OPTIMAL SOFTENING FOR N-BODY HALO SIMULATIONS

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ABSTRACT

We propose to determine the optimal softening length in N-body halo simulations by minimizing the ensemble-average acceleration error at a small radius \( r_0 \). This strategy ensures that the error never exceeds the optimal value beyond \( r_0 \). Furthermore, we derive semianalytic formulæ for calculating the acceleration error due to the discreteness of particles and softened gravity, which are validated by direct N-body force calculations. We estimate that current state-of-the-art halo simulations suffer \( \gtrsim 6\% \) acceleration error at 1% of the halo virial radius. The error grows rapidly toward the center and could contribute significantly to the uncertainties of inner halo properties.

Subject headings: galaxies: halos — methods: analytical — methods: n-body simulations

1. INTRODUCTION

N-body simulations use discrete particles to trace the phase-space evolution of a continuous density field under the influence of gravity. They have broad applications in modern cosmology that range from structures beyond galaxy clusters (e.g., Padilla & Baugh 2002; Bahcall et al. 2004) to Earth-mass dark matter halos emerging as the first objects in the universe (Diemand et al. 2005).

Because of their Monte Carlo nature, N-body codes have to soften the gravity to subdue destructive effects of strong two-body scatterings and to increase numerical efficiency (Dehnen 2001). Although softening reduces the variance of the force from discrete particles, it also introduces a bias (Merritt 1996). The bias increases with the softening length, while the variance does the opposite. As such, there must exist an optimal softening length that reaches the best compromise between the bias error and variance error.

Suitable softening lengths are often searched for through convergence tests with N-body halo simulations (Navarro et al. 1996; Moore et al. 1998; Splinter et al. 1998; Knebe et al. 2000; Fukushige & Makino 2001; Power et al. 2003). It should be emphasized that a proper softening length must be matched with other simulation parameters such as the time step. For example, with a poor combination of the softening length and time step, the inner halo profile could become corelike (Fukushige et al. 2004, hereafter FKM04). It is not practical to search for every possible softening length and its matching simulation parameters using N-body simulations. Thus, the resulting softening length may not be optimal, and it is not clear what physical error bounds this softening length imposes.

Merritt (1996) devised a more efficient and objective method that requires the optimal softening length to minimize the mean integrated square error (MISE) of the force,

\[
\text{MISE} = \int \rho(r) \left\langle \left| F(r) - F^{\text{true}}(r) \right|^2 \right\rangle \, dr,
\]

where angle brackets denote an ensemble average and \( \rho(r) \) is the continuous density. The true force refers to the Newtonian result in the continuous density field. The MISE is effectively a sum of mass-weighted square bias and variance, i.e.,

\[
\text{MISE} = \int \rho(r) \left( \left| F(r) - F^{\text{true}}(r) \right|^2 \right) \, dr + \int \rho(r) \left( \left( F^2(r) - \langle F(r) \rangle^2 \right) \right) \, dr.
\]

For halo simulations, the bias error is significant only at the center of the halo, while the variance error decreases relatively slowly outward. Hence, by minimizing the MISE one tends to allow large bias errors in the center in order to match small variance errors integrated over the whole halo, which may not be desirable for halo simulations. To ensure the accuracy of the density profile beyond a small radius \( r_0 \), one may require that the bias and variance errors, rather than the integrated ones, both be less than a threshold for \( r > r_0 \). This is the basis of our approach for optimizing the softening length.

The MISE method has been implemented for halos with N-body force evaluations at all radii (e.g., Merritt 1996; Athanassoula et al. 2000; Dehnen 2001), which demands much less run time than full N-body halo simulations. For a very large number of particles, however, a direct N-body summation of forces could still be time consuming. To improve the efficiency, we derive semianalytic expressions for the ensemble-average bias and variance errors assuming a Poisson sampling of the halo density profile with particles. In this work, we use spherically symmetric halos as targets for calculating the acceleration error and optimizing the softening length. Our method may be generalized for broader applications.

