Introducing Enzo, an AMR Cosmology Application

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Abstract. In this paper we introduce Enzo, a 3D MPI-parallel Eulerian block-structured adaptive mesh refinement cosmology code. Enzo is designed to simulate cosmological structure formation, but can also be used to simulate a wide range of astrophysical situations. Enzo solves dark matter N-body dynamics using the particle-mesh technique. The Poisson equation is solved using a combination of fast fourier transform (on a periodic root grid) and multigrid techniques (on non-periodic subgrids). Euler's equations of hydrodynamics are solved using a modified version of the piecewise parabolic method. Several additional physics packages are implemented in the code, including several varieties of radiative cooling, a metagalactic ultraviolet background, and prescriptions for star formation and feedback. We also show results illustrating properties of the adaptive mesh portion of the code. Information on profiling and optimizing the performance of the code can be found in the contribution by James Bordner in this volume.

1 Introduction

In astrophysics in general, and cosmology in particular, any given object of interest can have many important length and time scales. An excellent example of this is the process of galaxy formation. When studying the assembly of galaxies in a cosmological context, one wants to resolve a large enough volume of the universe to capture enough large-scale structure (a box with length on the order of several megaparsecs⁵). However, in order to adequately resolve

⁵ 1 parsec = 3.26 light years = 3.0857 × 10^{18} cm
structure in an individual galaxy one wants to have resolution two orders of magnitude smaller than the ultimate size of the objects of interest (a dwarf galaxy is on the order of $\sim 1$ kiloparsec). This typical cosmological problem requires roughly five orders of magnitude of dynamical range, which is prohibitively expensive when done using a single grid. Many other astrophysical phenomena, such as the study of molecular clouds and the formation of stars and galaxy clusters, require similarly large dynamical range. Many scientists have adopted Lagrangean techniques such as smoothed particle hydrodynamics (SPH)\textsuperscript{[1]} to address these issues. However, this type of method suffers from several drawbacks, including poor shock resolution and fixed mass resolution in regions of interest. The use of grid-based techniques with structured adaptive mesh refinement avoids many of these problems, and additionally allows the use of higher-order hydrodynamics schemes.

In this paper we present Enzo, an MPI-parallel 3D Eulerian adaptive mesh refinement code. Though it was originally designed to study cosmological structure formation, the code is extensible and can be used for a wide range of astrophysical phenomena. For more information on the performance and optimization of the Enzo code, see the contribution by James Bordner in this volume. The Enzo web page, which contains documentation and the source code, can be found at \url{http://cosmos.ucsd.edu/enzo/}.

2 Methodology

2.1 Application and AMR Implementation

Enzo is developed and maintained by the Laboratory for Computational Astrophysics at the University of California in San Diego. The code is written in a mixture of C++ and Fortran 77. High-level functions and data structures are implemented in C++ and computationally intensive lower-level functions are implemented in Fortran. Enzo is parallelized using the MPI message-passing library\textsuperscript{6} and uses the HDF5\textsuperscript{7} data format to write out data and restart files in a platform-independent format. The code is quite portable and has been ported to numerous parallel shared and distributed memory systems, including the IBM SPs and p690 systems, SGI Origin 2000s and numerous Linux Beowulf-style clusters.

The code allows hydrodynamic and N-body simulations in 1, 2 and 3 dimensions using the structured adaptive mesh refinement of Berger & Colella\textsuperscript{2}, and allows arbitrary integer ratios of parent and child grid resolution and mesh refinement based on a variety of criteria, including baryon and dark matter overdensity or slope, the existence of shocks, Jeans length, and cell cooling time. The code can also have fixed static nested subgrids,

\textsuperscript{6} http://www-unix.mcs.anl.gov/mpi/
\textsuperscript{7} http://hdf.ncsa.uiuc.edu/HDF5/
allowing higher initial resolution in a subvolume of the simulation. Refinement can occur anywhere within the simulation volume or in a user-specified subvolume.

