Mem. S.A.It. Suppl. Vol. 4, 69

Memorie della
Supplementi

Adaptive grid-based gas-dynamics and Poisson solvers for gravitating systems

P. Londrillo

INAF-Osservatorio astronomico di Bologna, via Ranzani 1, 40126 Bologna, Italy
e-mail: `londrillo@bo.astro.it`

Abstract. A short analysis on existing numerical methods and related code implementations for astrophysical gravitating systems, where gas-dynamical and N-body (collisionless) components are both represented, is first presented. By taking into account recent numerical and mathematical advances, a project to construct new codes allowing high accuracy and higher computational efficiency is then outlined.

Key words. Computational methods–Gas-dynamics

1. Introduction

In recent years a relevant number of codes to simulate gravitating systems has been constructed, in the effort to assure increasing space and mass resolution to simulate cluster and galaxy formation. Starting from a Cold Dark cosmological setting, where only gravitational interactions have been considered, new physical processes related to gas-dynamics of the baryonic components have then been taken into account. To cite only a few referenced codes, I mention here GADGET,(Springel et al. 2001), ENZO,(Bryan & Norman. 1997), FLASH, (Fryxell et al. 2000) and the recent RAMSES(Teyssier 2001) based on ART(Kravttsov et al. 1997) experience. In spite of a great spread of numerical recipes and technical aspects characterizing these and related works, the underlying physical and numerical models are only a few, allowing then a broad evaluation of advantages but also of the limitations of the proposed computational methods. In fact, while Gadget (as a prototype) is based on a strictly lagrangian N-body model where also gas-dynamics is represented by particles using Smooth Particle Hydrodynamics (SPH) schemes, all other codes rely on the eulerian (or grid-based) framework enforced with adaptive multigrid procedures, to represent both gas-dynamics and gravitational interactions. In these eulerian codes, since collisionless components are still described as N-body system, the Particle-Mesh (PM)(Hockney & Eastwood 1988) method is then applied to blend a particle representation with the grid based field (density and potential) variables.

As a first evaluation, it is apparent that all the referenced codes adopt *a same* computational framework (either of N-body or of grid-based type) to model *different* physical components, mostly for reasons of implementation simplicity. However, looking at general arguments one would require that also different numerical modelings should apply. In fact, conservative Euler (and MHD) equations have a natural representation on grid-based upwind schemes, enforced with Adaptive

Mesh Refinement (AMR) techniques to handle highly inhomogeneous systems. On the other hand, collisionless components interacting only via gravity forces, have a well posed and experimented representation in terms of lagrangian particles, where error estimates and convergence results rely only on the particle number N, under the condition it is sufficiently large, $N >>$.

Fast and accurate schemes of grid-based AMR type for gas-dynamics and of lagrangian type (Poisson solvers and symplectic integrators) for collisionless systems are today available. Therefore, it seems worthwhile to design and experiment a new class of N-body codes relying properly on these two main building blocks. It the following, I shall present more detailed motivations and a first outline of this computational project.

2. The Poisson solver algorithms for N-body systems

As anticipated, to compute gravitational forces two different numerical schemes can be used, depending of the adopted framework. A first class of schemes are based on the integral form

$$\Phi(x) = G\int \rho(y)K(|x-y|)\,dy,\ \ \mathbf{F} = -\nabla\Phi \quad (1)$$

where the kernel $K(|x-y|) = !x-y!^{-1}$ is the Green function of the Newtonian two-body interaction and $x, y \in R^3$ denote space coordinates. In this form, gravitational forces are expressed by the analytical derivative of the Green function. If a collisionless system is then discretized as a set of N representative particles having masses $\{m_i\}$, this gives

