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DEMONSTRATING DISCRETENESS AND COLLISION ERROR IN COSMOLOGICAL *N*-BODY SIMULATIONS OF DARK MATTER GRAVITATIONAL CLUSTERING

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ABSTRACT

Two-body scattering and other discreteness effects are unimportant in cosmological gravitational clustering in most scenarios since the dark matter has a small particle mass. The collective field should determine evolution; two-body scattering in simulations violates the Poisson-Vlasov equations. We test this result in PM, P^{3}M, Tree, and NGPM codes, noting that a collisionless code will preserve the one-dimensional character of plane-wave collapse. We find collisionality vanishing as the softening parameter approaches the mean interparticle separation. Solutions for the problem are suggested, involving greater computer power, PM-based nested grid codes, and a more conservative approach to resolution claims.

Subject headings: cosmology: miscellaneous — dark matter — gravitation — hydrodynamics — methods: numerical

1. INTRODUCTION

In the limit of small particle masses, a system of self-gravitating masses is described by the Poisson-Vlasov equations: the particle-particle scattering becomes unimportant, and the evolution approaches that of a continuous system with a time-dependent potential (Chandrasekhar 1942; Sellwood 1987). *N*-body codes have a small number of high-mass particles λ as compared to a universe of unclustered dark matter. It is not clear whether the ensemble converges to some or all of the properties of the solution of the real problem (Melott 1981). In fact, one may conclude that if "… much of the mass in the universe comprises an invisible component (the missing mass) there is no guarantee that the galaxies have ever acted as point particles. If this were the case, the results from *N*-body experiments would not apply to the real universe." (Hockney & Eastwood 1981, p. 454). The purpose of the Letter is to present preliminary results from a longer study in order to warn of possible problems with numerical codes.

The mean-field approach is typified by the particle-mesh, or PM, method (Doroshkevich et al. 1980; Melott 1981, 1982b; Klypin & Shandarin 1983). In this method, the particles move in a gravitational potential computed on a mesh. The shortcoming of the method is that there are no valid results below the mesh scale since potential and density are smoothed over that scale. So far, no errors have been reported other than this (rather serious) limitation.

Short-range forces may be added to preserve the r^{-2} force law in close encounters. P^{3}M (particle-particle-particle mesh) (Hockney & Eastwood 1981; Efstathiou & Eastwood 1981) and Tree codes (Suginohara et al. 1991) are two examples, although more recently codes based on adaptive mesh refinement (Pen 1995; Suisalu & Saar 1995; Gelato, Chernoff, & Wassermann 1996; Kravtsov, Klypin, & Khokhlov 1996) have been used. Generally, this approach improves resolution of the Green's function for the Poisson equation without improving the resolution of the source term. For this reason we call such codes HFLMR (high-force, low mass-resolution) codes. Roughly isotropic contraction of clumps is often used to justify this approach. Tests made by Kuhlman, Melott, & Shandarin (1996) on generic smooth initial perturbations do not support isotropic collapse. To prevent the formation of tight binaries that slow down execution, all codes resort to force softening, so that on scales less than ϵ the force law is softer than $1/r^2$. Values of ϵ (in units of the mean interparticle separation $n^{-1/3}$) of 0.01 to 0.2 are common, and results are usually presented down to ϵ. We will show that $\epsilon \sim 1$ is needed to maintain a collisionless, quasi-continuous system.

Computer codes are often cross-checked for convergence, but a common assumption may lead to a common error. Agreement with exact solutions is a better method of checking, but is not easy. One classic test for two-body scattering error is mass segregation. Particles of higher mass settle to inner parts of bound systems because of the equipartition resulting from two-body scattering. Efstathiou & Eastwood (1981) found strong segregation in P^{3}M. This result appears to have been largely ignored. Peebles et al. (1989) verified that segregation could be suppressed in PM with $\epsilon \sim 1$. In an equal-mass system, like most cosmological simulations, this error may exist but not result in segregation. Suisalu & Saar (1996) examined deflections and found an indication of trouble in a P^{3}M code, but their original method was unable to show whether the scattering was due to mean-field or two-body fluctuations.

2. PLANE-SYMMETRIC COLLAPSE

We suggest a new type of test (symmetry breaking) for codes in the nonlinear regime without an exact solution. We use a simple system with a clear prediction: plane-wave collapse. (Of course, we could use spherical collapse, two-dimensional collapse onto a filament, or any other type of symmetric collapse.) This situation has an exact solution up to shell crossing (Zeldovich 1970; Shandarin & Zeldovich 1989) and was used by Efstathiou et al. (1985) in code testing. However, these authors worked only in the precollapse regime and along

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coordinate axes so that no collisions were possible. Obviously, a collisionless system with only one-dimensional perturbations should remain one-dimensional. This fact is the basis of our test; its violation means the code is collisional or that it otherwise erroneously scatters particle orbits.

