Projects in Astrophysical and Cosmological Structure Formation (M. Norman, P. Padoan, A. Kritsuk UCSD)

A Renewal of NRAC Proposal MCA098020

Abstract

This group proposal from the Laboratory for Computational Astrophysics, UCSD requests additional resources to continue our numerical studies of structure formation in cosmological and astrophysical systems. Significant improvements and extensions of the Enzo adaptive mesh refinement code in the past year, as well as the expanded SDSC DataStar cluster and the NCSA Altix create new opportunities to increase the realism and dynamic range of simulations of cosmological structure formation, interstellar turbulence, and star formation via turbulent fragmentation of molecular clouds. This proposal requests resources to carry out the first 2048^3 uniform grid simulations of the Lyman alpha forest and supersonic turbulence, and the first 512^3 globally refined AMR simulations of galaxy clusters. Resources are also requested to continue our studies of the formation and feedback effects from the first stars, the chemical enrichment of the intergalactic medium, and protostellar core formation in magnetized molecular clouds.

I. Introduction

This is a renewal of our three-investigator (Norman, Padoan, Kritsuk) proposal “Projects in Astrophysical and Cosmological Structure formation.” The rationale for the group proposal is that we are all members of the Laboratory for Computational Astrophysics at UCSD, we all collaborate, we use a common code base (Enzo [1]), and we share a common need for 3D simulations of large spatial dynamic range. For example, cosmological structure formation in the large poses a minimum spatial dynamic range requirement of 10^5 for collapsed objects such as galaxies or galaxy clusters in large statistical volumes. This we achieve through the use of adaptive mesh refinement (AMR) (Fig. 1). An even larger dynamic range is required to follow the evolution of gravitationally collapsing protostellar cores in turbulent molecular clouds (Fig. 2). Other applications, such as the mildy overdense Lyman alpha forest or MHD turbulence, prefer the use of large uniform Cartesian grids for power spectrum analysis. Our largest previous simulations have been limited to 1024^3 resolution, which while not insignificant, falls far short of traversing the range of important physical scales.

This year, advances in the Enzo application software as well as hardware upgrades at the NSF centers create new opportunities to increase the realism and dynamic range of our simulations of cosmological structure formation, interstellar turbulence, and star formation via turbulent fragmentation in molecular clouds. Our research is supported by three NSF grants and one NASA grant to us. This proposal requests additional resources to carry out the first 2048^3 uniform grid simulations of the Lyman alpha forest in order to better constrain the matter power spectrum, supersonic turbulence to better understand the structure of molecular clouds, and the first 512^3 globally refined AMR simulations of galaxy clusters, to make predictions for upcoming Sunyaev-Zeldovich effect surveys. Resources are also requested to continue our studies of feedback effects from the first stars, structure and evolution of the intergalactic medium, and protostellar core formation in magnetized molecular clouds.

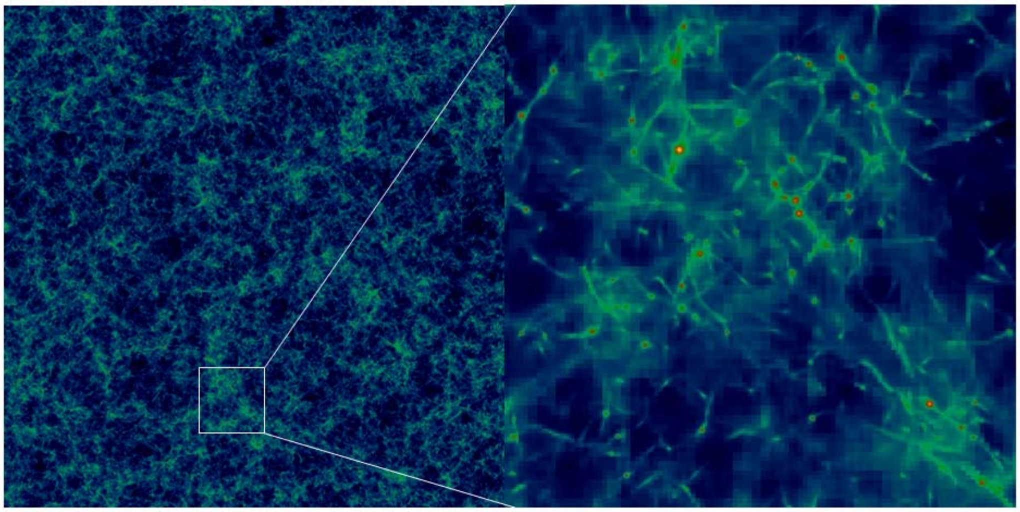

Fig. 1. AMR simulation of the distribution of baryons in the universe on a scale of 700 Mpc. Spatial dynamic range of the simulation is 65,536 within galaxy clusters.

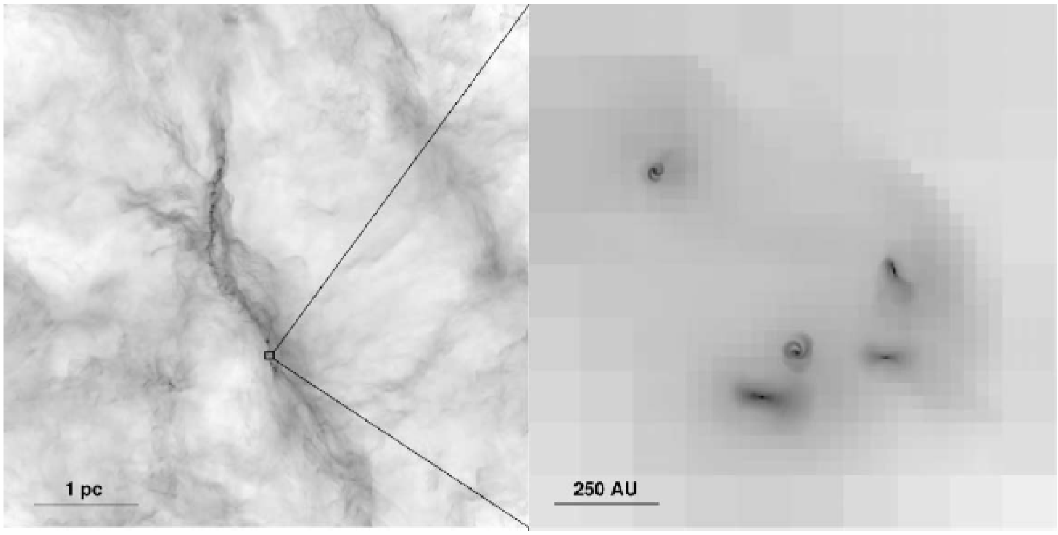

Fig. 2. AMR simulation of collapsing protostellar cores in a turbulent molecular cloud. Spatial dynamic range is >500,000. From Padoan et al. (2005).

