

# Performance characteristics of a parallel treecode

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**Abstract.** I describe here the performances of a parallel treecode with individual particle timesteps. The code is based on the Barnes-Hut algorithm and runs cosmological N-body simulations on parallel machines with a distributed memory architecture using the MPI message passing library. For a configuration with a constant number of particles per processor the scalability of the code has been tested up to  $P = 32$  processors. The average CPU time per processor necessary for solving the gravitational interactions is within  $\sim 10\%$  of that expected from the ideal scaling relation. The load balancing efficiency is high ( $\gtrsim 90\%$ ) if the processor domains are determined every large timestep according to a weighting scheme which takes into account the total particle computational load within the timestep.

**Key words.** Numerical methods – Cosmological simulations – Parallel treecode

## 1. Introduction

Numerical simulations play a fundamental role for improving the theoretical understanding of structure formation. This approach has received a large impulse from the huge growth of computer technology in the last two decades. Cosmological N-body simulations are now widely used as a fundamental tool in modern cosmology for testing viable theories of structure formation. A popular approach for solving the gravitational forces of the system is the tree algorithm (Appel 1985; Hernquist 1987). The particle distribution of the system is arranged into a hierarchy of cubes and the force on an individual particle is computed by a summation over the multi-

pole expansion of the cubes. An important point in favor of tree codes is that individual timesteps for all of the particles can be implemented easily, this allows a substantial speed-up of the force evaluation for a clustered distribution.

An important task is the improvement of the dynamic range of the simulations. Large simulation volumes are required for statistical purposes, but at the same time modelling the formation and evolution of each individual galaxy in the simulated volume requires that a realistic simulation should be implemented with  $10^8 \sim 10^9$  particles. This computational task can be efficiently solved if the code is adapted to work on a parallel machine where many processors are linked together with a communication network. This has led a number of

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authors to parallelize treecodes (Salmon 1991; Warren 1994; Dubinski 1996; Davé, Dubinski & Hernquist 1997; Lia & Carraro 2000; Springel, Yoshida & White 2001; Miocchi & Capuzzo-Dolcetta 2002). In this paper I present a parallel implementation of a multistep treecode based on the Barnes-Hut (1986, BH) algorithm. The code is cosmological and uses the MPI message library.

## 2. Parallelization of a treecode

The BH algorithm works by subdividing a root box of size  $L$ , which contains all of the simulation particles, into 8 subvolumes of size  $L/2$ . This procedure is then repeated for each of the subcubes and continues until the remaining cells or nodes are empty or have one particle. After the  $k$ -th iteration the size of the subcubes is  $l_k = L/2^k$ . After the tree construction is complete the multipole moments of the mass distribution inside the cells are computed starting from the smallest cells and proceeding up to the root cell. The moments of the cells are typically approximated up to quadrupole order. For each particle the acceleration is evaluated by summing the contribution of all of the cells and particles which are in an interaction list. The list is constructed starting from the root cell and descending the tree down to a required level of accuracy. At each level a cell of the tree is accepted if it satisfies an accuracy criterion. If the cell fails this criterion then it is opened, the particles contained are added to the interaction list and the accuracy criterion is applied again for the remaining subcells. The following acceptance criterion has been used (Barnes 1994; Dubinski 1996)

$$d > l_k/\theta + \delta, \quad (1)$$

where  $d$  is the distance between the center of mass (c.o.m.) of the cell and the particle position,  $\theta$  is an input parameter that controls the accuracy of the force evaluation, and  $\delta$  is the distance between the cell c.o.m. and its geometrical center.

### 2.1. Domain decomposition

The spatial domains of the processors are determined according to the orthogonal recursion bisection (ORB, Salmon 1991). The computational volume is first cut along the x-axis at a position  $x_c$  such that

$$\sum_{i <} w_i \simeq \sum_{i >} w_i, \quad (2)$$

where the summations are over all of the particles with  $x_i < x_c$  or  $x_i > x_c$  and  $w_i \propto N_{OP}(i)$  is a weight assigned to each particle proportional to the number of floating point operations (i.e. the computational work) which are necessary to compute the particle force.

