation domination onward. Yet, while they and other evidence, such as the Bullet Cluster (Clowe et al. 2006), strongly suggest that the dark fraction be well-approximated by dust, the composition and precise distribution of this dark matter is far from clear. While numerous particle dark matter candidates (e.g. Bertone et al. 2005) are theoretically popular at present, conflicting exclusions from possible detections and increasingly stringent constraints from lack of direct detection (e.g. Akerib et al. 2014) at cosmologically desirable mass scales continues to motivate investigation in novel directions.

With the growing wealth of high-precision astrophysical data (e.g. Ahn et al. 2012; Hinshaw et al. 2013; Planck Collaboration et al. 2014) and the absence of a “bottom-up” understanding of dark matter, cosmological N-body simulations have become essential for comparison against highly non-linear theoretical predictions in structure formation over many decades of spatio-temporal scale. In the past twenty years, the sophistication of these simulations both in physical scope and technical implementation has undergone unprecedented growth (c.f. Bagla & Padmanabhan 1996; Springel et al. 2005; Genel et al. 2014). Yet, the essential feature of N-body cosmological simulation, that well below the horizon scale it is appropriate to regard matter distributions as Newtonian (weak) perturbations to a Robertson-Walker background assumed to be a solution to Friedmann-like equations, has remained unchanged. While significant literature exists on the use of N-body methods to explore standard structure formation scenarios, there exist proposed exotic scenarios which are also amenable to N-body methods. In a particularly intriguing case, Hohmann & Wohlfarth (2010) proposed to model Dark Energy as a repulsive gravitational interaction between matter belonging to distinct copies of the Standard Model. That this model should make very strong predictions for weak-lensing observations and could be readily adapted to the dark matter problem motivates the extension of existing simulation tools to investigate and constrain more general cosmological models.

One well-established and versatile simulation tool is GADGET-2: a massively parallel, hybrid Tree and Particle Mesh (PM) software, with heavy memory and speed optimizations employed both algorithmically and in code (e.g. cache utilisation). Collisionless forces are computed through recursive traverse of a spatial oct-tree, with contributions from distant branches approximated by their monopole moments. Optionally, long-range collisionless forces can be computed efficiently with Fourier techniques, with tree computations restricted to near interactions. Fully periodic boundary conditions can be realised through the Fourier techniques or through the method of Ewald summation. Collisional dynamics are computed by smooth particle hydrodynamics (SPH). Particle data and computational load are distributed across computing nodes in a manner consistent with the recursive spatial decomposition. Not only does this
minimise interprocess communication, but such distribution gives force computations that are independent of the computing topology.

We have chosen to extend GADGET-2 to support D distinct species of gravitationally interacting particles. With this ngrav extension, GADGET-2 simulations may now conveniently define, in general, $D^2$ distinct gravitational force laws. In the following, we will discuss our implementation of this extension, assuming the reader is familiar with the goals, construction, and operation of modern $N$-body codes. We then compare the code’s performance, both in force accuracy and runtime, against a stock version of GADGET-2. For a comprehensive, though slightly dated discussion of $N$-body simulation techniques, we refer the reader to portions of the classic text by Hockney & Eastwood (1988). To complement this background, we enthusiastically suggest the lucid and modern discussion of the original gadgert-2 code by Springer (2005). Throughout this paper, $D$ will always refer to the number of distinct gravitationally interacting species, while $N$ will refer to the number of bodies considered in any particular simulation. Stock will refer to the unaltered GADGET-2.0.7, while ngrav will refer to our augmented version of GADGET-2.0.7.

### 2 IMPLEMENTATION

The approach we have taken toward extension of GADGET-2 is minimally intrusive and straightforward. Fortunately, the GADGET-2 code is engineered so that tree and mesh force computations are nearly decoupled from the more intricate SPH, time integration, domain decomposition, and IO routines.

