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A NEW METHOD TO FIND THE POTENTIAL CENTER OF *N*-BODY SYSTEMS

F. Cruz,[1] L. A. Aguilar,[1] and D. D. Carpintero[2]

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RESUMEN

Se presenta un método rápido para encontrar el centro del potencial de una distribución de *N*-cuerpos. El método usa un algoritmo iterativo que aprovecha el hecho de que el gradiente del potencial es nulo en su centro; emplea asimismo un radio de suavizado para evitar quedar atrapado en mínimos locales. Se ha probado el método con modelos de King (cuyos núcleos, de densidad relativamente constante, hacen particularmente difícil la determinación numérica de este centro), y se ha comparado su eficiencia y precisión con un método más directo, aunque de cálculo intensivo, basado en mallas cartesianas de resolución espacial creciente. En todos los casos, ambos métodos convergen al mismo centro dentro de la resolución de la malla, aunque el método iterativo es dos órdenes de magnitud más rápido.

Utilizamos este método en un problema astronómico: la evolución de un modelo de King de 10^5 partículas, en órbita alrededor de un potencial fijo representativo de nuestra Galaxia. Se utilizó un código de *N*-cuerpos con expansión en armónicos esféricos, en el que la determinación del centro del potencial es esencial para un cálculo correcto de las fuerzas. Se comparó esta simulación con el mismo código pero con un método empleado anteriormente para determinar el centro de expansión (White 1983). Con nuestra rutina se obtienen mejores resultados en la conservación de energía y de la masa.

ABSTRACT

We present a new and fast method to find the potential center of an *N*-body distribution. The method uses an iterative algorithm which exploits the fact that the gradient of the potential is null at its center: it uses a smoothing radius to avoid getting trapped in secondary minima. We have tested this method on several random realizations of King models (in which the numerical computation of this center is rather difficult, due to the constant density within their cores), and compared its performance and accuracy against a more straightforward, but computer intensive method, based on cartesian meshes of increasing spatial resolution. In all cases, both methods converged to the same center, within the mesh resolution, but the new method is two orders of magnitude faster.

We have also tested the method with one astronomical problem: the evolution of a 10^5 particle King model orbiting around a fixed potential that represents our Galaxy. We used a spherical harmonics expansion *N*-body code, in which the potential center determination is crucial for the correct force computation. We compared this simulation with another one in which a method previously used to determine the expansion center is employed (White 1983). Our routine gives better results in energy conservation and mass loss.

Key Words: **GLOBULAR CLUSTERS: GENERAL — METHODS: *N*-BODY SIMULATIONS, NUMERICAL**

[1]Instituto de Astronomía, Universidad Nacional Autónoma de México, Ensenada, B. C., México.

[2]Observatorio Astronómico, Universidad Nacional de La Plata and CONICET, Argentina.

1. INTRODUCTION

An important class of N-body simulation techniques relies on a potential representation by means of an expansion in harmonic functions suitable to the global symmetry of the model (Clutton-Brock 1973; Villumsen 1982; McGlynn 1984; Syer 1995). Harmonic expansion codes have been used to simulate N-body system dynamics like the dynamical friction on satellite systems (White 1983), the stability of spherical galaxies (Merritt & Aguilar 1985), the evolution of cold spherical collapses (Villumsen 1984; Aguilar & Merritt 1990), and galaxy mergers (Villumsen 1982). The accurate determination of the potential center for the harmonic expansion is of paramount importance to get good energy conservation and the correct simulation of the dynamics. Some authors have used the center of mass of a subset of the system (Villumsen 1982), others a weighted center of mass (McGlynn 1984) and yet others have used a "live" particle (i.e., a dynamical moving particle originally in the center of the system, White 1983) to anchor the center of the harmonic expansion. A fixed expansion center is not suitable for situations where the N-body system moves as a whole. The use of the center of mass as the center of the potential is inherently problematic, as the former is most affected by particles at large distance from the center while the latter is not; this has compelled some authors to use the center of mass of just the fraction of the system that is most bound. The last approach—the use of an active particle to designate the center of the expansion—requires the use of additional softening to dampen the irregular motion of the marker (White 1983). One additional consideration is that most of the simulated systems in the quoted references have a density distribution with a central cusp (e.g., a de Vaucouleurs profile) which eases the difficulty of locating the appropriate center for the expansion. The use of a model with a flatter core, like a King model, makes the problem much harder and it has not been investigated in the past.

