Snowmass2021 - Letter of Interest

Simulations and Modeling for the Cosmic Frontier

Thematic Areas: (check all that apply □/■)
□ (CompF1) Experimental Algorithm Parallelization
■ (CompF2) Theoretical Calculations and Simulation
□ (CompF3) Machine Learning
□ (CompF4) Storage and processing resource access (Facility and Infrastructure R&D)
□ (CompF5) End user analysis
□ (CompF6) Quantum computing
□ (CompF7) Reinterpretation and long-term preservation of data and code

Contact Information:
Salman Habib (Argonne National Laboratory) [habib@anl.gov]
Zarija Lukić (Lawrence Berkeley National Laboratory) [zarija@lbl.gov]

Authors:
Salman Habib (Argonne National Laboratory), Katrin Heitmann (Argonne National Laboratory), Zarija Lukić (Lawrence Berkeley National Laboratory)

Abstract: Next-generation cosmological modeling will focus on physically rich simulations to enable scientific discovery from future sky surveys spanning multiple wavebands. These simulations will have unprecedented resolution and volume coverage and must deliver guaranteed high-fidelity results for individual surveys as well as for the cross-correlations across different surveys. Contemporary computational resources have the potential to supply the needed capability, provided a number of obstacles can be circumvented. In this LOI we list the opportunities and challenges for cosmological simulations on next-generation high-performance computing (HPC) platforms.

1 Introduction

The next generation of cosmology experiments are aimed at exploring some of the most exciting questions in fundamental science – the twin mysteries of dark energy and dark matter and the origin of primordial fluctuations, along with the use of cosmology as a probe of particle physics (e.g., studies of the neutrino sector). Interpreting the results of many of these experiments involves solving an inverse problem, where given the observational results one wishes to unearth the details of the underlying physics. Modeling the effects of changes in parameter values as well as in the physical assumptions and establishing a direct connection to the observations across multiple surveys is a complex and challenging task. Cosmological simulations are the only way to approach this problem, simultaneously addressing the myriad issues associated with dynamical complexity, cross-correlations, and strict requirements on error control.

The required ability to create simulated "virtual universes" on demand is the fundamental computational challenge faced by the Cosmic Frontier. Indeed, it is not an exaggeration to say that the ultimate scientific success of the next generation of sky surveys hinges critically on the success of the underlying modeling and simulations.

The generation of these virtual universes can be accomplished in different ways. Large gravity-only simulations are used as the backbone for building sky maps that closely resemble the observations from large surveys. This approach requires careful modeling to establish the "galaxy-halo" connection[1]. The modeling strategies range from simple methods that take limited information into account and rely on empirical modeling assumptions to elaborate schemes that try to model galaxy formation processes as closely as possible but without taking into account computationally expensive gas physics and feedback effects directly. Hydrodynamics simulations attempt to model galaxy formation in cosmological volumes including gas physics and feedback effects. They employ phenomenological subgrid models whenever the dynamical range needed to resolve the physics of interest is too vast to start from first principles. The ultimate aim is to advance these different methods such that they all converge to the same answer – faithfully describing our Universe in all observable wavebands.

With the advent of exascale computing resources, several opportunities will arrive, but taking full advantage of them will not be straightforward. The high-performance computing (HPC) system architectures, associated software ecosystem, and data infrastructure will be substantially different from that of the previous generation. Adjusting to this computational environment, along with its variety and rapid evolution, will require special attention and substantial human resources.

The resolution and volume of gravity-only simulations will enable the creation of ever more detailed synthetic sky catalogs. Hydrodynamics simulations in large cosmological volumes with a rich set of well-tuned subgrid models will be feasible. These simulations will allow us to study and mitigate possible systematic effects that might obscure fundamental physics insights. Synthetic skies will be developed across multiple wavebands and surveys. In order to realize this vision, we have to fully exploit the next generation of HPC resources for these large-scale simulations, develop efficient analysis approaches and connect the simulations closely to observational data. This LOI aims to outline some of these challenges and possible solutions for the next-generation of cosmological simulations.

2 Challenges and Opportunities

2.1 Next-generation Supercomputing Platforms

The arrival of the first generation of exascale supercomputers, Aurora and Frontier, at the Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories provides an extraordinary opportunity to push scientific simulations to the next level. In cosmology, they enable two classes of simulations relevant to cosmological surveys: gravity-only simulations with unprecedented volume coverage and resolution and hydrodynamics simulations with exceptionally detailed and realistic modeling of baryonic physics in the Universe. The Exascale Computing Project (ECP) led by the Office of Advanced Scientific Computing Research (ASCR) in collaboration with other DOE science program offices has made tremendous strides to prepare scientific applications for these resources and will continue to do so. As part of this effort, important challenges have been identified, including the efficient use of computational accelerators, performance portable programming models and scalable algorithms. For gravity-only simulations, some of these challenges have already been successfully addressed by a subset of codes[2], for hydrodynamics simulations, these challenges are far more complex. Continuous developments on these fronts are extremely important in order to enable full exploitation of exascale systems and ones that will follow them.