GADGET-2 implements 6 distinct particle types, one of which features additional force computations from collisional dynamics. Let $D \leq 6$ be the number of distinct gravitational species. ngrav permits consideration of distinct gravitational interactions under all operational modes. For particle types $n, m$, the following map is established between 0 ≤ $n, m ≤ D – 1$

$$
F_{nm}(r) \propto \frac{\hat{r}}{r^2} \rightarrow \vec{F}_{nm}(r, N_\perp) \propto \begin{pmatrix} f_{00} & \cdots & f_{0D} \\ \vdots & \ddots & \vdots \\ f_{D0} & \cdots & f_{DD} \end{pmatrix} \hat{r}.
$$

Here were regard $n$ as the passive gravitational type and $m$ as the active gravitational type. $N_\perp$ represents the number of source particles contributing to the monopole approximation. In the direct force case, $N_\perp \equiv 1$. This extension to multiple force laws was implemented through function pointer tables. Note that analogous function pointer tables defining the softened interaction must also be provided. Tables for the gravitational potential, $\hat{k}$-space Greens’ functions, and lattice sum corrections may also be populated as necessary depending on the desired GADGET-2 operating mode.

Performance comparisons can be found in Table 1 where we find an ∼20% decreased runtime compared to stock. It should be noted that the uncertainties in Table 1 are rather large, ∼15% for reasons discussed in §4. Thus, in $D = 1$ cosmological scenarios, the ngrav extension does enable convenient investigation of a single, globally modified force law; if one can afford modestly longer runtimes. More importantly, the structures containing data on all $N$ simulation particles are unchanged and so the favourable memory storage requirements of GADGET-2 are maintained.

For cosmological simulations of metric theories of gravity, the evolution of the scale factor is determined by the full field equations. Contributions to the weak field equations atop this Robertson-Walker background are then determined by first order perturbation theory. While one can now investigate quite arbitrary force laws below the horizon scale, if the background expansion is significantly altered from the Friedmann equations, an additional straightforward adjustment to the timestep routines will be required to obtain meaningful simulations on cosmological scales.
2.1 Timesteps

The determination of a suitable timestep for the numerical integration is a subtle problem (e.g. Springel et al. 2001). On the one hand, it is desirable to use the largest possible timestep to speed the simulation, but one must do so while maintaining force accuracy. GADGET-2 employs the following collisionless particle timestep

$$\Delta t_{\text{grav}} = \min \left( \Delta t_{\text{max}}, \left( \frac{2\eta}{|\mathbf{a}|} \right)^{1/2} \right)$$

with $\eta$ specifying a desired accuracy, $|\mathbf{a}|$ the particle’s acceleration, and $\Delta t_{\text{max}}$ determined from global dynamical considerations. An undesirable feature is that an unphysical quantity, the gravitational softening length $\epsilon$, enters the timestep computation. While this has been argued robust through numerical investigations (e.g. Power et al., 2003), for more general force laws, it may be the case that softening is not required. In these situations, the softening specified to $n\text{grav}$ will continue to be used for timestep computation. For monotonically softening forces, this is reasonable because adjustments to the velocity always diminish as the interparticle separation approaches zero.

2.2 Tree forces

In keeping with our approach, the existing tree routines were extended simply by vectorising over the monopole positions, velocities, and mass centres. This additional data increases tree memory consumption by $\sim 0.3(D - 1)$ from stock. In order to accommodate more exotic force laws where the interaction scale is related to the active gravitational mass in more complicated ways, the tree structure and construction were augmented to optionally track $N_\Sigma$ for all contributing types. This quantity can then be used to suitably correct computation of the monopole moment.

Stock periodic computations in pure tree mode proceed with the method of Ewald summation (e.g. Hernquist et al. 1991). Though this method is only applicable to $\sim 1/r^2$ forces, this technique is an elementary application of methods from the broader topic of lattice sums (e.g. Glasser & Zucker 1980). There exist generalisations to quite arbitrary spherically symmetric forces through straightforward adjustments to the method of Bertaut. $n\text{grav}$ will compute and tabulate given corrections from an infinite image lattice for each of $D^2$ direct forces, and interpolates to actual particle positions in the same manner as stock.

