Parallel P3M with exact calculation of short range forces

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Abstract

A P3M (Particle-Particle, Particle-Mesh) algorithm to compute the gravitational force on a set of particles is described. The gravitational force is computed using Fast Fourier Transforms. This leads to an incorrect force when the distance between two particles is of the order of a grid cell. This incorrect force is subtracted exactly from all particles in parallel using convolution with the appropriate Green's function in real space in a time of order $N_T$, irrespective of the degree of clustering of particles. Next, the correct $1/r^2$ force is added for all neighbouring particles in parallel, leading to an accurate algorithm which runs efficiently on a highly parallel computer. A full force calculation for 128$k$ particles on a 128$^3$ grid in a mildly clustered situation requires approximately 196 seconds on a 8$k$ Connection Machine 2 with 8MHz clock. This decreases to an estimated 9.8 seconds on a full-sized 64$k$ CM200.
1. Introduction

In many fields of computational astronomy it is necessary to compute the gravitational force on a set of massive particles. The optimum algorithm to do this depends on what one wants to learn from the results.

The particle-particle (PP, or direct summation) method (Aarseth [1]) gives the highest accuracy, necessary for simulations where encounters between particles are real and are to be calculated accurately. (Such is the case in for example star cluster simulations.) The method is expensive since computer time \( \tau \) scales rather steeply with particle number \( N_T \): \( \tau \propto N_T^{1.6} \), where the exponent depends somewhat on the actual particle distribution computed upon. The PP scheme can be implemented very efficiently on many computer architectures.

The particle-mesh (PM) method (e.g. Hockney and Eastwood [2], chapter 5) uses a grid to compute interactions between particles in three steps: (1) compute a density distribution on the grid that faithfully represents the density distribution of the particles, (2) solve Poisson’s equation on the grid and compute the associated grid forces and (3) interpolate these forces back to the particles. Operations involving particles occur only in steps (1) and (3) and they scale linearly with \( N_T \). The solution of Poisson’s equation in step (2) is independent of \( N_T \). All three steps require many fewer operations than the PP method and consequently many more particles can be used in a simulation for the same amount of CPU time spent. Unfortunately, this grid-mediated force \( f \) computed between two particles which are only a few grid cells away from each another is inaccurate: it is both anisotropic and not translationally invariant. Consequently, the method is useful when the force on a particle is mainly determined by the smooth density distribution of all other (distant) particles—that part of the force being calculated accurately, and not so much by the irregular distribution of near neighbours (for example the force on a star in a galaxy). The solution of Poisson’s equation in step 2 can be done very efficiently using Fast Fourier Transforms (FFT’s), an algorithm which many computer vendors supply and which runs at near maximum machine speed. The PM method allows for a trivial implementation of periodic boundary conditions. Isolated boundary conditions can also be treated using FFT’s, but at rather a high cost (James [3]).

The particle-particle, particle-mesh (P3M, Hockney and Eastwood [2], chapter 8, Efstathiou et al. [4]) tries to combine the best of both PP and PM methods, namely use FFT’s on a grid to compute forces between distant particles efficiently (PM step) and use direct summation to compute forces between near particles accurately (PP step). Hence, forces are computed in three steps: (1) the PM step, to compute forces between distant particles using FFT’s, (2) a correction step, to subtract the inaccurate PM force for particles close to one another and (3) the PP step, to add the correct \( 1/r^2 \) force between those near neighbours. The correction force subtracted in step 2 is computed as a function of interparticle distance using the Green’s function used to solve Poisson’s equation on the grid. However, the applied correction is not exact since this grid-force is neither isotropic nor translationally invariant which means that the correction is not a function of interparticle distance alone. The Green’s function is smoothed on small scales to decrease the difference between correction term and grid-force in the least squares sense. This algorithm has the advantage over the PM one in that the resolution of the calculation is not limited by the size
of the grid cells, an important factor in simulations where the amount of clustering is not constant in time (e.g. in simulations of large scale structure formation). Both the correction force in step 2 and the PP force in step 3 are calculated on a per pair basis, hence required CPU time scales with $N_b^2$ for both, where $N_b$ is the average number of neighbours to be corrected. This leads to a slowdown of the speed of the program as the amount of clustering increases. This undesirable feature may be partly compensated for by introducing multiple grids (Villumsen [5]).

