Dynamic Work Distribution for PM Algorithm

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Abstract

Although poor for small dynamic scales, the Particle–Mesh (PM) model allows in astrophysics good insight for large dynamic scales at low computational cost. Furthermore, it is possible to employ a very high number of particles to get high mass resolution. These properties could be exploited by suitable parallelization of the algorithm.

In PM there are two types of data: the particle data, i.e. position and velocity, which are stored in one–dimensional arrays of \( N \) elements, and the grid data, i.e. density and force, which are stored in three–dimensional arrays \( M \times M \times M \) in size. Since individual particles can change cell under the action of gravitational force, parallelization is a real challenge on parallel machine and must account for the machine architecture.

We have implemented a dynamic work distribution through agenda parallelism. By subdividing the work in small tasks, the implementation is well balanced, scalable and efficient also for clustered particle distributions.

In this contribution we describe this efficient, load balanced, parallel implementation of PM algorithm on Cray T3E at CINECA and show its performances on cosmological simulation results.

1 Introduction

N–body simulation codes are powerful tools to study the non–linear evolution of gravitational systems. They are used in cosmology to study the evolution of the large scale structure of the universe and formation and evolution of galaxy clusters.

Starting from linear initial condition described by cosmological models, N–body codes provide the actual distribution of a N-particle system due only to gravitational interaction.

In the study of the large-scale structure it is important to perform simulations with a high number of particles, because higher mass resolution can be achieved.

Being the fastest of all known algorithms, the PM algorithm (Hockney & Eastwood, 1981; Birdsall & Langdom, 1985) can be effectively used to study the cluster and large-scale evolutions, where we want to consider the contributes of the very-large scales in the universe.

At the moment, massive parallel processors (MPPs) are the most powerful computers available. Implementing parallel PM algorithm is thus needed in order to make simulations with as high as possible number of particles (Ferrell & Bertschinger, 1994; Pearce & Couchman, 1997; MacFarland et al., 1998; Carretti, 1999).

MPP machines offer very different architectures and require different parallelization strategies in order to achieve high efficiency.

We have performed a dynamic parallel implementation of the PM algorithm on the Cray T3E at CINECA Computing Center. We have used the Cray proprietary shmem library, which performs message-passing among processors by fully exploiting the machine hardware.
2 PM Algorithm

The PM algorithm solves the gravity field equations

\[ \nabla^2 \phi = 4\pi G \rho, \quad (1) \]

\[ F = -\nabla \phi, \quad (2) \]

on a grid. We will call \( N \) the particle number and \( M \) the one-dimensional grid point number. The total grid point number is \( M^3 \).

The PM algorithm computation steps can be summarized as follows:

- given particle coordinates, field source values are assigned to the grid points, using some interpolation scheme;
- field equations are solved on the grid and then forces are computed on the grid;
- the force components are interpolated back to the particles and velocities and positions are updated.

In the first step each particle distributes its mass to \( N_g \) grid points according to a polinomial interpolation. The most popular are the Cloud in Cell (CIC) and the Triangular Shaped Cloud (TSC) schemes. The first one performs a linear interpolation and scatters the particles to the 8 nearest grid points. The second one (a quadratic interpolation) to the 27 nearest grid points. In general, \( N_g = (n+1)^3 \), where \( n \) is the order of the interpolation scheme. In particular, in our simulations we use the CIC scheme and the same number of particles and grid points (\( N = M^3 \)).

In the second step the field equations on the grid is solved. The fastest way is to perform a Fast Fourier Transform (FFT) which requires an operation number of the order \( O(M^3 \log M^3) \). The force can be easily computed in Fourier domain and then on the grid points, after anti-transformation.

In the third part of PM the force field sampled on the grid is interpolated back to particles. To reduce the errors, the interpolation scheme must be the same of density assignent (Hockney & Eastwood, 1981; Birdsall & Langdon, 1985). Finally, positions and velocities of the particles are updated.

The deposition of field-source values on the grid points and the interpolation of the force back to the particles are the most time consuming part of codes based on PM model: more than 60% of the computation time can be required for these steps.

Furthermore, when the system under analysis reaches strong nonlinear regimes, in few time steps and even starting with homogeneously distributed particles, it is possible to reach a state with highly clustered particles in very few cells, almost uniform distribution of particle in some fraction of the cells and no particles in the remaining ones.

The first and the third part have \( O(N) \) operation number, whereas the second one has \( O(M^3 \log M^3) \) operation number. Since the particle number \( N \) is proportional to \( M^3 \) (typically \( N = M^3 \) or \( N = (M/2)^3 \)), the total operation number is \( O(N \log N) \).