Among the Enzo software advances which enable the new simulations is a fast subgrid neighbor search algorithm and packed AMR file I/O using HDF5. These enhancements allow us for the first time to do global, adaptively refined simulations with >100,000 grid patches (e.g., Fig. 1). This capability will be used to simulate a statistical population of galaxy clusters on the light cone including gas dynamics. A second Enzo advance is the conversion to 64-bit integer addressing throughout, which supports simulations with 10 billion particles or more. A third Enzo advance is the incorporation of ideal MHD into our parallel AMR framework. This advance opens the door to many new applications. This year we will perform the first high dynamic range simulations of protostellar cloud core formation including the effects of magnetic fields.

II. Project Descriptions and SU Request

The project description is divided according to the three principal application areas. A summary of progress, new project description, and resource justification is provided in each section. A summary of the projects and the resource request is given in Table 1. Enzo performance and scaling is given in the Methodology section. Publications resulting from last year's allocation are also listed.

Project	**SUs**	**Preferred Machine**	**Alternate Machine**
First Stars and Feedback	266,000	SDSC DataStar p655	TeraGrid cluster
Chemical Enrichment of IGM	150,000	SDSC DataStar p655	TeraGrid cluster
Lyman α Forest	360,000	SDSC DataStar p655	None
Cluster Light Cone	180,000	NCSA Altix	None
Supersonic Turbulence	384,000	SDSC DataStar p655	None
Inertial Particles in Turbulence	406,000	SDSC DataStar p655	TeraGrid cluster
Core Formation via Turbulent Fragmentation	400,000	TeraGrid cluster	SDSC DataStar p655
Structure of MHD Protostellar Cores	220,000	NCSA Altix	None
Data analysis	50,000	SDSC DataStar p690	TeraGrid IBM p690

Table 1. Summary of projects and SU request.

II.1 Cosmological Structure Formation

Research described in this section is funded by an NSF grant to Norman and Hernquist entitled "The Galaxy/IGM Connection" and an NSF grant to Norman and Tytler entitled "Precision Studies of the Intergalactic Medium".

Project 1: Formation and Feedback from the First Stars

Progress. Using last year's allocation, Brian O'Shea completed his Ph. D. thesis entitled "The Formation of Population III Stars and Their Affect on Structure Formation in the Early Universe." One paper has appeared in the Astrophysical Journal based on this work, one has been submitted, and five more are in preparation. We used a suite of extremely high dynamical range (3×10^8) simulations of Population III (hereafter Pop III) star formation in a ΛCDM universe to study the ensemble properties of collapsing primordial protostellar cores. We confirm the results of Abel, Bryan and Norman (2002), but find a large scatter in the accretion rates onto the primordial protostars, implying a large range of possible initial stellar masses. The implied stellar mass function is still extremely top-heavy when compared to that of stars in the galaxy today, however. Additionally, we studied the formation of Pop III stars in the presence of a photodissociating background and also using a generic warm dark matter (WDM) particle model and discovered that both a soft UV background and a decreased dark matter particle mass serve to delay the onset of protostar collapse and increase the halo mass at the time of collapse. This agrees well with previous work. Using several extremely high dynamical range simulations of Pop III star formation we discovered that the evolution of angular momentum in the cores of collapsing Pop III protostars is due primarily to the turbulent transport of angular momentum. We also used simulations with Lagrangian "tracer particles" to confirm that angular momentum "segregation" is an important secondary effect.

Simulations of chemical and radiative feedback from Pop III stars have also been performed with the Enzo AMR code. We have conducted preliminary calculations of the effects of Pop III HII regions on the formation of later generations of structure, and have also examined the metal feedback and enrichment from Pop III supernovae.

New project description.

1) Effect of Collisionally Induced Emission

Simulations of Pop III star formation have made significant progress in the past year. Previous work by members of this collaboration has shown that Pop III protostars have a wide range of accretion rates onto the protostellar core (O'Shea & Norman 2006a), and that turbulence is responsible for much of the transport of angular momentum in these cores (O'Shea and Norman 2006b). However, these simulations have been terminated when the central baryon density in the collapsing core reaches 10^{15} particles/cm^3, which is approximately 8 orders of magnitude below stellar density. These simulations were stopped because the assumption of optically thin radiative cooling breaks down, indicating that further calculations will need to include full radiation transport to reach to stellar densities. However, work by Ripamonti & Abel (2004) on the opacity of primordial gas due to collisionally induced emission indicates that one can modify the existing primordial gas cooling algorithms in Enzo to make the cooling/heating rates accurate for several more orders of magnitude in density without explicitly including radiation transport. This modification has already been implemented in the Enzo code, and agrees with the Ripamonti & Abel result for preliminary calculations. However, in order to follow the collapse of the gas cloud to higher densities, we need to use extended-precision (128 bit) arithmetic for particle and grid position information to ensure numerical stability. This capability also currently exists in the Enzo code (Bryan, Abel & Norman 2001). We will perform a half dozen extended-precision Enzo runs using the Ripamonti & Abel cooling fix in several different cosmological realizations to study the collapse of a primordial protostellar cloud to higher densities. These calculations will investigate whether CIE induces fragmentation of the cloud core, and also will be used to provide initial conditions for ZEUS-MP radiation transport calculations which will study the shutoff of accretion onto the Pop III protostar.

2) Ensemble study of Population III accretion rates

In previous work we have examined the accretion rates onto Pop III protostars using a variety of box sizes and random realizations (O'Shea & Norman 2006a). However, each of these calculations is of the most massive halo in relatively small volumes, and may represent a skewed sample of Pop III protostellar cores (Barkana & Loeb 2004). A more realistic sample of Pop III protostars would be taken from a single, large simulation volume, with halos representing a wide variety of formation redshifts and local environments simulated at extremely high resolution. This would allow us to disentangle environmental effects on protostellar accretion rates from box size and halo selection effects. We propose to simulate a volume of the universe approximately 2 comoving Mpc on a side. While this may seem small, it represents large scale structure at z=20. We will first perform a dark matter-only calculation to identify all dark matter halos where Pop III stars could conceivably form over a wide range of redshifts, and will then select approximately two dozen of these halos to re-simulate at higher resolution using both dark matter and baryon physics (including primordial chemistry and radiative cooling). The halos will be selected to sample a wide variety of formation redshifts and environments, which will provide increased insight on the accretion properties of Pop III protostars and the relationship of this local quantity with more global properties of the primordial halos.

3) Population III supernovae/cosmic metal pollution/second generation objects

One of the most important issues concerning the effects of Pop III stars is their feedback of heavy elements into the intergalactic medium. This addition of metals will profoundly affect the cooling properties of the gas, allowing it to cool to much lower temperatures, and consequently change the mass scale at which fragmentation and collapse occurs (Bromm & Loeb 2003). Preliminary work studying the dispersal of metals by Pop III supernovae in a cosmological context has been carried out by O'Shea and Norman (2006d), who examine the metal enrichment of a 30 solar mass Type II supernova using a spherically symmetric Sedov-Taylor blast wave as an initial condition. We propose to extend these calculations with the addition of more realistic initial conditions, including asymmetric (i.e. non-spherical) supernova models, and also examine the properties of much more massive (~250 M_{solar}) pair instability supernovae in order to give reasonable upper and lower bounds on metal enrichment patterns from Pop III supernovae. We will continue the simulation until the metals are incorporated into a more massive second generation object. We will study the metallicity distribution in these objects for some insight into what the mass and metallicty distributions second generation stars will have.