These difficulties have motivated us to seek an alternative, in the form of a fast algorithm that can locate the center of the potential with good accuracy, within the finite spatial resolution imposed by the discreteness of the N-body distribution. In § 2 we describe the method and its optimization. In § 3 we present results of tests in which the potential center has been determined with the proposed method and with a more computer intensive method that relies on the evaluation of the potential at Cartesian meshes of increasing spatial resolution. In § 4 we apply our new method to one astronomical problem: the evolution of a globular cluster in a fixed galactic potential using a spherical harmonics expansion code, and compare these results with the live particle method. Finally we compare the performance of this code with a tree code.

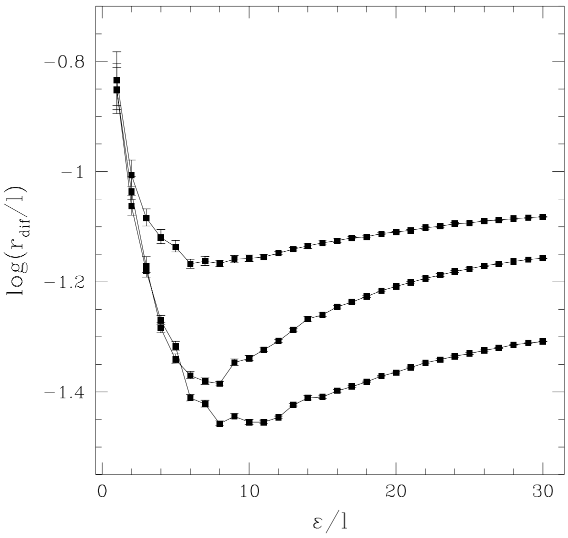

Fig. 1. Logarithmic median separation $r_{\rm dif}$, between the potential centers found with the iterative method and with the mesh method, versus the softening parameter ε. Both are shown in units of the mean particle separation l, within the half-mass radius. Each line corresponds to a different 10^5 particle random realization of the same King model. Each point represents the median of an ensemble of 1,000 experiments made at a fixed softening, but with different random starting points, for the iterative method. The error bars indicate the interquartile span of the distribution.

2. METHOD

The potential Φ at a point $\mathbf{r}$ due to a collection of N softened particles is given by

$$\Phi(\mathbf{r}) = -G \sum_{i=1}^{N} \frac{m_i}{[(\mathbf{r}_i - \mathbf{r})^2 + \varepsilon^2]^{1/2}}, \qquad (1)$$

where m_i and $\mathbf{r}_i$ are the mass and position of the $i^{\rm th}$ particle, respectively, ε is the softening length, and G is the gravitational constant.

The critical points $\mathbf{r}_c$ of the function $\Phi(\mathbf{r})$, defined by the condition