2. ACCELERATION BIAS

For convenience, we consider the acceleration bias and variance and express lengths in units of the halo virial radius \( r_v \). We set the mass of the halo within \( r_v \) to 1, so that the mass of each particle is \( m_p = N^{-1} \), where \( N \) is the number of particles within \( r_v \).

The gravitational attraction between two particles can be generalized as \( F = m_p^2 f(r, \epsilon) \), where we have dropped Newton’s constant. For Newtonian gravity \( f(r, \epsilon) = r^{-2} \), and for Plummer softening \( f(r, \epsilon) = (r^2 + \epsilon^2)^{-1} \). We also use the S2 softening (Hockney & Eastwood 1981), which treats particles as spheres of radius \( \epsilon/2 \) with density decreasing linearly from the maximum at the center to zero at \( \epsilon/2 \). The S2 softening is often used in particle-particle particle-mesh codes (e.g., Couchman 1991; Jing & Fang 1994).

Suppose that a particle is located at a distance \( r \) from the center of the halo, as illustrated in Figure 1. The mean radial acceleration of the particle is

\[
\langle a_r \rangle = \left\langle \int f(d, \epsilon) \cos \theta \, dm \right\rangle,
\]
where \( dm = m_p n(R) \, dV \) and \( n(R) \) and \( dV \) are the particle number density and volume element at \( R \), respectively. By definition, we have

\[
\rho(R) \simeq m_p \left[ n(R) \right]_{\rho=\rho(R)} \tag{3}
\]

where \( \rho(R) \) is the spherically symmetric halo density. The number of particles \( n(R) \, dV \) within the volume \( dV \) follows approximately the Poisson distribution, so that its mean and variance are both the density times \( dV \). The accelerations are evaluated with direct summations over 10,000 random realizations of a Navarro-Frenk-White (NFW; Navarro et al. 1997, hereafter NFW97) halo, which has a concentration number \( c \) of 5. As expected, the acceleration bias error does not depend on the number of particles within the virial radius

\[
\delta \rho(R) \, dV \quad \text{is solved for Newtonian gravity, whereas for Plummer softening (FKM04), the Plummer softening performs worse than the S2 softening at the same quoted softening length, because it has a broader softening kernel than S2 does.}

For better comparisons, we present fractional bias errors \( \frac{b_{\text{f}}}{a_{\text{f}}^\text{true}} \) in Figure 3, which includes \( N = 10^7 \) results from 10,000 realizations of the same halo. There is a good agreement between direct \( N \)-body force summations (open symbols) and the semianalytic results of equation (6) (solid lines). Note that the bias error does not depend on the number of particles within the virial radius.

### 3. ACCELERATION VARIANCE

At a fixed position, the acceleration fluctuates from one realization to another because of the discrete sampling of the halo

\[
a_{\text{r}} = \langle a_r \rangle - a_{\text{r}}^\text{true}. \tag{6}
\]

Figure 2 shows a few examples of \( \langle a_r \rangle \) under softened gravity. The accelerations are evaluated with direct \( N \)-body force summations over 10,000 random realizations of a Navarro-Frenk-White (NFW; Navarro et al. 1997, hereafter NFW97) halo, which has a concentration number \( c = 5 \). As expected, the acceleration bias is significant only at \( r \) less than a few \( r_c \) and is small at larger radii even where particles can be, on average, closer than the softening length in the S2 case.

