LUSciD Cosmology Status Report, 3Q2007

Milestones and Deliverables

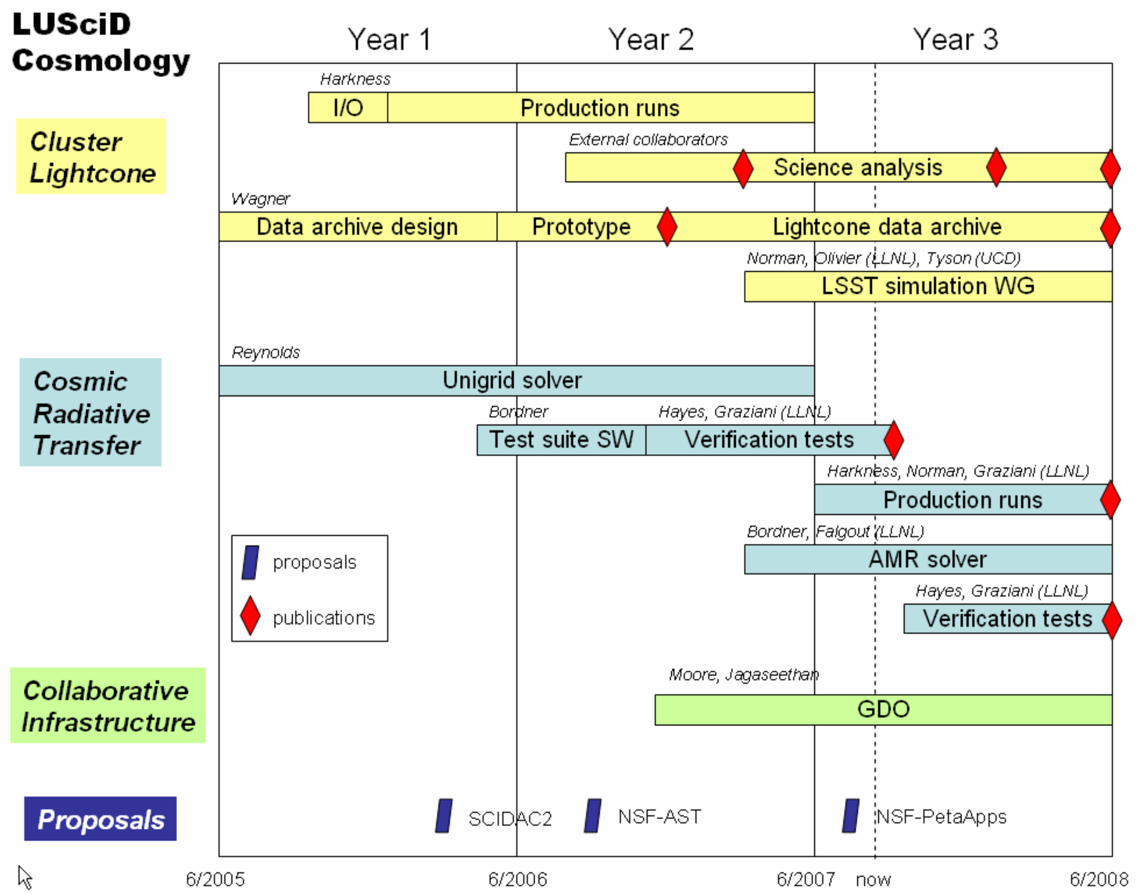

Fig. 1. Cosmology project timeline.

The project timeline shown above summarizes the main activities within the cosmology project. Progress is as follows. Names in parenthesis without affiliations are at UCSD and funded by the LUSciD project.

Production runs (Harkness)

The production runs for the Lightcone simulations have been completed on Thunder. Table 1 summarizes their properties. Fig. 2 shows a striking volumetric rendering of Tile 16 done at NCSA. Production runs exercising our new cosmic radiation transfer scheme have not begun as we are completing verification tests at the present time.