3 Parallelization Strategy

In PM there are two types of data: the particle data, i.e. position and velocity, which are stored in one-dimensional arrays of \( N \) elements, and the grid data, i.e. density and force, which are stored in three-dimensional arrays \( M \times M \times M \) in size. Since individual particles can change
cell under the action of gravitational force, parallelization is a real challenge on parallel machine and must take into account the machine architecture.

In a naive approach, it is possible to perform a static work distribution taking as reference the particles or the grid points. In the first case, the machine work is well balanced (each PE has the same number of particles), but many remote communications are required, when the gravitational system is strongly non-linear. In the CIC scheme, for instance, each particle scatters its mass to 8 nearest grid points and therefore can require up to 16 remote communications. Due to this overhead, the code is inefficient.

In the second approach the grid points are uniformly distributed to the processors and each processor performs all computational steps for the particles which belong to its grid points. This implementation is well balanced if particles are unclustered and uniformly distributed in the simulation box, but becomes quickly unbalanced as the particles start to cluster.

Since gravitational force has to be studied in non-linear regime, these naive approaches are unsuitable.

We approach the problem by a suitable block decomposition of data. In this scheme each processor allocates $N/N_{PE}$ particles and $M 	imes M 	imes (M/N_{PE})$ grid points, where $N_{PE}$ is the number of the processors (see figure 1). In this way the first and second dimensions of grid arrays are local while the third one and the particles are distributed. A dynamic work distribution is then implemented to treat this block data. In this case we will see that the implementation is well balanced, scalable and efficient.

We describe now the main strategies followed to optimize the parallelization on Cray T3E, which are atomic update, agenda parallelism and data transfer rate.
3.1 Atomic Update

Parallel codes need sometimes to lock a block data to perform atomic operations. For example a block data updated by more processors must be updated by the processors in turn. Before a processor updates the block data, it must lock them. If another processor wants to update the same data and finds them locked, it has to wait for their unlocking. As data are unlocked by the first processor, the second can proceed to lock and to process the block data.

The *shmem* library on Cray (CRAY) contains a routine to implement the locking: *shmem_swap* routine performs an atomic swap among two data on two different processors.

The *shmem_swap* prototype is

\[
\text{integer} \ ires, \ value, \ pe, \ target \\
ires = \text{shmem_swap} (\text{target}, \ value, \ pe)
\]

This routine puts in variable *target* of processor *pe* the parameter *value* and gets in local variable *ires* the previous value of *target*. The following scheme realizes the lock–update:

```
real  a(N)
integer ires, value, pe, target
integer lock
lock = 0
call barrier()
ires = 1
do while (ires == 1)
    ires = shmem_swap(lock, 1, 0)
enddo
call sub1(a)
ires = shmem_swap(lock, 0, 0)
```

*sub1(a)* is a routine which updates the block-data *a*. To update the block–data *a*, the variable *lock* on PE 0 behaves as a semaphore. If *lock = 0* or *lock = 1* block data are unlocked or locked, respectively. Initially its state is set to unlock. The barrier allows all processors to know the initial state of block data. *ires* contains the value of *lock*.

To update *a*, a processor has to wait *lock = 0*. After the updating the processor set *lock = 0* and allows the update of another processor. In this way call *sub1(a)* is executed in turn by the processors.

3.2 Agenda Parallelism

Agenda parallelism is a well known parallel paradigm (Carriero & Gelernter, 1990). The work is subdivided in an agenda of subworks, *N_{SW}*, in number. Each subwork can be marked to notify if it has been performed or not. Each processor scrolls the agenda, takes an unmarked subwork and marks it. This prevents that another processor performs the same subwork. We use the locking procedure to implement the agenda parallelism, through a lock–array of size *N_{SW}*, initially set to 0. When the work has to be performed, a processor scrolls the lock–array of PE 0 and executes any free subwork according to the scheme below:
integer  i, ires, value, pe, target
integer  lock(NSW)

lock = 0
call barrier()
do i = 1, NSW
    ires = shmem_swap(lock(i),1,0)
    if (ires == 0) call subwork(i)
endo
call barrier()

where subwork(i) routine performs the $i^{th}$ subwork.

Agenda parallelism is a good paradigm as the work may be divided in subwork with very different computing time. A processor performing computationally expensive subworks takes charge of few subworks, whereas a processor performing computationally less expensive subworks takes charge of many subworks. This procedure is self-balancing and each processor spends about the same time to complete the whole work. Therefore the agenda parallelism is a good approach to implement a dynamic work distribution.