$$\Phi(x_j) = \frac{1}{2}G\sum_{i>j}^{N} m_i K(|x_i - x_j|), \qquad (2)$$

plus some softening for near interactions $|x_i - x_j| < \epsilon$, allowing to smooth out small scale fluctuations and unwanted two-body relaxation effects. A careful discussion of the relevance of so ftening to mimic collisionless fluids has been given, for example, in(Dehnen 2000) and (Knebe et al. 2003). For large $N >>$, the $O(N^2)$ sum in Eq. (2) can now be evaluated in efficient way and to a prescribed order of accuracy, via a multipole expansion of the Green function. A general theory of this method and a proper design of fast summation algorithms have been developed by(Greengard & Rokhlin 1987). In the astrophysical context, a specific implementation of this method has been introduced by (Barnes & Hut 1985) (the widely used BH tree-code) having $O(N \log N)$ computational complexity. Recently, (Dehnen 2002) developed new algorithms assuring effective $O(N)$ complexity and uniform accuracy in the range (a relative mean force error $\simeq 10^{-3} - 10^{-4}$), considered quite acceptable for most astrophysical problems.

In the second kind of numerical models, the potential, forces and density variables are represented as eulerian fields, and the Poisson equation is then solved using the differential (or local) form:

$$\nabla^2\Phi(x) = 4\pi G\rho(x),\ \ \mathbf{F} = -\nabla\Phi, \qquad (3)$$

equipped with the far field (or periodic) boundary conditions. In this form, variables are discretized on a grid and differential operators are then approximated by finite differences or spectral methods. In the finite differences approximation, the Poisson equation can be solved using relaxation methods and multigrid techniques, to assure efficiency and to improve local resolution. In any case, a Poisson solver on a grid costs $O(N_g \log N_g)$ floating operations, where now N_g denotes the total number of grid points.

The main limitation of this method, when applied to a collisionless fluid, is that grid based variables have to be related to finite-size lagrangian particles by some form of local interpolation. As carefully discussed in (Hockney & Eastwood 1988), the resulting PM schemes carry over unwanted effects (grid anisotropy, aliasing, etc.) and error analysis becomes now quite involved and extremely sensitive to the local particle distribution.

3. AMR schemes for Euler equations.

The AMR framework is a rapidly developing set of numerical procedures designed to increase spatial (and temporal) resolution of numerical simulation of fluid-dynamics (and MHD) equations on both structured and unstructured meshes. In astrophysical applications cartesian structured meshes are usually adopted and two main approaches have been proposed. In the standard approach, first introduced by (Berger & Oliger 1984), the computational domain is covered by a set of local grids or ' patches' of cells, with different degree of local refinement, starting from a base coarse grid. The resulting grid hierarchy is then organized as a tree and Euler equations are solved on each grid patch, at a time. To a second (alternative) approach belongs a rather broad class of schemes where now grid cells (or blocks of cells) having different level of refinement are organized as an oct-tree, as in the standard BH N-body code. The resulting scheme has the following main features:

- in a nested grids system, at each level of refinement, unrefined cells (the leaves of the tree) have particular meaning. Flux derivatives and time integration of the gas-dynamic equations are computed only on this set of cells.

-the totality of leaves covers spatially the entire computational domain in a unique way;

-no difference greater than one in grid refinement is allowed for neighboring cells.

Several AMR schemes based on this second approach have been proposed recently, like PARAMESH in the FLASH code, and the Fully Threaded Tree (FTT,(Khoklov, 1998) as in the ART and in the RAMSES codes. Moreover, a more general class of schemes where adaptivity is based on the Harten Multiresolution Analysis method (Harten, 1994)(hereafter, HMRA), have been designed by (Cohen et al. 2002) and applied by (Roussel et al. 2003). The latter developments, in particular, appear as most promising, since HMRA provides a rigorous mathematical support for error estimates.

4. A computational project to blend N-body to AMR gas-dynamics

The previous analysis on the state of art of numerical modeling suggests a strategy to develop codes where efficient and accurate N-body schemes, like those exploiting Dehnen's algorithms, are used for collisionless components while eulerian grid-based adaptive schemes, like in the HMRA framework, are used for gas-dynamics.