$$\boldsymbol{\nabla}\Phi(\mathbf{r}_c) = \mathbf{0}, \qquad (2)$$

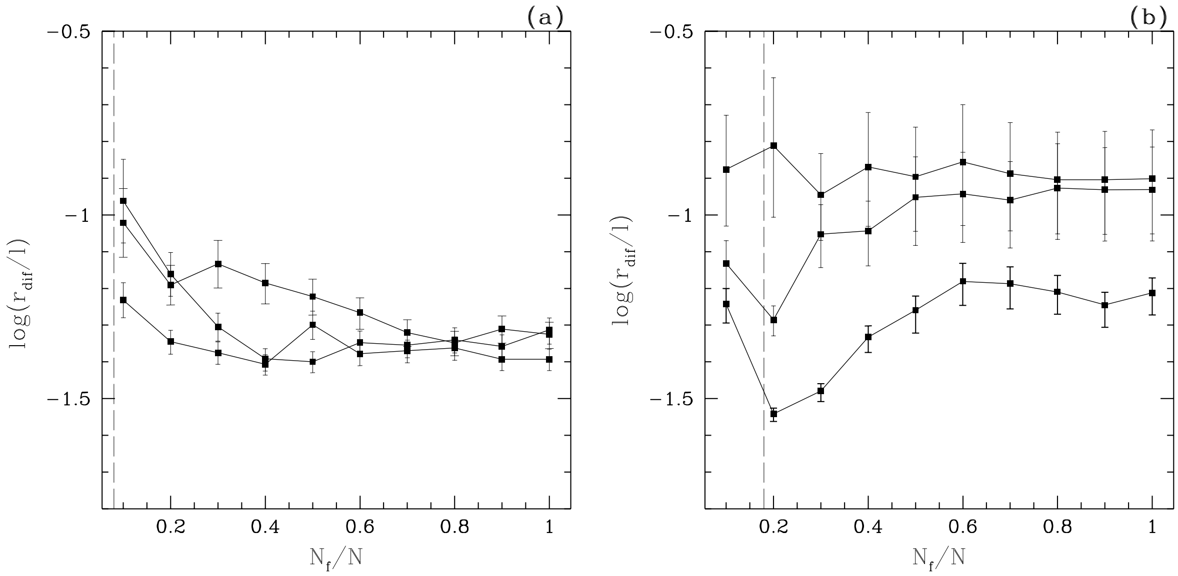

Fig. 2. Logarithmic median separation $r_{\rm dif}$, between the potential center found with our method and that obtained with the mesh method, in units of the mean inter-particle separation l, inside the half mass ratio, versus the fraction $N_{\rm f}/N$ of particles used in the iterative method. The panels correspond to King models with concentration parameters (a) $c = 1.5$ and (b) $c = 1$. Each line corresponds to experiments with different initial random realizations for each concentration. The error bars correspond to the interquatilic intervals for the 25% and the 75% of the distribution. The dashed line show the corresponding value of N_f/N for the core radius for this realizations.

include all maxima, minima and saddle points of Φ. It is clear that, at every $\mathbf{r}_i$, we have a (local) minimum of Φ. (In fact, were it not for the softening parameter, we would have a pole at every $\mathbf{r}_i$.) Besides these minima, the function Φ will have an overall concave shape with its own global minimum, $\mathbf{r}_{\rm c}^*$, due to the entire set of particles. The latter is the *center of the potential*, i.e., the critical point searched for—we do not expect global maxima or saddle points unless Coriolis accelerations are present. It is worth noting that the global minimum is not necessarily an *absolute* minimum, since the bottom of the well of a particle may be lower than $\mathbf{r}_{\rm c}^*$.

Let us solve first for any critical point; we will narrow down the search later to the $\mathbf{r}_{\rm c}^*$. Combining equations (1) and (2), we have

$$\sum_{i=1}^{N} \frac{m_i(\mathbf{r}_i - \mathbf{r}_{\rm c})}{[(\mathbf{r}_i - \mathbf{r}_{\rm c})^2 + \varepsilon^2]^{3/2}} = \mathbf{0}. \qquad (3)$$

Since this equation cannot be solved analytically for the critical points $\mathbf{r}_{\rm c}$, we revert to a numerical solution. To this end, we rewrite the last equation as

$$\mathbf{r}_{\rm c} = \frac{\displaystyle\sum_{i=1}^{N} \frac{m_i\mathbf{r}_i}{[(\mathbf{r}_i - \mathbf{r}_{\rm c})^2 + \varepsilon^2]^{3/2}}}{\displaystyle\sum_{i=1}^{N} \frac{m_i}{[(\mathbf{r}_i - \mathbf{r}_{\rm c})^2 + \varepsilon^2]^{3/2}}}. \qquad (4)$$

This equation allows us to compute $\mathbf{r}_{\rm c}$ by iteration.

To avoid being trapped in an undesired local minimum, and to drive the iteration to $\mathbf{r}_{\rm c}^*$, we may increase the softening parameter ε. It is clear that, the greater the softening parameter, the shallower the individual wells, and the less probability of ending up in one of them.