3.3 Data Transfer Rate

Parallel computing requires a good data transfer rate among processors. Cray’s shmem library provides some routines to transfer data between processors asynchronously. In particular, we use shmem_get and shmem_put routines which get/put data from/in a processor. This routines allow a very fast transfer rate, if many data are transfered simultaneously. If the data to transfer are few the transfer rate is worse: the transfer time is led by latency time and is independent of the data number.

In table 1 it is reported the transfer time between 2 processors obtained when shmem_get and shmem_put routines are used.

| N    | t(get)   | t(put)   |
|------|----------|----------|
| 1    | 9.30 $10^{-6}$ | 8.80 $10^{-6}$ |
| 4    | 1.00 $10^{-5}$ | 1.00 $10^{-5}$ |
| 16   | 1.05 $10^{-5}$ | 1.00 $10^{-5}$ |
| 64   | 1.15 $10^{-5}$ | 1.15 $10^{-5}$ |
| 256  | 1.60 $10^{-5}$ | 1.70 $10^{-5}$ |
| 1 K  | 3.60 $10^{-5}$ | 3.60 $10^{-5}$ |
| 4 K  | 1.06 $10^{-4}$ | 1.08 $10^{-4}$ |
| 16 K | 4.00 $10^{-4}$ | 3.94 $10^{-4}$ |
| 64 K | 1.56 $10^{-3}$ | 1.54 $10^{-3}$ |
| 256 K| 6.20 $10^{-3}$ | 6.24 $10^{-3}$ |
| 1 M  | 2.50 $10^{-2}$ | 2.50 $10^{-2}$ |
| 4 M  | 1.00 $10^{-1}$ | 1.00 $10^{-1}$ |

Table 1: Transfer time for shmem_get (t(get)) and shmem_get (t(put)) routines: $N$ is the number of transfered data and $t$ is the transfer time in second. 4 processors are in use and the communications are between processor 0 and processor 3.
The latency time is very important until when 100 data are transferred simultaneously. Therefore, as the data are few, it is important to transfer them by means of one only instruction. It is better to group data in a unique structure and to transfer this structure, rather than data separately. Transferring \( N \) data with \( N \) operations requires about \( N \) times the time to transfer all the data simultaneously.

The implementation of density computation and force interpolation could require many remote-load operations, therefore it is important to reduce their number.

We introduce a new derived type, which contains all the particle information: position and velocity. We call it \( \text{part3D} \) and it is described as:

\[
\begin{align*}
\text{TYPE} & \quad \text{part3D} \\
\text{real} & \quad :: \quad x, y, z \\
\text{real} & \quad :: \quad vx, vy, vz
\end{align*}
\]

In this way all 6 data of a particle are in adjacent memory locations and can be loaded by means of one remote-load operation. For example, if we need all data of particle \( j \) of processor \( \text{pe} \), we can use

\[
\text{call shmem\_get(XLOC, X(j), 6, pe)},
\]

where \( \text{XLOC} \) is a local variable of TYPE \( \text{part3D} \) and \( X \) is a one-dimensional array of TYPE \( \text{part3D} \) and size \( N \).

4 Parallel Implementation

4.1 Density Computation

Density computation is the first step of PM. The particles scatter their mass to the nearest grid points according to a polinomial interpolation.

It is not an easy task to perform a well balanced parallel implementation of density computation in PM algorithm. There are two types of data structures. The first one is related to particles and is organized in \( N \)-element vectors. Particle positions and velocities are represented by this data type. 3-dimensional arrays are used to represent values on the grid, as density and force fields. Particles move with respect to the grid and can cluster around few grid points. This behaviour is a strong source of load unbalancing in a naive parallel implementation.

To avoid load unbalancing we use a dynamic work distribution through agenda parallelism (Carriero & Gelernter, 1990). We define tasks by dividing the 3-dimensional density arrays allocated to each processors \( (M \times M \times (M/N_{PE})) \) in \( N_{C} \) chunks of dimension \( M \times (M/N_{C}) \times (M/N_{PE}) \) (see figure 2).

Particles are locally sorted so that they are grouped according to the global chunks they belong to. A local vector contains the information on the address of the first particle and on the particle number for each chunk. In this way for each processor the particles of a chunk are stored in adjacent memory location and can be remote-loaded together in one operation.

To compute the density, each processor selects a task which has not yet been executed and locks it. Since particles have been ordered according to the chunks they belong to, this processor can collect all the particles which give a contribution performing \( N_{PE} \) remote-load operations and then compute the contribution to the grid density.
Figure 2: The $N_{PE}$ local array (each of dimension $M \times M \times (M/N_{PE})$) are subdivided in $N_C$ chunks each. Thus the global 3-D array consists of $N_{PE} \times N_C$ chunks. In the figure each local array is divided in 8 chunks.