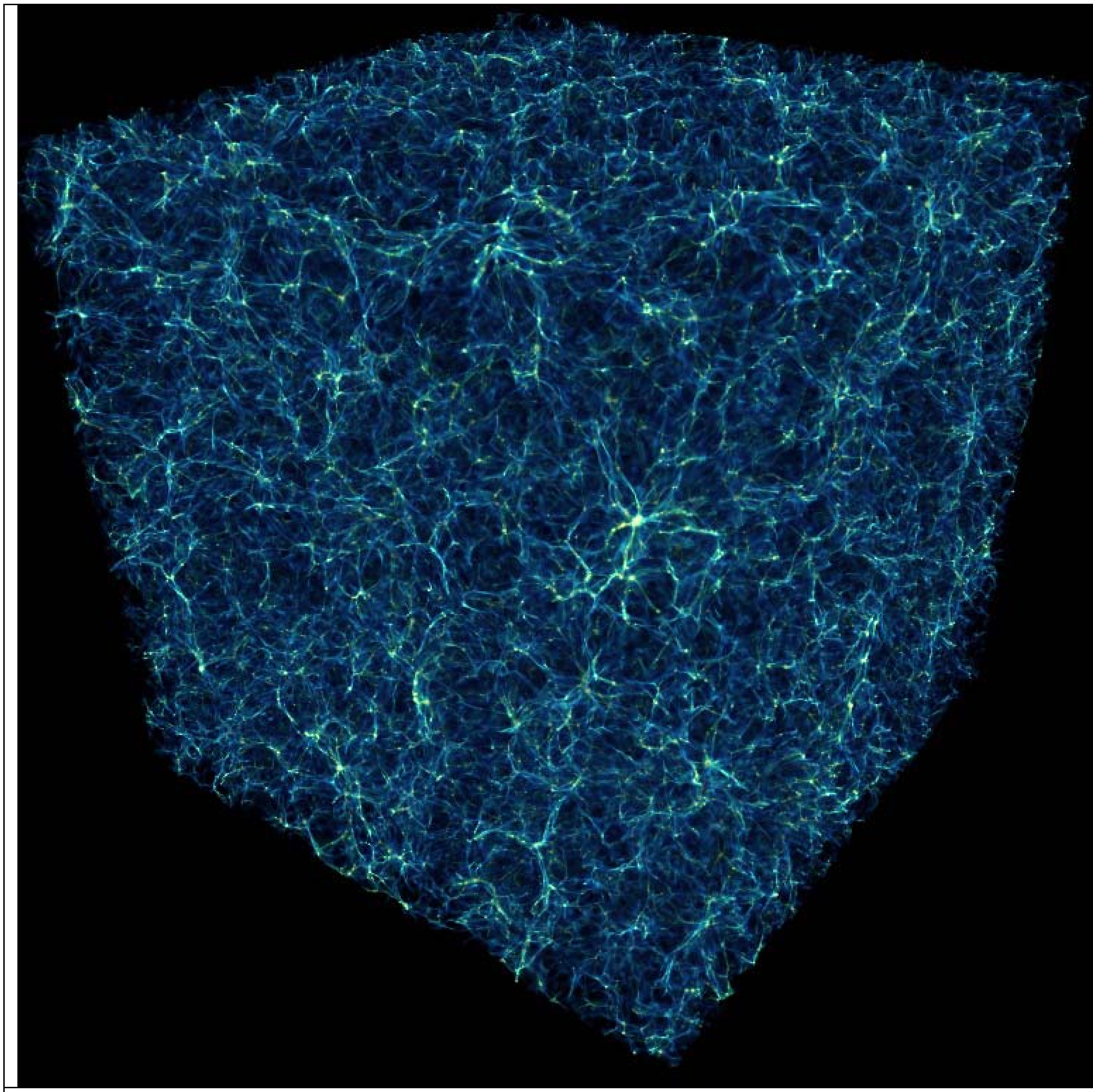

Fig. 2. Volumetric rendering of cosmological structure in a portion of the Lightcone simulation carried out at LLNL as a part of the LUSciD project. The AMR code Enzo was used to simulate the distribution of galaxy clusters in a volume 2 billion light years on a side with an effective resolution in the cluster cores of a $(65{,}536)^3$ grid.

