Mem. S.A.It. Suppl. Vol. 1, 120

Memorie della
Supplementi

N-body simulations for structure formation from random initial conditions

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Abstract. We present the results of an extensive series of high-performance simulations of the evolution of self-gravitating systems with periodic boundary conditions. The main aim of the project is to investigate the role of gravitation and of initial conditions and boundary conditions into the following evolution toward a metastable equilibrium, in a way such to distinguish the role of the various ingredients in the overall dynamics. In particular, we compare the evolution of spatially infinite self-gravitating systems embedded in an expanding universe with that of systems in a static frame. We discuss the differences and the similarities in several statistical quantities, as the density profiles of clusters and the two point autocorrelation function.

Key words. Numerical methods - Parallel treecode - Galaxies: halos

1. Introduction

In 1692, replying to a letter by Richard Bentley, Master of the Trinity college, Newton wrote: "... if the matter was evenly disposed throughout an infinite space, it could never convene into one mass; but some of it would convene into one mass and some into another, so as to make an infinite number of great masses, scattered at great distance from one to another throughout the infinite space...." (I.Newton,1692, quoted in Saslaw, 2000)

Since Newton, the origin of structures in the Universe is a fundamental issue in physics. The understanding of this process is relevant not only for the uncovering of the mechanisms of the formation of cosmic structures. It is also a way to constrain the values of cosmological parameters and to investigate the physical properties of what

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seems to be a fundamental component of the universe, i.e. the dark matter.

Actually, in the simulation of the formation of galaxies and clusters of galaxies the standard paradigm considers two different ingredients: dark matter and barionic matter. The evolution of dark matter clustering is usually calculated using N-body techniques,as P^3M (Efstathiou et al. 1985), AP^3M (Couchman et al. 1995) or tree codes (Barnes & Hut 1986); the evolution of the gaseous component is usually followed by combining hydrodynamics code with N-body code.

In these proceedings, we consider simulations of the first type, i.e. a system made of particles which interact only though gravitation. However, we focus on the statistical properties of the evolution of infinite gravitating systems due to gravity alone. For this reason, we study in details the simplest example of an infinite gravitating systems: a set of points placed at random in a cubic volume with periodic boundary conditions. Particles have the same mass, and usually no initial velocity. No cosmological expansion is included in the model, since it introduces further dynamical aspects in the evolution (which also depend on the choice of cosmological parameters), that we intend to study separately.

We consider this system a prototype model, a simple system which can give interesting indications for the understanding of more complex and realistic systems.

Static and expanding gravitating systems are expected to show similarities as well as differences. In particular, it is interesting to discuss wheter statistical properties which have been found to be "universal", i.e. the same in systems with different initial conditions, in the expanding case, still retain their universality in gravitating systems without expansion. A well known example of such properties is the density profile of virialised clusters (Navarro, Frenk & White 1997).

We study the properties of such system through an extensive series of accurate N-body simulations. Our code has been parallelised using the OMP paradigm to achieve a larger numerical accuracy. We show and discuss the perfomances of our code on the ORIGIN 3800 hosted at CINECA.

2. The model

We study in details the dynamical evolution of infinite gravitating systems in a very simple model, in which N particles with equal mass are placed at random in a cubic volume. To mimic the effect of an infinite system, periodic boundary conditions are used both for the motion and for the force. Therefore a particle actually feels the force due both to the particles in the cubic volume and to their infinite replicas. This is accomplished by the use of Ewald formula, a standard prescription to implement periodic boundary conditions in electrostatics, which has been used in simulations of gravitating systems since the work of Hernquist et al. (1991). Thus, the system is in fact infinite, since it is periodic; however, at variance with realistic infinite systems, the number of degrees of freedom is actually finite, and finite size effects can affect the results. To cope with this, we study systems with different number of particles N, keeping the mass and number density constant. This allows to study the properties of the system in the "thermodynamic limit"(see e.g. Bottaccio et al. 2002).