When the root  $x_c$  has been determined the particles are then exchanged between the processors, until all of the particles with  $x_i < x_c$  belong to the first  $P/2$  processors and those with  $x_i > x_c$  are in the second  $P/2$  processors. The whole procedure is repeated recursively, cycling through the cartesian dimensions, until the total number of subdivisions of the computational volume is  $\log_2 P$  (with this algorithm  $P$  is constrained to be a power of two). At the end of the domain decomposition the subvolumes will enclose a subset of particles with approximately an equal amount of computational work. The calculation of the forces is then approximately load-balanced among all of the processors.

### 2.2. Construction of the local essential tree

A BH tree is constructed by each processor using the particles located in the processor subvolume. However, the local tree does not contain all of the information needed to perform the force calculation for the processor particles. For these particles a subset of cells must be imported from the trees of the other processors according to the opening angle criterion applied to the remote cells. Each processor then receives a set of partial trees which are merged with the local tree to construct a local essential tree

(Dubinski 1996). The new local tree contains all of the information with which the forces of the local particles can be consistently calculated.

The communications between processors of nodes from different trees implies that in order to graft the imported cells onto the processor local trees it is necessary to adopt an efficient addressing scheme for the memory location of the nodes. This is easily obtained if the construction of the local trees starts from a root box of size  $L$ , common to all of the processors. The main advantage is that now the non-empty cells of the local trees have the same position and size in all of the processors. Each cell is then uniquely identified by a set of integers  $\{j_1, j_2, \dots\}$ , with each integer ranging from 0 to 7 which identifies one of the 8 subcells of the parent cell. These integers can be conveniently mapped onto a single integer word of maximum bit length  $3k_{max}$ , where  $k_{max}$  is the maximum subdivision level of the tree. For a 64 bit key  $k_{max} \leq 21$ . This integer word represents the binary key of the cell. When a cell of the tree is requested from a remote processor to construct its local tree, the associated key is sent together with the mass, c.o.m. and multipole moments of the cell. The receiving processor then uses this key to quickly identify the cell location in the local tree and to add the new cell to the local tree. A similar addressing scheme has been implemented, in their version of a parallel treecode, also by Miocchi & Capuzzo-Dolcetta (2002). An efficient construction of the local essential tree is thus obtained as follows.

i) Once the ORB has been completed and each processor has received the particle subset with spatial coordinates within its spatial domains, the local trees are constructed according to BH in each of the processors  $P_k$ , where  $k$  is a processor index ranging from 0 to  $P - 1$ .

ii) The communications between processors can be significantly reduced if one adopts the following criterion to construct the partial trees that will be exchanged between processors. After the local trees

have been constructed, each processor applies the opening angle criterion between the nodes of its local tree and the closest point of the volume of another processor  $P_k$ . The partial tree obtained contains by definition all the nodes of the local processor necessary to evaluate the forces of the particles located in the processor  $P_k$ . This procedure is performed at the same time by each processor for all of the remaining  $P - 1$  processors. At the end, each processor has  $P - 1$  lists of nodes which are necessary for the construction of the local essential trees in the other processors. The processor boundaries are determined during the ORB and are communicated between all of the processors after its completion. Therefore the main advantage of this procedure is that all of the communications between processors necessary for the construction of the local essential trees are performed in a single all-to-all message passing routine. The drawback of this scheme is the memory overhead, because each processor imports from another processor a list of nodes in excess of those effectively needed to perform the force calculation. As a rule of thumb it has been found that for  $\theta = 0.4$  a processor with  $N_p$  particles and  $N_c$  cells imports  $\sim N_p/8 - N_p/4$  particles and  $\sim N_c$  cells. The number of imported nodes is independent of the processor number. The value  $\theta = 0.4$  is a lower limit that guarantees reasonable accuracy in the force evaluation in many simulations. In the communication phase between processors mass and position are imported for each particle, and the mass, c.o.m., quadrupole moment and the binary key are imported for each cell.