Table 1. Light-cone simulations details

Tile	**Z_stop**	**L_box** (Mpc/h)	**N_part**	**N_cpu**	**N_levels**	**Δx_min (kpc/h)**	**M_dm (Msol/h)**
1	3	851.71	896^3	1372	3	119	$2x10^{10}$
2	2.63	851.71	896^3	1372	3	119	$2x10^{10}$
3	2.29	730.04	768^3	1728	3	119	$2x10^{10}$
4	1.99	730.04	768^3	1728	3	119	$2x10^{10}$
5	1.72	608.36	640^3	1000	3	119	$2x10^{10}$
6	1.48	608.36	640^3	1000	3	119	$2x10^{10}$
7	1.26	486.69	512^3	512	3	119	$2x10^{10}$
8	1.07	512	512^3	512	7	7.8	$7.2x10^{10}$

9	0.91	512	512^3	512	7	7.8	7.2×10^{10}
10	0.76	512	512^3	512	7	7.8	7.2×10^{10}
11	0.63	512	512^3	512	7	7.8	7.2×10^{10}
12	0.52	512	512^3	512	7	7.8	7.2×10^{10}
13	0.42	512	512^3	512	7	7.8	7.2×10^{10}
14	0.32	512	512^3	512	7	7.8	7.2×10^{10}
15	0.22	512	512^3	512	7	7.8	7.2×10^{10}
16	0.11	512	512^3	512	7	7.8	7.2×10^{10}

Science analysis (Norman, Harkness, Wagner, Skory)
Harkness, Wagner and Skory are developing software to analyze the massive volumes of Lightcone data. Harkness is developing a parallel version of Enzo's AMR (adaptive mesh refinement) halo finder HOP. Wagner is developing a parallel AMR ray caster for applications to weak lensing. Skory is developing software to generate LSST mock galaxy catalogs from the Lightcone data that will be used to generate simulated LSST sky maps.

Lightcone data archive (Wagner)
Rick's stuff here.

LSST simulation working group (Norman, Olivier (LLNL collaborator), Tyson (LSST PI))
The LSST simulation working group is a standing working group whose goal is to carry out an end-to-end simulation of the LSST telescope, camera, and analysis pipeline in realistic usage scenarios as proof-of-concept. Up until now, the WG has focused mainly on simulating the light path from the top of the Earth's atmosphere to the CCD detector. Beginning in February Norman began participating in WG telecoms to consider how one could simulate the light path from cosmological distances to the top of the atmosphere.

Norman visited Olivier and the LLNL data management team in June, and interacted with Olivier, Tyson and Croton by telecom in July. The outgrowth of those discussions is detailed plan for the next 12 months to produce LSST mock galaxy catalogs and from them, simulated LSST sky images. This plan is attached as an appendix. SDSC staff scientist Robert Harkness and UCSD graduate students Rick Wagner and Stephen Skory embarked on this plan starting October 1.

Radiation transport code development (Reynolds, Hayes (LLNL collaborator), So (ISCR summer intern))
Progress in radiation transport in Enzo over the last 6 months has proceeded along two main paths: (1) setting up and running various radiation, radiation-hydrodynamics, and radiation-chemical ionization test problems, and (2) implementing software enhancements to enable these and future simulations in these regimes.