As the task is executed, the processor releases the chunk and selects another one from the agenda and then repeats the same operation. This goes on until all tasks are executed.

In this way each processor manages about the same number of particle and the load is well balanced. If particles are uniformly distributed, the chunks have about the same number of particles and the processors work the same number of chunks with a well balanced load. If particles are strongly clustered, some chunks have many particles and some few. A processor that grabs such chunks with many particles, will spend much more time to perform computation and will take few chunks. On the other hand, a processor which grabs chunks with few particles, will spend a shorter time to perform related computations and will take many chunks. If the total chunk number is much greater than $N_{PE}$, each processor will treat about the same number of particles and the load will be well balanced again.

This implementation is dynamic: the processors do not perform the same work at each time–step and the computational load adapts itself to the particle distribution.

Since particles distribute their mass to the nearest grid points, a particle near the edge of a chunk updates the grid points of its chunk and of the next chunks (up to a maximum number of 3) and a grid point at the edge of a chunk is updated by particles of its chunk and of nearest chunks (up to a maximum number of 3). In this way more processors can update simultaneously the same grid point.

If this happens, some contribution to density field could be lost. To avoid this we perform an atomic updating of density array (see section 3.1). The processors use a local auxiliary chunk and scatter the particles on it. It consists of a chunk of the global density array and of the boundary grid points which the chunk particles can update. As the chunk computation is performed, the processor locks in sequence all the chunks of the global density array, which can be updated by the chunk particles, and updates them by means of the values stored in the
auxiliary one. In this way another processor cannot update the same grid points. Finally it unlocks the chunks and makes them available to the other processors.

4.2 Force Interpolation

Force interpolation is the third step of PM algorithm. In this step the force on each particle and then the particle velocity are computed. It is the inverse operation of density computation, and we apply the same parallel implementation.

However there are two main differences. First, the force arrays must not be updated during force interpolation. Therefore the lock of atomic updating is no more required. Second, this operation updates the particle velocity, and the three velocity components must be loaded, updated and stored. By means of derived type part3D we load velocity and position in one operation. So we do not add remote operation to load velocity. However, to store the updated velocity we must perform a remote–store operation. Therefore force interpolation requires two times more communications than the density computation.

4.3 FFT

Our algorithm solves the field equations by Fast Fourier Transform (FFT). There are parallel 3–dimensional FFT routines in Cray’s scilib library. They operate on 3D array distributed to the processors. They are very fast but require a lot of workspace memory. For example, the real–to–complex and complex–to–real FFTs applied to a 3D array of $M \times M \times M$ size require a complex workspace of $2 \times M \times M \times M$ size.

We have implemented a 3D–FFT for distributed arrays, which is a bit slower than Cray’s implementation, but requires a smaller workspace.

An analytic three–dimensional Fourier transform (FT) is equivalent to 3 one–dimensional ones,

$$\int f(\mathbf{x}) e^{-ik\cdot x} \, dx = \int dz \, e^{-ik_x z} \left( \int dy \, e^{-ik_y y} \left( \int dx \, f(x, y, z) e^{-ik_z x} \right) \right).$$

Each transformation is performed with respect to one of the 3 variables $x, y, z$. The first one performs 1D–FFTs on column vectors along the array $x$ axis. The second and the third one perform them on column vectors along the $y$ and $z$ axis.

In our data distribution the 3D array are distributed between the processors with respect to the third dimension, whereas the first and the second one are local. Therefore, each processor performs the 1D–FFT on all its column vectors along the $x$ and $y$ axes and the computation is totally local. The third dimension is distributed and the column vectors along the $z$ axis are distributed between all processors. To perform it, we assign the same number of columns to processors. As a processor computes a Fourier transform for an assigned column, collects it from all processor by shmem_get routine and stores it in a local vector. Then the processor performs the 1D–FFT on the local vector and scatters it to the processors by shmem_put routine and stores it on the distributed array.

To perform the 1D–FFTs we use the routines of scilib library, which work on local vectors. To execute them we need a real workspace of $8 \times M$ size per processor. Furthermore we need a complex auxiliary vector of size $M$ per processor. So our 3D–FFT implementation requires only a real workspace of size $10 \times M \times N_{PE}$, which is much less than the $4 \times M \times M \times M$ real workspace of Cray’s implementation.