We consider both models where initial velocities of particles are zero and models where they are gaussian distributed, with given velocity dispersion σ. The latter case is particularly suited for the study of phase transitions in a gravitating gas. This is not an easy topic to investigate by the standard thermodynamics because of the long range nature of the potential (Padmanabhan 1990).

No cosmological expansion is included in the model. However, the absence of cosmological expansion raises theoretical issues which are worth to be addressed briefly. First of all, expansion allows an infinite gravitating system to be stable, while it is well known that a non-expanding universe is unstable (see e.g. Peebles 1980). In our model, stability is artificially ensured by periodic boundary conditions, which prevent the system from collapsing on its center of mass. Since we are studying a prototype model, realism is not a central issue.

From the physical point of view, it is interesting to discuss other differences between a system with and without cosmological expansion.

- The most immediate consequence is related to the typical times for structure formation. Structure formation proceeds exponentially fast without expansion, but it is slowed down by expansion, which counters gravitational collapse. As a reference, in a universe with $\Omega_{om} = 1$, $\Omega_{o\Lambda} = 0$ structure formation rate is a power law in first approximation.
- stability of structures: in the expanding scenario, one can formulate a stable clustering hypothesis, i.e. for a structure with appropriate physical properties the Hubble expansion can balance exactly gravitational collapse, so that the structure is stable. In the absence of expansion, on the other hand, structures can only stabilise via an effective pressure due to internal velocity dispersion.
- Another interesting question is related to the definition of the potential in a non-expanding infinite system with respect to an expanding one. It is well known that, contrary to the expanding case, the potential is ill-defined. Usually, the arbitrary constant is such that the potential energy in a point is the work required to take the particle far from any other. In an infinite system such energy is of course infinite. However, it is easy to show that the *force* acting on a particle in such systems is (conditionally) convergent, as well as in the expanding case, under quite general conditions for the spatial distribution of particles. Therefore in such cases, the differences of potentials between two points in the system are also well defined. For this reason, the definition of the arbitrary constant for the gravitational potential is not relevant for the dynamics (Bottaccio 2001).

3. Numerical codes

We follow the evolution of the system by means of N-body simulations. The long range nature of the gravitational potential and its short range divergence conjure up to require a careful implementation of the numerical techniques involved. The long range nature implies that an exact forces evaluation among N 'particles' needs an amount of computation $O(N^2)$. When a large number of particles is required (of the order of $N > 10^4$), as in our case and in most cosmological and astrophysical simulation, efficient and faster methods for approximate force evaluation are needed.

For this reason, in our code we chose to employ a 'tree' algorithm (see Barnes & Hut 1986; Hernquist 1987; Miocchi & Capuzzo Dolcetta 2002), which speeds up the force evaluation by means of a hierarchical and recursive subdivision of the space occupied by the system into cubic boxes. Each box is subdivided into 8 cubic boxes beginning from a given cube (the 'root' box) that contains all the system and stopping at boxes with only one particle inside. Various multipolar coefficients related to the potential produced by the particles within a box are evaluated and properly stored for each box. This is done in the 'tree-construction' stage. The logical scheme of such a structure corresponds to an octal tree graph, which the name of the algorithm comes from.

Then, in the 'tree-walking' stage, the force evaluation on each particle is performed using a multipolar expansion (truncated at the quadrupole moment) of the potential produced by the set of particles contained into sufficiently distant boxes, while for those within closer boxes a direct summation is used (the distance is checked according to the 'open-angle' parameter). In this way the computational time scaling reduces significantly from $O(N^2)$ to $O(NlogN)$.