Test problems and results:
Three verification problems were implemented to test the radiation diffusion module under the assumption of two-temperature grey diffusion in media with a constant (and

spatially uniform) ionization state. The first of these, due to Turner and Stone [1], initializes a spatially homogenous medium with different matter and radiation temperatures and follows the subsequent evolution to the final equilibrium state. Material properties are chosen such that the specific heat of the material is much lower than that of the radiation, so that the radiation temperature remains virtually unchanged and the material simply equilibrates to this value. Figure 1 shows results for two cases, in which the initial matter temperature is much higher/lower than the radiation temperature. In both cases the material equilibrates to the correct value, shown by the dashed line.

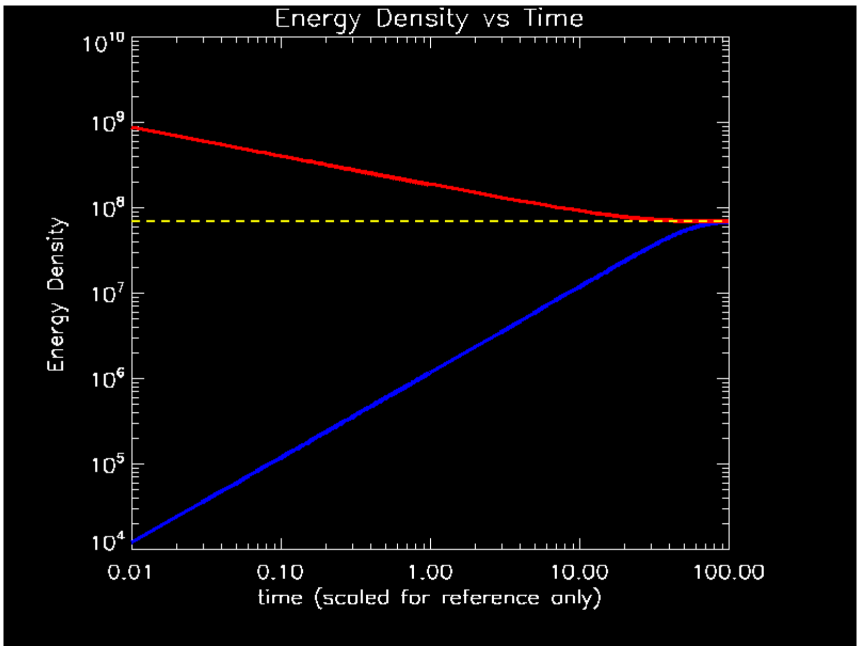

Figure 1: Turner & Stone test problem of matter-radiation equilibration in a spatially homogeneous medium.

Because all material and radiation properties remain spatially uniform, the Turner & Stone problem tests the matter-radiation terms in isolation. Our second problem is a classic diffusion test due to Su and Olson [2], in which a constant flux is incident on an initially uniform medium on the left boundary. A radiation wave therefore propagates across the domain; this radiation wave is initially far out of equilibrium with the material. The medium is assumed to remain static, so this problem tests the diffusion operator in combination with matter coupling, but without hydrodynamics. The problem is constructed so that an exact semi-analytic solution for the radiation and material temperatures, as functions of space and time, may be derived. The exact solution is formulated in terms of dimensionless radiation and gas energies (U and V), a dimensionless length coordinate (X), and dimensionless time (tau). The strength of the matter-radiation coupling is controlled by a dimensionless parameter, epsilon. The Su and Olson paper tabulates exact values of U and V on a grid of X-tau values for epsilons of 0.1 and 1.0. Figure 2 shows Enzo results for the case of epsilon = 0.1 at tau values of 1, 3, 10, 30, and 100, with exact solution values provided by the black points.