With softening lengths of a few percent of the virial radius\(^1\) (e.g., NFW97; Navarro et al. 2004, hereafter N04; see Table 1),

\[^1\] The softening splines in NFW97 and N04 differ from S2, but we do not expect such differences to alter the result qualitatively.

| Simulation   | \( \bar{\epsilon} \) (%\(^4\)) | \( N \) | \( \frac{b_{\text{f}}}{a_{\text{f}}^\text{true}} \) (%) | \( \sigma_{\text{f}}a_{\text{f}}^\text{true} \) (%) |
|-------------|----------------|-----|----------------|----------------|
| NFW97      | 20             | \( 10^4 \) | 30             | 30             |
| M99         | 1              | \( 10^6 \) | 0.07           | 8              |
| N04         | 10             | \( 10^6 \) | 7              | 5              |
| FKM04      | 0.3            | \( 10^7 \) | 0.2            | 6              |

Notes.—The acceleration errors are estimated at 1% of the virial radius. For spline softening (NFW97, M99, and N04), \( \bar{\epsilon} \) equals the scale beyond which the gravity is Newtonian, whereas for Plummer softening (FKM04), \( \bar{\epsilon} \) is their reported softening length. The number of particles \( N \) within \( r_c \) is approximate.
These fluctuations impose a sample variance error on particles’ acceleration, and they depend on both the number of particles and softening. With the help of equation (4), we find the acceleration variance

$$
\sigma_a^2 = \langle a^2 \rangle - \langle a \rangle^2 = \frac{2\pi}{N} \int_0^\pi \sin \theta \, d\theta \int_0^{d_{\text{cut}}} f^2(d, \epsilon) \rho(R) d^2 d,
$$

(7)

where $d_{\text{cut}}^2 + 2d \epsilon \cos \theta + \epsilon^2 = R_{\text{cut}}^2$ and $R_{\text{cut}}$ formally extends to infinity. Since the result within the virial radius converges very quickly for $R_{\text{cut}} \geq \text{a few } r_v$, we set $R_{\text{cut}} = 2r_v$ to be consistent with $N$-body calculations.

We calculate fractional variance errors $\sigma/a_{\text{true}}$ for the same set of configurations as for the fractional bias errors in § 2. The variance errors of direct $N$-body force summations are plotted in Figure 3 with solid symbols. One sees that the $N$-body results are very well traced by equation (7) in solid lines. For a fixed $N$, a smaller softening length results in larger variance errors, while for a fixed softening length, the variance error scales as $N^{-1/2}$.

Plummer softening has smaller variance errors than the S2 softening with the same $\epsilon$ and $N$ because of its broader softening kernel.

To access the effect of the halo profile, we calculate acceleration errors using different concentration numbers and using a Moore et al. (1999, hereafter M99) profile, which has a stronger cusp of logarithmic slope $-1.5$. The bias error does not change.
much with the profile. On the other hand, the variance error is reduced by a factor of 2–3 by boosting the concentration from \(c = 5\) to \(c = 20\). The variance error of M99 halos is a factor of 1.6 smaller than (roughly the same as) that of the corresponding NFW halos at \(r = 0.01\) (\(r \sim 1\)), when the concentration number is adjusted to \(c(M99) = c(NFW)/1.7^{0.5}\) (Peacock & Smith 2000).

4. OPTIMAL SOFTENING

As seen in Figure 3, the bias error increases much faster toward the center of the halo than the variance error. Minimizing the MISE (Merritt 1996) may not be optimal for studying inner halo properties, because the MISE method prefers a relatively large softening length so that small variance errors spread over the entire halo are matched by large bias errors confined in the center.

We propose to optimize the softening length by minimizing the mean acceleration error \(\mathcal{E}_a = (\theta_a^2 + \sigma_a^2)^{1/2}\) at a small radius \(r_0\). In this way, one ensures that \(\mathcal{E}_a\) never exceeds the optimal value at larger radii. Conversely, one could set an error budget at \(r_0\) and determine the number of particles needed for a particular softening.