A strict lagrangian representation of collisionless components has well documented advantages, since hamiltonian properties are preserved by symplectic, time reversal integration schemes. Once a fast Poisson solver is available as in the multipole expansion of Eq.(2), the local (in space) adaptivity of a lagrangian flow is also achieved in a natural way, without the recourse to hybrid PM procedures. Moreover, multipole expansion allows uniform high order accuracy (for example, the referenced Dehnen scheme provides a fourth oreder accurate potential at any point inside a tree cell), while multigrid solutions of the Eq. (3) can be efficiently constructed only at a second order level and adding particle-mesh interpolation further limits the resolution demands.

On the other hand, to integrate gas-dynamic (and MHD) equations, eulerian grid-based methods should be preferred since they assure the conservative form and then the application of well experimented shock-capturing schemes. Moreover, as a viable alternative to SPH, here numerical diffusivity can be better controlled and constrained to sufficiently low levels in a way physical processes requiring small scale resolution, like kinetic transport and turbulence, can then be better described. In the same AMR framework where gas density on a grid cell is represented, typically, to second order accuracy, gravity potential can be evaluated to four-*th* order by implementing fast multipole expansion, as in the scheme proposed by(Greengard & Lee 1996).

The price to be paied having different numerical modelings does not seem to be significant, in my opinion, and no particular implementation difficulties may arise as long as a common data structure (the tree organization of cells) and and effective $O(N)$ complexity (N being the particle number or the active grid points) hold for both frameworks.

5. Adaptive gas-dynamics under HMRA

N-body codes exploiting Dehnen's fast algorithms are documented elsewhere(Londrillo et al., 2003). Here I consider only some preliminary results on the implementation of HMRA schemes for grid-based gas-dynamics. Extension to MHD is under development, following the general method presented in(Londrillo & Del Zanna, 2003)

The basic principle underlying the Harten approach can be roughly summarized by reversing the popular statement: *adaptive methods are designed to improve resolution where it is needed*, into the statement *multiresolution information of grid data allows to save memory and cpu time whenever the highest available resolution is redundant.* This allows to put error analysis of any adaptive scheme in to a rigorous framework, as shown in the AMR procedures designed by(Cohen et al. 2002).

Following this design, I have then implemented in Fortran90 AMR scheme having the following main features.

5.1. The tree data structure

The set of nodes defining the tree structure is organized in octal blocks of cubic cells, similar to the octs of the FTT scheme. Any block is a logical unit holding informations on the eight ordered cells it represents (flow variables and space coordinates). To assure connectivity among cells, as needed to compute flux derivative and time evolution, each oct-cell of a given level L holds a pointer to the $L+1$ level oct containing its children (if any). As usual, cells with no children are leaves of the tree. Moreover, each oct holds pointers to the parent cell and to the eight octs which are neighbors of the parent cell. In a Fortran implementation, octs are represented by an array of structures, $Oct(k)$, $k = 0, 1, ...,$ and pointers by integers k_n addressing an array element, $Oct(k_n)$, or integers $k_c = 0, 1, .., 7$ addressing an oct-cell, $Oct(k_n)\%cell(k_c)$. It is now easy to check that this simple form of data organization requires a minimum of memory storage to assure connectivity and fast tree traversal.