In table 2 we report the execution time for our and Cray’s 3D–FFT implementation on a 256$^3$ array. Our implementation is only slightly slower than Cray’s one. Both routines have a good scalability till 64 processors. As the processor number is near to $M$, the number of remote
communications increases and the performance decreases. Therefore we have implemented a parallel 3D–FFT which requires much less workspace and is slightly slower than the Cray’s one.

| \(N_{PE}\) | 16   | 32   | 64   | 128  |
|-----------|------|------|------|------|
| Cray      | 0.83 | 0.47 | 0.30 | 0.22 |
| user      | 1.00 | 0.51 | 0.36 | 0.29 |
| Cray/user | 0.83 | 0.92 | 0.83 | 0.76 |

Table 2: Computation time for real–to–complex 3D–FFT routines applied to a \(M^3 = 256^3\) 3D array. \(N_{PE}\) is the processor number. Cray is the routine of Cray’s scilib library and user is our implementation described in section 4.3. Cray/user is the ratio between the computation time of Cray’s and our implementations. Results are reported for 16, 32, 64 and 128 processors. Time is in second.

5 Performances

We have implemented our code on a Cray T3E at CINECA (Bologna). This T3E has 256 processing elements (PE) with a 600 MHz DEC Alpha EV5 each. 128 PEs have a 256 MByte memory and the other 128 a 128 MByte memory.

We have compared the result of our implementation with a serial version of the code (Moscardini, 1990). The two codes produce results which are the same up to the machine accuracy.

We performed a cosmological simulation with \(N = M^3 = 256^3\) and \(100h^{-1}\)Mpc box-size (\(h\) is the Hubble constant in \(100Km s^{-1} Mpc^{-1}\) unit) to test the performances of the parallel implementation with both homogeneous and clustered particle distributions.

Following Ferrell & Bertschinger (1994) we measure the clustering with the homogeneity parameter \(FracOC = N_{oc}/M^3\), where \(N_{oc}\) is the number of mesh cells with at least one particle in them. \(FracOC\) is the fraction of mesh cells with at least one particle in them.

At the beginning the particle distribution is quite homogenous. The gravitational evolution induces clustering and at the end the particles are clustered.

Table 3: Computing time for the components of PM in the test simulation. Table reports results for 32, 64 and 128 processing elements (PEs) at the begin (homogeneous) and the end (clustered) of the simulation. For all test simulations \(N = M^3 = 256^3\).

Table 3 shows the computing time for the components of PM at the beginning (homogeneous particle distribution) and at the end (clustered particles). Density Computation and Force Interpolation are described above in previous sections. Sorting is the required time to sort the particle. FFT is the required time to compute Fast Fourier Transform, 1 forward e 3
backward. Force Computation collects the routine to compute the gravitational potential and the 3 force components in Fourier space. Force Interpolation is performed 3 times per time–step to compute the 3 force components. Therefore, Force Interpolation time is about 3 times greater than Density Computation time.

The balancing properties of the code are shown in figure 3, where we plot the computing time per step of our test simulation for 32, 64 and 128 processors. The computing time is quite constant for all simulations and all processor numbers. The small fluctuations are due only to sorting routine. Therefore our implementation is very well balanced during the clustering evolution and it is not affected by the clustering.

The scalable properties are reported in table 4 that shows the speed-up for the components of PM. All components have a speed–up near 2, which is the ideal values, and scale very well. Only FFT do not scale well, as we have shown above in section 4.3. The sorting routine has a speed–up greater than 2 because the number of particles per processor decreases by increasing the processor number. The speed-up of the whole PM routine is slightly smaller than 2, but this is due to the FFT routine.

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Table 4: Speed-up for the indicated components of PM in the test simulation. Table reports results for the indicated processor scaling at the begin (homogeneous) and at the end (clustered) of the simulation. For all test simulations $N = M^3 = 256^3$.

References

[1] Birdsall C. K., Langdon A. B., 1985, Plasma Physics, (McGraw–Hill)
[2] Carretti E., 1999, PhD thesis, Università di Bologna
[3] Carriero N., Gelernter D., 1990, How to Write Parallel Programs, MIT Press
[4] CRAY, Application Programmer’s Library Reference Manual, publication SR-2165
[5] Ferrell R., Bertschinger E., 1994, Int. J. Mod. Phys. C, 5, 933
[6] Hockney R. W., Eastwood J. W., 1981, Computer Simulation Using Particles (New York: McGraw-Hill)
[7] MacFarland T., Couchman H. M. P., Pearce F. R., Pichlmeier J., 1998, New Astr., 8, 687
[8] Moscardini L., 1990, PhD thesis, Università di Bologna
[9] Pearce F. R., Couchman H. M. P., 1997, New Astr., 5, 411