The hierarchical tree algorithm (Appel [6], Barnes and Hut [7]) groups distant particles and uses a multipole expansion to decrease the number of terms occurring in the calculation of the force on one particle from $N_T$ to $\log N_T$. Forces between neighbouring particles are computed on a particle-particle basis. The algorithm allows the use of individual time-steps which improves its efficiency substantially in some situations. The tree traversal algorithm can be vectorized efficiently on architectures favouring small vectors (Hernquist [8]), however, such codes run rather inefficient on highly parallel computers that require long vectors (Makino and Hut [9]).

In this paper we discuss a P3M implementation that differs on two grounds from the P3M discussed in Efstathiou et al. [4]: (1) the method uses convolution in real space to subtract the grid-mediated force on neighbour particles exactly in a time of order $N_T$, irrespective of the particle distribution and (2) sorts particles in cells to efficiently compute the PP part on a highly parallel computer (in our case on a 8192 nodes Connection Machine 2 (CM2)). Both the PM part, using FFT’s and the PP part, using a scan-copy approach, run very efficiently on the CM2. The convolution part that corrects the short range force is described in section 2. The parallel PP part is described in section 3. Final remarks can be found in section 4. The Appendix describes some properties of the CM2 and in addition gives some optimization and algorithmic design considerations for the operations needed in both the PM and PP calculations.

2. Correcting the short range force

The computation of the grid-mediated interaction consists of the following steps (see e.g. Hockney and Eastwood [2], chapter 5 or Efstathiou et al. [4] for more details): (1) given the distribution of particles, compute the density on the grid, (2) compute the grid potential by convolving the density distribution with the Green’s function and difference it to obtain the grid forces, and (3) interpolate these forces to the particles. In the following we assume that the assignment of mass to the grid and of forces to particles uses cloud-in-cell assignment (i.e. linear interpolation in all three Cartesian directions) but other assignment schemes can be considered as well.

The density $\rho(i,j,k)$ at vertex $(i,j,k)$ of the 3D grid due to particles $n = 1 \ldots N_T$ with masses $m(n)$ and coordinates $(x(n),y(n),z(n))$ is:

$$
\rho(i,j,k) = \frac{1}{V_c} \sum_{n=1}^{N_T} m(n) f(X_i,x(n)) f(Y_j,y(n)) f(Z_k,z(n)),
$$

where we have defined:

$$
f(x,y) = \begin{cases} 
0; & \text{if } |x-y| > c; \\
1 - |x-y|/c, & \text{otherwise.}
\end{cases}
$$
Here, \( c \) is the size of a grid cell, \( V_c = c^3 \) its volume and \((X_i, Y_j, Z_k)\) its Cartesian coordinates. Given this density distribution, one next calculates the potential \( \Phi(i, j, k) \) by convolving \( \rho \) with the Green’s function \( G \):

\[
\Phi(i, j, k) = \sum_{p, q, r} \rho(p, q, r) G(i - p, j - q, k - r). \tag{3}
\]

The convolution in Eq. (3) can be done very efficiently by means of FFT’s. Given the potential \( \Phi \) one needs to compute the forces on the grid. This can be done, for example, using the following centered difference expression:

\[
F_X(i, j, k) = (\Phi(i + 1, j, k) - \Phi(i - 1, j, k))/2c. \tag{4}
\]

Finally, these forces are interpolated back to the particles, using an equation similar to Eq. (1):

\[
F_x(n) = \sum_{i,j,k} F_X(i, j, k) f(X_i, x(n)) f(Y_j, y(n)) f(Z_k, z(n)). \tag{5}
\]

Note that a particle \( n \) receives forces from the eight vertices nearest to it in Eq. (5), just as it contributes mass to only eight vertices in Eq. (1). This completes the calculation of the PM forces.

The force \( F_x(n_1) \) on a particle \( n_1 \) will have a contribution to it from a particle \( n_2 \), say. If the distance between \( n_1 \) and \( n_2 \) is small compared to the cell size \( c \), then this contribution is a poor approximation to the correct force. However, we now show that we can use equations (1)-(5) to compute these inaccurate forces due to particles close to one another. Once the inaccurate interparticle force is subtracted, one can add the correct force on \( n_1 \) due to \( n_2 \). (The latter PP calculation is described in section 3.) It is convenient to subtract forces from particles \( n_2 \) which are either in the same cell as \( n_1 \) or in one of the (26, in 3D) neighbouring cells. The algorithm works for particles any number of cells away from \( n_1 \), but the amount of computer time needed for the subtraction of the inaccurate force and especially for the addition of the correct force in the PP part becomes rapidly prohibitively large.