The AMR grid patches are the primary data structure in Enzo. Each individual patch is treated as an individual object, and can contain both field variables and particle data. Individual patches are organized into a dynamic distributed AMR mesh hierarchy using arrays of linked lists to pointers to grid objects. The code uses a simple dynamic load-balancing scheme to distribute the workload within each level of the AMR hierarchy evenly across all processors.

Although each processor stores the entire distributed AMR hierarchy, not all processors contain all grid data. A grid is a real grid on a particular processor if its data is allocated to that processor, and a ghost grid if its data is allocated on a different processor. Each grid is a real grid on exactly one processor, and a ghost grid on all others. When communication is necessary, MPI is used to transfer the mesh or particle data between processors. The tree structure of a small illustrative 2D AMR hierarchy – six total grids in a three level hierarchy distributed across two processors – is shown on the left in Figure 1.

![Figure 1. Real and ghost grids in a hierarchy; real and ghost zones in a grid.](image)

Each data field on a real grid is an array of zones with dimensionality equal to that of the simulation (typically 3D in cosmological structure formation). Zones are partitioned into a core block of real zones and a surrounding layer of ghost zones. Real zones are used to store the data field values, and ghost zones are used to temporarily store neighboring grid values when required for updating real zones. The ghost zone layer is three zones deep in order to accommodate the computational stencil in the hydrodynamics solver (Section 2.3), as indicated in the right panel in Figure 1. These ghost zones can lead to significant computational and storage overhead, especially for the
smaller grid patches that are typically found in the deeper levels of an AMR grid hierarchy.

For more information on Enzo implementation and data structures, see references [3], [4], [5] and [6].

2.2 N-body Dynamics

The dynamics of large-scale structures are dominated by “dark matter,” which accounts for \( \sim 85\% \) of the matter in the universe but can only influence baryons via gravitational interaction. There are many other astrophysical situations where gravitational physics is important as well, such as galaxy collisions, where the stars in the two galaxies tend to interact in a collisionless way.

There are multiple ways that one can go about calculating the gravitational potential (which is an elliptical equation in the Newtonian limit) in a structured AMR framework. One way would be to model the dark matter (or other collisionless particle-like objects, such as stars) as a second fluid in addition to the baryon fluid and solve the collisionless Boltzmann equation, which follows the evolution of the fluid density in both physical space and velocity space (referred to collectively as “phase space”. This is computationally prohibitive due to the large dimensionality of the problem and because the interesting portion of the solution to the equation does not tend to occupy a small volume of the computational domain, which makes this approach unappealing in the context of an AMR code.

Enzo uses a totally different approach to collisionless systems, namely, the N-body method. This method follows trajectories of a representative sample of individual particles and is much more efficient than a direct solution of the Boltzmann equation in most astrophysical situations. The particle trajectories are controlled by a simple set of coupled equations (for simplicity, we omit cosmological terms):

\[
\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \tag{1}
\]

\[
\frac{d\mathbf{v}_p}{dt} = -\nabla \phi \tag{2}
\]

Where \( \mathbf{x}_p \) and \( \mathbf{v}_p \) are the particle position and velocity vectors, respectively, and the term on the right-hand side of the second equation is the gravitational force term. The solution to this can be found by solving the elliptic Poisson’s equation:

\[
\nabla^2 \phi = 4\pi G \rho \tag{3}
\]

where \( \rho \) is the density of both the collisional fluid (baryon gas) and the collisionless fluid (particles).
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These equations are finite-differenced and for simplicity are solved with the same timestep as the equations of hydrodynamics. The dark matter particles are sampled onto the grids using the triangular-shaped cloud (TSC) interpolation technique to form a spatially discretized density field (analogous to the baryon densities used to calculate the equations of hydrodynamics) and the elliptical equation is solved using FFTs on the triply periodic root grid and multigrid relaxation on the subgrids. Once the forces have been computed on the mesh, they are interpolated to the particle positions where they are used to update their velocities.