We made the test more relevant by tilting the plane of collapse relative to the simulation cube. We set up a single perturbation wave $\boldsymbol{k} = (2, 3, 5)k_f(|\boldsymbol{k}| = 6.16k_f$, where k_f is the fundamental mode) by Fourier transform on a grid of 64^3 particles. We began with an amplitude $\delta \equiv (\rho - \bar{\rho})/\bar{\rho} \sim 0.1$ and evolved for an expansion factor of 7.7 after the first shell crossing, during which collisions are permitted by theory. While the physical system should have no scattering, near misses may generate scattering numerically. The role of the symmetry simply makes scattering detectable. To perform the comparison we used a PM code (Melott 1981, 1986), a P^3M code (kindly supplied by H. Couchman), and a Tree code (Suginohara et al. 1991). We also tested a nested-grid particle-mesh (NGPM) code (Splinter 1996). All runs had identical (publicly available) initial conditions. The initial conditions for the NGPM code were generated in the manner described above for both the coarse and the fine grid. We also made cross-check runs in which the perturbation $\boldsymbol{k} = (0, 0, 6)k_f$ was *not* tilted with respect to the cube.

The PM run was performed on a 64^3 mesh and duplicated on a 128^3 mesh to emulate a modification sometimes used, as well as to verify the code independence of our results. PM tests were made using traditional two-point differencing and the Melott (1986) improved–force-resolution staggered-mesh scheme. There was no significant difference in scattering, as we report here. We performed otherwise identical P^3M and Tree tolerance parameter $\theta = 0.2$ runs with $\epsilon = 0.1$ and 1.0, as well as a transitional P^3M run with $\epsilon = 0.5$. In the P^3M code, we used two choices of time-integration variable and varied the time step greatly, assuring satisfaction of both Courant and leapfrog stability conditions. The PM and NGPM codes automatically test and adjust time steps as needed. The adaptive smoothing length capability of the P^3M code was turned off, as suggested by Gelb & Bertschinger (1994). The NGPM code had a refinement factor of 8, putting it close in spatial resolution to the $\epsilon = 0.1$ P^3M run, but with 512 times increased mass resolution (making it an HFHMR code). Results of a much more extended study will be presented elsewhere.

Figure 1 shows the overall configuration of the PM system after collapse. All runs look roughly similar. Differences between tilted runs are shown in Figure 2, in which slices of one collapsed planar region are projected along the initial perturbation axis. The only inhomogeneity should be projection of the initial lattice onto this plane. Some runs show clumping, suggesting scattering error. All the erroneous HFLMR runs (the P^3M and Tree code runs with $\epsilon < 1$, and the 128^3 mesh PM run) share softening lengths shorter than the mean interparticle separation. The runs that performed well (normal PM, P^3M and Tree with $\epsilon = 1$, and NGPM) all have softening comparable to this distance; of course, for NGPM this distance is considerably smaller, but at no collision penalty. (Axis-aligned PM and P^3M runs show the lattice, with no clumping visible.)

We use as one quantitative measure the distribution of particle velocities, which should be strictly normal to the planes; we separate the velocities into components along the normal and in the plane, $V_{\rm plane} = (V_{p1}^2 + V_{p2}^2)^{1/2}$. Figure 3 shows scatter plots for 1000 randomly selected particles from each of our runs. Many particles are hidden by superposition. The correct result is a line along the $V_{\rm norm}$ axis. This line is approached only by nonsparse PM and NGPM, by P^3M and Tree as the short-range force is turned off, and by axis-aligned runs that have only head-on collisions. With $\epsilon = 0.1$, the most common choice, the error is large.