Resource justification

Effect of CIE: A standard Enzo Pop III star formation calculation with a 128^3 root grid, 3 static nested grids and 28 total levels of refinement uses approximately 1400 SUs on SDSC DataStar. However, using the code in its extended precision (128-bit) mode approximately doubles the computation time. Also, resolving the Jeans length at all scales by 64 cells significantly impacts the computational cost, also by approximately a factor of two above the standard calculation of this type. As extended precision is available only on SDSC DataStar, we estimate that each of these high-precision runs will cost approximately 6,000 SUs on DataStar. We would like to do 6 of these runs, varying cosmological realizations, for a total of 36,000 SUs.

Ensemble study of Population III accretion rates: In this calculation we will use a single cosmological volume, but re-simulate multiple small sub-volumes at extremely high precision. As discussed above, each standard Enzo Pop III star formation calculation uses approximately 1400 SUs on DataStar. However, we will be using a much larger simulation volume (~2 Mpc instead of 300 kpc comoving) and will use more static nested grids, increasing the computational cost. Test simulations done with larger box sizes and more nested subgrids suggest that the overall computational time for each simulation in the ensemble will cost approximately 3,000 SUs on DataStar. The initial survey calculation will be a relatively low- resolution AMR calculation with a 256^3 root grid and 8 levels of refinement (refining everywhere), which will cost approximately 8,000 SUs. With 1 survey calculation at 6,000 SUs and 24 calculations in the ensemble at 3,000 SUs apiece, this comes to 80,000 SUs total for this project.

Population III supernovae/cosmic metal pollution: Preliminary Enzo calculations of a 30 solar mass Pop III supernova in a standard setup indicate that the evolution of the supernova remnant from a simple Sedov blast wave requires approximately 5,000 SUs on 32 processors of DataStar. We will do multiple simulations of a 30 solar mass Type II supernova, varying asymmetries and orientation of the supernova. Initial calculations of a 250 solar mass pair instability supernova (PISN) show that this calculation is much slower, by approximately a factor of 5, which is due to the increase in ejecta velocity in a 250 solar mass supernova compared to a 30 solar mass supernova. We wish to do five Type II solar supernovae (which will cost 5,000 SUs apiece) and five higher mass PISN (at approximately 25,000 SUs apiece) for a total request of 150,000 SUs for this project. Our best realization for both the Type II and PISN will be evolved until their ejecta is incorporated into a higher mass protogalactic halo.

Project 2: Chemical Enrichment of the Intergalactic Medium by Protogalaxies

Progress: Observations show that the intergalactic medium at redshifts z~3 is chemically enriched to a metallicity of about $Z/Z_{solar}=10^{-3}$ with a positive dependence on gas overdensity (Schaye et al. 2003). There is a dichotomy of opinion about the typical mass of the protogalaxies contributing most of the metals to the IGM. On the one hand, Madau, Ferrara and Rees (2001) argue that it is the more numerous, low mass protogalaxies of mass 10^{8-9} M_{solar} that contribute most of the metals at $5 < z < 12$. Monte Carlo simulations by Scannapieco, Ferrara and Madau (2002) seem to bear this out. These galaxies, however, are not yet observable at these high redshifts, and so we have no hard data about the outflows themselves. On the other hand, we have observations of Lyman break galaxies (LBG; Steidel et al. 1999, Adelberger et al. 2002) at z=3-4 from which wind velocities and mass loss rates can be measured. The masses of LBG galaxies are estimated to be 10^{10-11} M_{solar} --much higher than the putative 10^{8-9} M_{solar} polluters of Madau et al. This makes them much rarer in terms of number density at this redshift, but more energetic. No doubt galaxies of all mass contribute to the pollution of the IGM. We would like to quantify how.

With last year's allocation we used the NSF teragrid to carry out the first billion cell hydrodynamic cosmological simulations designed to assess the relative contributions and unique signatures of feedback from galaxies in the mass range 10^{8-10} M_{solar}. We simulated an 8 Mpc survey volume with 1024^3 uniform cells without and with star formation and feedback (Fig. 3). These simulations capture every 10^8 M_{solar} halo in the volume, but do not resolve the individual galaxies. Using a parameterized star formation and feedback algorithm constrained by the observed cosmic star formation history, we simulate the energy and metal feedback into the IGM at z=3. We have completed analyzing the Lyman α forest absorption statistics in the two simulations and find them to be virtually indistinquishable in all statistics employed. This result is surprising considering 25% of the volume and 55% of the mass is disturbed in the feedback simulation. A preliminary analysis of the metallicity-overdensity relation in the feedback simulation is in good agreement with the results of Schaye et al. (2003). This provides strong support to the Madau et al. hypothesis that it is the lower mass galaxies that enrich the IGM with metals. We are preparing a letter and a longer paper to the Ap J describing these results.

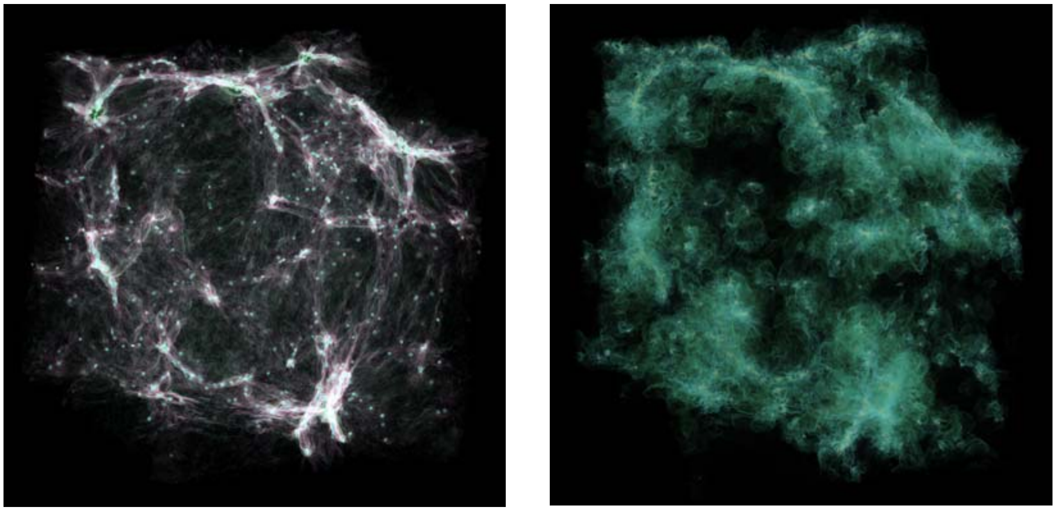

Fig. 3. The effect of galaxy feedback on the intergalactic medium. Left: distribution of neutral hydrogen in a 8 Mpc volume which gives rise to the Lyman α forest absorption in the absence of galaxy feedback. Right. With galaxy feedback. Both simulations used 1024^3 cells and dark matter particles, and were performed on the NSF TeraGrid.