The code integrates the equations of motion using an improved second order *leap-frog* algorithm with individual and variable time-steps. These features are needed in order to take into account the presence of a wide set of time scales, typical of astrophysical self-gravitating systems that are subject to the gravothermal collapse which, in turn, leads to very non-homogeneous density distributions. Moreover, the important evolutive role played by 2-body collisions (and even by higher order collisions) requires very accurate time-integration for close encounters as well. In practice, the time integrator has to be flexible enough to integrate carefully close encounters while saving computational time on "soft" collisions. Indeed, in our code the time steps of the i-th particle is determined by evaluating a time τ according to its cinematic properties computed in its first-neighbour's reference frame. Then the particle time step is $\Delta t_i = \Delta t/2^b$, with b positive integer such that Δt_i is as close as possible to τ. Δt is a fixed small fraction of the dynamical time, i.e. the time scale of the 'global' evolution of the system (driven by mean-field potential). This scheme —the block-time method firstly proposed by Aarseth (1985)— was furtherly improved by ensuring the local third order accuracy, even during the change of the particle time step (when time simmetry is lost). Further details can be found in Miocchi & Capuzzo Dolcetta (2002).

The short range divergence of the gravitational interaction would also imply, in principle, that arbitrarily close encounters could give rise to arbitrarily large accelerations. By consequence, this would require a vanishing time step in the integration of the particle motion. However, very close encounters are quite rare and not very relevant for the purposes of our statistical study, as we have explicitely checked. Therefore we have chosen to "smooth" the potential at scales smaller than an appropriate smoothing length (determined by the smaller time step that the code is able to use a priori), by means of a β-spline function, as in Hernquist (1987).

Moreover, a suitable way to evaluate forces with periodical boundary conditions (see Hernquist et al. 1991) has been implemented employing the Ewald summation formula (Ewald 1921). This required the development of a separate code to produce a table of values for the computation of long-range forces, and of a few subroutines to handle these values properly and consistently.

4. Parallelisation of the code

The parallelisation of codes devoted to the study of self-gravitating systems, is intrinsecally much more difficult than for other problems in computational physics, because of the long range nature of the interaction and of the presence of very different time scales. Since each particle in principle interacts with each other, each processor must communicate the positions of the particles it holds in its memory to *any* other processor involved in the simulation. Thus, the amount of communications between processors can seriously affect the efficiency of the parallelisation. Therefore, the architecture of the parallel computer is a relevant feature to be considered, together with algorithmic aspects. We have put in evidence such difficulties in Pietronero et al. (2002), where we describe our attempt to run N-body simulations of gravitating systems on CRAY T3E at Cineca, with a code written using PGHPF directives for parallelisation. In that case we succeded to run simulations up to 64^3 for short times. We identified the physically distributed memory architecture of the machine, as the main source of CPU-time overhead.

We have therefore tried to overcome these obstacles by running the simulations on a parallel machine with memory phys-

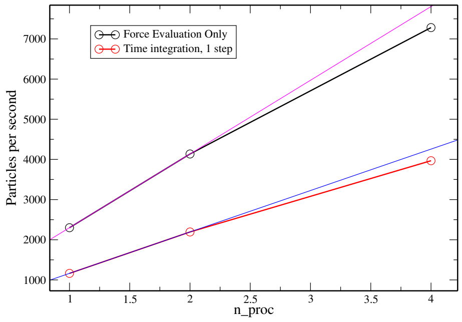

Fig. 1. Efficiency of the code in particles per second vs. the number of processors for 1 timestep (red line) and for force computation only (black line), compared to a linear behaviour (magenta and blue lines) in a simulation with 64^3 particles.

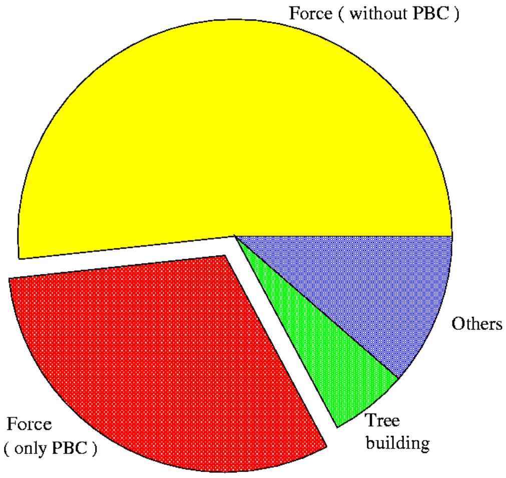

Fig. 2. Use of Cpu time in 1 step of time integration. The evaluation of the force (yellow + red) accounts for 82.8% of the time, 31.1% (red) is due to periodic boundary conditions. Tree-building (green), initialization, time integration and load unbalancing only take 17.2% of time.