Assume for the purpose of explanation that the system is one dimensional and number the vertices of the grid \( 1 \cdots N_g \). We will say that a particle is in cell \( i \) if the left vertex of the cell this particle is in, is \( i \). Particles in cell \( i \) receive forces from vertices \( i \) and \( i + 1 \). In turn, the force \( F_X(i) \), on vertex \( i \), depends on the potential on vertices \( i - 1 \) and \( i + 1 \). Since we want to correct the force on vertex \( i \) and \( i + 1 \) due to particles in cells \( i - 1, i \) and \( i + 1 \), we need to calculate the potentials on vertices \( i - 1, \cdots, i + 2 \), due to those particles.

For this purpose, calculate the quantity \( \rho_L(i) \) defined by

\[
\rho_L(i) = \frac{1}{V_c} \sum_{n=1}^{N_T} m(n) g(X_i, x(n)), \tag{6}
\]

where

\[
g(x, y) = \begin{cases} 
0, & \text{if } |x - y| > c, \text{ or } x > y; \\
1 - |x - y|/c, & \text{otherwise}. 
\end{cases} \tag{7}
\]

Comparing Eq. (6) with Eq. (1), it is clear that \( \rho_L(i) \) is the density at vertex \( i \) due to all particles in the cell \( i \) (the left (L) vertex), whereas \( \rho \) (defined by Eq. (1) for the 3D case) is the density at vertex \( i \) due to particles in cells \( i - 1 \) and \( i \). In an analogue way we compute the density \( \rho_R(i) \),
which is the density at vertex $i+1$ due to particles in cell $i$. (Consequently, $\rho(i) = \rho_L(i) + \rho_R(i-1)$.)

Given $\rho_L$ and $\rho_R$, we compute the densities $\rho_{-1}$, $\rho_0$, $\rho_1$ and $\rho_2$ defined by:

\begin{align*}
\rho_{-1}(i) &= \rho_L(i-1) \\
\rho_0(i) &= \rho_R(i-1) + \rho_L(i)(\equiv \rho(i)) \\
\rho_1(i) &= \rho_R(i) + \rho_L(i+1)(\equiv \rho(i+1)) \\
\rho_2(i) &= \rho_R(i+1).
\end{align*}

These densities are the ones that determine the forces in cell $i$ due to particles in cells $i-1$, $i$ and $i+1$. We then use these densities to compute the potentials $\Phi_{-1}(i), \cdots, \Phi_2(i)$ using the convolution in real space:

\[ \Phi_l(i) = \sum_{m=-1}^{2} \rho_m(i)G(l-m), \]

for $l = -1, \cdots, 2$. Note that the convolution (9) contains only four terms whereas the full convolution (3) contains $N_g$ terms (in 1D). $G$ denotes the Green’s function in real space, as before. Finally, we compute the forces $F_{X_L}(i)$ and $F_{X_R}(i)$ as

\begin{align*}
F_{X_L}(i) &= (\Phi_1(i) - \Phi_{-1}(i))/2c \\
F_{X_R}(i) &= (\Phi_2(i) - \Phi_0(i))/2c,
\end{align*}

which are the correction forces to be interpolated to the particles in cell $i$ from the left ($L$) and right ($R$) vertices of cell $i$ respectively.

The forces between two particles, obtained using this procedure, are exactly equal to the forces computed using the PM algorithm if these particles are either in the same or in neighbouring cells. If particles are further away from each other, then these forces are exactly zero.

Our implementation uses circular shifting (see Appendix) of the grid arrays (like e.g. $\rho_L$ and $\rho_R$) in all three Cartesian directions to compute the neighbour forces to subtract. This has the advantage that the same boundary conditions are imposed in PM and correction part if the same grid is used in both parts (i.e. if the FFT computes the forces for periodic boundary conditions, then also the subtraction of neighbour forces will be done as if the system were periodic). The same is true for isolated boundary conditions.