The memory required by a single processor to construct the local essential tree is then approximately a factor  $\sim 2$  larger than that used in the implementation of the local tree. This memory requirement can be efficiently managed with dynamic allocation, and is not significantly larger than that required with other schemes used to construct the local essential tree (e.g., Dubinski 1996).

### 2.3. Force calculation

After the construction of the local essential trees has been completed, each processor proceeds asynchronously to calculate up to the quadrupole order the forces of the active particles in its computational volume. The code has incorporated periodic boundary conditions and comoving coordinates. Therefore the forces obtained from the interaction lists of the local essential trees must be corrected to take into account the contribution of the images. (Davé, Dubinski & Hernquist 1997; Springel, Yoshida & White 2001). These correction terms are calculated before the simulation using the Ewald method. The corrections are computed on a cubic mesh of size  $L$  with  $50^3$  grid points and stored in a file. During the force computation a linear interpolation is used to calculate, from the stored values, the correction terms corresponding to the particle positions.

In a cosmological simulation the evaluation of the peculiar forces in the linear regime is subject to large relative errors. This is because for a nearly homogeneous distribution, the net force acting on a particle is the result of the cancellation of the large partial forces determined from the whole mass distribution. From a set of test simulations Davé et al. (1997) found that in the linear regime, when  $\theta = 0.4$  and the cell moments are evaluated up to the quadrupole order, the relative errors in the forces are  $\lesssim 7\%$ . This problem is not present at late epochs, when the clustering of the simulation particles is highly evolved and even for  $\theta \simeq 1$  the relative errors in the forces are small ( $\lesssim 1\%$ ). This imposes in the simulation the necessity of varying  $\theta$  according to the clustering evolution, since the computational cost of evaluating the forces with a small value of  $\theta$  is wasted in the non-linear regime. In this regime the forces can be evaluated with an accuracy as good as that obtained in the linear regime, though using an higher value of  $\theta$ .

After several tests it has been found that a good criterion to control the value

of  $\theta(t)$  is that at any given simulation time  $t$  the energy conservation must be satisfied with a specified level of accuracy. The Lyzer-Irvine equation is

$$a^4 T + aU - \int U da = C, \quad (3)$$

where  $a = a(t)$  is the expansion factor,  $T$  is the kinetic energy of the system,  $U$  is the potential energy and  $C$  is a constant. The accuracy of the integration can be measured by the quantity  $err(t) = |\Delta(C)/\Delta(aU)|$ , where  $\Delta f$  denotes the change of  $f$  with respect its initial value. The time evolution of  $err(t)$  has been analyzed for different test simulations. The cosmological model considered is a flat CDM model, with a vacuum energy density  $\Omega_\Lambda = 0.7$ , matter density parameter  $\Omega_m = 0.3$  and Hubble constant  $h = 0.7$  in units of  $100 Kmsec^{-1} Mpc^{-1}$ . The power spectrum of the density fluctuations has been normalized so that the r.m.s. mass fluctuation in a sphere of radius  $8h^{-1} Mpc$  takes the value  $\sigma_8 = 1$  at the present epoch,  $a(t) = a_{fin} = 11$ . The simulations are run in a  $L = 200h^{-1} Mpc$  comoving box with  $N_p = 84^3$  particles. For a simulation with  $\theta = const = 0.4$  one has  $err(t) \lesssim 10^{-3}$  even in non-linear regimes, when  $a(t)$  approaches its final value. The distribution of the relative root mean square errors in the force components of the particles can be reproduced if during the simulation  $\theta = \theta(t)$  increases with time, provided that its value never exceeds an upper limit implicitly defined for  $\sigma_8 \geq 0.2$  by the constraint

$$\Delta C/\Delta(aU) \leq 0.025/[1 + (0.4/\sigma_8)^3]^{1.7}. \quad (4)$$

An additional constraint sets an upper limit  $\theta \leq 0.9$ . This criterion can therefore be profitably used to constrain the value of  $\theta(t)$  according to the clustering evolution, and at the same time to maintain the relative errors in the forces below a fixed threshold ( $\lesssim 3\%$ ). This allows a substantial increase in the code performances. The computational cost of evaluating the forces depends on  $\theta$  and for the considered runs

at  $a(t) = 11$  it is significantly reduced by a factor 10 to 20 when  $\theta$  is increased from 0.4 to  $\sim 0.9$ .