2.3 Hydrodynamics

The primary hydrodynamic method used in Enzo is based on the piecewise parabolic method (PPM) of Woodward & Colella [7] which has been significantly modified for the study of cosmology. The modifications and several tests are described in Bryan et al. [8], but we provide a short description here.

PPM is a higher-order-accurate version of Godunov’s method with third-order-accurate piecewise parabolic monotonic interpolation and a nonlinear Riemann solver for shock capturing. It does an excellent job capturing strong shocks and outflows. Multidimensional schemes are built up by directional splitting, and produce a method that is formally second-order-accurate in space and time and explicitly conserves energy, momentum and mass flux. The conservation laws for fluid mass, momentum and energy density are written in comoving coordinates for a Friedman-Robertson-Walker spacetime. Both the conservation laws and Riemann solver are modified to include gravity, as calculated in Section 2.2.

There are many situations in astrophysics, such as the bulk hypersonic motion of gas, where the kinetic energy of a fluid can dominate its internal energy by many orders of magnitude. In these situations, limitations on machine precision can cause significant inaccuracy in the calculation of pressures and temperatures in the baryon gas. In order to address this issues, Enzo solves both the internal gas energy equation and the total energy equation everywhere on each grid, at all times. This dual energy formalism ensures that the method yields the correct entropy jump at strong shocks and also yields accurate pressures and temperatures in cosmological hypersonic flows.

As a check on our primary hydrodynamic method, we also include an implementation of the hydro algorithm used in the Zeus astrophysical code. [9, 10] This staggered grid, finite difference method uses artificial viscosity as a shock-capturing technique and is formally first-order-accurate when using variable timesteps (as is common in structure formation simulations), and is not the preferred method in the Enzo code.

2.4 Additional Physics Packages

Several physics packages are implemented in addition to dark matter and adiabatic gas dynamics. The cooling and heating of gas is extremely important...
in astrophysical situations. To this extent, two radiative cooling models and several uniform ultraviolet background models have been implemented in an easily extensible framework.

The simpler of the two radiative cooling models assumes that all species in the baryonic gas are in equilibrium and calculates cooling rates directly from a cooling curve assuming $Z = 0.3 Z_\odot$. The second routine, developed by Abel, Zhang, Anninos & Norman [11, 12], assumes that the gas has primordial abundances (ie, a gas which is composed of hydrogen and helium, and unpolluted by metals), and solves a reaction network of 28 equations which includes collisional and radiative processes for 9 separate species ($H, H^+, He, He^+, He^{++}, H^-, H_2^+, H_2, e^-$). In order to increase the speed of the calculation, this method takes the reactions with the shortest time scales (those involving $H^-$ and $H_2^+$) and decouples them from the rest of the reaction network and imposes equilibrium concentrations, which is highly accurate for cosmological processes. See Anninos et al. [12] and Abel et al. [11] for more information.

The vast majority of the volume of the present-day universe is occupied by low-density gas which has been ionized by ultraviolet radiation from quasars, stars and other sources. This low density gas, collectively referred to as the “Lyman-α Forest” because it is primarily observed as a dense collection of absorption lines in spectra from distant quasars (highly luminous extragalactic objects), is useful because it can be used to determine several cosmological parameters and also as a tool for studying the formation and evolution of structure in the universe (see [13] for more information). The spectrum of the ultraviolet radiation background plays an important part in determining the ionization properties of the Lyman-α forest, so it is very important to model this correctly. To this end, we have implemented several models for uniform ultraviolet background radiation based upon the models of Haardt & Madau [14].

One of the most important processes when studying the formation and evolution of galaxies (and to a lesser extent, groups and clusters of galaxies and the gas surrounding them) is the formation and feedback of stars. We use a heuristic prescription similar to that of Cen & Ostriker [15] to convert gas which is rapidly cooling and increasing in density into star “particles” which represent an ensemble of stars. These particles then evolve collisionlessly while returning metals and thermal energy back into the gas in which they formed via hot, metal-enriched winds.