The computational expense of this correction step is not dramatic. In a 3D system, one has to compute corrections from all eight vertices of the cell the given particle is in, hence the force assignment requires the same amount of computation as in the PM part: $\approx 9 \times 3 \times 8 N_T = 216 N_T$ operations. However, for each of these eight vertices one needs to compute corrections due to all eight vertices a particle assigns mass to, i.e., the mass assignment needs to be done eight times more often than in the PM part. (This can be reduced, but then one needs to introduce many more temporary variables to store the grid density for all eight vertices separately, in the 1D example one needs to store $\rho_L$ and $\rho_R$ separately, whereas in the PM part one needs to store only the sum $\rho_L(i) + \rho_R(i-1)$.) Mass assignment takes $\approx 11 \times 8 N_T = 88 N_T$ operations. One convolution like Eq. (9), requires many fewer operations than the PM part: as Eq. (9) shows, one needs to multiply the densities $\rho$ with the central four values of the Green’s function. These parallel statements require computer time scaling linearly with the total number of vertices and in addition are executed at near top speed on a parallel computer since the amount of communication required
to complete them is virtually zero. (The PM convolution Eq. (3) requires of order $21N_g^3\log N_g^3$ operations.) On the other hand, one needs to perform the convolution (9) 1728 times in order to correct for all contributing vertices, thus making this part of the algorithm responsible for most of the CPU time needed for the correction step, notwithstanding the extremely high execution speed with which Eq. (9) is computed (close to 500 MFlops on the 8k CM2). We will show in section 3 that the PP calculation requires a comparable amount of CPU time.

Some timings of the PM and correction algorithm on a 8192 processor CM2 running at 8 MHz are given in Table 1. These timings were obtained using the CM2 vendor supplied timer and are reproducible to within 10%. The CPU time required is given for the mass and force assignments during the PM step (column 3), the FFT step (column 4), the mass assignment and force assignment part in the correction step (column 5), the convolution of Eq. (9) (column 6) and the total calculation (column 7) for the given number of particles $N_T$ ($k$ stands for 1024) and grid vertices $N_g$ (in 1D, i.e. the timed 3D system has $N_g^3$ vertices). The time stated for the FFT part includes the computation of the Green’s function and the extraction of its central region, needed in the convolution part of the correction step, in addition to the actual FFT calculation. We reiterate that all these times are independent of the actual particle distribution.

| $N_T$ | $N_g$ | PM assignments | FFT | Correction assignments | Convolution | Total |
|-------|-------|----------------|-----|------------------------|-------------|-------|
| 8k    | 32    | 0.2            | 0.12| 0.8                    | 1.8         | 3.0   |
| 64k   | 32    | 0.9            | 0.12| 5.5                    | 1.8         | 7.3   |
| 64k   | 64    | 1.4            | 0.93| 6.0                    | 10.8        | 19.1  |
| 64k   | 128   | 6.2            | 7.26| 16.7                   | 73.2        | 103.4 |
| 128k  | 128   | 6.9            | 7.26| 22.1                   | 73.2        | 109.5 |

Figure 1 illustrates the accuracy of the PM force obtained in the way just described. The figure shows the deviation of the radial force, the tangential force and the potential from their Newtonian values for randomly distributed massless test particles in a $16^3$ grid with unit cell size. The forces are due to eight equal mass particles that were also randomly distributed in cell (8,8,8). The truncated Green’s function appropriate for an isolated system was used and the PM FFT calculation was computed on a grid of doubled size (in each direction) to avoid aliasing, as described in Hockney and Eastwood ([2], p. 213). Deviations of the force of order 6% occur up to six cells away, and the force never quite reaches it’s $1/r^2$ behaviour (a deviation $\leq 1\%$ remains). The latter is probably due to differencing errors in obtaining the force from the potential since the potential is more accurate than the force, as Fig. 1 shows.

In summary, the result of the two steps, the PM and the correction step is the following: for two particles $n_1$ and $n_2$ more than two cells apart, the force is computed using the PM algorithm. If these particles are in the same cell or in neighbouring cells, the force between them is exactly zero. In the next section, we describe a parallel algorithm to compute the forces due to these neighbouring particles.
3. Parallel Particle-Particle part

The PP part becomes increasingly time-consuming as the degree of clustering of particles increases and consequently more PP forces need to be computed. Hence it is important that the algorithm deals efficiently with such clustered particle distributions. The algorithm we propose is a variant of that discussed in Theuns and Rathack ([10]), in the context of a parallel SPH (Smoothed Particle Hydrodynamics) implementation. It uses large vectors and a minimum of inter-processor communication to run efficiently on a massively parallel computer like the CM2. In addition, it is written in such a way that densely populated cells interact very efficiently with sparsely populated ones.