#### 2.4. Multiple timesteps and particle update

After the force calculation is complete, particle velocities and positions are updated in each processor. In the individual timestep scheme (Hernquist & Katz 1989) the particle timestep of particle  $i$  is defined as  $\Delta t_i = \Delta t_o / 2^{n_i}$ , where  $n_i \geq 0$  is an integer. The particle timesteps are determined according to several criteria. The first is important at early epochs and requires that

$$\Delta t_i \leq \Delta t_{exp} = 0.03 \frac{2}{3} H(t), \quad (5)$$

where  $H(t)$  is the Hubble parameter at the simulation time  $t$ . The other two criteria are

$$\Delta t_i \leq 0.3(\varepsilon_i a^3(t)/g_i)^{1/2} \quad (6)$$

$$\Delta t_i \leq 0.3(\varepsilon_i/v_i), \quad (7)$$

where  $\varepsilon_i$  is the comoving gravitational softening parameter of the particle  $i$ ,  $g_i$  is the peculiar acceleration and  $v_i$  its peculiar velocity. These criteria are similar to those adopted by Davé et al. (1997). At the beginning of the integration  $t = t_{in}$ , the forces are evaluated for all of the particles and their positions are advanced by half of the initial timestep, which is common to all the particles. In this integration scheme the forces are evaluated at later times  $t > t_{in}$  only for those particles for which is necessary to maintain the second-order accuracy of the leapfrog integrator. The particle positions are advanced using the smallest timestep  $\Delta t_{min}$ , as determined by the above constraints. In the parallel implementation, each processor determines the individual particle timesteps and the smallest timestep  $\Delta t_{min}^{(pr)}$  of its particle subset,  $\Delta t_{min}$  is then the smallest of these  $\Delta t_{min}^{(pr)}$  and is used by all the processors.

After that particle positions have been updated, it may happen that a fraction

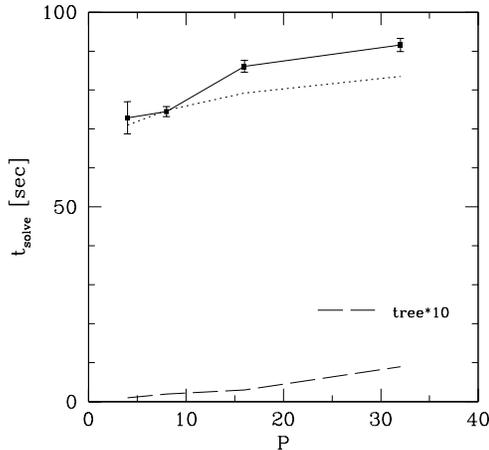
of the particles assigned to a given processor have escaped the processor subvolume. At each timestep the particles that are not located within the original processor boundaries are migrated between the processors. In principle the computational cost of locating the processor to which the escaped particle belongs scales as the processor number  $P$  (Davé et al. 1997, sect. 5.1). However, if during the ORB the processors are partitioned according to the procedure described in sect. 2.1, the final processor ordering makes it possible to reduce to  $\sim \log_2 P$  the number of positional tests of the particle. This is not a significant improvement in pure gravity simulations, where the fraction of particles that leave a processor at each step is small ( $\sim 5\%$ ), but is important in a future implementation of the code that will incorporate smoothed particle hydrodynamic (Davé et al. 1997, Springel et al. 2000). In such a scheme gas properties of a particle are estimated by averaging over a number of neighbors of the particle; in a parallel implementation an efficient location of the particle neighbors located in the other processors is important in order to improve the code performances.

