Parallelization of a Code for the Simulation of Self-gravitating Systems in Astrophysics. Preliminary Speed-up Results.

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Received: accepted
ABSTRACT

We have preliminary results on the parallelization of a Tree-Code for evaluating gravitational forces in N-body astrophysical systems. For our T3D CRAFT implementation, we have obtained an encouraging speed-up behavior, which reaches a value of 37 with 64 processor elements (PEs). According to the Amdahl’law, this means that about 99% of the code is actually parallelized. The speed-up tests regarded the evaluation of the forces among \( N = 130,369 \) particles distributed scaling the actual distribution of a sample of galaxies seen in the Northern sky hemisphere. Parallelization of the time integration of the trajectories, which has not yet been taken into account, is both easier to implement and not as fundamental.
1. Introduction and Scientifical Motivations

Super computers are allowing a rapid development of numerical simulations of large $N$–body systems in Astrophysics. These systems are generally composed by both collisionless matter (such as: stars, galaxies, ...) and collisional matter (i.e. gas). Both phases are usually characterized by being self–gravitating, that is the dynamics of the bodies (stars or fluid elements) is strongly influenced by the gravitational field produced by the bodies themselves.

This self–influence is what makes the evaluation of the long–range gravitational force the heaviest computational task to perform in a dynamical simulation. In fact, the number of terms which has to be considered in a direct and trivial evaluation of all the interactions between bodies grows like $N^2$, and since many astrophysically realistic simulations require very large $N$ (greater than $10^5$), such a direct numerical evaluation seems hard to face with presently available computers.

To overcome this problem various approximate techniques to compute gravitational interactions have been proposed. Among them, the Tree–code algorithm proposed by Barnes & Hut\(^1\) is now widely used in Astrophysics because it does not require any spatial fixed grid (like, for example, methods based on the solution of Poisson’s equation). This makes it particularly suitable to follow very inhomogeneous and variable (in time) situations, typical of self–gravitating systems out of equilibrium. In fact its intrinsic capability to give a rapid evaluation of forces allows spending more CPU-time to follow fast dynamical evolution, in contrast to other higher accuracy methods that are more suitable for other physical situations, e.g. dynamics of polar

\(^1\) Barnes J., Hut P. “A hierachical $O(N \log N)$ force calculation algorithm”. *Nature*, vol. 324, p. 446 (1986).
fluids, where the Coulomb term is present.

With the help of the parallelization of our codes, we intend to increase by one or two order of magnitude the number of particles we can use to represent physical systems, in respect to that generally adopted on serial computers ($\sim 10^4$). In particular our first scientifical aim is the study of close encounters between massive black holes and globular clusters. These latter are systems formed by more than $10^5$ stars gravitationally bounded in a spherical peaked distribution. Such a problem is important in the effort to understand better the nature and formation mechanisms of the Active Galactic Nuclei. We hope parallelization makes possible to represent each star with a single particle, in a one-to-one correspondence. This fact clearly will make simulations much more physically meaningful.

2. The Tree–code

We built our own serial implementation of the Tree–code. We give here only a very brief description of the algorithm.

First, the entire system of particles (which can represent stars, single galaxies as well as fluid elements of a gaseous self-gravitating phase) is enclosed in a cubic box (the “root” box). This box is then subdivided into eight sub-cells of half size. The subdivision continues recursively for each of these sub-cells until one obtains cells with

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2 Capuzzo-Dolcetta R., Miocchi P., “Galactic Nuclei Activity Sustained by Globular Cluster Mass Accretion”, PaSS (1998) in press.

3 For more details see Miocchi, P. “Costruzione di un codice numerico per lo studio della dinamica e idrodinamica di sistemi auto–gravitanti in Astrofisica”, Graduation Thesis, Univ. of L’Aquila (1994).
only one particle inside (called terminal cells). In this way the subdivision is *locally* as refined as the particle density is high. Moreover empty cell are not subdivided further.

Then, for each box various multipolar coefficients (total mass, position of the center of mass, quadrupole mass tensor, and so on) are calculated. They will be useful to evaluate the gravitational field that the box produces on a particle. Such coefficients, plus other useful data, are stored into pointed arrays which are structured as a *tree* graph: the root box points to its non-empty sub-cells, which point to their non-empty sub-sub-cells and so on; terminal boxes are the “leaves” in this tree structure. We refer to the above steps as the ‘Tree-setting’ phase. Furthermore, we say that the root box is at the level 0 of subdivision, its sub-cells are at level 1, and so on.