During force computation, tree walks may be significantly optimised by suitable choice of opening criteria. For collisionless force computations in stock, the tree is walked at most twice, once for the usual particle-particle interaction, and once again for any periodic correction from a presumed infinite lattice of simulation volumes. The latter lattice walk can proceed more efficiently, as the opening criteria is significantly different: corrections to near particles are very low. We considered performing $D$ separate tree walks, but stock employs a very effective relative opening criteria during the tree walk, where the acceleration previously computed is compared to a Newtonian estimate of the new acceleration to determine whether to open further the node. These previous accelerations, however, are stored on a per-particle basis and the amount of memory required to store $D - 1$ additional accelerations produced an undesirable increase in memory consumption. Further, to accurately compute this quantity for each gravitational type, temporary tree structures accumulating gravitational accelerations due to the tree and the mesh also needed to be vectorised. Since these quantities are computed internally at double precision, data for $D$ relative opening criteria leads to unacceptable memory consumption by the tree. It was decided that, since many alternative force-laws cannot deviate too strongly from the Newtonian force, any gains in speed due to decreased depth within the tree would not be offset by the additional memory requirements. Instead, we vectorised within the single tree walk that gadget-2 already performs, and continue to employ the Newtonian relative opening criteria. This opening criteria is conservative, provided that the alternative force-laws are dominated by the usual Newtonian interaction, and results in slightly improved force errors. This improvement is easily understood: the mass distribution is now characterised by $D$ distinct monopoles. Overall, the expected tree walk runtime is decreased approximately by a constant factor of $1/D$, indeed such behaviour is found in Figure 1.

2.3 Mesh forces

In order to minimise surface to volume ratio, stock does not attempt to overlap local PM computation with local particle distribution. Instead, density data is exchanged between all tasks according to an optimal slab decomposition determined by the Fourier routines of Frigo & Johnson (2000), and the resulting potential is exchanged back. Since the identities of all the particles which contribute to any given slab are unknown, the PM routine must iterate $D^2$ times.
At present, particle interactions under force laws with mass-dependent scale are only accurately computed in pure tree, non-periodic modes. This is due to the Fourier computation’s use of a single momentum-space Greens’ function for all contributing mass, and to the necessary precomputation of force and potential correction tables for direct infinite space boundary conditions, for \( D = 3 \) ngraus (blue, dashed), all interactions Newtonian. Residuals computed against stock (pink, solid). Note that an erroneous softening scale of 600kpc in the included stock ΛCDM initial condition was decreased to 50kpc to keep the softening scale below the cutoff for use of the PM computation. (instead of \( D(D + 1)/2 \) and exploiting symmetry), so that each gravitational type can be both the passive and active gravitational mass. Though more sparse, the exchanged data is of the same dimensionality and the mesh runtime is approximately decreased by a constant factor of \( 1/D^2 \). This performance hit is of little concern, however, as the Fourier computation runtime continues to be heavily subdominant to that of the Tree algorithm.

In GADGET-2, one may optionally enable Peano-Hilbert sorting of particle data on each local processor. This was found by Springel (2005) to often give substantial (but architecture dependent) improvements in runtime as spatial proximity translates to memory proximity. To enable processing of the entire local particle content with only a single traversal of the data, if \( D > 1 \) and TreePM mode is enabled, we have implemented an additional sort by gravitational type before the Peano-Hilbert sort. Subsequently, each gravitational type is then Peano-Hilbert sub-sorted. As is done in stock, both sorts proceed so that only one reordering of the particle data memory is required. For compatibility with the collisional code of GADGET-2, collisional particles must be mapped to gravitational type 0.

2.4 Limitations

At present, particle interactions under force laws with mass-dependent scale are only accurately computed in pure tree, non-periodic modes. This is due to the Fourier computation’s use of a single momentum-space Greens’ function for all contributing mass, and to the necessary precomputation of force and potential correction tables for direct infinite lattice contributions. Even in non-periodic pure tree mode, due to the monopole averaging procedure, considerable force errors could result given situations where a node contains comparable numbers of differently massed particles. The efficient and accurate computation of such interactions is an open question.

In GADGET-2, collisional forces are only computed for one type of particle. While it is possible to alter the gravitational force law between these “gas” particles, it is not presently possible to have distinct “gasses” interacting under separate gravitational force laws. Most observational signatures of modifications to gravity manifest at the level of large-scale structure formation. Since these processes are dominated by collisionless dynamics, we do not believe this restriction to be a serious impediment.

3 TEST PROBLEMS

As is it impossible to formally verify the correctness of the ngraus extension, we instead perform force accuracy comparisons against the well-vetted stock version. All the following tests, including the profiling results presented in Table 1 and Figure 1 were carried out on the Amazon EC2 service, with a dedicated two virtual machine (VM) cluster on the same Placement Group to gauge performance over a 10 Gigabit local network. Each machine provided 16 of 32 available cores for computation with 60 gigabytes of RAM (the c3.8xlarge instance) for a total of 32 cores and 120 gigabytes of RAM across the cluster. It should be noted that EC2 does not guarantee dedicated processor access, which leads to a large variance in runtime performance.

