"Alleviating the scaling problems of cosmological hydrodynamic simulations"

Blue Waters Subaward NEIS-P^2 Final Project Report
Report Period: 10/1/2012 -- 9/30/2013

PI: K. Nagamine (University of Nevada Las Vegas), Co-PIs: G. Bryan (Columbia), R. Cen (Princeton), J. P. Ostriker (Princeton / Columbia), T. Naab (MPA), L. Oser (Columbia)
(the *CAGE* team)

1. Background and Activities:

This is the final project report of the NSF Blue Waters Subaward NEIS-P2. The intermediate report was also submitted to NCSA in June 2013, describing the first half of the progress.

In Feb 2012, Drs. Ludwig Oser and Thorsten Naab from the Max Planck Institute for Astrophysics (MPA), Germany, joined the CAGE team. Co-PI Ostriker has been collaborating with them for the past several years, and they brought an important skill to the CAGE team to perform zoom-in simulations. Using the support of this NEIS-P2 fund, we have been reformulating and extending the method of performing multiple zoom-in runs for cosmological galaxy formation. The NEIS-P2 fund was issued to Columbia University, and it used to support the salary of Dr. Oser.

The delivery of the NEIS-P2 fund to Columbia Univ. was delayed by a few months, and we were only able to hire Dr. Oser from Nov. 1, 2012 at Columbia. This delayed the start of our NEIS-P2 project by a few months, and we submitted the intermediate report in June, 2013.

In addition to a few tele-cons, we had an in-person CAGE meeting at Princeton Univ. during Sep. 24-28, 2012, where we discussed our research strategies, physics to implement in our codes, and the plan for NSF-AST proposal submission. We submitted the NSF-AST proposal (PI: R. Cen) for scientific projects, however, it was unsuccessful unfortunately. A few conference presentations were given, as summarized in the last section.

2. Major research and education activities, and findings

In the field of cosmological galaxy formation, the load-balancing and scaling of cosmological hydro codes to large core counts have been one of the major problems. To alleviate these problems, we have been developing the *HECA (Hierarchical Ensemble Computing Algorithm)* technique.

In HECA, we carry out an ensemble of zoom-in simulations concurrently, which allows us to avoid the communication overhead in computation, and the problem becomes close to `embarrassingly parallel'. The idea is that it might be faster to carry out multiple zoom-in simulations separately for many refined regions, rather than performing a full cosmological simulation for the entire volume, if the communication overhead is relatively high. We have performed some test runs with GADGET-3 on

Blue Waters and a few other machines to test this hypothesis. The HECA can be applied to both GADGET and Enzo codes.

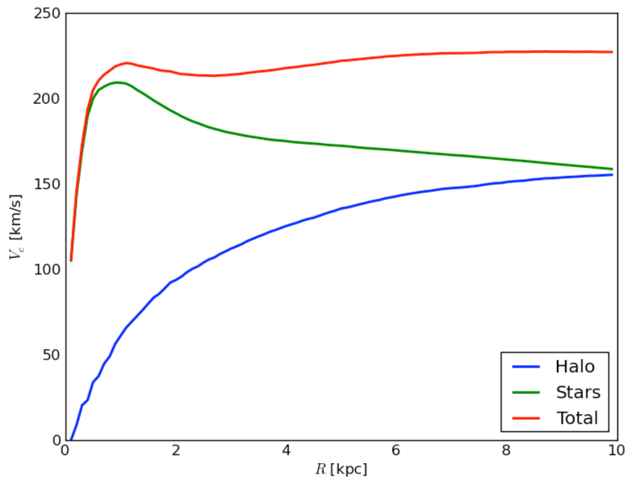
The results of the HECA test runs with GADGET-3 on BW were summarized in the intermediate report, so we will not repeat it here. In short, Dr. Oser ran several sets of simulations concurrently, achieving more efficient usage of larger computational resources. In the largest test run, he performed 1,909 zoom-in simulations concurrently using 61,088 CPUs with no observable slowdown of the individual runs, demonstrating that we can scale HECA up to large processor counts.

To run these HECA test runs, Dr. Oser developed python scripts to spawn multiple jobs concurrently within a single queue. The same software scheme should be applicable to Enzo, however, it is not as simple as GADGET-3 to set up the initial condition file for the zoom-in simulations for Enzo. Therefore we have not reached the point where we can test the Enzo HECA run to a similar scale. We also intend to test a hybrid version of GADGET-3 (OpenMP+MPI), which might give ~20% increase in performance.