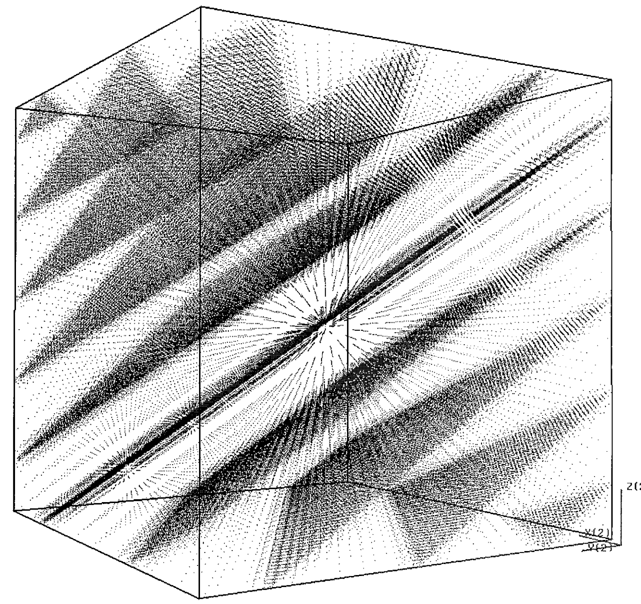

FIG. 1.—Configuration of particles at the end of our PM simulation. The other simulations look much the same, except for more inhomogeneity in some cases.

The relative error can be made quantitative by comparing the median speed in the plane to the median speed along the normal, as shown in Table 1. Another measure is the kinetic energy; the mean in the plane and along the normal are also shown in Table 1. Lastly, we show the median value of $d_{\rm plane}$, the distance in mesh units by which particles have strayed off the normal trajectory. All values are the mean or median of 10,000 particles (subgrid particles in NGPM). Our axis-aligned PM and P^3M runs had *zero* off-normal velocity (within computer precision).

Figure 4 shows a phase-space diagram of a single sheet, including the normal displacement and velocity, with the other four phase-space dimensions suppressed. The correct solution is a spiral (Doroshkevich et al. 1980; Melott 1982a; Bond, Szalay, & White 1983). The codes that preserve this pattern are those with softening comparable to the mean interparticle separation.

We can verify that scattering occurs from encounters, not from the initial gravity fields, by noting that off-normal components are small until shell crossing in all codes; they increase strongly in the inclined HFLMR codes as particles pass each other.

3. DISCUSSION

We have shown that HFLMR computational methods in widespread use for gravitational clustering in cosmology perform incorrectly on a simple test problem because they try to model a continuous system with discrete masses. The PM and NGPM methods (as normally used) are able to handle this test because there is no evasion of the discreteness limitation. PM