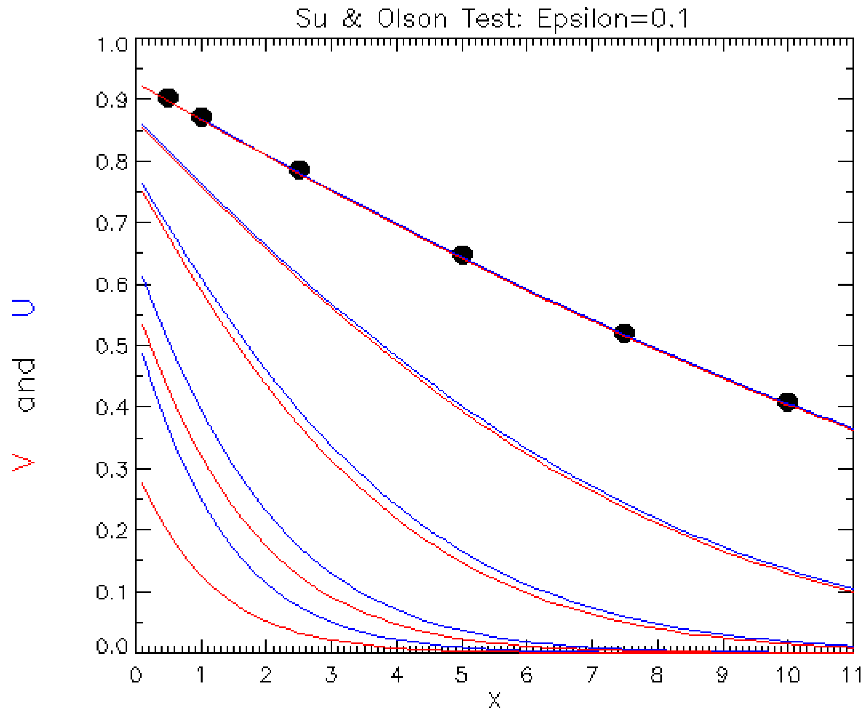

Figure 2: Su & Olson test problem, radiation diffusion interacting with matter coupling.

Our third and most general test that excludes chemistry is a subcritical radiating shock wave; this test thus combines the full grey radiation machinery with Enzo's PPM-based hydrodynamic solver. The shock wave is generated by imposing a steady inflow of material against a reflecting boundary. The parameters of the problem are taken from a preprint by Lowrie and Edwards [3], who describe both the test problem and a procedure for generating an exact semi-analytic solution that assumes 2-T grey radiation diffusion. Construction of the semi-analytic solution is a non-trivial exercise and is a "work in progress" as of this writing. Figure 3 shows results for a Mach-2 subcritical radiating shock wave. The height and shape of the "spike" in the gas temperature is extremely sensitive to the Mach number, and its detailed structure is precisely specified by the exact solution. As noted in [3], higher Mach numbers require extremely high spatial resolution to capture the detailed structure of the temperature spike; simulations at higher Mach numbers will therefore provide excellent tests once the radiation module is fully interfaced with the adaptive mesh refinement algorithm.