Given the basic requirements of the CM2 as discussed in the Appendix, the main idea of the algorithm is to construct two vectors, a Bottom (B) vector and a Top (T) vector, which are organized such that interaction can occur between a particle $B(i)$ and a particle $T(i)$. Such an interaction can be computed very efficiently on a parallel computer since $B(i)$ and $T(i)$ are in the private memory of the same processor. After this calculation, $T$ is reorganized so that $B(i)$ interacts with another particle in $T$ and these two steps are repeated until all interactions have been computed. The task is now to make this reorganization as efficient as possible.

The algorithm we use is different for interactions between particles in the same cell and interactions between particles in neighbouring cells. In the first step, we want to calculate all interactions between a particle and all other particles in the same cell. We do this by loading all particles in $B$ such that particles in the same cell are in consecutive array locations (which we will call `segments`). $T$ starts out as being a copy of $B$ which we CSHIFT by one to the left (see the Appendix which discusses CSHIFT): every particle $B(i)$ has now a (different) particle $T(i)$ above it which is in the same cell and so we can compute their mutual interaction. We then CSHIFT $T$ left one more step and compute another interaction. We repeat the process until all interactions have been computed. Remark that, as the process advances, particles will be shifted into $T$ which do not belong to the same cell as $B(i)$, since not all cells have the same number of particles in them. Consequently, the algorithm becomes less and less efficient in calculating forces as more and more cells have been processed and valid interactions occur in only the most populated cells. Figure 2a illustrates this processing of intra-cell interactions.

Next we describe how to compute interactions between cells. Again we load particles into segments in array $B$. The segments themselves are organized in such a way that particles of two cells that interact are in the same locations in $B$ and $T$, i.e., if a cell is found in locations $B[i_1 : i_n]$ then the particles of a neighbour cell are in locations $T[i_1 : i_m]$. Of the interacting cells, we always send the larger one to $B$, i.e. $n \geq m$. Array $B$ will contain of order $13/2$ times the number of particles, since each cell interacts with 13 neighbouring cells (because of symmetry we don’t need to process all 26 neighbouring cells). The algorithm now proceeds as follows: (1) copy the first particle of each of the segments in $T$ to all particles in its corresponding segment in $B$, (2) compute the interactions between this particle and all particles in the bottom segment, (3) sum the force contributions of the copied particle along the segment and store the sum, (4) shift the particles in $T$ by one position to align a new, unprocessed particle of $T$ with its corresponding segment in $B$, (5) repeat steps (1)-(4) until all interactions have been computed. Finally, the results of all 13 cellular interactions are added to the force due to particles in the same cell to obtain the neighbour force for each particle. The copying in step (1) and the summing in step (3) are done using special
routines called scanning routines, supplied by the vendor (see Appendix). Figure 2b illustrates this part of the algorithm.

We want to stress the high level of parallelization thus obtained: all cells are processed in parallel in the intra-cell calculation and in addition, all 13 directions are processed in parallel during the inter-cell calculation. The copying of particles from $T$ along segments in $B$ has the advantage that the time required to compute the forces depends only on the maximum number of particles in a segment in $T$ and not on the number of particles in segments of $B$. Since we take care always to put the densest cells in $B$ we can also compute uneven particle distributions rather efficiently.

Table 2 presents timings of the PP algorithm to illustrate the overall efficiency. The triply periodic system which was timed was set-up in the following way: $N_T$ particles were distributed in cells using a random number generator such as to give a prescribed value of the dispersion of cell occupation numbers $\sigma \equiv (N_c - < N_c >)^2 > 1/2 / < N_c >$, where $< N_c >$ is the average number of particles per cell. Table 2 gives the values for $N_T$, $\sigma$ and the maximum number of particles in a given cell, $N_{\text{max}}$ in columns 1-3. The next four columns give the required CPU-time (in seconds) for (4) the organization associated with the intra-cell computation, (5) the intra-cell computation itself, (6) the organization associated with inter-cell communication and (7) the inter-cell computation itself. The $32k$ system consisted of $16^3$ cells and so had $< N_c > = 8$, while the $128k$ system had $32^3$ cells and $< N_c > = 4$. We want to stress that in this part of the calculation, computer time is less when more vertices $N_g$ are used, since fewer PP forces need to be computed in this case.