### 3. Performances

The treecode described here uses the BH tree algorithm to compute the gravitational forces. The implementation of this algorithm is identical to that of Dubinski (1996) and Davé et al. (1997). The dependence of the errors in the force evaluations on a number of input parameters has been discussed previously by these authors, therefore an error analysis of the forces will not be presented here.

#### 3.1. Scalability

The computational speed of the code is defined as the particle number divided by the elapsed CPU wall-clock time  $t_{solve}$  spent in the force computation of the particles. For a specified accuracy and particle dis-



**Fig. 1.** The averaged elapsed CPU time  $t_{solve}$  spent in the force evaluation as a function of the number of processors  $P$ . The value of the opening angle parameter is  $\theta = 0.4$ , quadrupole moments are taken into account. The tests have been performed on an IBM SP3 machine, the error bars are the dispersions over the  $P$  processors. The total particle number of a test is  $N_p = 32^3 P$ . The dashed line is the CPU time for constructing the tree scaled up by a factor 10. The initial particle configuration is determined from a uniform distribution perturbed according to a CDM power spectrum (see text). The dashed line is the expected  $t_{solve}$  from the ideal scaling relation  $\propto \log(N_p)$ .

tribution, the CPU time  $t_{solve}$  of a parallel treecode with maximum theoretical efficiency is a fraction  $1/P$  of that of the serial code.

The scalability of the parallel treecode has been tested by measuring  $t_{solve}$  using a different number of processors  $P$ . The initial positions of  $32^3 P$  particles in a  $L = 11.11h^{-1}Mpc$  comoving box have been perturbed according to a CDM model with  $\Omega_m = 1$ ,  $h = 0.5$  and power spectrum normalization  $\sigma_8 = 0.7$  at the present epoch. The value of the opening angle is  $\theta = 0.4$  and forces have been computed at

redshift  $z = 39$ . The number of particles  $N_p = 32^3 P$  scales linearly with  $P$ . This dependence of  $N_p$  on  $P$  has been chosen in order to consistently compare the force solving CPU time  $t_{solve}$  with the one necessary for the construction of the local essential tree. With the choice  $N_p/P = const$  the CPU time  $t_{solve}$  scales ideally as  $t_{id} \propto \log N_p \propto \log P$ . The results are shown in Fig. 1, where  $t_{solve}$  is plotted (continuous line) up to  $P = 32$ . For a configuration of  $P$  processors  $t_{solve}$  is defined as the average of the values of the individual processors. The tests have been performed on an IBM

SP3 machine. The dotted line shows the ideal scaling relation. In the large  $P$  limit  $t_{solve}$  is approximately 10% higher than the ideal scaling relation. This is probably due to cache effects of the machine which arise when  $N_p \gtrsim 10^5$  during the tree descent necessary to calculate the forces. An important result is the time  $t_{tree}$  required to construct the local essential trees. The dashed line of Fig. 1 shows that this time is always a small fraction ( $\lesssim 5\%$ ) of the time required to compute the gravity. It is worth stressing that the communication part is efficiently handled by the all-to-all routine and the corresponding time is a negligible fraction of  $t_{tree}$ . The computational speed is  $\sim 32^3/t_{solve} \sim 500P$  *part/sec*. This is valid for  $\theta = 0.4$ . If  $\theta$  is increased the particle interaction list will have a smaller number of terms and  $t_{solve}$  will be smaller. It has been found that  $t_{solve}(\theta)$  is well approximated by  $t_{solve}(\theta \leq 1) \propto 10^{-5\theta/3}$ . If  $\theta = 1$  the CPU times of Fig. 1 will then be reduced by a factor  $\sim 10$ . A comparison of the code performances with those of other authors is difficult because of different algorithms, particle distributions and machines. An educated guess that the code has performances fairly comparable with those of the Springel et al. code (2000) is given by Fig. 12 of their paper. In this figure the gravity speed as a function of the processor number is shown for a cosmological hydrodynamic SPH simulation in a comoving box size of  $50h^{-1}Mpc$  with  $32^3$  dark matter particles and  $32^3$  gas particles. The cosmology is given by a  $\Lambda$ CDM model with  $\Omega_m = 0.3$  and  $h = 0.7$ . The simulations are evolved from an initial redshift  $z_i = 10$ . The plotted speeds have been measured on a CRAY T3E (300MHz clock). From Fig. 12 the computational speed of gravity for  $P = 32$  is  $\sim 7500$  *part/sec*. The cosmological model is not that adopted in the tests of Fig. 1, but at early redshifts the computational cost of the gravity force calculation is not strongly dependent on the assumed model. For  $P = 32$  and  $\theta = 0.4$  the results of Fig. 1 give a gravity speed of  $\sim 12 \cdot 10^3$  *part/sec* for a CDM model at  $z_i =$