This, however, has its cost: the increase of ε will also yield a shallower overall potential, resulting in a higher global minimum (the limiting case being $\varepsilon \to \infty$, with no individual wells, but also no potential at all!) Nevertheless, the global potential becomes shallow at a rate that is always less than those individual minima, so we can safely increase ε up to a certain amount to avoid getting trapped.

Besides these considerations, we want the algorithm to be fast. To this end, we can take advantage of the fact that the contribution to the potential from particles lying far away from the center of the system is small. Thus, we may remove these particles from the computation without affecting noticeably the position of the potential center. This can be achieved by simply reordering the particles in ascending order from nearest to farthest from one initial central position, and performing the summations in equation (4) up to a certain $N_{\rm f}$, the new total number of particles to be considered.

Finally, we introduce a convergence criterion η defined as

$$\eta \equiv |\mathbf{r}_{\rm c}^{k-1} - \mathbf{r}_{\rm c}^{k}|\,, \qquad (5)$$

where $\mathbf{r}_{\rm c}^{k-1}$ and $\mathbf{r}_{\rm c}^{k}$ are sequentially computed values for $\mathbf{r}_c^*$. When the desired convergence is achieved the iteration is stopped.

To optimize the algorithm, we need to find the best values for the three parameters $N_{\rm f}$, ε, and η. To this end, we performed extensive numerical experiments, comparing the results of our method with the potential center computed by directly interpolating in a cubic mesh. To improve the precision of the latter method, we first used a low resolution mesh to find an approximate minimum of the potential; then, centered on this position, we put a higher resolution mesh and repeated the process several times. The resolution of the last mesh was 0.001 times the mean inter-particle separation l inside the half mass radius of the distribution. We show the results of these experiments in the next section.

3. RESULTS

The first parameter we tune is ε, used to avoid getting trapped in local minima. We arbitrarily set the other two parameters to be $\eta = 10^{-3}$ and $N_{\rm f}/N = 0.5$; we show below that these values represent a good choice. Figure 1 shows the results obtained, gauged by the discrepancy between the iterative and the mesh methods as a function of softening. The discrepancy is measured by the distance between the potential centers found by the iterative and the mesh methods $r_{\rm dif}$, in units of the mean particle separation within the half-mass radius l. Each line corresponds to experiments with a different 10^5 particles random realization of a King model of concentration $c = 1.5$. For each one, we have tested our procedure at softenings in the range $1 \leq \varepsilon/l \leq 30$. At each softening we have tried the iterative method 1000 times starting from different random initial points. The dot at each softening value marks the median of the ensemble distribution and the error bar its interquartile range. We see that softenings in the range $10 \leq \varepsilon/l \leq 20$ are optimal, with differences among random realizations being dominant. The agreement

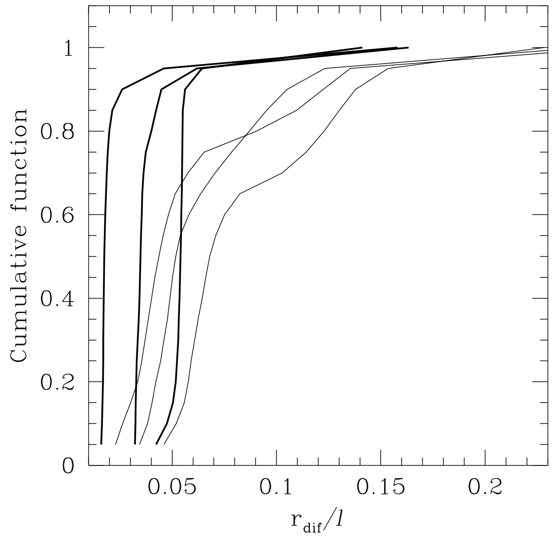

Fig. 3. Cumulative function of $r_{\rm dif}/l$ for three realizations of a King model with $c = 1.5$. The thick lines correspond to the experiments with $\eta = 10^{-4}$; the thin lines to $\eta = 10^{-3}$.