ically shared among processors. In such a way, the communication overhead becomes actually negligible, and there is no need for time consuming algorithmic solutions, which aim at distributing the computational domain such to minimize data exchange among processors. The machine we use is a SGI Origin3800, hosted at Cineca, with 128 processors RISC14000, grouped in nodes of four processors each. Such nodes have a physically shared memory.

5. Performances (OMP)

The performances of the code on this machine are illustrated in figs. 1, 2. The tests have been performed on simulations with 64^3 particles. In fig. 1 we show the efficiency

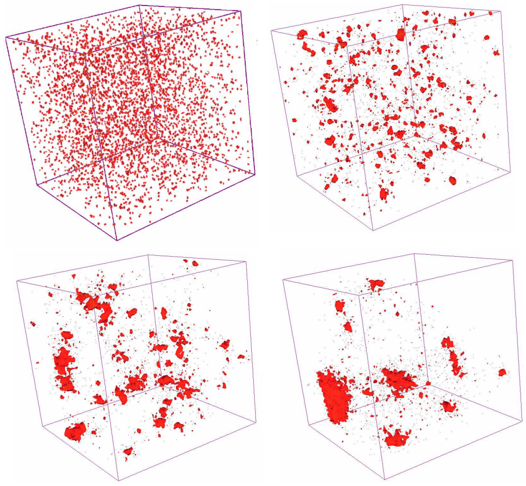

Fig. 3. Evolution of structures in simulation of the model described in sec. 2 with 64^3 particles. Structures are identified by isodensity contours. Time flows from left to right and from top to bottom. Small structures merge to form larger ones, in a way which is fairly independent on the actual number of particles used, until very few large structures are left.

of the code in particles per second, i.e. the number of particles which are evolved in one second, versus the number of processors for force computation only (black) and the whole integration of one time step (red), compared to the "ideal" linear behaviour. The number of particles per second *per processor* is of approximately 2200 for 1 processor and 7200 for 4 processors. Therefore the overall speed up (the gain in computational velocity) with four processors is ≈ 3.3. We consider this result quite good, since it is not so far from ideal optimal speed up of 4.

The pie chart in fig. 2 illustrates the relative time consumption for different sections of the code, during the integration of one time step. It is interesting to put in evidence that the amount of time spent for force evaluation ($\approx 83\%$ of the total!), is by far the most time consuming part of the code. In particular, a relevant part of this time (31,1%) is due to the inclusion of periodic boundary conditions in force evaluation.

Other specific features of the model we study which affect the total computational time are:

- zero initial velocities: very 'collisional' regime at the beginning of the evolution, that implies very short time steps at early times;
- rather small smoothing lengths: great chance of close encounters;
- no cosmological expansion (which slows down the dynamics);
- integration up to asymptotic times.

With this code we were able to run a simulation with 112^3 particles for several dynamical times (approx 10000 CPU hours).

6. Static and expanding gravitating systems: similarities in selected statistical properties

As we have mentioned in the previous sections, static and expanding gravitating systems are expected to show similarities as well as differences. In particular, it is interesting to discuss whether statistical properties which have been found to be "universal", i.e. the same in systems with different initial conditions, in the expanding case, still retain their universality in gravitating systems without expansion. A well known example of such properties is the density profile of virialised halos. Navarro, Frenk & White (1997) have been the first to show by N-body simulations that such profiles where well fitted by a single functional form in a variety of simulations with very different choice of initial particle distributions and cosmological parameters. They have therefore suggested the existence of a universal density profile of the kind:

$$\rho(r) = \frac{A}{(r/r_s)^{\alpha}(1+r/r_s)^{2-\alpha}} \qquad (1)$$

with $\alpha = 1$, where A is a constant depending on the central density of the halo, and r_s is a scale radius. The existence of universal density profiles is an intriguing issue, although it had been recently debated both for the exact value of α (e.g. Fukushige & Makino 2001), and for the universality itself Jing & Suto (2000).