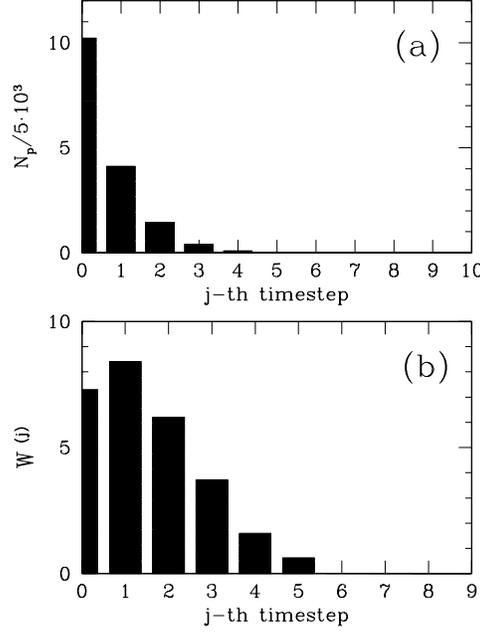
39. The measured speed must be reduced by  $\sim 20\%$  to take into account the higher clock rate of the IBM SP3 (375MHz). The final value ( $\sim 9500$  *part/sec*) is similar to the one obtained by Springel et al. (2000).

### 3.2. Load balancing

An important characteristic of a treecode is load balancing. An ideal code should have the computational work divided evenly between the processors. This is not always possible and code performances will be degraded when the load unbalancing between the processors becomes large. At any point of the code where synchronous communications are necessary there will be  $P - 1$  processors waiting for the most heavily loaded one to complete its computational work. Load balancing can then be measured as

$$L = \frac{1}{P} \sum_p 1 - (t_{max} - t_p)/t_{max}, \quad (8)$$

where  $t_p$  is the CPU time spent by the processor  $p$  to complete a procedure and  $t_{max}$  is the maximum of the times  $t_p$ . A treecode spends most of the CPU time in computing gravitational forces, and so it is essential to have good load balancing ( $\gtrsim 90\%$ ) with the gravity routine. This task is not obviously achieved with a multistep treecode. The number of active particles for which it is necessary to compute the gravitational forces at  $t_n^{(k)}$  varies wildly with the timesteps. The current simulation time  $t_n^{(k)}$  is defined  $k$  steps after  $t_n = n\Delta t_0$  as  $t_n^{(k)} = t_n + \sum_{j=1}^{j=k} \Delta t_j$ , the summation is at  $t > t_n$  over the past timesteps  $\Delta t_j$ . At a certain step the ORB procedure described in sect. 2.1 can be used to obtain load balancing, but at later steps the unbalancing can be substantial. This problem has prompted some authors to consider more complicated approaches (Springel, Yoshida & White 2001; Miocchi & Capuzzo-Dolcetta 2002). Here a simpler route is followed which starts from the observation that in a multistep integration scheme, a better measure of the