As mentioned in Section 1, Enzo can be downloaded from the web at http://cosmos.ucsd.edu/enzo/ Vigorous code development is taking place, and we are in the process of adding ideal magnetohydrodynamics and a flux-limited radiation diffusion scheme to our AMR code, which will significantly enhance the capabilities of the code as a general-purpose astrophysical tool.
3 Adaptive Mesh Characteristics

The adaptive nature of grid cells in the AMR simulations results in a wide range of baryon mass scales being resolved. Figure 2 shows the distribution of cells as a function of overdensity for a range of Enzo simulations in a simulation volume which is $3 \, h^{-1}$ megaparsecs on a side. These simulations use either a $64^3$ or $128^3$ root grid and either 5 or 6 levels of refinement (such that $L_{\text{box}}/e = 4096$, where $L_{\text{box}}$ is the box size and $e$ is the smallest spatial scale that can be resolved). All grids are refined by a factor of 2.0, and grids are refined when dark matter density (baryon density) exceeds a factor of 4.0 (2.0) times the mean density of cells at that level. In addition, a simulation is performed where the overdensity threshold is doubled. Initial conditions are generated using power spectra and methods common to cosmological simulations. Examination of Figure 2 shows that the entire density range in the simulations is covered by large numbers of cells. In particular, cells at low densities are well-resolved in these simulations, which is in stark contrast to simulations performed using Lagrangian methods, which are typically undersampled at low density. Raising the overdensity threshold for refinement decreases the total number of cells but their relative distribution as a function of overdensity is unchanged. In all simulations the total number of cells at the end of the run has increase by a factor of $\sim 8 - 10$ from the number of cells in the root grid.

Figure 3 shows the distribution of number of cells at the end of a simulation as a function of the mass of baryons in that cell. Arrows indicate the mean cell mass contained on the root grid at the onset of the simulation for simulations covering the same spatial volume as the simulations described above with a $64^3$, $128^3$ or $256^3$ root grid (labelled N64, N128 and N256, respectively). Over the course of the simulation the mean mass resolution, as indicated by the peak of the distribution, increases by almost an order of magnitude relative to the initial mass resolution, though the distribution of cell masses is quite large. Figure 3 shows that the mean cell mass as a function of overdensity (at the end of the simulation run) stays fairly constant, which lower mean cell masses in underdense regions and higher mean cell masses in highly overdense regions (presumably due to the limitation on the number of levels of adaptive mesh refinement allowed). The mean cell mass over the entire density range is between $\sim 5 - 10$ times better than the starting mass resolution for all simulations. Runs with lower overdensity criteria for refinement have somewhat better mass resolution overall.

4 Summary

In this paper we have presented Enzo a cosmology code which combines collisionless N-body particle dynamics with a hydrodynamics package based on the piecewise parabolic method, all within a block-based adaptive mesh refinement
algorithm. Several other physics packages are implemented, including multiple models for gas cooling and ionization, a uniform ultraviolet background model for gas heating, and a prescription for star formation and feedback.

**Enzo** is being released to the public as a community astrophysical simulation code. This code is being modified and documented to be as widely useful as possible, and can be found at [http://cosmos.ucsd.edu/enzo/](http://cosmos.ucsd.edu/enzo/). Active development is taking place, centering on the addition of magnetohydrodynamics and a diffusive radiative transfer algorithm.

Further information concerning the performance of the **Enzo** code (including a package of performance monitoring and visualization tools) is described in a contribution by James Bordner in this volume, and on the **Enzo** website.
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Fig. 3. Number of cells as a function of baryonic mass (normalized to bin size) for several Enzo simulations with \( L_{\text{box}} = 3h^{-1}\)Mpc. The arrows correspond to the mean mass resolution of the root grid for simulation volumes with the same volume but root grids with \( 64^3, 128^3 \) or \( 256^3 \) cells (labelled N64, N128 and N256, respectively). See Figure 2 for a description of the line labels.