5.2. The refinement-derefinement procedures

The crucial point of any AMR scheme is provided by the refinement-derefinement rules and by the related numerical representation of grid data, at any refinement level, needed to get information on the smoothness properties of the discretized flow variables. Let then $\{u_i\}^{L-1}$ represent cell averaged data of the numerical solution at a cell $[C_i]^{L-1}$ belonging to the $(L-1)$ level of refinement, $L = 1, 2, ..., L_{max}$. In the HMRA framework, the prolongation of the reference function defined by the $\{u_i, u_k\}^{L-1}$ data (u_k belonging to neighbors of C_i), at any point inside the cell and then at the centers of the children cells $[C_j]^L$, is provided by local polynomials based on wavelets. The corresponding prolongation operator $P : \{L-1 \rightarrow L\}$ acting on cell averaged variables is defined as the exact inverse of the cell averaging operator $A : \{L \rightarrow L-1\}$. If now $[\hat{u}_j]^L$ denote the resulting approximated values under prolongation and $[u_j]^L$ the local solution, the error norm $D(L) \equiv ||\hat{u}_j - u_j||$, for $L = 2, ..., L_{max}$ measures the smoothness properties of the numerical $u(x)$ function and provides then the basic tool to decide refinement (or derefinement) of the leaf cells during the integration steps. Following Harten's analysis, for given thresholding error ϵ, the estimate

$$D(L) \leq 2^{3(L-L_{max})}\epsilon, \; L = 1, 2, .., L_{max} \qquad (4)$$

provides the basic condition for cell refinement, assuring that errors introduced by the refinement-derefinement procedures keep within the ones introduced by the base integration scheme.

This accuracy demand poses new challenging problems, which have to be fully considered in the numerical experience, yet. In particular, the refinement condition in Eq. (4) requires that, to keep second order accuracy, the same of the base integration schemes, the prolongation polynomial must be third order (i.e. quadratic in all space coordinates), while existing AMR codes routinely use linear interpolants.

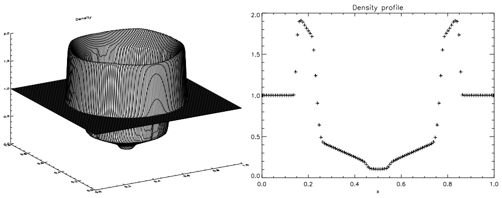

Fig. 1. Left panel: the surface plot of the density for the propagating pressure jump test problem, at time $t = 0.1$. Grid data : $N_x = N_y = 128$ Right panel: the density profile along the x coordinate, at $y = 1/2$, for the same test problem.

5.3. The integration step on leaves

For assigned refinement criteria, leading to a tree structure as outlined in Sec. 3, at each level L, only leaf cells and then only a subset of the grid data (as defined by the cardinality of the most refined grid), enter the time integration step. To reconstruct flux variables at the cell interfaces and then to evaluate flux derivatives, upwind schemes require an appropriate stencil of $2r - 1$ data along each space coordinate, where r denotes the formal order of the scheme. To date, AMR numerical experiences are essentially limited to second order (in space and time) schemes, where a set of 26 neighboring cells are needed to assure a three-point stencil along any direction (diagonals included). In the present implementation, I used the Godunov-type *positive* scheme proposed by(Liu & Lax 199), which is already well experimented also for MHD problems.

5.4. A simple test problem

A two-dimensional test problem is presented here, to check first how condition in Eq. (4) works. In a square cartesian domain $0 \leq x, y \leq 1$ the initial conditions are given by a circular spot $r \leq r_0$ filled with higher pressure fluid $p = 10$, while the ambient fluid $r > r_0$ has uniform pressure and density $p = \rho = 1$. Initial velocities are set to zero everywhere. The initial presure jump produces then a propagating circular shock, and an exapansion wave inside the perturbed region.

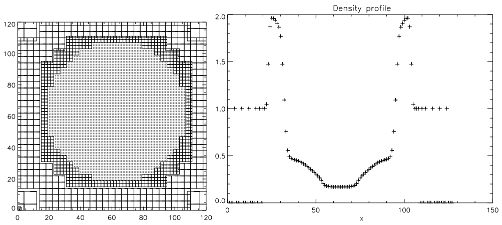

Fig. 2. Left panel: the distribution of leaf cells, in the adaptive grid, for the same problem as in Fig.1. Square symbols of different sizes correspond to different levels of refinement. Right panel: the density profile along the x coordinate, at $y = 1/2$, in the adaptive grid (four levels of refinement).