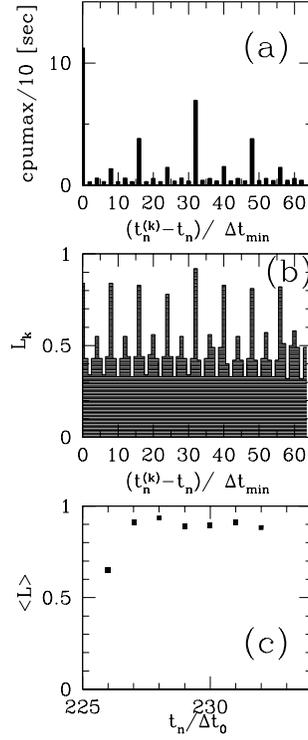


**Fig. 2.** (a): Number of particles with timesteps  $\Delta t_j = \Delta t_0 / 2^j$  at the end of a macrostep  $\Delta t_0$ . The simulation is that of sect. 3 with  $N_p = 2 \cdot 32^3$  particles,  $\Delta t_0 = t_{fin}/424$ ,  $\Delta t_{min} = \Delta t_0/32$ , and simulation time  $t_n = n\Delta t_0 = 225\Delta t_0$ . (b): For the same particle distribution the corresponding computational loads  $W^{(j)} = \sum_{i \in \Delta t_j} W_i$  are shown, the summation is over all the particles  $i$  with timesteps  $\Delta t_j$ . The individual particle weight used in the ORB is  $W_i = \sum_k w_i^{(k)}$ , here  $w_i^{(k)}$  is the single-step particle work at the  $k$ -th step after  $t_n$  and the summation is over the steps between  $t_n$  and  $t_{n+1}$ .

computational work done by each particle  $i$  is given by  $W_i = \sum_k w_i^{(k)}$ , where  $w_i^{(k)} \propto N_{OP}(i)$  is the number of floating point operations of particle  $i$  necessary to calculate the gravitational forces of the particle at the simulation time  $t_n^{(k)}$ . If the particle  $i$  is not active at  $t_n^{(k)}$ ,  $w_i^{(k)} = 0$ . The summation is over the steps between  $t_n$  and  $t_n + \Delta t_0$ , the weights  $W_i$  are now used at each large step  $\Delta t_0$  to subdivide the computational volume according to the ORB procedure. Theoretically this weighting scheme does not guarantee a perfect load balance, nonetheless it has been found

to yield satisfactory results ( $L \gtrsim 90$  %) in many typical applications. The reason lies in the shape of the distribution function  $F(\Delta t_i)$  of the particle timesteps  $\Delta t_i$ , for a simulation with an evolved clustering state. The number of particles with timesteps in the interval  $\Delta t_j, \Delta t_j + \Delta t$  is given by  $n_j = F\Delta t$ . The particle timesteps are determined according to the criteria defined in sect. 2.4; another parameter which determines the shape of the distribution function is the minimum timestep  $\Delta t_{min}$ .

The optimal choice for  $\Delta t_{min}$  requires that the number of particles of the binned distribution  $n_j$  in the last time bin should



**Fig. 3.** The load balancing scheme is tested for a parallel run with  $P = 4$  processors. The simulation is that of Fig. 2. **(a):** The top panel shows, between  $t_n$  and  $t_{n+1}$ , the maximum of the CPU times of the  $P$  processors at the simulation time  $t_n^{(k)}$ ,  $n = 225$ . The corresponding load balancing  $L_k$  is plotted in the mid panel **(b)**. The bottom panel shows the load balancing at the end of each macrostep  $\Delta t_0$ . The goodness of the weighting scheme is shown by the first point, where the ORB procedure has been performed setting  $w_i = \text{const.}$

be a small fraction of the total particle number ( $N_{opt} \sim 10\% N_p$ ). The distribution  $n_j$  of a test simulation is shown as a function of the particle timesteps  $\Delta t_j$  in Fig. 2a at the end of a large timestep  $\Delta t_0$ , when the particle positions are synchronized. The simulation is that of sect. 3.1 with  $N_p = 2 \cdot 32^3$  particles,  $\Delta t_0 = t_{fin}/424$ ,  $\Delta t_{min} = \Delta t_0/32$  and simulation time  $t_n = n \Delta t_0 = 225 \Delta t_0$ .