In the present work we investigate whether and to which extent such universality is preserved in non expanding systems. This can be helpful in estabilishing the *minimal requirements* for a model which tries to explain the emergence of such universality. Only few attempts have been done in this direction even in the cosmological context. Assuming the ratio between mass density and velocity dispersion is a power law, Taylor & Navarro (2001) have shown hydrostatic equilibrium is satisfied by a family of density profiles which includes a profile of the kind of eq.1. They also argue that a key element in the formation of such profile is the repeated merging of smaller clusters at earlier time, which eventually give raise to the final cluster. Although partially speculative, this suggestion would explain why the universal profile is not found in simulations of isolated systems; actually in this case the dynamics is dominated by the collapse onto the center of mass rather than by repeated merging.

We compare some statistical quantities measured both in our simulations and in cosmological ones. In particular we refer to the analysis of simulations where initial conditions are similar to ours. To make the comparison, we rescaled the spatial scales, since the unit length is different.

In fig. 4 we compare the density profile $\rho(r)$ of a virialised cluster in different simulations. Our simulation has $N = 112^3$ particles, while we refer for the cosmological ones to the data from Crone et al. (1994) ($N = 64^3$) and Navarro, Frenk & White (1997) (halos extracted from a simulation with 10^6 particles, then risimulated with a higher mass resolution.). There is a substantial agreement at large scales (and of course with the formula in Fukushige & Makino 2001), which implies that expansion has little or no influence on those scales. On small scales, instead, $\rho(r)$ is considerably different: our profile is shallower and its amplitude is smaller than in the cosmological simulations. The reason for such difference is still not clear, but it could be due to the expansion.

Actually, the total number of particles N appears to be not relevant, since cosmological simulations with larger and smaller N have similar $\rho(r)$, but very different from ours.

A different comparison between static and expanding systems can be performed by looking at two-point correlations. The study of the evolution of correlations in the system provides a quantitative way to describe the features of structure formation. Therefore it plays a key role in testing theoretical models. In fig. 5 we compare the measure of two-point autocorrelation function $\xi(r)$ in an expanding system (data taken from Weinberg & Cole (1992); Suginohara et al. (1991)) and in one of our simulations. The three systems have the same initial conditions (apart from the velocity distribution) and the same number of particles ($N = 64^3$).

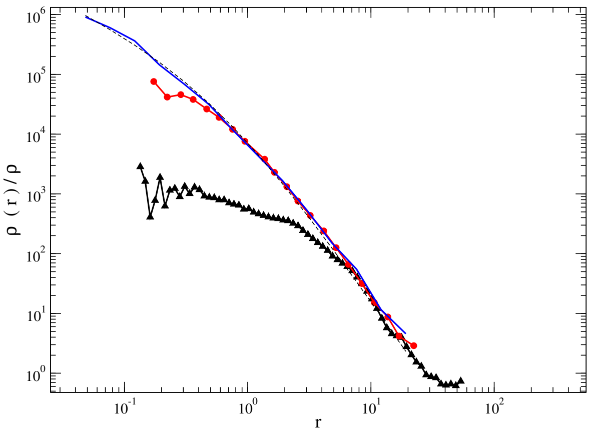

Fig. 4. Density profile $\rho(r)$ of a virialised cluster in expanding (red and blu lines) and non-expanding systems (black line) with similar initial conditions for particles. The black line with filled triangles refers to one of our simulations with $N = 112$ particles and smoothing length $\epsilon = 0.028$. The red line with filled circles refers to data from a simulation by Crone et al. (1994), with $N = 64^3$ particles, smoothing length $\epsilon \approx 0.25$, $\Omega = 1$. The red line with filled circles refers to data from a simulation by Navarro, Frenk & White (1997) (the halo is resimulated from a simulation with $N = 10^6$ particles), smoothing length $\epsilon = 0.077$, $\Omega = 1$. The dashed line is the expression in eq. 1