In the ‘Force-evaluation’ phase, for each particle one considers all the cells previously found, “ascending” the tree structure, starting from the root cell, in the following way: given a cell, if it is sufficiently distant from the particle, then the field at the particle position is evaluated by means of a truncated multipolar expansion (using the coefficients stored for this cell in the previous phase). Otherwise one “opens” the cell, passes to the next subdivision level and considers its sub-cells. The field produced by terminal cells are evaluated just by summing directly the contribution due to the particle contained there.

While the direct evaluation of forces scales as $N^2$, in the Tree–code the CPU-time requirement scales as $N \log N$, making possible simulations with high $N$. Moreover the main advantage of this *gridless* method is its adaptability to any geometrical configuration of the masses and its Lagrangian nature. It is based on a particle representation of the density field, which permits, for example, to calculate easily gravitational self–interaction among the various parts of a fluid, just by representing
its fluid elements with particles as well. This gives the possibility of using Lagrangian methods such as the SPH for simulating hydrodynamical evolution. A disadvantage is the needing to re-execute all the phases previously described at every time-step during the simulation, even if the particles had small displacements.

Recently a new method has been proposed; it is called Fast Multipole Algorithm (FMA). Its CPU-time is claimed to scale as $N$, at least in quasi-homogeneous 2-D particle distributions. Were this linear behavior confirmed in 3-D highly non-uniform cases, the FMA would really be appealing for use in astrophysical simulations. For this reason we compared CPU times of our own serial implementations of an adaptive 3-D FMA and a Tree-code to evaluate gravitational forces among $N$ particles in several (uniform and clumped) spatial configurations. These comparison tests (see [1] and [2]) indicates the Tree-code as faster than the FMA in all the situations considered for $N$ up to $2 \cdot 10^5$. This convinced us to concentrate our efforts in the parallelization of the Tree-code.

3. The Parallelization

Tree-code is difficult to parallelize mainly because the evaluation of all the interactions among bodies is not completely separable into a set of independent tasks. The difficulties are due mainly to the following peculiarities:

1. gravitation is a long-range interaction: inter-processor communications are inevitable;

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4 Monaghan J.J., *ARA&A*, vol. 30, p. 543 (1992)

5 Greengard L., “The Rapid Evaluation of Potential Field in Particle Systems”, PhD Thesis, MIT Press (Cambridge, MA, London, UK) (1987).
2. non-uniform distributions (very frequent in Astrophysics) mean great differences in the amount of contributions to the force on each particle: a good load balancing is hard to be achieved.

Point 2 means that we should perform an appropriate domain decomposition among PEs in order to minimize inter-communications. This is generally obtained with a domain subdivision which assigns to PEs domains which are as spatially contiguous as possible. This consideration is particularly important in a message passing context. We will face with this kind of parallelization in the future. At present we want to exploit the great transfer rate of the T3D/E machines, parallelizing our serial code on the T3D using CRAFT language without caring too much of reaching an optimal data locality. Anyway we must pay attention to point 2 which, in a message passing approach, implies that the domain decomposition should be “weighted” in order to take into account the work load for each PE.

We found that the greatest difficulties in getting good performances are in the Tree-setting phase, in which is not easy to avoid load unbalancing and overhead times due mainly to barriers and critical regions. In order to eliminate such synchronization “bottlenecks” we adopted the following scheme:

1. All PEs work together to build the tree data and pointers structure starting from the root and up to a certain level of subdivision, say $L$. This is the lowest level such that the number of non-empty cells found (they have size $l/2^L$, being $l$ the root cell size) is greater than $kp$, with $p$ the number of PEs and $k > 1$ a coefficient. In this phase we have reached a well balanced work load, exploiting the fact that the maximum number of non-empty cells at the level $L$, about $8^L$, is not too large from the point of view of the memory occupation. This cannot be done for the complete tree structure because, in general, astrophysical
distributions are very clumped and one can easily reach more than 10 levels of subdivisions, which means to have, at least in principle, more than $8^{10}$ possible cells with their corresponding memory locations! We won’t give here further details on this argument, anyway the interested reader can find some explications in [3].

2. At this point, a work distribution is performed by means of do-shared loops distributed on the cells of level $L$. In this way each PE works *independently* on its cells and it builds, for them and all their descendants, the related tree structure. In this phase, the work load for a PE exploring a cell, is determined by the total number of non-empty descendants it finds. Thus, load balancing is guaranteed by fixing $k$ high enough such that every PE has a total work load which is constant and equal to all other PEs, apart from statistical fluctuations (see next section).