The conclusion of the HECA test run is that we can achieve a higher resolution in HECA than in full-box cosmological hydro simulations, and it is now possible to scale up to arbitrarily large processor counts. By running multiple zoom-in runs concurrently, we can simulate a statistically relevant sample of galaxies at high resolution, alleviating the earlier problem of small samples for zoom-in simulations. Furthermore, because each zoom-in simulation is much cheaper than the full-box cosmological run, we can also implement and test different physical models.

Dr. Oser has also worked on some of the new implementation of various physical modules. He implemented the density independent SPH formalism proposed by Saitoh & Makino (2013) as well as an entropy diffusion formalism as brought forward by Price (2008) into GADGET-3. In addition, he integrated a more accurate Wendland kernel. This alleviates the known problems to resolve hydrodynamical instabilities with standard SPH codes. The updated code has passed all relevant tests (shear flow, Gresho-vortex, 'blob-test', Sedov-explosion) with excellent scaling behavior.

Furthermore he included the metal enrichment, cooling and diffusion formalism described in Aumer et al. (2013), as well as a novel algorithm to follow stellar feedback. He included the effect of energy feedback from young massive stars onto the interstellar medium, i.e., the gas particles around a newly formed stellar population will receive energy according to the expectations from stellar synthesis models (~10^{51} erg per 100 solar masses). Additionally the stellar populations formed in the simulation will lose a significant fraction of their mass due to SNII, SNIa and stellar mass loss (from AGB stars) over time. Therefore instead of just increasing the internal energy of the surrounding gas we also transfer mass, metals, and momentum. This form of kinetic feedback allows us to efficiently drive winds from the center of the galaxies alleviating the problem of too centrally peaked circular velocity curves often seen in simulations with weak feedback. In the Figure below, circular velocity of a simulated galaxy with a stellar mass of 7.4 x 1010 Msun at redshift z=0. The circular velocity curve of the stellar component remains flat and close to the peak value up to large radii similar to the Milky Way.



The described feedback mechanism already improves the well known overcooling problem, i.e., that the stellar mass of simulated galaxies is in general higher than predicted by abundance matching models (Moster et al. 2010). We also include the effect of feedback from supermassive black holes which will help to get an even better agreement of simulated to predicted galaxy masses in the most massive halos.

Development of the Enzo code has progressed on a number of fronts. Some of the new physics implementations were already described in the intermediate report. Here we only highlight the new paper by the Enzo Collaboration that describes the code in detail: “Enzo: An Adaptive Mesh Refinement Code for Astrophysics” (submitted to ApJS, arXiv:1307.2265). The code is available at http://enzo-project.org

3. Opportunities for training, development and mentoring

The CAGE collaboration is mentoring a large number of postdocs and graduate students, who work on related projects. During this report period, **PI Nagamine** has worked with one postdoc (A. Kashi, UNLV), two graduate students (R. Thompson, K. Todoroki, UNLV), and five undergraduates who work on projects related galaxy formation at UNLV. **Co-PI Bryan** has been supervising 3 graduate students (C. Hummels, Y. Li, C. Simpson) and two postdocs (R. Joung, M. Turk) at Columbia. **Co-PI Cen** supervised one graduate student, two undergraduate students, and worked with one postdoc (S. Tonnesen). **Co-PI Ostriker** worked with one postdoc (L. Oser), two graduate students at Princeton (E. Choi, J. Li), and one graduate student (A. Nunez) at Columbia. **Co-PI Naab** has supervised a few postdocs and graduate students at MPA.

4. Conference Presentations

• “Alleviating the scaling problems of cosmological hydrodynamic simulations with HECA” Oser, Nagamine, et al., *XSEDE13 conference*, San Diego, CA, July 2013.

• "Alleviating the scaling problems of cosmological hydrodynamic simulations with HECA"   Cen, Oser, Nagamine, et al., *Blue Waters Workshop*, NCSA, IL, May 21, 2013.

• "Alleviating the scaling problems of cosmological hydrodynamic simulations with HECA"   Oser, Nagamine, et al., *Extreme Scaling Workshop*, Chicago O'hare, IL, July 16-17, 2012.

• "Weak scaling results of the GADGET-3 cosmological SPH simulations and HECA" Nagamine, Oser, et al. *XSEDE12 conference*, Chicago, IL. July 17-19.