The intra-cell calculation scales linearly with $N_T N_{\text{max}}$, since the required time is proportional to both the maximum number of particles in a cell and the total number of particles. The time required to compute the inter-cell interactions increases with increasing clustering $\sigma$ at first but then becomes nearly constant, because fewer cells take part in the calculation with increasing clustering at that stage. This is probably pathological to our chosen particle distribution, so we generated another particle distribution where each cell contained at least one particle.

Table 2

| $N_T$ | $\sigma$ | $N_{\text{max}}$ | set-up 1 | intra-cell | set-up 2 | inter-cell |
|-------|----------|------------------|---------|------------|---------|-----------|
| 32k   | 0.0      | 8                | 0.22    | 0.04       | 2.5     | 3.6       |
| 32k   | 0.9      | 21               | 0.22    | 0.13       | 2.3     | 7.2       |
| 32k   | 2.1      | 65               | 0.25    | 0.38       | 1.8     | 10.8      |
| 32k   | 4.9      | 294              | 0.27    | 1.75       | 1.0     | 10.5      |
| 128k  | 0.0      | 4                | 1.40    | 0.07       | 12.2    | 10.7      |
| 128k  | 0.9      | 10               | 0.8     | 0.19       | 11.3    | 15.8      |
| 128k  | 2.1      | 33               | 0.8     | 0.54       | 8.4     | 13.1      |
| 128k  | 4.1      | 106              | 0.8     | 2.3        | 7.1     | 15.9      |

Results for this distribution are presented in Table 3 and illustrate the load-balancing problem that occurs for this more realistic particle distribution. The first set of four lines are appropriate for
the algorithm as described so far, the next four are for the load-balanced algorithm to be described next, using the same particle distribution. Table 3 shows that the old algorithm becomes very much less efficient as the degree of clustering increases from 0 to 5. The reason for this is as follows: most of the interactions between cells involve calculations in which at least one of the cells is sparsely populated and only a few involve interactions between two densely populated cells. Although those sparsely populated cells finish their interactions soon, they still remain active in the calculation since all cells are processed in parallel. (The calculation finishes when the densest cell has been processed.) Clearly, one could avoid this load-balancing problem by processing in parallel cells which have about the same number of particles in the Top segments and hence all cells processed in parallel finish their interactions at the same time. As the algorithm is set-up to interact cells, this step is rather easy to implement and the load-balanced algorithm is indeed much more efficient, as Table 3 testifies.

Table 3

| Load-balanced | $\sigma$ | $N_{max}$ | set-up 1 | intra-cell | set-up 2 | inter-cell |
|---------------|---------|-----------|----------|------------|----------|------------|
| no            | 0.0     | 4         | 1.40     | 0.07       | 12.2     | 10.7       |
| no            | 0.8     | 10        | 0.88     | 0.29       | 16.1     | 30.8       |
| no            | 1.8     | 30        | 0.76     | 0.69       | 15.3     | 65.3       |
| no            | 5.0     | 204       | 0.92     | 4.30       | 15.0     | 353.0      |
| yes           | 0.0     | 4         | 1.10     | 0.07       | 11.8     | 10.6       |
| yes           | 0.8     | 10        | 0.77     | 0.19       | 19.2     | 19.0       |
| yes           | 1.8     | 30        | 0.77     | 0.59       | 29.1     | 26.9       |
| yes           | 5.0     | 204       | 0.83     | 4.10       | 43.5     | 38.0       |

4. Summary and conclusions

We have presented a parallel P3M algorithm which corrects exactly for inaccurate grid-induced PM forces between neighbouring particles. The PM step uses FFT’s to compute the gravitational force between distant particles and convolution of the density with the central part of the Green’s function to subtract grid-induced forces between neighbouring particles in a time $\propto N_T$. Although this corrections step requires a large number of operations to be executed on the grid, the algorithm is still economically viable since these parallel statements are executed extremely fast on the CM2 (running at $\approx 500 - 600$ MFlops). The PP step uses parallel processing of cells and duplication of particles to efficiently compute neighbour forces in situations where the particle distribution is clustered. The PP step uses the same boundary conditions (i.e. isolated or periodic) as the PM step does. A full force calculation in a triply periodic system for 128k particles on a 128$^3$ grid with a rather high degree of sub-clustering takes about 196 seconds (14 seconds for the PM calculation, 95 for neighbour force subtraction and 86 for PP calculation) on a 8k CM2. Scaling the timings from the 8k nodes CM2 to a 64k nodes CM200, this becomes an estimated 9.8 seconds.
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Appendix. CM2 optimization considerations

The Connection Machine 2 (CM2) is a massively parallel SIMD computer consisting of thousands of simple processors, each having its own private memory and interconnected with a hypercube topology. The user interacts with this hypercube through a front end computer which is a conventional workstation. The computer at the Scuola Normale has 8192 processors and a total of 256MBytes of internal memory (i.e. 8192 single precision real numbers per processor).