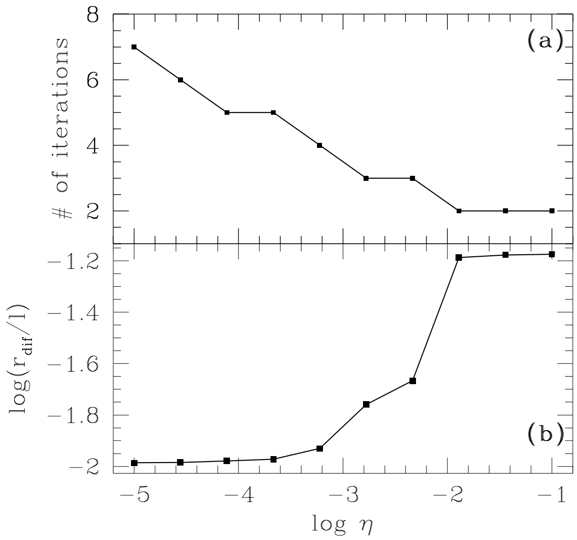

Fig. 4. (a) Number of iterations as a function of the convergence criterion η. Each point corresponds to the mean of 1000 different computations of the potential center for a King model with $c = 1.5$. (b) Discrepancy $r_{\rm dif}/l$ between the iterative and mesh method, as a function of η, for the same set of experiments as in (a).

between the iterative method and the mesh method, used as our control, is better than $0.1l$ in this region. From now on, we fix the softening at $\varepsilon = 15\,l$.

For the number of particles used in the iterative method, $N_{\rm f}$, we have done a similar series of experiments as with ε, but using two King models with concentrations of $c = 1.5$ and 1.0. The results are shown in Figure 2. Again, three random realizations were used and an ensemble of 1000 experiments were done for each $N_{\rm f}$. The starting points for each experiment were chosen randomly from the region defined by $[r_{\rm h}, 5\,r_{\rm h}]$, with $r_{\rm h}$ the half-mass radius of the system (i.e., the starting points were well outside the core of the system). We see that the coincidence with our control method improves as more of the cluster is included, but with a weak dependence. We settled on a value of $N_{\rm f}/N = 0.40$.

In order to assess the effect of the convergence criterion η, we performed 10^4 computations of $r_{\rm dif}/l$ in the $c = 1.5$ King model, each with a different starting point chosen from the interval $[r_{\rm h}, 5r_{\rm h}]$; we then arranged the resulting values in ascending order and formed the corresponding cumulative function. Figure 3 shows this cumulative function for two values of η. We can see that 80% of the results fall inside $0.05\,l$ for $\eta = 10^{-4}$, and 70% of the results fall inside $0.08\,l$ for $\eta = 10^{-3}$. We conclude that any value in this range would be a suitable choice for η.

For a further tuning of the parameter η, which controls when the iterative method should stop at the desired accuracy, we must find a balanced choice between precision and computing time. Figure 4*a* shows the mean number of iterations required to reach a desired convergence η. As expected, the number of iterations grows as η decreases. It is worth noting that the number of iterations is very low, ranging from 2 to 7 when η takes values between 10^{-1} and 10^{-5}. However, we note that changing η from 10^{-3} to 10^{-4} yields an increase from 3 to 5 in the number of iterations, i.e., a code 60% more expensive in time. On the other hand, Figure 4*b* shows the achieved accuracy $r_{\rm dif}/l$ as a function of the convergence criterion, η. We can see that shifting from $\eta = 10^{-3}$ to $\eta = 10^{-4}$ increases the accuracy a mere 30%, as compared with a 60% degraded performance in time.

From the previous results we conclude that $10^{-4} < \eta < 10^{-3}$, $N_{\rm f} \geq 0.4N$, and $\varepsilon \geq 15l$ are good choices for the three parameters involved for these particular N-body models (King Models with 10^5 particles).

4. AN ASTRONOMICAL PROBLEM

We use our iterative algorithm in a harmonic expansion N-body code (White 1983) to follow the evolution of a globular cluster in orbit in a galactic potential. For a globular cluster, the determination of the center of this expansion is difficult, because of a central core where the density is roughly constant and the corresponding potential is very shallow. We compared this simulation with another one done with the same harmonic expansion code, but using the *live particle* method used originally by White (1983) and subsequently by other authors (e.g., Aguilar & White 1985; Merritt & Aguilar 1985; Aguilar & Merritt 1990) to find the center of expansion.