<u>New project description</u>.

The simulation in Fig. 3 right used a uniform mesh of 8 comoving kpc spatial resolution (=2 kpc at z=3). This is inadequate to resolve the internal structure of the galactic wind bubbles themselves. Moreover, this is inadequate to resolve the gravitational potential well of the host galaxy, which is important for determining the escape fraction of hot gas (Fujita et al. 2004). We propose to resimulate select subvolumes of the 8 Mpc 1024^3 unigrid simulation performed in 2005 using AMR to achieve much higher spatial resolution than in the previous calculation but at the same superb mass resolution. We will then vary star formation and feedback parameters for these simulations examining the efficiency with which high-redshift galaxies eject metals into the intergalactic medium and the distance to which they are propelled. We will compare our results to previous analytic estimates (Fujita et al. 2004). We will construct synthetic metal absorption line spectra for species of C, Si and O assuming local ionization equilibrium and compare these to observations.

Resource Justification

These simulations will use similar setups to Enzo Pop III star formation calculations (namely, a relatively coarse root grids with multiple static nested grids, with AMR taking place only within a small volume), so it is reasonable to assume that the overall computational cost neglecting star formation and feedback will be similar (1500 SUs apiece). Previous simulations have shown that, depending on the choice of star formation and feedback parameters, the overall simulation time can increase by an order of magnitude due to shorter timesteps imposed by stellar energy injection. Therefore, we estimate that each of these calculations will require 15,000 SUs. We would like to perform 10 such simulations, choosing several different galaxy environments as well as varying the star formation efficiency parameter. The total request is therefore 150,000 SUs on SDSC Data Star.

Project 3: A Precise Measurement of the Matter Power Spectrum using the Lyman α Forest

The Lyman α forest (LAF) in the absorption spectra of high redshift quasars (Rauch 1998) has emerged as an attractive tool for cosmological measurements. This is because we now understand that the LAF directly samples matter fluctuations in the intergalactic gas and hence dark matter on scales $10^2 > \lambda > \sim 0.1$ Megaparsecs (Croft et al. 2002). This understanding has been achieved by virtue of high resolution hydrodynamical cosmological simulations of the structure of the high redshift intergalactic medium (IGM). The PI took part in the initial discovery of the nature of the LAF (Zhang, Anninos & Norman 1995; Zhang et al. 1997, 1998), explored the convergence properties of our numerical models (Bryan et al. 1999), and investigated its use as a cosmological probe (Machacek et al. 2000; Tytler et al. 2004; Jena et al. 2005).

The key to extracting cosmological information from the Ly α forest is to understand how the absorption relates to the underlying matter power spectrum. Mathematically, it is assumed that if $P_F(k)$ is the flux power spectrum, and $P(k)$ is the matter power spectrum, then the two are related by $P(k)=b^2(k)\, P_F(k)$, where b(k) is the scale-dependent *bias factor* (Croft et al. 2002). If one knew b(k) by some means, then one could infer the matter power spectrum by measuring $P_F(k)$. The approach to evaluating b(k) is to carry out a large suite of hydrodynamical cosmological simulations of the Ly α forest varying P(k), the cosmological, and astrophysical parameters. From these outputs synthetic absorption spectra are generated by passing lines of sight through the volume. An ensemble of such spectra are used to derive $P_F(k)$ and hence b(k). Croft et al. (2002) used this approach to measure P(k) to ~20% accuracy over a range of scales 1.5 orders of magnitude smaller than current CMB measurements.

Progress: Our goal is to improve on the Croft et al. (2002) result using better simulations, more and better observations, and a better handle on systematics. Recently, working with a team of observers at UCSD led by David Tytler, we have established a concordance model for the LAF (Jena et al. 2005) which is in agreement with other measurements, and in addition constrains two astrophysical parameters which describe the metagalactic UV background radiation field. To do this, we ran a large parameter survey on NSF resources on numerical grids of 128^3, 256^3, 512^3, and 1024^3 cells in size with our hydrodynamic cosmology code *Enzo*. Although the 1024^3 simulations are the largest of their kind to date, they fall short by a factor of at least 2 per dimension to permit a precision measurement of the matter power spectrum. The reason for this is that a minimum resolution of 40kpc is required to resolve the LAF absorbers (Bryan et al. 1999). Adopting this, 1024^3 cells takes us to a box size of 40 Mpc. However the largest Fourier mode in the box assuming periodicity—the standard approach—is only 20 Mpc, and this is far short of the peak of the concordance ΛCDM power spectrum. Such a simulation lacks large scale power. This will bias the estimate of the matter power on large scales.

New Project Decription: In Jena et al. (2005) we showed that we could correct for grid resolution effects using a cell size as coarse as 100 kpc. Employing a 2048^3 grid with 100 kpc cells takes us to a 200 Mpc volume. Assuming the box is periodic, it would include power on scales up to 100 Mpc. This is an order of magnitude improvement over Croft et al. (2002). Using SDSC's expanded Data Star cluster, we propose to carry out a single 2048^3 simulation of our concordance model of Lyman α forest. This plus our existing survey will allow us to measure b(k) defined above over the range of scales required for precision measurements of the matter power spectrum from the LAF.

Resource Request: SDSC Data Star is the only machine in the NSF system with enough memory to accommodate a 2048^3 simulation of the LAF (~4 TB). Enzo performance results on grids up to 2048^3 cells and processor counts up to 2048 are given in the Methodology section. On 2048 processors, Enzo sustains 620 GF for this calculation, which is about 6% of peak. One timestep at the beginning of the run requires 130 wall-sec = 2048 x 130/3600 ~75 SUs. 2000 timesteps will thus consume 150,000 SUs. This estimate is substantially low for two reasons. First, based on our experience with 1024^3 simulations, I/O and restart roughly doubles the execution time. In addition, structure formation at lower redshifts causes the timesteps to drop somewhat, increasing the number of timesteps needed to reach our stopping redshift. Applying factors deduced from our 1024^3 simulations, we estimate we need 360,000 SUs to perform this simulation.

Project 4: Galaxy Cluster Lightcone

Large, deep surveys of galaxy large scale structure; galaxy clusters traced by X-rays, the Sunyaev-Zeldovich effect, and weak lensing; and the intergalactic HI absorption (the Lyman alpha forest) offer substantial promise to improve the precision measurement of the cosmological parameters, the matter power spectrum, and probe the dark energy equation of state. Increasingly, the interpretation of massive amounts of observational data relies on comparison and calibration with equally massive numerical simulations of cosmic structure formation. In the precision era, these simulations must model both baryons and dark matter over a large dynamic range in length scale. At UCSD we are developing the Enzo code with these applications in mind.