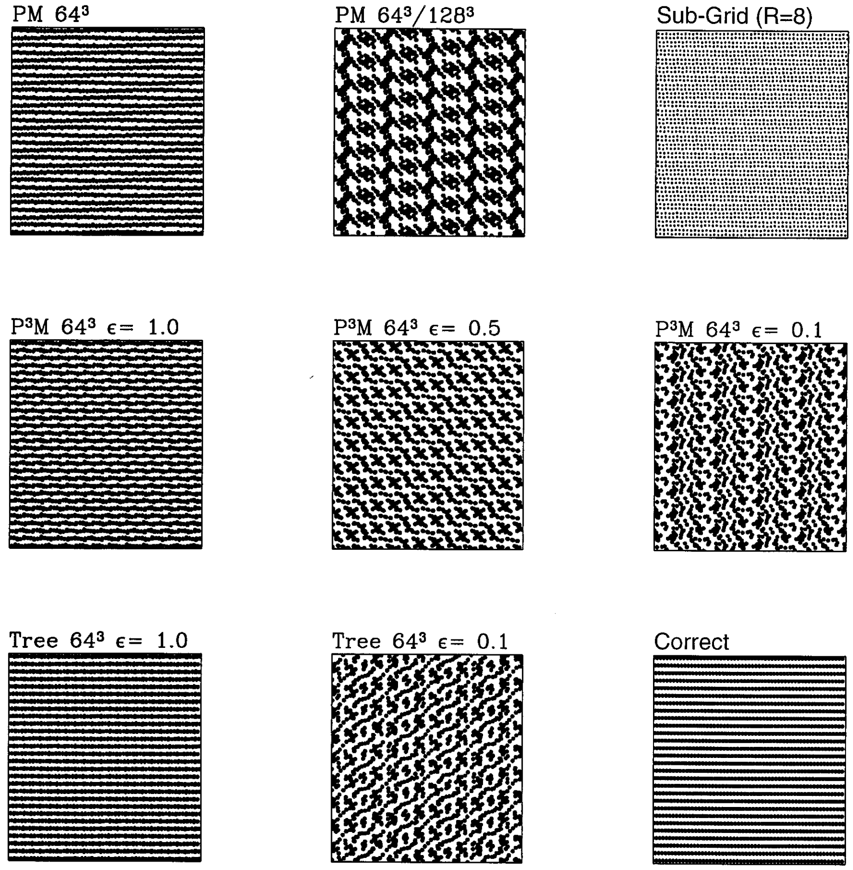

FIG. 2.—A slice of one of the planes from each cube, seen projected along the normal to the plane. The dimensions of the slice are $16 \times 16 \times 4$. To construct the NGPM slice, a slice of size $4 \times 4 \times 1$ was extracted from the subgrid particles and repeated periodically to produce a slice of size $16 \times 16 \times 4$. This slice was then sampled to reduce the number of particles to roughly that of the other runs. *top row*: PM with one particle per cell, PM with one particle per 8 cells (a common "resolution-increasing" procedure), and NGPM (subgrid). *Middle row*: P^3M with various values of ϵ. *Bottom row*: Tree code with various values of ϵ, and the correct result, which was constructed by propagating particles along normals to the plane; the lines come from the tilted projection of the cubic lattice. This projection represents the standard of comparison for all the codes except NGPM, which shows the correct appearance.

can be forced to fail by increasing the lattice resolution beyond appropriate limits. HFLMR methods work properly if the short-range force is turned off or if they are forced to align with the coordinate axes.

Since convergence to the proper behavior is very slow (e.g., Hockney 1971), past comparisons by varying particle number have not revealed this problem (e.g., Efstathiou & Eastwood 1981). Coupling these incorrectly evolved systems to hydrodynamics will guarantee that the simulation is done in the wrong background gravitational potential. We do not claim that the effect occurs on larger scales. Melott & Shandarin (1990), Little, Weinberg, & Park (1991), and Melott & Shandarin (1993) have shown that small-scale effects scarcely propagate to large scales, but more quantitative study is needed. However, errors would only stop growing in voids or in regions where the particle density exceeds ϵ^{-3}.

Questions may be raised about the relevance of our example. Galaxies are not infinite planes. However, the first collapse on any scale is expected to be sheetlike (Shandarin et al. 1995; Kuhlman et al. 1996; Gouda 1996), so there is ample opportunity for our test situation to arise. Furthermore, collisionality operates in the absence of symmetry; our planar collapse study simply makes it starkly obvious. One may argue that since collapsed pancakes are unstable to small-scale perturbations, the HFLMR codes model them correctly, justifying the results they give for small ϵ. On the other hand, since there is no small-scale power in the initial conditions, these codes are artificially producing power on small scales by the growth of shot noise. The results of a simulation should be a consequence of initial conditions that were imposed. This point is illustrated in the orientation dependence of the HFLMR codes. Since we get two completely different results depending on orientation, one must ask which result is correct. Most importantly, our results serve to raise the question of whether a code performs well overall in a complex nonlinear problem when it cannot replicate a simple test case. As this Letter was going to press, the authors learned of the work of Park (1997), in which spherical collapse is studied, producing conclusions close to ours. Values $\epsilon = 0.01$ or even smaller are used in clustering studies.

One might hope that realistic cosmological scenarios with power on all scales avoid this problem. Impressed perturbations might overwhelm discreteness if the spectrum is normalized to the shot-noise level at the particle Nyquist frequency (Efstathiou et al. 1985). We tested this possibility by putting in an inclined plane wave close to the particle Nyquist frequency at the white-noise amplitude. Again we found strong scattering in a $\epsilon = 0.1$ P^3M run and essentially none in PM. At this short wavelength the resolution limitations of PM show themselves

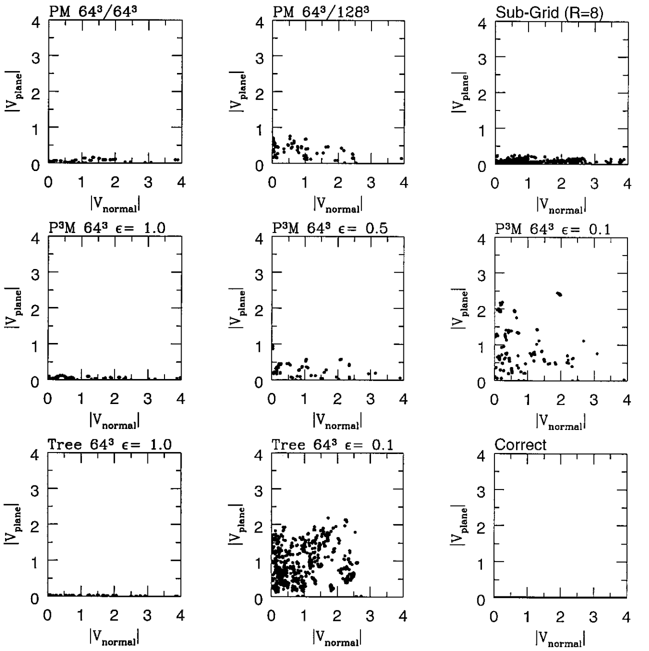

FIG. 3.—Scatter plots of the absolute value of velocity components for 1000 particles randomly selected from each of the simulations, projected both along the normal to the plane of collapse and in the plane. For correct physical modeling, all points should lie along the x-axis. Each plot contains the same number of points; many are superimposed. The panels are arranged as in Fig. 2. Velocity units are the Hubble velocity across one cell.