Fig. 4. Mean baryonic mass in cells as a function of baryon overdensity (normalized to bin size) in Enzo simulations. These are the same simulations (with the same labels) as in Figure 2. Horizontal lines correspond to the initial mean mass resolution of simulations with the same volume but \( 64^3, 128^3 \) and \( 256^3 \) root grid cells (labelled N64, N128 and N256, respectively).
References

[1] J. J. Monaghan. Smoothed particle hydrodynamics. *Annual Review of Astronomy & Astrophysics*, 30:543, 1992.

[2] M. J. Berger and P. Colella. Local adaptive mesh refinement for shock hydrodynamics. *J. Comp. Phys.*, 82:64–84, 1989.

[3] G. L. Bryan and M. L. Norman. A hybrid amr application for cosmology and astrophysics. In N. Christochoines, editor, *Workshop on Structured Adaptive Mesh Refinement Grid Methods*, page 165. IMA Volumes in Mathematics No. 117, 2000.

[4] G. L. Bryan and M. L. Norman. In D. A. Clarke and M. Fall, editors, *Computational Astrophysics; 12th Kingston Meeting on Theoretical Astrophysics*, proceedings of meeting held in Halifax; Nova Scotia; Canada October 17-19; 1996. ASP Conference Series # 123, 1997.

[5] G. L. Bryan. Fluids in the universe: Adaptive mesh in cosmology. *Computing in Science and Engineering*, 1:2:46, 1999.

[6] M. L. Norman and G. L. Bryan. Cosmological adaptive mesh refinement. In Kohji Tomisaka Shoken M. Miyama and Tomoyuki Hanawa, editors, *Numerical Astrophysics : Proceedings of the International Conference on Numerical Astrophysics 1998 (NAP98), held at the National Olympic Memorial Youth Center, Tokyo, Japan, March 10-13, 1998.*, page 19. Kluwer Academic, 1999.

[7] P. R. Woodward and P. Colella. A piecewise parabolic method for gas dynamical simulations. *J. Comp. Physics*, 54:174, 1984.

[8] G. L. Bryan, M. L. Norman, J. M. Stone, R. Cen, and J. P. Ostriker. A piecewise parabolic method for cosmological hydrodynamics. *Comp. Phys. Comm.*, 89:149–168, 1995.

[9] J. M. Stone and M. L. Norman. Zeus-2d: A radiation magnetohydrodynamics code for astrophysical flows in two space dimensions. i - the hydrodynamic algorithms and tests. *ApJ*, 80:753, 1992.

[10] J. M. Stone and M. L. Norman. Zeus-2d: A radiation magnetohydrodynamics code for astrophysical flows in two space dimensions. ii. the magnetohydrodynamic algorithms and tests. *ApJ*, 80:791, 1992.

[11] T. Abel, P. Anninos, Y. Zhang, and M. L. Norman. Modeling primordial gas in numerical cosmology. *New Astronomy*, 2:181–207, August 1997.

[12] P. Anninos, Y. Zhang, T. Abel, and M. L. Norman. Cosmological hydrodynamics with multi-species chemistry and nonequilibrium ionization and cooling. *New Astronomy*, 2:209–224, August 1997.

[13] M. Rauch. The Lyman Alpha Forest in the Spectra of QSOs. *Annual Review of Astronomy and Astrophysics*, 36:267–316, 1998.

[14] F. Haardt and P. Madau. Radiative Transfer in a Clumpy Universe. II. The Ultraviolet Extragalactic Background. *ApJ*, 461:20—+, April 1996.

[15] R. Cen and J. P. Ostriker. Galaxy formation and physical bias. *ApJL*, 399:L113–L116, November 1992.