2.2 Scalable Analysis Approaches

Scalable analysis approaches are as important as the development of the simulation codes. In principle, many petabytes of data can be easily generated by current and next-generation HPC systems, in pratice, however, storage capacities are limited and the handling and processing of very large data sets would require large supercomputing resources in their own right. Consequently, carefully designed analysis routines have to be instantiated on-the-fly while the simulation codes themselves are running ("in situ" analysis). The development of these analysis routines faces the same challenges as the simulation codes, and scalability and efficient usage of the available architectures are mandatory. A successful cosmological simulation program therefore needs to ensure that the development of the codes and the analysis routines go hand in hand. This task is complicated by the fact that cosmological simulations aim to provide predictions for a wide range of observations. A carefully orchestrated analysis approach has to be developed with cosmological surveys in mind – close collaboration between simulators and observers is essential for its success.

2.3 Verification and Validation

The accuracy requirements for cosmological simulations are very stringent. As outlined above, the simulations provide the foundation for the analysis of current and next-generation cosmological surveys. Given the aim to constrain, e.g., dark energy parameters at the percent level, simulations and the coupled analysis and modeling approaches have to deliver results at the same accuracy. The community has made good progress with regard to code verification in the last few years by carrying out rigorous comparison projects[3–6] and convergence studies[7]. However, not all differences between the codes and analysis tools have been fully resolved and/or understood. In particular, in the area of hydrodynamics simulations, much more work is needed to obtain the desired levels of robustness.

Validation (confirming the accuracy of the simulation predictions by direct comparison against observations) is another crucial area that requires a concerted effort between different code and analysis development teams and observers. Fortunately, the upcoming surveys will provide a rich data set for this effort. A delicate issue is how to control errors coming from empirical modeling used within the setup of the simulations. The detailed connection between the simulations and the survey observables has to be tightened up considerably as this is the most problematic aspect of the validation program from the simulation perspective.

3 Summary

Science with future cosmological surveys will require close coupling to a state-of-the-art simulation campaign that not only provides a complete and robust modeling platform for each survey about also provides a facility to simultaneously model a number of observations including their cross-correlations. Next-generation HPC systems promise to provide a capability that can help achieve these goals; getting to the desired results will require a concerted effort in implementing new algorithms/models, and evolving the simulation codes and associated analysis tools. Additionally, close collaborations with survey teams will be an essential element for success.

Note: The list of references is far from complete and is not meant to be representative.

References

[1] For a recent review see: R.H. Wechsler and J.L. Tinker, Ann. Rev. Astron. Astrophys. **56**, 435-487 (2018)

[2] S. Habib, A. Pope, H. Finkel, N. Frontiere, K. Heitmann, D. Daniel, P. Fasel, V. Morozov, G. Zagaris, T. Peterka, V. Vishwanath, Z. Lukić, S. Sehrish and W.k. Liao, New Astron. **42**, 49-65 (2016)

[3] K. Heitmann, P. M. Ricker, M. S. Warren and S. Habib, Astrophys. J. Suppl. **160**, 28-58 (2005)

[4] A. Schneider, R. Teyssier, D. Potter, J. Stadel, J. Onions, D.S. Reed, R.E. Smith, V. Springel, F.R. Pearce and R. Scoccimarro, JCAP **04**, 047 (2016)

[5] J. Onions, A. Knebe, F.R. Pearce, S.I. Muldrew, H. Lux, S.R. Knollmann, Y. Ascasibar, P. Behroozi, P. Elahi, J. Han, M. Maciejewski, M.E. Merchan, M. Neyrinck, A.N. Ruiz, M.A. Sgro, V. Springel and D. Tweed, Mon. Not. Roy. Astron. Soc. **423**, 1200-1214 (2012)

[6] O. Agertz, B. Moore, J. Stadel, D. Potter, F. Miniati, J. Read, L. Mayer, A. Gawryszczak, A. Kravtsov, J. Monaghan, A. Nordlund, F. Pearce, V. Quilis, D. Rudd, V. Springel, J. Stone, E. Tasker, R. Teyssier, J. Wadsley and R. Walder, Mon. Not. Roy. Astron. Soc. **380**, 963-978 (2007)

[7] K. Heitmann, M. White, C. Wagner, S. Habib and D. Higdon, Astrophys. J. **715**, 104-121 (2010)