A particularly exciting new challenge in observational cosmology is to measure the expansion history of the universe to sufficient precision to see whether the cosmological constant is truly constant, or whether the vacuum energy density responsible for accelerated expansion has changed with lookback time. There are two basic routes to doing this; the challenge is so difficult both will be required. The traditional route is to measure the luminosity distance to a standard candle such as Type Ia supernovae as a function of redshift. The resulting Hubble diagram is fit to different world models, and a best fit is found. This is how the accelerating universe was discovered (e.g., Perlmutter 2003). The second route is to use observations of the growth of cosmic structure to define a standard ruler or to measure the growth factor of density perturbations with redshift. In the later approach, galaxy clusters offer the most promise because their space density is extraordinarily sensitive to cosmology over the redshift range 0-1.5 when cosmic acceleration becomes dominant (Carlstrom et al. 2003). Large samples of high redshift galaxy clusters will be detected soon using the Sunyaev-Zeldovich effect (SZE) in blind surveys with a variety of radio telescopes nearing completion.

Progress: The key to deriving cosmology parameters from impending SZE surveys is to relate a cluster's SZE signal to its dynamical mass. In the past few years M. Norman working with collaborators J. Burns, P. Motl and E. Hallman at the University of Colorado have shown that the SZE provides the most accurate and least biased mass estimate when compared with X-ray methods alone (Motl et al. 2005, Hallman et al. 2006, Norman 2006). We used Enzo to simulate a large sample of galaxy clusters at a variety of redshifts which were then numerically "observed" in X-ray and SZE wavebands. The synthetic images were then analysed as if they were real data. The result of our analysis is as stated above provided one can observationally resolve the cluster's SZE radial profile and measure its emission weighted temperature (Hallman et al. 2006).

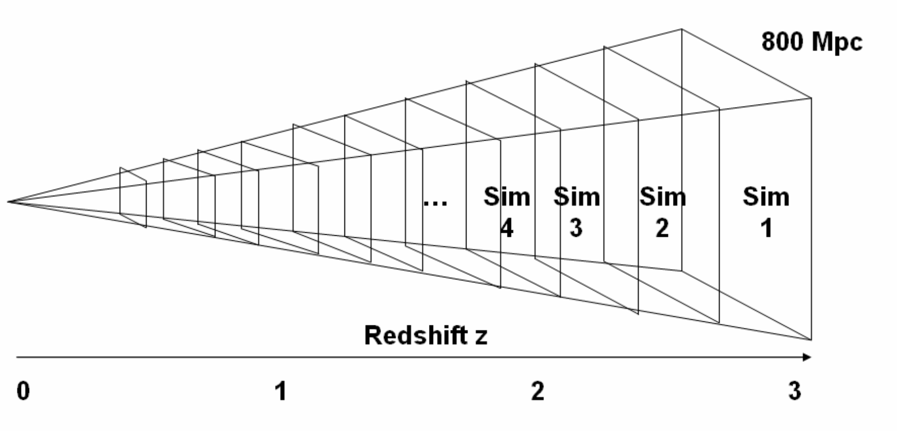

Fig. 4. Tiling the lightcone with high resolution AMR simulations for analysis of weak lensing shear, SZ clusters, etc. The benefit of this strategy is high spatial resolution and constant angular resolution within a large survey volume.

New Project Description: We have established the reliability of using X-ray and SZE data to measure cluster masses as a function of redshift. This was based on hydrodynamic cosmological simulations of galaxy clusters in relatively small volumes simulated one at a time (Loken et al. 2002, Motl et al. 2005). Our recent software advances (cf. Fig. 1) now allow us to simulate entire samples in larger volumes at high resolution. We propose to use Enzo's unique AMR capabilities to simulate a complete sample of galaxy clusters on the light cone $0<z<3$ for a large area of the sky, comparable to what is planned for the South Pole Telescope. The lightcone is tiled in redshift space with a dozen or so high resolution AMR simulations each subtending the same solid angle (Fig. 4). The box sizes are varied to achieve constant angular resolution in the observer frame. A lightcone covering 100 square degrees would require simulation volumes as large as 800 Mpc on a side at $z=3$. In order to achieve the spatial, mass, and angular resolution requirements in galaxy clusters with a completeness limit of 10^{14} M_{solar}, AMR simulations with a root grid resolution of 512^3 cells and 3-5 levels of adaptive refinement will be needed. Because of the large amount of total memory required as well as the variable and sometimes large memory requirement per node due to AMR, the only machine within the NSF system where we can run such simulations is the NCSA Altix system Cobalt with 2 TB of RAM.

Resource Request. Our detailed lightcone design for 100 square degrees, 10 arcsec angular resolution consists of 16 AMR simulations with box sizes ranging from 256 to 800 comoving Mpc. This year we are requesting resources for four simulations out of the sixteen in order to better estimate the total requirements. A separate LRAC proposal will be submitted for the full lightcone. The four are the tiles with stopping redshifts 3, 2 ,1 and 0.1 in boxes of size 800, 650, 400 and 256 Mpc, respectively. The maximum level of refinement to achieve our angular resolution requirement is 3, 3, 3 and 5, respectively. The CPU estimates are based on a single 512^3 2-level AMR simulation we are currently running on Cobalt. The wall clock time on 256 processors to reach $z=3$, 2, 1, 0.1 is 2000, 5000, 33,000 and 200,000 (est.) sec. respectively (Fig. 6). The 3-level simulations will at most double the execution time: 2x(2000+5000+33000)=80,000 sec on 256 processors = 5690 SUs. The 5-level simulation will increase the execution time at most 8-fold, and thus we estimate that will require 8x(200000)=1.6 Msec on 256 processors = 20 x 5690 SUs = 113,800 SUs. The four simulations total 120,000 SUs. Increasing this by 50% for data I/O (Fig. 6 is without I/O), we reach 180,000 SUs on the NCSA Cobalt system.

II.2 Interstellar Turbulence

Projects 5-8 are supported by NSF and NASA grants to P. Padoan (PI), Norman and Kritsuk (co-investigators).

Project 5: Application of AMR to Supersonic Turbulence

Progress: Kritsuk, Norman & Padoan (2006, hereafter KNP06) have demonstrated that adaptive mesh refinement (AMR) yields savings of computer resources for numerical simulations of isotropic supersonic turbulent flows with high Reynolds numbers. The statistical properties of turbulence simulated with AMR and on uniform grids with resolution up to 1024^3 agree surprisingly well. The KNP06 simulation was the first AMR simulation of isotropic turbulence, and also the highest resolution simulation of supersonic isothermal turbulence in molecular clouds. With last years LRAC allocation, we have completed a set of 1024^3 turbulence simulations on uniform grids at Mach numbers in the range from from 6 to 12 which produced more than 20TB of data. This state-of-the-art data set allowed us to derive time-average statistics for supersonic turbulence with unprecedented accuracy. Two Phys. Rev. E papers are in preparation describing these results.