The corresponding distribution of particle computational loads  $W_i$  is shown in panel (b). The plotted distribution is  $W^{(j)} = \sum_{i \in \Delta t_j} W_i$ , the summation being over all of the particles  $i$  with timesteps

$\Delta t_j$ . About  $\sim 90\%$  of the particles are in the first three time bins, it can be seen that for these bins the variations in the load distribution are within  $\sim 20\%$ . For example the number of particles  $n_j$  with timestep  $\Delta t_3 = \Delta t_0/8$  is  $\sim n_0/10$ . The choice of a simple weighting scheme  $w_i \propto N_{OP}(i)$  would have given a shape of the load distribution similar to that of  $n_j$ . The reason for the shape of the load distribution of Fig. 2b is that in a multistep integration scheme the particle forces are calculated within a large timestep  $\Delta t_0$  when their positions must be synchronized. An optimal choice of the constraints on the

particle timesteps yields a binned distribution  $n_j$  with a hierarchy  $n_{j+1} \sim n_j/2$ . A weighing scheme that sums the number of floating point operations over a large timestep  $\Delta t_0$  takes into account the fact there are few particles with  $\Delta t_j \ll \Delta t_0$  but that these particles have forces calculated a number of times  $\propto \Delta t_j^{-1}$ . This weighting scheme leads, at the end of a large timestep  $\Delta t_0$ , to particle loads with a distribution which can be considered for practical purposes roughly constant for a large fraction of the simulation particles ( $\sim 90\%$ ). An ORB domain decomposition is then applied every large timestep  $\Delta t_0$  according to the calculated weights of the particles. The subdivision of the computational load that follows from this ORB among the processors it is still unbalanced, but within a large timestep  $\Delta t_0$  the unbalancing is higher when the computational work is minimal. This is clearly illustrated in the example of Fig. 3. The simulation of Fig. 2 has been used at the same simulation time, with  $N_p = 2 \cdot 32^3$  particles divided among  $P = 4$  processors. The processor domains have been found as previously discussed. Panel (a) shows the elapsed CPU wall-clock time spent by the parallel code to compute the gravitational forces. The CPU time is plotted between  $t_n$  and  $t_{n+1}$  versus the simulation time  $t_n^{(k)}$  and is the maximum of the single processor values. There is a large burst of CPU work when the particles synchronized at  $t_n^{(k)}$  are those with timesteps  $\Delta t_0$ ,  $\Delta t_0/2$  and  $\Delta t_0/4$ . The instantaneous load balancing  $L_{(k)}$  is calculated using Eq. 8 between  $t_n^{(k)}$  and  $t_n^{(k+1)}$ . It can be seen that  $L_{(k)}$  drops to very inefficient values ( $\lesssim 0.3$ ) when  $t_n^{(k)}$  corresponds to a small number of active particles and it reaches a high efficiency ( $\gtrsim 0.9$ ) with the highest CPU times. The overall load balancing is measured by applying Eq. 8 between every ORB domain decomposition: panel (c) shows  $\langle L \rangle$  versus the simula-

tion time  $t_n$  for ten large timesteps  $\Delta t_0$ . To show how well the method is working the ORB procedure has been performed setting for the first step  $w_i = const$ , yielding  $\langle L \rangle \sim 0.5$ . This proves that the load balancing performances are sensitive to the chosen weighting scheme and that the procedure previously described is optimal to achieve a good load balance for the parallel tree code described here.

Preliminary results show that this weighting scheme for the ORB domain decomposition can still be successfully used to obtain an efficient load balancing ( $\gtrsim 90\%$ ) when the number of processors is higher than that of the tests performed here ( $P = 32$ ). This confirms that the load balancing efficiency of the adopted weighting scheme is robust for a variety of clustering states in cosmological simulations.

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