DEVELOPMENT OF A SCALABLE GRAVITY SOLVER FOR ENZO–E

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EXECUTIVE SUMMARY

Blue Waters was used to develop and profile a highly scalable version of the Enzo cosmological adaptive mesh refinement (AMR) code called Enzo–E (E for extreme scale) [4]. In this project, the research team illustrated the weak scaling results of the domain-decomposed AMR Poisson solver using a suite of dark matter clustering simulations.

RESEARCH CHALLENGE

Improved computational models of the intergalactic medium (IGM) are needed to extract information encoded in the high-resolution optical spectra of distant quasars. That information includes the physical state of the mostly primordial gas pervading the Universe but also the dark matter that shapes the gas into discrete intergalactic absorption line systems (the Lyman-α forest). Standard computational models are discrepant with respect to certain aspects of the observational data [1] suggesting there is some key ingredient missing in the models. Previously, the research team explored whether modeling the population of quasars that provide a photoionizing bath of ultraviolet radiation as discrete point sources rather than a homogeneous background could improve agreement with observations. The team found it does not, using the Enzo hydrodynamic cosmology code [2] enhanced with multigroup flux-limited diffusion radiative transfer. The team is, therefore, investigating its next hypothesis: that dense gas bound to galaxies that is unresolved in the Enzo simulations supplies significant absorption of the quasar light and modifies the key observables in such a way as to improve agreement with observations.

METHODS & CODES

Including galaxies in simulations of the IGM poses severe resolution requirements that can be addressed using adaptive mesh refinement (AMR) around galaxies. However, Enzo's AMR capability is not sufficiently scalable to permit a full frontal assault on this problem. For this reason, the research team has been developing a successor to the Enzo code called Enzo–E built on an entirely new highly scalable AMR framework called Cello [3]. The combined code—Enzo–E/Cello—uses the Charm++ parallel object framework for parallelization. The team has implemented the proven-scalable Forest-of-Octrees AMR algorithm [4] on top of Charm++ and has obtained excellent parallel scaling results on Blue Waters as a prelude to the target application.

Solving the elliptic Poisson equation on the Forest-of-Octrees adaptive mesh is a prerequisite for cosmological applications. In the past year, the team has developed such a solver and profiled it on Blue Waters. Fig. 1 shows its application to a pure dark matter N-body simulation. The left side shows the projection of the dark matter density onto the adaptive mesh at redshift 7.5 in a cubic volume 6 comoving megaparsecs on a side. The right side shows the projection of the adaptive mesh, with levels of refinement encoded in color: root grid = dark blue; levels 1, 2, 3, 4 = light blue, green, yellow, and red, respectively. Each square is the projection of a block of 16 x 16 x 16 computational cells, on which the gravitational potential was solved using the following method.

First, the dark matter particle masses were assigned to the grid block that contains them using Cloud-In-Cell interpolation. Second, the matter densities were projected to the root grid (level 0). Third, the global gravitational potential was computed on the root grid using a V-cycle multigrid solver. Fourth, the gravitational potential was interpolated from the root grid to the faces of each octree. Fifth, the gravitational potential was computed for each octree using a multilevel iterative solver (BiCGStab). Finally, the potential was smoothed across all the leaf nodes of all octrees using Jacobi smoothing.