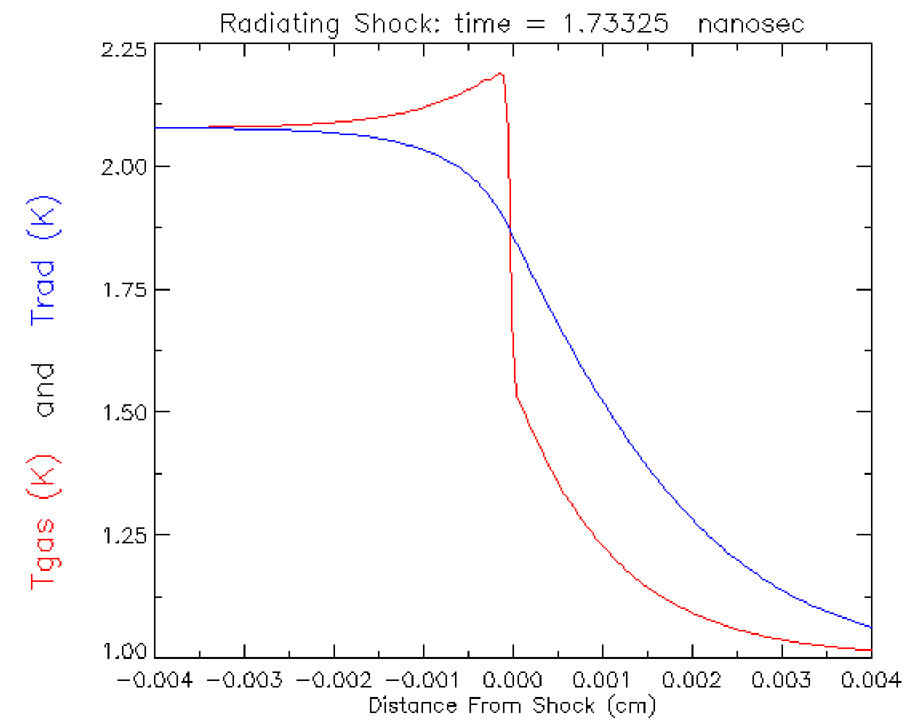

Figure 3: Lowrie & Edwards test problem of a Radiating shock wave.

Our final test problem performed during this time period is that of isothermal chemical ionization of an initially-neutral Hydrogen region due to radiation emitted from a point source; this test thus combines the full grey radiation machinery with chemical model of Hydrogen ionization. The problem parameters are taken from paper by Iliev et al. [4] , in which a number of cosmological radiative transfer codes have been compared on a variety of test problems. The problem performed here allows an analytical solution for the propagation of both the radiation through the domain, as well as the HII ionization front.

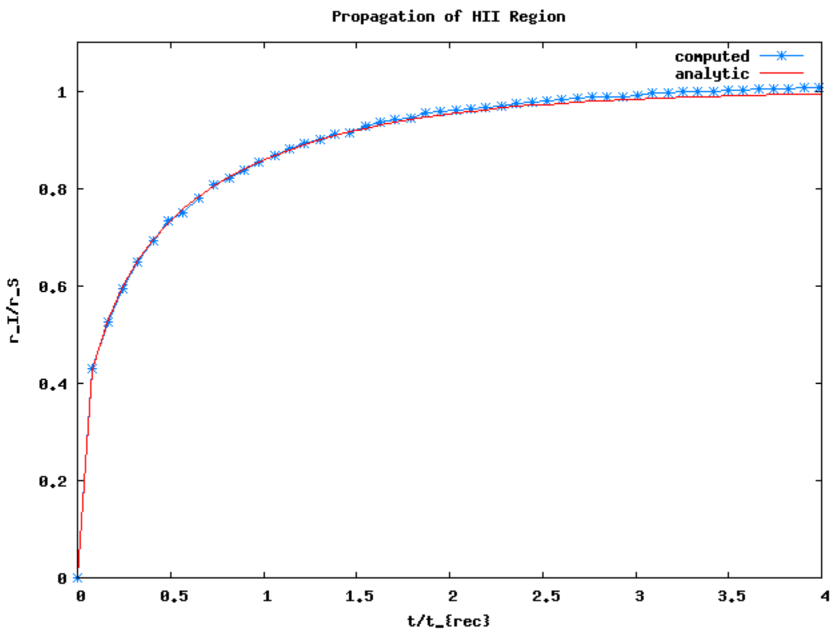

Figure 4: Iliev et al. test of isothermal radiation-induced ionization of an initially neutral Hydrogen region.

Figure 4 provides comparisons of the computed ionization front location (blue, starred curve) with the analytically predicted solution (red curve), in which the ionization front expand until it approaches the Strömgren radius r_s, at which point the HII -> HI recombinations balance the HI -> HII ionizations. The results shown in Figure 4 were performed on a very coarse 32^3 uniform spatial discretization, whereas the simulations in the comparison paper were performed on a resolution of 256^3. We therefore are using this problem as a suitable test for examining scalability of the fully implicit nonlinear solver infrastructure, as well as the inner linear solver provided by the HYPRE library (here given by their SMG solver). In addition, we are currently implementing the second of the tests from this paper, in which the same problem is performed while allowing the gas temperature to vary due to heating and cooling interactions with the radiation and chemical fields.