New Project Description: We are currently running an AMR turbulence simulation on NCSA's Altix with effective resolution of 2048^3 and a root grid of 512^3 points, refining on regions with strong shocks and shear. This simulation will be completed by the expiration of our current allocation. In order to convincingly demonstrate the utility of AMR for modeling supersonic turbulent flows at high Reynolds numbers, it is important to directly compare the 2048^3AMR simulation with a uniform grid simulation of the same resolution, focusing especially on features that are strongly resolution dependent. In order to achieve this goal, we propose a unigrid 2048^3 simulation of driven Mach 6 turbulence on SDSC DataStar system. We will start the simulation with a re-gridded 1024^3 premixed box as the initial condition and then will evolve it for three dynamical times to achieve sufficient relaxation. The resulting dataset will be also used to derive time-average statistical properties of this turbulent flow and compare those with model predictions.

Resource Request and Justification: Our request of 384,000 SU is based on one of our 1024^3 unigrid run performed in 2005 on 64xP655+ new nodes of DataStar. An 18-hour job running on 512 processors at resolution of 1024^3 points followed the flow evolution for 1.2 dynamical times at a rate of (18hours*512procs)/1.2t_dyn = 8,000 SU per dynamical time. Our estimate for the proposed run SU = $8000*2^4*3$ = 384,000. With the required memory of 1.7TB (2048^3*21field*8byte*1.1ghost) we will be able to perform this run on 64+ new nodes with 32GB per node.

Project 6: Inertial Particles in Turbulent Flows

Progress: The properties of interstellar dust are crucial for many astrophysical processes, but the evolution and spatial distribution of dust in turbulent interstellar clouds has not yet been extensively studied. Dust grains in turbulent interstellar clouds behave much like aerosols in the atmosphere or plankton in the oceans. The turbulence tends to organize the grains in clusters, strongly affecting their coagulation rates. Using time from last year's allocation, we have implemented inertial particles within Enzo, and carried out pilot simulations of 128^3 and 256^3 particles and cells. Results are very encouraging and interesting, deviating strongly from analytic predictions. A paper is nearing completion on our first results.

New Project Description: We are sufficiently intrigued by our first results, that in order to study the process of dust coagulation in realistic clouds, we propose to run 512^3 and 1024^3 hydrodynamic simulations of supersonic turbulence with 512^3 and 1024^3 embedded inertial particles, respectively. These simulations will be used to compute the collision frequencies of particles of the same or different sizes and their spatial distribution. Results of these simulations will be crucial for many astrophysical applications, including dust opacity in planetary and brown dwarf atmospheres, chemistry and observational properties of star forming clouds, radiation pressure on accreting gas around massive protostars, formation of planetesimals. Because the clustering of dust grains depends on the turbulence, if we will succeed in detecting the observational evidence of clustering we will be able to constrain some properties of interstellar turbulence. In parallel to these simulations, we are developing an observational program based on dust scattering of the near-IR interstellar radiation field, which should allow us to probe the dust distribution in star forming clouds to scales as small as the Kolmogorov dissipation scale.

SU Request and Justification: We will evolve a 512^3 model of Mach 4 turbulence with inertial particles for 10 dynamical times and then double the linear resolution and continue the simulation for another three dynamical times. Our completed 512^3 Mach 1 simulation was running on 64xP655+ new nodes of DataStar at 7,000 SU per dynamical time. Thus, the first stage of the proposed simulation will require SU = 70,000, while the second will take SU = 16*3*7,000 = 336,000. The total request is SU 406,000. The memory required for the final high-resolution part of this project includes (1024^3 *21field*8byte*1.1ghost) = 200GB for the hydro part, (1024^3*10*8) = 86GB for the inertial particles, and 86GB for the tracer particles. The total is about 0.4TB. We plan to run the simulations using 64xP655+ nodes of DataStar, although we could also attempt it on the TeraGrid cluster.

II.3 Star Formation

Project 7: Formation of Self-gravitating Protostellar Cores via Turbulent Fragmentation

Supersonic MHD turbulence is the dominant fragmentation mechanism in star-forming clouds (Padoan & Nordlund 1999). The statistics of the turbulence determine the statistics of the initial conditions of the gravitational collapse of protostellar cores, in particular the core mass distribution (Padoan & Nordlund 2002). In interstellar clouds the turbulence is scale-free over a huge range of scales, from 10^{14} to 10^{20} cm, so a very large range of scales is required also in the simulations. We propose to run 1024^3 supersonic MHD simulations of turbulent flows, which would be the largest ever carried out. The largest published simulations are 512^3 resolution by Li & Norman (2004). We will drive the turbulence for approximately 4 dynamical times, until it is statistically relaxed. Then we will turn on self-gravity to study the nonlinear evolution of gravitationally unstable cores created by the turbulent flow. The main results of these simulations will be a computation of the mass distribution of protostellar cores, to be compared with the observed mass distributions of both starless cores and stars. The data cubes will also be used for radiative transfer calculations to produce maps of molecular emission lines and dust emission, extinction and scattering. These maps will be the most realistic models of star forming clouds (including collapsing protostellar cores) ever generated and will be compared directly with observational data. These unigrid simulations will also be used to generate initial data for the AMR MHD simulations described below designed to resolve the internal structure of the self-gravitating cores.

SU Request and Justification: For these simulations we will use the ZEUS-MP MHD code developed by the Laboratory for Computational Astrophysics (Hayes et al. 2005).

ZEUS-MP is better suited for large unigrid runs than our newly developed MHD option in Enzo. A super-Alfvenic 1024^3 MHD turbulence simulation runs on DataStar at a rate of 12,000 SU per dynamical time. A run with higher initial value for the magnetic field (i.e., lower Alfvenic Mach number) requires proportionally more resources. We plan 3 runs with an average rate of 33,000 SU/dynamical time, covering a total of 12 dynamical times. Therefore SU = 33,000x12 = 400,000. Our memory estimate for a 1024^3 simulation is (25 fields)x1024^3x8x1.1=240GB. In 2005 we have been successfully running simulations of this kind using 64xP655+ nodes on DataStar. We plan to run these simulations on the TeraGrid cluster.

Project 8: Structure of Magnetized Protostellar Cores from Turbulent Fragmentation

New Project Description: For past two years UCSD graduate David Collins has been working to incorporate ideal MHD into the Enzo AMR code. This work is now complete and ready for application. As a part of Collins' PhD dissertation we wish to simulate the formation and collapse of protostellar cores resulting from turbulent fragmentation of the parent molecular cloud. The goal is to simulate with high spatial resolution the internal structure of cores thus produced to see whether they differ in significant ways from cores produced by ambipolar diffusion theory (Mouschovias et al. 2005).