We present force accuracy comparisons between stock and \( D = 3 \) ngraus for three of the four stock included test initial conditions in Figures 2, 3, and 4 under Newtonian interactions. The figures display the fraction of \( N_f \) force com-
computations with force error $\Delta f/f$ in excess of that fraction. These initial conditions test the full range of GADGET-2 capabilities, including pure tree mode and tree-particle mesh mode, both with and without periodic boundary conditions. The collapsing gas sphere was excluded as the present implementation of ngravs requires that all collisional particles be of the same gravitational species. Note that the force accuracies are virtually identical; the residuals indicating relatively minor improvements due to three multipole moments per node.

3.1 Internal consistency

To verify the newly introduced optional tracking of contributing particle counts in tree computations, we investigate the colliding galaxy scenario with two distinct gravitational species. The first species, denoted as 0, interacts via the usual Newtonian interaction

$$\Phi_{00}(r) = -\frac{M m_0}{r}. \tag{3}$$

We use uppercase to denote the active gravitational mass and lowercase to denote the passive mass. The second species, denoted 1, is characterised by a dimensionless scale $\beta$ and interacts as

$$\Phi_{11}(r) = -\frac{2 M_1 m_1}{\pi r} \tan^{-1} \left( \frac{4 \pi \beta r}{M_1/N_\perp + m_1} \right). \tag{4}$$

Note that the interaction is Newtonian at large $r$, but softens to a constant as $r \rightarrow 0$. This is the exact potential between two hypothetical, spherically symmetric, cored densities of the following form

$$\rho(r, M) = \frac{M^2}{4 \pi \beta^2} \frac{1}{(M/2 \beta r)^2 + r^2} \quad \tag{5}$$

in units where $G \equiv c \equiv 1$ and $M$ is the total mass enclosed by such an object. Interactions across species are of the same functional form as Eqn. 4 apart from the softening scale continuing to be set by the cored object

$$\Phi_{01}(r) = -\frac{2 M_0 m_1}{\pi r} \tan^{-1} \left( \frac{4 \pi \beta N_\perp r}{m_1} \right), \tag{6}$$

$$\Phi_{10}(r) = -\frac{2 M_1 m_0}{\pi r} \tan^{-1} \left( \frac{4 \pi \beta N_\perp r}{M_1} \right). \tag{7}$$

Note that Newton’s third law is not violated, the distinct Eqs. 6 and 7 distinguish between the passive and active mass for correct computation. One may think of this interaction as a preference for phenomenological cored halos (e.g. Walker et al. 2009; de Blok 2010) having motivated an actual new class of hypothetical object. For our purposes, it serves as an example where tracking the number of a contributing species to the monopole approximation yields an exact correction to the force law. The results in Figure 5 exhibit the force accuracy achieved through this novel $N_\perp$ feature.

4 CONCLUSION

We have detailed the ngravs extension to the massively parallel hybrid Tree and mesh $N$-body code GADGET-2, which permits consideration of $D$ distinct forms of gravitational interaction between particle species. Our implementation vectorizes over the existing monopole moments within the oct-tree structure, and distinguishes between active and passive gravitational mass within the mesh computations. Memory consumption remains favourable: particle data storage is unchanged from GADGET-2, tree storage is increased by $\sim 0.3(D-1)$, and Fourier storage requirements are unchanged. We subject the code to numerous tests to gauge performance both in runtime and in force accuracy. We verify that runtime is dominated by tree performance and scales as $1/D$. Though runtime performance is diminished from that of stock GADGET-2, the ngravs extension is a viable choice for preliminary investigation of a globally modified ($D=1$) force law. We find qualitatively identical, slightly improved, force accuracies compared to GADGET-2: behaviour expected from our particular implementation. We also have introduced and verified a novel feature which tracks the number of contributing particles of all species to any given monopole approximation, which can then be used to correct exotic force laws with dynamic softening lengths. We believe that the ngravs extension will facilitate investigation and constraint of exotic gravitational scenarios and have released ngravs publicly to the research community.

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Figure 5. Force accuracy comparison in pure tree mode between two distinct gravitationally interacting species: one Newtonian, the other as described with $\beta \equiv 1.31 \times 10^{-6}$. Note that force accuracy comparable to GADGET-2 is maintained when the number of particles contributing to monopole approximations, $N_\perp$, is tracked (yellow, solid) and used to adjust the force. Without such tracking, the force errors increase by an order of magnitude (orange, dashed).
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