In order to make a good distribution not only of the work but also of the data, the vectors and the various arrays which reproduce the tree data structure into the memory, have to be shared. This means that, since each PE which is working on its cells has to update frequently such shared arrays, in order to avoid race conditions one should use *atomic updating* or even critical regions. This would give a very bad speed-up, as we verified. Thus we prefer to use an alternative approach which we can call “double passing”.

In such a scheme, in the first passage all PEs explore their cells as they should stored and updating arrays, but without doing it. They just find how many locations they use in these arrays. Then they subdivide arrays and vectors into segments, such that each PE will use exclusively its own segment. Obviously, the PEs have to communicate one each other the respective boundaries of the array segments used,
but this is done only once. Then, in the second passage, each PE repeats the scanning of the cells storing proper data and pointers only on its own memory locations. This permits to avoid any atomic updating of shared pointers, race conditions, critical regions, and so on.

4. Results and Future Prospects

To test the speed-up of our parallelized code, we distributed $N = 130,329$ particles scaling the density distribution of a sample of galaxies in the Northern galactic hemisphere (see Fig.1), taken from the Leda catalog\(^6\). As one can see, this is a very clumped distribution which constitutes a good benchmark for a test of the code.

Moreover, we fixed $k = 30$ and the ‘tolerance’ parameter $a = 0.7$ in the force calculation. This latter parameter regards the criterion to establish whether or not in the Force-evaluation phase, a cell is ‘sufficiently distant’ from a particle, as we have described.

In Fig.2 we show the speed-up results obtained on the T3D. We give the total speed-up, that regarding the Tree-setting and that regarding the Force-evaluation. The curves in Fig.2 confirm the Tree-setting as the most difficult part of the algorithm to be well parallelized, while the Force-evaluation speed-up has a very good behavior in spite of the fact it uses intensively remote reading. In fact, this latter phase has

\(^6\) Di Nella M., Paturel G., *Comptes Rendue de l’Acad. des Sciences de Paris*, Sec. II, t319, p. 57 (Paris, FR, 1994).
been trivially parallelized distributing work among PEs, by means of a do-shared loop on the particles. Each PE calls its private subroutine to evaluate the force acting on its own particles. To do this it has to read the data of the various cells which are stored, in general, in the memory of another PE.

In Fig. 3 the work load distribution is shown for the run with 8 processors, during both phases. The work load has been normalized to the average over all PEs. For the Tree-setting phase it has been calculated as proportional to the total number

Fig. 1.— *Observed distribution of a sample of galaxies in the sky Northern hemisphere (Leda catalog). The axes units correspond to about 80 Mpc.*
Fig. 2.— Measured speed-up for the Tree-setting phase (blue), the Force-evaluation phase (green) and total (red). The test refers to the evaluation of gravitational forces among $N = 130,139$ particles (see text).

of non-empty descendants each PE finds starting from its own cells at the level $L$. In the Force-evaluation phase it has been deduced from the total number of force contributions each PE has to sum in considering all the particles in its domain. Note how load balancing is very good for this latter phase, while for the Tree-setting there are differences among PEs work load which, in any case, do not exceed the 20% of the average.

To conclude, the results are rather good: the total speed-up is high enough and it does not show any flattening, at least for $p \leq 64$. According to the Amdahl’s law, this indicates that the effective parallelized portion of the code (whose CPU-time
Fig. 3.— Normalized work load distribution over 8 processors in both phases: Tree-setting (red) and Force-evaluation (green).

scales like $1/p$) is about 99% of the total. One has to consider also that for $p > 16$ the amount of particles per processor is not that high (less than 5,000). We think that using more particles we would get even better results. This drives us to extend the parallelization also to the time integration of particles trajectories and to the SPH routines for the numerical simulation of hydrodynamics of a self-gravitating fluid. In any case these latter goals are quite easier to be reached than that of the proper parallelization of the Tree-code we have done here.

5. Acknowledgments

This work has been supported by the grant k90rmzz1 at the CINECA Supercomputing center (Bologna, Italy). We thank warmly dr. M. Voli (CINECA) for his valuable help and suggestions and dr. M. Montuori (Univ. “La Sapienza”) for
giving us the data sample of galaxies positions.
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This manuscript was prepared with the AAS LaTEX macros v4.0.