Software enhancements:

Several algorithmic refinements were required in support of these verification tests. The boundary conditions for the Su & Olson problem require special attention. The problem specifies that the incident flux remain constant on the left boundary, which implies a time-varying radiation energy density in the boundary zone to satisfy that constraint. The radiation energy on the boundary is set by evaluating the semi-analytic solution for U (which must be computed numerically) for X = 0, and mapping to code coordinates appropriately. The outer boundary is specified to be a vacuum boundary with zero incident flux. The correct outward flux is achieved by modifying the diffusion coefficient on the boundary so that the diffusive flux matches that predicted by a transport solution for a hot "infinite plane" abutting a vacuum. Neither a simple "zero energy" Dirichlet nor "zero flux" Neumann condition captures this physics correctly. The appropriate treatment for vacuum boundary conditions on the diffusion equation will be documented in the forth-coming Enzo method paper [5].

In addition to adjusting the relevant boundary conditions for the Su & Olson problem, we have added a number of algorithmic enhancements to the nonlinear solver and coupled PDE infrastructure during this time period. The first among these is that we have derived and implemented analytical Jacobian computations for use within the Newton nonlinear solver algorithm, for a number of relevant RT modeling systems (two temperature only, radiation plus chemistry, etc.). Previous to this enhancement, Jacobian elements for the Newton system were approximated using finite differences, allowing rapid prototyping of various modeling problems, but at the expense of decreased accuracy and increased computational work. With these new analytical Jacobians, the solver is more efficient in both its construction and convergence.

We have also incorporated user-control over solution units in these calculations, and have adjusted the solvers to use these units to non-dimensionalize the implicit systems of equations. Such an improvement allows the solver to better balance the amount of computational effort used in solving such coupled PDE systems involving variables with highly varying solution magnitudes (e.g. the Iliev et al. problem involved radiation energy densities on the order of 1e-15, chemical species densities on the order of 1e-27, and specific gas energy densities on the order of 1e+12).

Also for the Iliev et al. ionization problem, we extended the physics capabilities of the radiation module and associated equations to allow for solution to the monochromatic radiation energy equation (as opposed to the integrated, Grey, radiation energy equation). Additionally, we have adjusted the formulae for computation of the flux limiter used within the radiation diffusion coefficient to allow for extremely small opacities (e.g. 1e-26), as are prevalent in cosmology applications.

An additional solver enhancement is the ability to prescribe one of a variety of methods to generate an initial guess for the nonlinear solver at a given time step. It is well known that gradient-based nonlinear solvers (like Newton's method) are very sensitive to the initial guess – a good initial guess can guarantee extremely-fast quadratic convergence of the solver, whereas a bad initial guess can lead to divergence of the algorithm. We have incorporated a number of popular and novel initial guess strategies, with user control over the algorithm to be used. We plan to investigate the benefit of these and other strategies on the target reionization problems, when we have reached the point of production runs.

Due to the increased freedom in choosing time steps within implicit simulations (no CFL stability restriction), we have also incorporated a rather simple adaptive time step selection strategy. This strategy chooses time step sizes based on anticipated change in the solution values over the course of an individual time step, reducing or increasing the time step size during the simulation in an attempt to obtain the largest step possible while keeping the anticipated change in solution to within a user-specified tolerance.

In anticipation of very large scale simulations, we have restructured our communication routines for implicit problem data as well as the overall nonlinear solver algorithm to better interleave communication and computation, in hope of achieving increased scalability and defraying the additional inter-processor communication cost inherent to implicit solver algorithms.

Lastly, while our target applications involve 3D simulations, we have also begun implementation of reduced-dimensionality capabilities in the module for 2D and 1D problems, allowing for more efficient simulations of analytical test problems and nightly regression tests, as well as investigations of implicit solver scalability and efficiency due to time step stability as problems are highly refined in space. Such studies will allow us to estimate the potential benefit of such fully implicit simulations for 3D AMR calculations, which will also involve highly refined spatial regions.