Resource Request: Two AMR runs aimed at studying a few, individual cores at extremely high resolution are planned. A key control parameter is the mass-to-magnetic flux ratio in the gravitationally bound core. These runs will take the afore mentioned ZEUS-MP simulations as initial conditions, but using 6 levels of AMR on a few collapsing cores, using density as a refinement criterion. This will allow us to predict the core angular momentum, density, and magnetic field profiles to predict the effects of self-gravitating MHD turbulence on core properties. These profiles will then be compared to both observations and to the predictions of the ambipolar diffusion model of star formation. Each of these deep, high resolution runs will take an estimated 110,000 SUs. This timing estimate is made by taking the measured time to do the hydrodynamic run shown in Fig. 2, which has the same dynamic range and root grid size, and multiplying by a factor of 2, which is the relative speed of the MHD and HD solvers. The total request is therefore 220,000 SUs on the NCSA Altix system Cobalt.

III. Numerical Methodology

III.1 The Enzo Code

Our AMR code Enzo [1] (Bryan & Norman 1997; Bryan 1999; Norman & Bryan 1999; Bryan, Abel & Norman 2001) is a grid-based hybrid code (hydro + N-body) which uses the algorithm of Berger & Collela (1989) to improve spatial resolution in regions of large gradients, such as in gravitationally collapsing objects. The method is attractive for cosmological and astrophysical applications because it: (1) is spatially- and time-adaptive, (2) uses accurate and well-tested grid-based methods for solving the hydrodynamics equations, and (3) can be well optimized and parallelized. The central idea behind AMR is to solve the evolution equations on a grid, adding finer meshes in regions that require enhanced resolution. Mesh refinement can be continued to an arbitrary level, based on criteria involving any combination of overdensity (dark matter and/or baryon), Jeans length, cooling time, etc., enabling us to tailor the adaptivity to the problem of interest. The code solves the following physics models: collisionless dark matter and star particles, using the particle-mesh N-body technique; gravity, using FFTs on the root grid and multigrid relaxation on the subgrids; cosmic expansion; gas dynamics, using the piecewise parabolic method (PPM); multispecies nonequilibrium ionization and H_2 chemistry, using backward Euler time differencing; radiative heating and cooling, using subcycled forward Euler time differencing; and a parameterized star formation/ feedback recipe. An ideal AMR MHD solver has been implemented in the past year which combines the TVD ideal MHD solver of Ryu, Jones & Frank (1995), the constrained transport (CT) algorithm of Balsara & Spicer (1999) and the AMR conservative reconstruction of Balsara (2001).

Enzo is implemented in a combination of C/C++ and Fortran, and is parallelized using the MPI message-passing library. The code can run on any distributed memory parallel supercomputer or PC cluster, although 64-bit architectures are required for applications using the implicit kinetic solver. Enzo is used in two basic modes. In unigrid mode, AMR is switched off, and parallelization is used for block-decomposing the root grid. Unigrid simulations as large as 2048^3 using as many as 2048 processors have been successfully carried out on SDSC's IBM DataStar. In AMR mode, the root grid is typically smaller (e.g., 256^3 or 512^3), but still block decomposed for parallel execution. AMR typically generates tens to hundreds of thousands of subgrids, which are dynamically load-balanced across the processors. In general, the computational load increases with level of refinement up to some maximum which can be 10-100 times that required to advance the root grid one timestep. Due to variable memory per node requirements, the largest AMR simulations can only be done on the NCSA Altix system Cobalt using its shared memory feature.

III.2 Performance and Scaling

Because Enzo has so many physics and gridding options, there is no compact way of presenting its performance and scaling. It is problem dependent. Unigrid (uniform, static Cartesian grid) runs are easily analyzed for performance and scaling since the workload and decomposition is static. One can run a problem at full scale for a few timesteps, measure the performance, and from that estimate the time required for the full run. The latest unigrid benchmarks are shown in Fig. 5 and discussed below. This approach is not possible for AMR (adaptive mesh refinement) runs since every performance characteristic (e.g., CPU, MEM, COMM) is both problem and time dependent. To make matters worse, it is also machine dependent, sensitive mostly to memory and network bandwidth rather than the speed of the CPU because Enzo in AMR mode makes a lot of memory references per computation. The only useful metric is *time to solution* for the full scale problem on the architecture and processor count of choice. The SU estimates for the AMR runs described above are based on measured time to solution for problems whose size and level of refinement we have already run, with some scaling to account for processor speedups. In cases where we have not run an AMR calculation to conclusion at full scale, we have run subvolumes of the full problem to completion, measured its execution time, and then scaled the result assuming fixed work per processor and 50% parallel speedup.

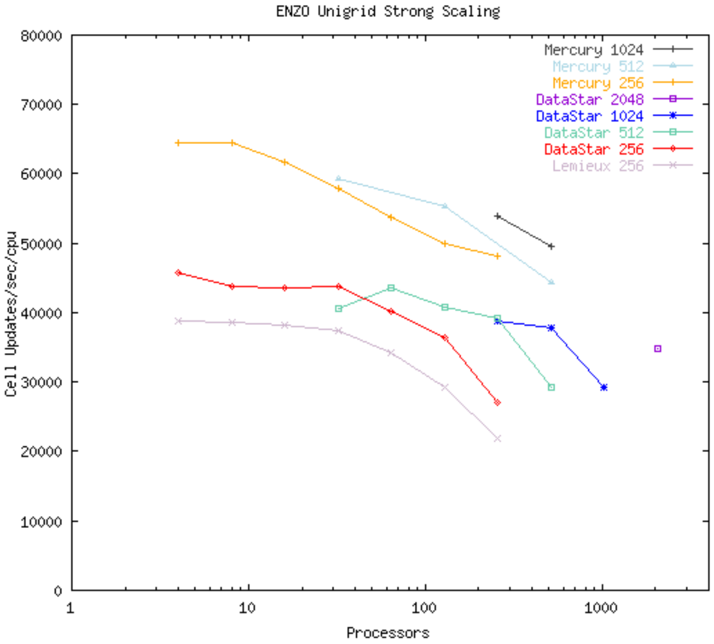

Fig. 5. Enzo performance and scaling for unigrid cosmology runs of size 256^3, 512^3, 1024^3 and 2048^3 on SDSC Data Star (DS), TeraGrid cluster (TG) and PSC TCS1 (TCS). Enabled physics: collisionless dark matter dynamics, 6 species hydrodynamics, self-gravity, nonequilibrium ionization and cooling. (Courtesy R. Harkness, SDSC).