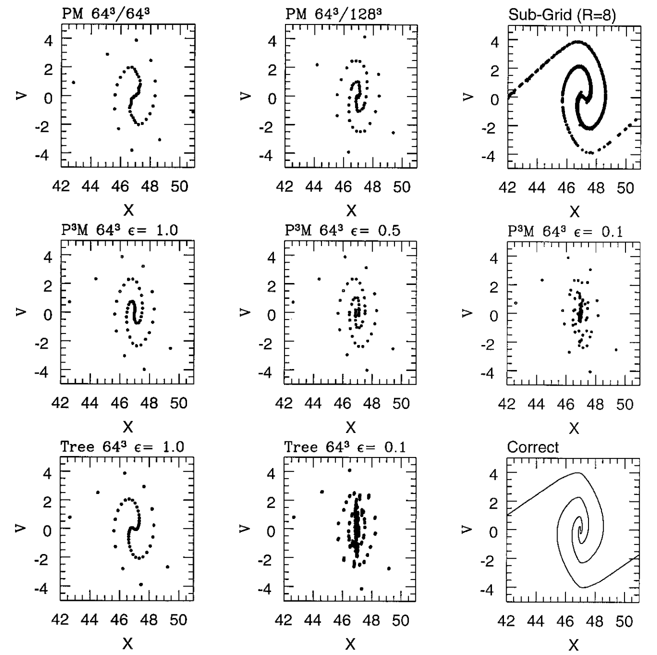

FIG. 4.—Scatter plots of the normal component of the velocity for all particles collapsed toward one of the pancake planes vs. particle displacement from the midpoint. The known solution is a spiral pattern whose development varies with resolution in some codes but which is totally disrupted in others. The arrangement and units are used as in Fig. 3.

in the code's lower velocity dispersion, so that both codes were performing badly. The accuracy of cosmological results from HFLMR codes remains an open question.

Suto (1991) examined the divergence of particle trajectories in a series of N-body cosmological simulations with varying ϵ. He found that the comoving trajectories diverged with time as $e^{\lambda t}$, fitting $\lambda \simeq 0.05(G\bar{\rho})^{1/2}\epsilon^{-1.2}$. By requiring $e^{\lambda t_{\rm H}} < \epsilon$, where $t_{\rm H}$ is the Hubble time, we require that deflection of nearby trajectories by shot noise is small. Enforcing such a condition gives $\epsilon \gtrsim 1$, similar to our results and to the results of Peebles et al. (1989) and Suisalu & Saar (1996).

One promising method of achieving better force and mass resolution while doing correct physics is nested-grid methods, which put more particles in the region of interest. Such methods are shown here to greatly reduce collisions and may allow the study of small-scale structure to progress (e.g., Villumsen 1988; Anninos, Norman, & Clarke 1994; Splinter 1996). Putting in a higher particle density shows only that one cannot get something for nothing by sidestepping the laws of physics.

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TABLE 1

CODE COMPARISON—PLANE WAVE TEST

Code	Median $V_{\rm norm}$	Median $V_{\rm plane}$	Kinetic Energy $\bar{T}_{\rm norm}$	Kinetic Energy $\bar{T}_{\rm plane}$	Median $d_{\rm plane}$
PM	0.75	0.03	1.82	0.001	0.01
PM ($N_c = 128^3$, $N_p = 64^3$)	0.91	0.44	2.53	0.22	0.80
Subgrid ($R = 8$)	0.77	0.05	1.84	0.02	0.003
P³M ($\epsilon = 1.0$)	0.70	0.05	1.99	0.004	0.03
P³M ($\epsilon = 0.5$)	0.82	0.27	2.00	0.15	0.12
P³M ($\epsilon = 0.1$)	0.78	0.62	2.10	0.76	0.53
Tree ($\epsilon = 1.0$, $\theta = 0.2$)	0.57	0.01	1.82	0.0003	0.02
Tree ($\epsilon = 0.1$, $\theta = 0.2$)	0.81	0.62	2.08	0.79	0.45

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