We plan to include descriptions of all of these algorithmic enhancements, as well as documentation of the fully coupled implicit formulation in the forth-coming method paper [5].

hypre-solve (Bordner)
Development has begun on "hypre-solve", in preparation for adding AMR radiation transfer support to Enzo. hypre-solve is designed to be a lightweight, flexible testing framework for setting up linear systems defined on AMR grids for realistic test problems, applying LLNL CASC's hypre linear solvers to the test problems, and analyzing solver performance, robustness, accuracy, and scaling.

Development will proceed in three stages: discretizing the Poisson equation (which is used in Enzo for computing self-gravity) and solving the resulting linear system with hypre's solvers. The scope of the test problems is an arbitrary collection of point masses and massive spheres discretized on a parallel distributed AMR hierarchy. I expect to finish implementing this first stage in a about month. Subsequent stages, which will build on the first stage, will be single-group RT problems, and multi-group AMR RT. After each stage is complete and solvers have been tuned, code will be migrated to the Enzo RT branch.

Bordner progress goes here.

Collaborative Interactions

Norman, Reynolds, and Bordner visited LLNL in early June to collaborate with Hayes and Falgout on aspects of the radiation transport component of the project, as well as to brief potential collaborators on its goals and progress. Norman visited with Olivier to discuss LSST image simulation progress. Bordner interacts with the Hypre group via email. UCSD physics graduate student was a LLNL summer intern, and was mentored by LLNL staff member John Hayes working on radiation verification tests.

Proposals

Norman submitted a proposal to the NSF Petascale Applications program (PetaApps), which is still pending. Norman and Moore plan to submit to the NSF CDI program directly building on the work begun here within the LUSciD project.

Publications

None in this quarter.

References

[1] Turner, N. & Stone, J., 2001, ApJ. Supp., 135, 95-107.
[2] Su, B. & Olson, G., 1996, JQSRT, vol. 56, No. 3, 337-351.
[3] Lowrie, R. & Edwards, J., 2007, Shock Waves, submitted.
[4] Iliev et al., Mon. Not. R. Astron. Soc., vol 371, 1057-1086.
[5] Bryan, G. et al., 2008, in preparation.

Appendix: LSST Lightcone Project Plan (Aug. 10, 2007)

Goal

Simulate LSST image fields containing lensed galaxies to a depth of z=3.

Approach

1. Simulate cosmic structure in a 100 sq. deg. lightcone to a depth of z=3 using AMR cosmology code Enzo.
    a. Status: completed (see Table 1).
    b. Issues: are additional higher-resolution simulations needed?
2. Generate mock galaxy catalogs using HOD+CLF methodology described in Yan, White and Coil, ApJ 607, 739 (2004), with SDSS, DEEP2 updates.
    a. Status: Oct. 1, 2007 start date
    b. Who: UCSD graduate student Stephen Skory (sskory@physics.ucsd.edu)
    c. Issue: need magnitude limits, source counts from LSST.org
    d. Issue: calibrating HOD+CLF at z>1
    e. Issue: galaxy colors?
    f. Issue: in what format would you like galaxy catalog?
3. Calculate gravitational shear/magnification for each galaxy using ray tracing through the lightcone
    a. Status: Oct. 1, 2007 start
    b. Who: UCSD graduate student Rick Wagner (rwagner@physics.ucsd.edu)
    c. Issue: is weak lensing approximation adequate?
    d. Issue: development and verification of lensing code
    e. Issue: currently lightcone stops at z=0.1; do we need z=0?
4. Generate simulated LSST sky maps (100 sq. deg.)
    a. Status: March 1, 2008 start
    b. Who: Skory, Wagner, and someone from LSST team who has done this
    c. Issue: galaxy morphologies
    d. Issue: how many images, and of what size?
    e. Issue: image format?