Unigrid performance

Sustained per processor performance for Enzo is best illustrated with the 256^3 speeds for NP=4. TG is nearly twice as fast as TCS1 and 50% faster than DS. Enzo sustains slightly over 1 GFlop/s on one processor of TG. For this small problem, all three architectures exhibit good parallel scaling up to NP=32, with a roll-off in parallel efficiency thereafter. TG shows the least roll-off, with only a 25% degradation in per processor performance out to NP=256. For 512^3 and 1024^3 problems, TG remains the fastest platform--some 20% faster than DS. However, DS's superior data handling capabilities and larger total RAM make it the preferred system for 1024^3 unigrid runs (or larger), with TG coming in a close second. Based on these findings, we target our large unigrid runs to DS and TG. Additionally, at present only DS is the only architecture capable of 2048^3 runs.

512^3 AMR performance

The performance of AMR codes is problem and machine dependent, as mentioned above. This year we are requesting time for the first 512^3 globally refined simulations of galaxy clusters (Project 4). These runs generate N>200,000 subgrid patches which is in a qualitatively new regime to anything we have done before. Here we simply present the measured resource requirements for a 512^3 2-level AMR simulation we have run on NCSA's Cobalt system, upon which we base our resource requirement estimates in

Project 4. Extensive optimizations have been implemented to make such calculations feasible. We have replaced Enzo's O(N^2) subgrid neighbor search with a O(N*NP) algorithm, which speeds up the calculation by a factor of 10 for large N.

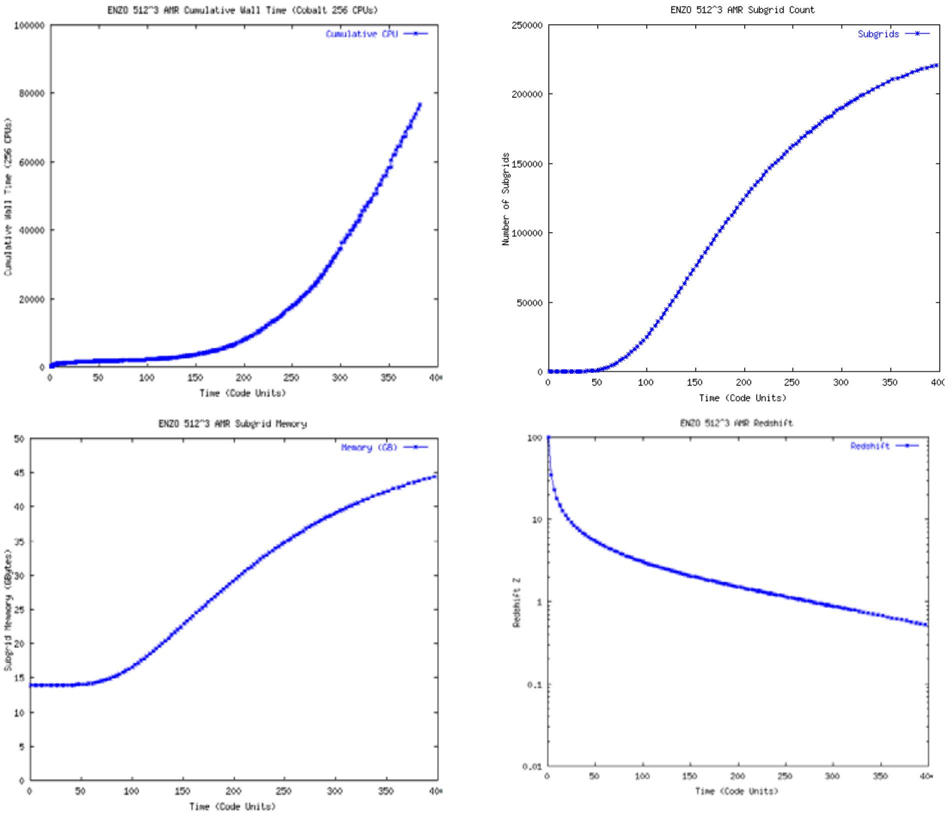

Fig. 6. CPU and MEM requirements for a 512^3 2-level Enzo simulation of galaxy cluster formation on NCSA Cobalt. Top left: Cumulative wallclock-sec on 256 processors versus timestep. Top right: number of AMR subgrids vs. timestep; Bottom left: subgrid memory vs. timestep; Bottom right: cosmological redshift vs. timestep. (Courtesy R. Harkness, SDSC).

IV. Publications Supported by Previous LRAC Award

1. Jena, T., Norman, M. L. et al. 2005. "A Concordance Model of the Lyman α Forest at z=1.95", MNRAS, 361, 70
2. Kritsuk, A., Norman, M. L. & Padoan, P. 2006, "Adaptive Mesh Refinement for Molecular Cloud Turbulence", Ap. J. Lett., in press
3. Kritsuk, A., Wagner, R., Norman, M. L. & Padoan, P. 2006. "Intermittency in Supersonic Hydrodynamic Turbulence: Density Statistics", PRL, submitted
4. Kritsuk, A., Wagner, R., Norman, M. L. & Padoan, P. 2006, "Intermittency in Supersonic Hydrodynamic Turbulence: Velocity Statistics", in preparation
5. Norman, M. L. 2006. "Hot Gas in Galaxy Clusters: Theory and Simulations", in *Background Microwave Radiation and Intracluster Cosmology*, proceedings of Varenna Summer School, eds. F. Melchiorri & Y. Rephaeli, Ital. Inst. Phys.

6. Norman, M.L., O'Shea, B.W., Paschos, P., and Harkness, R. 2006 “Metal feedback from high-redshift galaxies”,in preparation
7. O’Shea, B. W. 2005. “The Formation of Population III Stars and Their Affect on Structure Formation in the Early Universe”, Ph. D. thesis, UIUC
8. O’Shea, B.W., Abel, T., Whalen, D. & Norman, M.L., 2005, “Forming a Primordial Star in a Relic HII Region”, ApJ, 628, L5
9. O’Shea, B. W., & Norman, M. L. 2006 Population III Star Formation in a Lambda CDM Universe, I: The effect of environment on protostellar accretion rates, in preparation
10. O’Shea, B. W., & Norman, M. L. 2006 Population III Star Formation in a Lambda CDM Universe, II: Angular momentum evolution, in preparation
11. O’Shea, B. W., & Norman, M. L. 2006 Population III Star Formation in a Lambda CDM Universe, III: Effects of a photodissociation background, in preparation
12. O’Shea, B. W., & Norman, M. L. 2006 Population III Star Formation in a Lambda CDM Universe, IV: Metal dispersal by, in preparation
13. O’Shea, B. W., & Norman, M. L. 2006 Population III Star Formation in a Lambda WDM Universe, Ap. J., submitted
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15. Padoan, P., Kritsuk, A., Norman, M. L. & Nordlund, A. 2005. “A Solution to the Protostellar Accretion Problem”, Ap. J. Lett., 622, L61
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19. Whalen, D., & Norman, M. L., 2006, “A Multistep Algorithm for the Radiation Hydrodynamical Transport of Cosmological Ionization Fronts and Ionized Flows”, Ap. J., submitted, (astro-ph/ 0508214)

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