A new parallel TreeSPH code

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Abstract

In this report we describe a parallel implementation of a Tree-SPH code realized using the SHMEM libraries in the Cray T3E supercomputer at CINECA. We show the result of a 3D test to check the code performances against its scalar version. Finally we compare the load balancing and scalability of the code with PTreeSPH (Davè et al 1997), the only other parallel Tree-SPH code present in the literature.

1 INTRODUCTION

In Numerical Astrophysics there is nowadays a great need to increase the dynamical range of N-body simulations. This is mainly the case of large Scale Structures and Galaxy Formation simulations, the motivation being that one would be likely able to simulate volumes comparable to the dimension of the Universe, but resolving at the same time the regions in which many important physical processes -like star formation- occur. The involved dynamical range is of the order of $10^9$. The last decade has seen a huge effort to realize good codes -both eulerian and lagrangian- to study Galaxy Formation. In particular lagrangian codes, due to their spatial flexibility, have become a major tool in this kind of applications (Carraro, Lia and Chiosi 1998). In the case of lagrangian codes, the dynamical range is improved by using greater and greater numbers of particles. This fact also has the advantage to decrease the errors (which are poissonian) in the model predictions. Unfortunately scalar (and even vector) particle codes are not suitable to study

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with sufficient accuracy Galaxy Formation processes, because the dynamical range reachable is of the order of some thousands, using roughly half a million particles. Moreover such big simulations require enormous computing time. Therefore the use of massively supercomputers is the possible way out for these resolution problems. The first example of the parallelization of a particle code is PTreeSPH (Davé, Dubinski and Hernquist 1998). This code allows to run simulations with half a million particles in the reasonable time of 6000 node-hours. PTreeSPH is a C code which uses MPI communication package in a Cray T3D machine. In this report we describe a new implementation of a TreeSPH code realized using SHMEN libraries for the 128 nodes Cray T3E supercomputer hosted by CINECA. We are going to use this code to study individual galaxy formation and evolution. This approach allows us to decrease by several order the necessary dynamical range and to perform useful simulations by using some hundreds thousand particles.

2 THE CODE

Our TreeSPH is a F90 code, which is described in details in Carraro, Lia and Chiosi (1998). It is a gravity treecode combined with an SPH hydrodynamics. It uses variable smoothing lengths and individual time steps. The scalar version of the code contains a very good implementation of the baryons physics, i.e. cooling, star formation, feedback and chemical evolution (Lia, Carraro and Chiosi 1998; Carraro, Lia and Buonomo 1998).

To keep processors balanced, the parallel code utilizes a domain decomposition algorithm based on a particle workload criterion. At any time step we compute the particle workload on the basis of the particle timestep, which gives and idea of the amount of floating point operations (gravity plus hydro) of the particle itself. The procedure consists in deriving the center of mass of the workloads distribution and iteratively subdivide the volume distributing particles to the processors. The subdivisions are not necessarily performed along planes parallel to the reference frame axis, the only real goal being to render sub-volumes as more spherical as possible.

Communications are handled using Shared Memory paradigm with the SHMEm-library routines. This choice is advantageous in a number or way. First, these routines are provided by Cray Research itself to have the best use of the hardware remote memory access available on the Cray T3E (which
Figure 1: Adiabatic collapse of an isothermal gas sphere. Snapshots refer to $t = 0.88$ when the shock is most prominent. Left panels refer to the scalar version, right to the parallel one.
is the CINECA’s machine we used for our work); thus we have in turn the best performance for communication. Second, having no more need of synchronization for communication (an explicit receive for each sent message) our algorithm greatly gains in simplicity and the synchronization performance cost is eliminated too. The only drawback might be the portability, but the new version 2.0 of the standard MPI library already includes the On-Side Communication paradigm which implements a remote memory access much similar to the Shared Memory; this will allow us to easily port our program to the MPI 2 coding style, which should naturally grow in popularity thanks to the popularity already gained by its predecessor (MPI 1).

Communications are controlled using a data structure made of two trees. Any CPU builds at any timestep its own tree up, then it descends once all other trees to gather all the necessary information to compute SPH estimates of the physical quantities. We call this structure ghost tree. This has some similarities with the local essential tree. The descent allows simultaneously to compute gravity and to perform neighbors searching. Care is also payed to the memory necessary to maintain remote informations. In addition, if the domain decomposition is made efficiently, it is not necessary to descend entirely a remote tree, this descend being decided in obey to an opening criterion similar to the local tree opening criterion.

3 A 3-DIMENSIONAL TEST

In order to analyze the behavior and the performances of the code, we have run the adiabatic collapse test, which is an ideal test to check the response of the code to situations in which a large dynamic range in space and time is present. The comparison between the results of the scalar and parallel version is presented in Fig. 1, where left panels refer to the scalar version(red), right panels to the parallel one(green). The collapsing gas produces a shock most prominently at $t = 0.88$ (time is in code units, where total mass $M$, total radius $R$ and gravitational constant $G$ are set equal to 1), and for this time we show the comparison of density, pressure, internal energy and radial velocities profiles. This tests has been realized using 4000 particles distributed in 16 processors. The scalar test has been realized using 2176 particles. The results are quite good, except for the inner region of the sphere, which by the way is under the resolution, which is governed by the gravity softening parameter,
kept equal to 0.1 for consistency with Davé, Dubinski and Hernquist 1998. In Fig.2 we show energy conservation, which in this case is under 8%.

4 PERFORMANCE ANALYSIS

In this section we present the performance of the code in terms of load balancing and scalability. To this aim we performed the adiabatic collapse test at increasing number of processors, and computed the load balance according to Dave’, Dubinski and Hernquist (1998) equation (12):

\[ L = \frac{1}{N_p} \sum_{i=1}^{N_p} \frac{N_p}{t_{max} - t_i} \]  

(1)

The result is plotted in Fig. 3, where dashed line shows the mean load balance for the PTreeSPH code. Our global load balance is always greater than 90%, which means that the time a processor remains idle is always lower than 10%. This is mainly due to the asynchronous communications scheme used. Scalability means that any routine in the code should speed up linearly
Figure 3: Global Load Balance as given by equation 1. Dashed line represents PTreeSPH mean load balance.
Figure 4: Scalability of four subroutines using 8, 16, and 32 processors.
at increasing number of processors. Here we consider four routines: gravity, neighbors searching, hydrodynamics and ghost tree construction. The scalability is measured in terms of the time fraction spent by any subroutine. Fig. 4 shows that gravity, neighbors searching and ghost tree construction subroutines scale linearly with the number of processors. The computation of hydrodynamics does not decrease too much, this being less than a problem, due to the small time spent by this subroutine.

5 FUTURE PERSPECTIVES

At present our parallel code contains also an implementation of cooling phenomena. We are going to implement also star formation, feedback and chemical evolution (Lia, Carraro, Chiosi and Voli 1998). Some additional work is in progress to render the code more efficient implementing variable softening parameters and anisotropic smoothing lengths. By using half a million particles we hope to resolve regions of $10^4$ solar masses in a $10^{11}$ solar masses galaxy, or to easily resolve the stellar distribution in a $10^6$ solar masses globular cluster.

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