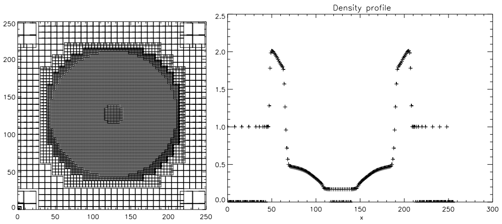

Fig. 3. Left panel: the distribution of leaf cells, in the adaptive grid, for the same problem as in Fig.1, now with $L_{max} = 8$. Square symbols of different sizes correspond to different levels of refinement. Right panel: the density profile along the x coordinate, at $y = 1/2$, in the adaptive grid (five levels of refinement now active).

In Fig.1, the surface plot(left) and the central x profile (right) of the fluid pressure, at a time $t = 0.1$ are shown. A uniform grid $N_x = N_y = 128$ ($L = L_{max} = 7$) is here chosen.

In the next Fig.2, the same run has been performed using the HMRA scheme, with $L_{max} = 7$ and tolerance value $\epsilon = 0.01$ The left pannel now shows the grid point distribution representing leaf cells (only the finest four levels of refinement contain leaves). As can be seen, to keep the prescribed accuracy, all the interior region, up to the shock, is covered by only the finest $L = L_{max}$ grid.

Finally, the same run has been repeated, now with $L_{max} = 8$ (corresponding to the finest grid size $\Delta x = \Delta y = 1/256$. The interior (smoother) region now is covered by leaf cells residing at the $L = L_{max} - 1$ refinement level, as shown in Fig.3.

6. Conclusions

I have presented a short analysis of the most referenced codes, designed to simulate collisionless and baryonic matter dynamics in the study of galaxy formation. Motivations to develop a new computational framework exploiting recent achievements in algorithm design have then been argumented and some preliminary implementation results of this project are finally documented.

References

Barnes, J. E. & Hut, P.,1986, Nature, 324,486(BH)

Berger, M. J. & Oliger, J.,1984, Journal of Computational Phys.,53, 484

Bryan, G. L.& Norman, M. L., 1997, Astro-ph/9710187

Cohen, A., Keber,S.M., Muller, S.,& Postel, M., 2002, Math. of Comp.,72,183

Couchmann, H.P., 1991,ApJ,368,L23

Dehnen, W., 2000,ApJ,536,L39

Dehnen, W.,2002, Journal of Computational Phys.,536,L39

Fryxell, B., Olson, K.,Ricker, P., Timmes, F.X.,Zingale, M.,Lamb, D.Q.,MacNeice,P., Rosner, R., Truran, J.W.& Tufo, H. 2000, ApJS, 131, 273

Greengard, L. & Lee, J-Y.,1996, Journal of Computational Phys., 125, 415

Greengard, L. & Rokhlin, V.,1987, Journal of Computational Phys., 73, 325

Harten, A., 1995, Comm. Pure Appl. Math., 48,1305

Hockney,R.W.& Eastwood,J.W.,(1988), *Computer Simulations Using Particles*, Bristol Adam Hilger.

Khokhlov, A.M.,1998, Journal of Computational Phys.,143,519

Knebe, A., Green, A. & Binney, J. 2003, MNRAS 313, 873

Kravtsov,A. V., Klypin,A. A. & Khokhlov, A. M., 1997, ApJS, 111, 73

Liu, X-D & Lax, P.D.,1996, Journ.Comput.Fluid Dyn., 5, 133

Londrillo, P., Nipoti, C.& Ciotti, L., 2003, Mem.S.A.it Supp., 1, 18

Londrillo, P. & Del Zanna, L., 2003, Journal of Computational Phys.(in press)

Roussel, O., Schneider, K. Tsigulis, A., Bockhorn, H., 2003, Journal of Computational Phys.,188,493

Springel, V., Yoshida, N. & White, S.D.M., 2001, New Astron., 6, 79

Teyssier, R., 2001, A&A,385, 337