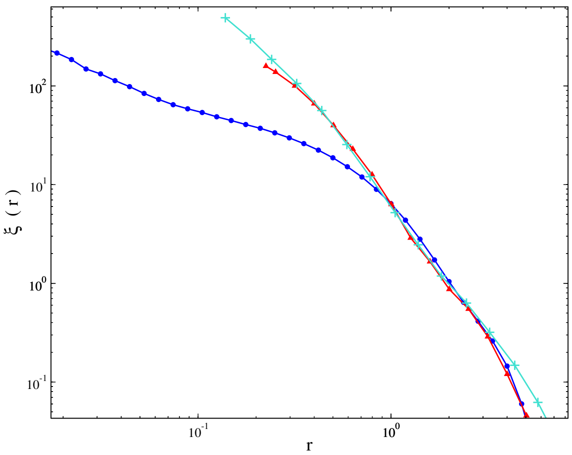

Fig. 5. Comparison between the two-point correlation function $\xi(r)$ in expanding and non-expanding systems with $N = 64^3$ particles. The red line with filled triangles refers to the simulations by Weinberg & Cole (1992). The turquoise line with pluses reports data from Suginohara et al. (1991), with smoothing length (in the current length units) $\epsilon = 0.05$. The blu line with filled circles refers to one of our simulations (it is the only without expansion of the three shown) with smoothing length $\epsilon = 0.028$.

The length scales of the expanding system are rescaled to match the non-expanding one. The agreement between the three measures is good at large scales. At small scales, however, $\xi(r)$ for the non expanding system is smaller and shallower, in a similar way as $\rho(r)$

It is well known that if a system is mainly made of clusters with density profile $\rho(r)$ and typical radius r_S, $\xi(r)$ is determined by $\rho(r)$ on scales $r \leq r_S$ (e.g. Scoccimarro et al. 2001). Therefore the measures shown in fig. 5 are consistent. The difference at small scales we observe in $\rho(r)$ and $\xi(r)$ should not be due to the value of the smoothing length. Actually, it has been observed that larger smoothing lengths give raise to shallower profile $\rho(r)$ (e.g. Crone et al. 1994). Here the data show a shallower $\rho(r)$ having a smaller smoothing length than the cosmological simulations.

7. Conclusions

In this paper, we report the performances of our parallel code for N-body simulations on SGI Origin 3800 at CINECA.

We put in evidence that the parallelisation is quite good and the total overhead is small. The performances of the code look similar to other codes presented in these proceedings (Valdarnini 2002). The most time consuming part, however, is still the force computation; taking into account periodic boundary conditions in such computation represents a large fraction of the time spent. Using the parallel code, we run a 112^3 particle simulation for several dynamical times, together with a numer of smaller simulations performed on serial computers.

We compare the results of our N-body simulations with standard cosmological simulations. Our system differs from the cosmological one because there are no cosmological expansion no initial velocities.

We observe that at small scales the density profile $\rho(r)$ of virialised haloes ad the two point correlation function $\xi(r)$ have smaller amplitude and are shallower. At larger scales, instead, all the simulations give comparable results. The difference at small scales does not depend on the total number of particles N, since we compare with cosmological simulations with smaller and larger N. Moreover, this difference should not be due to the value of the smoothing length; in fact, it has been noted (e.g. Crone et al. 1994) that smaller smoothing lengths as ours should give steeper profiles, while we observe the opposite. An interesting possibility is that such difference is due to cosmological expansion, which is absent in our case.

Acknowledgements. M.B. and M.M. thank INFM-SMC for financial suppport. The simulations were perfomed thanks to INFM grant for Parallel Computing. Fig. 1 was created by AstroMD visualisation tool (www.cineca.it/astromd/)

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