In this experiment we put an N-body King model with 10^5 particles and concentration $c = 1.5$, in a circular orbit in the fixed galactic potential from Bachall, Schmidt, & Soneira (1983), adapted by Cruz (1999, e.g., § 3) to compute the force and the potential in analytical form. We use $\eta = 5 \times 10^{-4}$, $N_{\rm f} = 0.4N$, and $\varepsilon \simeq 15\,l$ for our centering routine.

The cluster orbit is circular with a radius of 3 kpc, and we follow it for 10 orbital periods. To avoid large transient effects, the initial size of the cluster was $\sim 30\%$ smaller than the Roche lobe at this galactic radius. The simulation with our centering routine had an energy conservation error of 0.3% and the cluster lost 2% of its mass. The simulation with the live particle method conserved energy within 2% and the cluster lost 8% of the mass.

In Figure 5 we show the evolution of the Lagrangian radii corresponding to 0.1%, . . . , 0.9%, 1%, . . . , 9%, 10%, . . . , 90%, . . . , 91% . . . , and 99% of the mass of the globular cluster with our routine, top panel, and for the *live particle* method, bottom panel. We see that with the iterative method, the cluster structure does not vary significantly during the whole simulation (the radial variation of the half mass ratio was 0.5%). On the other hand, when using the live particle method, the cluster undergoes a large expansion just after the first orbital period (Fig. 5*b*). The half mass radius of the cluster expands 36% of its original size in the first orbital period, and continues expanding until it reaches 64% of its original size at the end of the simulation. This difference in the structure of the simulated cluster is presumably the result of the errors in the location of the expansion center by the live particle method. To verify the role of the potential centering in these simulations, we have followed the position of this center in both simulations. In Figure 6 we have plotted the time evolution of the variation of the radial position

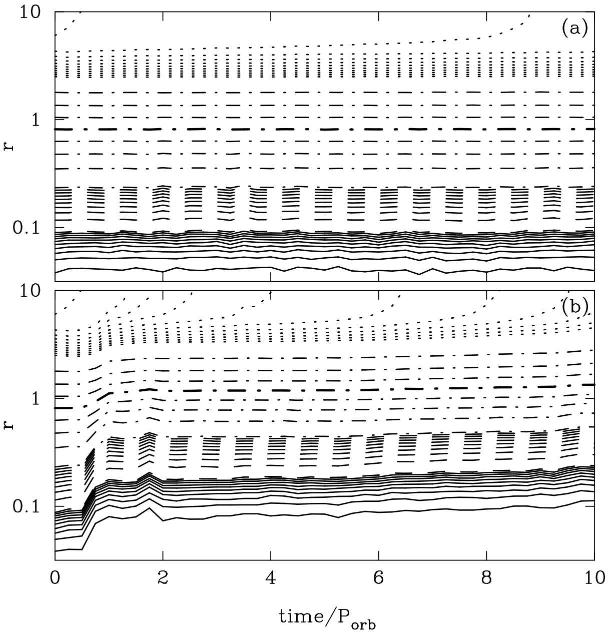

Fig. 5. Lagrangian radii for the cluster mass in the simulation with our centering routine (a), and the live particle method (b). The solid lines correspond to 0.1%, ..., 0.9%, the dashed lines to 1%, ..., 9%, the dashed and dotted lines to 10%, ..., 50% (thick line), ..., 90%, and the dotted lines to 91%, ..., 99% of the mass.