The top speed of this configuration is ≈1Gflop. High execution speeds (typically about half of the quoted maximum speed for applications written in high level language) are obtained when operations are done on operands which are in the local memory of each processor (i.e., when no communication between processors is necessary). In addition, the length of the vectors on which the operations are done should be at least 3-4 times the number of processors to amortize start-up costs. Figure 1 in Theuns and Rathsack ([10]) illustrates some typical execution speeds measured on this CM2.

CM Fortran contains some extensions that allow operations typical for parallel computers. One of these extensions, which we used extensively in this implementation, is the CSHIFT function which shifts all elements in an array over a specified number of positions in a given direction (e.g. $-x$, $+z$). This routine uses the underlying hypercube topology and is very fast. In addition, it allows for an easy implementation of periodic boundary conditions in both the PM and the PP part. Another routine which is essential for the PP part is a functionality called scanning. The scan routine allows the execution of an operation (e.g. copying, summing, etc.) along a 1D array. The scope of the operation is guided by logical vectors which define segments in the array. The scan functionality applies an operator to all values in a segment, and all segments are scanned in parallel. This routine allows for the copying of an element in a cell to all other elements in another (or the same) cell and for the summing of the contributions of those particles to the copied one. Finally, there is a very fast vendor supplied complex to complex FFT on the CM2.

CM Fortran permits arrays to be allocated dynamically with a size determined at run time. This allows one to optimize the size of the vectors on which the parallel operations are executed and in addition save on memory since arrays which are not used in a given subroutine can be deallocated. (For example, the grid arrays in the PM part are not used in the PP part and hence can be deallocated.) Consider for example the PP step: initially we interact cells which have few particles in the Top cell but potentially many in the Bottom cell: as a result, vectors $B$ and $T$ are very large and their size in practise is limited by the total memory available (512k in our case). Using such large vectors substantially reduces the communication overhead costs involved in loading them. As the PP calculation progresses, however, fewer and fewer cells are interacted, yet each cell requires more and more interactions to complete. Hence, efficiency is increased considerably by doing these interactions on much smaller matrices. Memory is freed at the end of a calculation when the dynamically allocated vectors are deallocated.
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Figure Captions

Fig. 1:
PM forces and potential on massless test particles randomly distributed in a $16^3$ grid due to eight massive particles randomly distributed in cell (8,8,8) as a function of the distance $|r|$ of the particle to vertex (8,8,8). Shown are the deviations (in %) of (a) radial, (b) tangential PM force and (c) PM potential with respect to their Newtonian counterparts in units of total Newtonian force and Newtonian potential respectively. Particles in cells not neighbouring cell (8,8,8) are denoted by crosses, whereas particles in cell (8,8,8) or one of it’s neighbouring cells are denoted by dots. For the latter particles, relative deviations have been divided by four. The forces and potential on these particles will be exactly equal to their Newtonian values after correction step and PP part.

Fig. 2a:
Illustration of the intra-cell calculation. Particles in the same cell are indicated with the same letter ($a,b,c,\cdots$) and particles in a given cell are numbered ($a_1, a_2, \cdots$). In the top panel, the Top array $T(1)$ is identical to $B$ but shifted to the left by one. Force calculation now occurs between different particles that are in the same cell: these pairs are underlined. Next, $T$ is shifted once more and again forces are calculated. The process finishes in step 4, when there are no more particles in $T$ that interact with particles in $B$.

Fig. 2b:
Illustration of the inter-cell calculation. Particles in the Bottom array are designated with lower case letters and particles in the Top array that belong to a neighbouring cell with the corresponding uppercase letter. Segments are delimited by vertical lines and empty array positions are denoted by a dot. The process starts by copying, for each cell in the $T$ array, its first element ($A_1, B_1, \cdots$) into array $I$ and next copying this particle into array $C$ over the whole segment delimited by
B. Forces are now calculated between all particles in $B$ which have their corresponding uppercase particle above them in $C$. Next, $T$ is shifted to the left and the process is repeated until all particles in $T$ have been processed.