Figure 4 illustrates the mean acceleration error at 1% of the halo virial radius (dotted lines) as a function of the softening length for different numbers of particles. For an NFW (\(c = 5\)) halo with S2 softening, we obtain, from the minimum of each error curve, \(\epsilon_{\text{opt}} = 0.11N^{-0.20}\) and \(\mathcal{E}_a = 14N^{-0.38}\). For the same halo but with Plummer softening, \(\epsilon_{\text{opt}} = 0.065N^{-0.26}\) and \(\mathcal{E}_a = 13N^{-0.36}\). The optimal softening lengths and minimum acceleration errors of corresponding M99 halos have nearly the same \(N\) dependence as those of NFW halos but with 15%–30% smaller prefactors, because they have smaller variance errors at the same softening length.

The \(N\) dependences of our results are consistent with those of MISE results in Athanassoula et al. (2000) and Dehnen (2001), despite the fact that our halos differ from theirs and that we prefer smaller softening lengths. For a closer comparison, we calculate the optimal softening length for a Hernquist (1990) sphere of \(10^5\) particles with Plummer softening. We find \(\epsilon_{\text{opt}} = 0.0049\) and \(\mathcal{E}_a = 30\%\) with \(r_0 = 0.01\), whereas Dehnen (2001) obtained \(\epsilon_{\text{opt}} = 0.016\) and a mass-weighted average error of 6.7%, which lead to \(\mathcal{E}_a = 55\%\) at \(r = 0.01\). With our \(\epsilon_{\text{opt}}\) the average error is 7.2%. This shows that our strategy is to trade slightly larger (yet tolerable) errors at large radii with smaller errors near the center (although \(10^5\) particles do not seem sufficient for studying inner halo properties no matter what softening length is used).

5. DISCUSSION AND CONCLUSIONS

The optimal softening lengths in this work are not truly optimal in the sense that they slightly depend on the assumed halo profile and that, in turn, the simulated halo profile could be affected by the softening length. Nevertheless, our strategy provides guidance for choosing the softening length and for evaluating acceleration errors of simulated halos. For example, we list in Table 1 error estimates for four sets of halo simulations ranging from one of the first claims of the universal profile (NFW97, \(N < 10^4\)) to the latest investigation (FKM04, \(N > 10^5\)). The errors are typically \(\geq 6\%\) at \(r = 0.01r_v\). Since the mass within \(0.01r_v\) is a few thousandths of the halo virial mass, even a few percent acceleration errors may contribute significantly to the uncertainties in the inner slope of the halo. In fact, N04 achieve convergent results only at \(r \geq 0.01r_v\). Hence, it may not be reliable to extrapolate to ever smaller radii and infer a central cusp.

Power et al. (2003) propose that the optimal softening length should satisfy the condition that the maximum stochastic acceleration \((\sim 1/r_v^2)\) be several factors smaller than the mean field acceleration at \(r_v (\sim 1/r_v)\). Roughly speaking, the acceleration variance arises from two sources: the stochastic acceleration as defined by Power et al. (2003) and Poisson fluctuations of particles in the halo. Since the latter increases toward the center, setting a small stochastic acceleration at \(r_v\) does not always guarantee small errors near the center.

Our criterion for the optimal softening length imposes a strict upper limit on the mean acceleration error at \(r > r_0\). Direct error bounds on halo properties may be more useful for interpreting simulation results, but to identify the most accurate simulation on which error estimates of other simulations can be based, one needs a gauge like the mean acceleration error.

To optimize the softening length for general density fields or halos with substructures or asymmetries, one must derive equations (5) and (7) without assuming spherical symmetry for the density. Moreover, one should generally minimize the acceleration error in high-density regions, where the error tends to be large.

From NFW97 to N04, the acceleration error at \(0.01r_v\) is reduced from \(42\%\) to \(8.6\%\), and one starts to see a continuously changing (logarithmic) central density slope instead of a constant slope of \(-1\) in an NFW halo. Hence, it will be interesting to see how the results evolve when the error is further reduced to well below \(1\%\) with \(N > 10^4\). A recent investigation on two-body relaxation also suggests that \(>10^6\) particles are required to faithfully model the very inner regions of halos (El-Zant 2005).

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