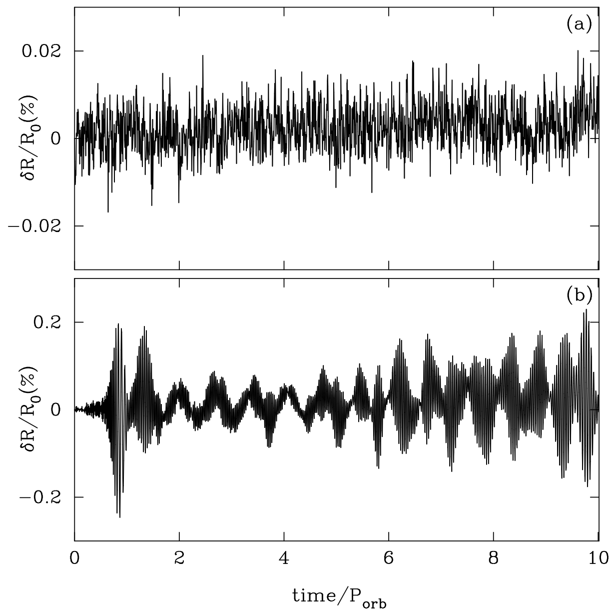

Fig. 6. Orbital variation for the same simulations of Fig. 5. In (a) we show the radial variation of the center of the potential with respect to the initial position when using our iterative method. In (b) we show the radial variation of the position of the *live particle*. Notice than in this case the y-axis is one order of magnitude larger than in (a).

of the expansion center with respect to the galactic center for our routine, top panel, and for the *live particle* method, bottom panel. In Fig. 6a the maximum variation of the position of the center is 0.01% from the original position. This is dominated by random fluctuations with only a small secular deviation. Instead, in Fig. 6b we can see that the oscillation of the *live particle* is one order of magnitude larger than in the previous case, and also note an increase of the amplitude of this oscillation during the last orbital periods. In particular, the first expansion seen in Fig. 5b is associated with the large oscillation in the live particle (Fig. 6b), before the first orbital period.

From these figures we conclude that the structural evolution of the cluster in our N-body simulation has a strong dependence on the correct choice of the center of expansion for the spherical harmonic code. If we want to study the evolution of a globular cluster due to the tidal field of the Galaxy, our method of finding the center of expansion results in a significant improvement, and ensures that the energy and mass variations in the cluster correspond to dynamical effects and not to numerical errors.

Finally, we followed the evolution of this cluster with the N-body code `GADGET` (Springer, Yoshida, & White 2001), in order to compare the performance of our code with a tree-type code, one of the most frequently used codes in the literature. We found that the tree code is 24 times more expensive in CPU time than the harmonic expansion code, at the same energy conservation. The cluster structure shows the same variation and mass loss in both simulations. In a situation like the one modeled here, where the N-body system retains its overall symmetry, it is clear that a harmonic expansion code with our centering routine is a more efficient simulation tool than a tree code.

5. CONCLUSIONS

We have presented a new method to find the potential center of an N-body distribution. This method has three parameters, which are easy to set for any stellar system, and they allow us to improve the accuracy and reduce the computational cost. The performance of this routine was found to be superior to that of the live particle method used by other authors to find the center of the potential. We followed the evolution of a globular cluster for 18,270 time steps, obtaining an energy conservation of 0.3%, whereas in previous works, in which a spherical harmonics expansion was used, an integration spanning 2000 time steps yielded an energy conservation of 3% (Villumsen 1982); another integration spanning 800 time steps yielded an energy conservation of 1% (Villumsen 1984), and yet another, spanning 2000 time steps, yielded an energy conservation of 1% (Aguilar & Merritt 1990). Although we cannot directly compare these simulations with our results, they give us an idea of the performance of our code as compared with other methods. Furthermore, considering that a King model was used in our simulations—a model with a flat core and therefore with a potential center rather difficult to determine—we conclude that our routine greatly improves the N-body simulations performed with harmonics expansion.

By using this new centering routing we can increase the number of particles in N-body simulations performed with the harmonic expansion method, allowing us to explore a larger range in the initial parameters of those N-body simulations.

The `FORTRAN` routine `CENTER` for computing the center of the potential (density) in an N-body model is available upon request from F. Cruz.

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Luis A. Aguilar and Fidel Cruz: Instituto de Astronomía, UNAM, Apartado Postal 877, 22860 Ensenada, B. C., México (aguilar, fidel@astrosen.unam.mx).

Daniel D. Carpintero: Facultad de Ciencias Astronómicas y Geofísicas, Universidad Nacional de La Plata, Paseo del Bosque S/N, 1900 La Plata, Argentina (ddc@fcaglp.unlp.edu.ar).