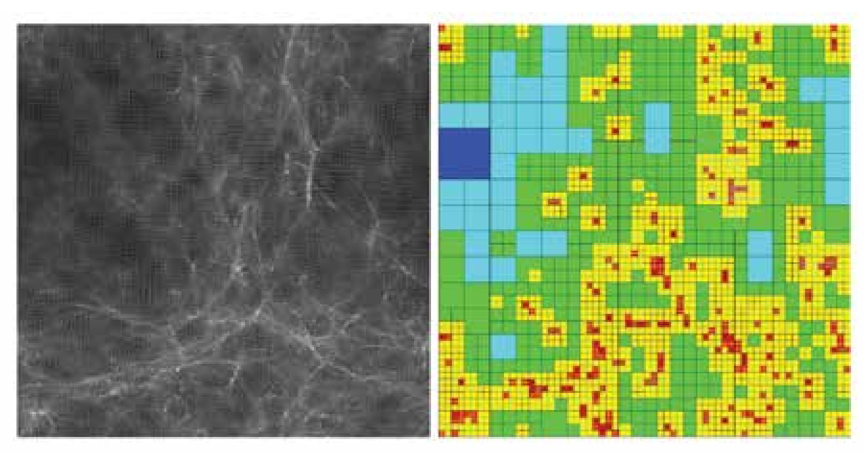

Figure 1: Left—The gravitational clustering of dark matter in a six megaparsec volume of the Universe. Right—The array-of-octree computational mesh. Each square is the projection of a cubic region of space resolved by 16 x 16 x 16 cells. This computation uses five levels of mesh refinement, color coded by level.

RESULTS & IMPACT

The DD (domain-decomposed) Poisson solver described above was implemented and tested on Blue Waters in the context of dark matter-only cosmological structure formation simulations. Weak scaling results are shown in Fig. 2. The research team plotted wall time per timestep versus timestep for four simulations in box sizes 3, 6, 12, and 24 comoving megaparsecs on a side, with root grid resolutions of 64^3, 128^3, 256^3, and 512^3 cells. These correspond to 4^3, 8^3, 16^3, and 32^3 arrays of blocks of 16^3 cells each. Each root grid block is the base of a separate octree, which refines as structure forms. With 8 root grid blocks per core, the simulations were run on 8, 64, 512, and 4,096 cores of Blue Waters. At early times, before cycle 100, mesh refinement had not begun, and the execution time was dominated by the global multigrid solver. At later times, up to a factor of 100 more refined blocks at all levels were created to resolve structure formation. Execution time was dominated by the BiCGStab tree solver. The fact that the curves from different runs bunch together at late times indicated favorable weak scaling of the DD solver.

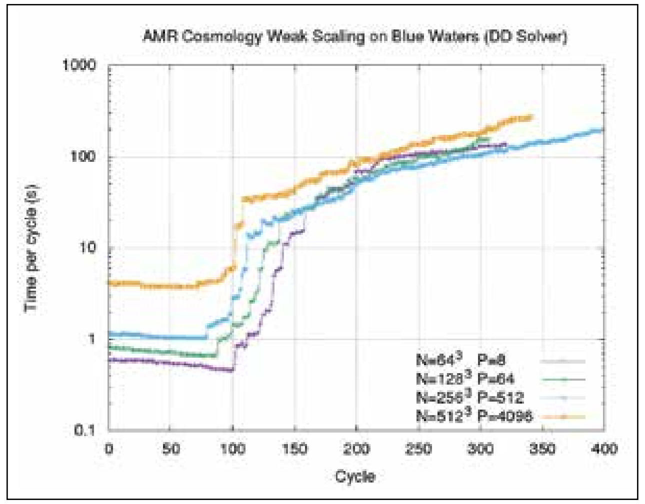

Figure 2: Wall time per timestep vs. timestep for four cosmological AMR simulations performed with Enzo–E comprising a weak scaling study. Growth in wall time reflects the creation of additional blocks as structure forms. The four simulations have 4^3, 8^3, 16^3, and 32^3 octrees, with eight octrees assigned to each core.

WHY BLUE WATERS

It is essential to have a petascale resource like Blue Waters to develop an application for exascale machines. The sheer size, the favorable queue structure, and the excellent throughput at large core counts were instrumental during the code development and test phase of this research. In the process of developing the DD solver, certain synchronization issues only showed up at large scale (P > 1,000). It was essential to be able to turn around large test runs quickly as the research team diagnosed the problem.

PUBLICATIONS & DATA SETS

J. O. Bordner and M. L. Norman, "Computational cosmology and astrophysics in adaptive meshes using Charm++," presented at the SC'18 PAW–ATM Workshop. [Online]. Available: https://arxiv.org/abs/1810.01319

Enzo –E GitHub repository. [Online]. Available: https://github.com/enzo-project/enzo-e