Large Scale Simulations of Sky Surveys

Abstract

Large-volume sky surveys have accessed the vast temporal and spatial expanse of the Universe via a remarkable set of measurements, and many more are sure to follow. To make new predictions for these cosmological observations, and to properly interpret them, large-scale numerical simulation and modeling has become an essential tool. Here we discuss HACC (Hardware/Hybrid Accelerated Cosmology Code), an extreme-scale N-body cosmology code and its associated analysis framework, focusing on the complexity of the analysis workflow, which is as important as running the underlying simulation.

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1. Simulating the Universe as Seen through Large-Scale Sky Surveys

Cosmologists have looked deeply at the Universe and found it to be ‘dark’. Detailed observations over the last three decades spanning the full range of the electromagnetic spectrum, from gamma rays to the radio sky, carried out from the ground and from space, persuasively suggest an astonishing picture: ~70% of the matter-energy content of the Universe is made up of a mysterious ‘dark energy’ component, potentially responsible for the Universe's accelerated expansion, 25% of the matter exists in the form of a yet unidentified ‘dark matter’ component, and only 0.4% of the remaining ordinary matter, happens to be visible. Understanding the physics of the mysterious dark sector is the foremost challenge in cosmology today. Major cosmological missions are ongoing and planned to create ever more detailed maps of how mass is distributed in the Universe. These maps hold the key to advancing our knowledge of the make-up and evolution of the Universe, enabling us to unlock its ‘dark’ secrets.

Unlike a science based on the experimental method, cosmology lacks investigations under the researcher’s control, performed under strict isolation, and allowing step-by-step progress towards solving a physical problem, however complex it may be. The task is instead to make a number of robust observations, where statistical and systematic errors can be bounded, and then to arrive at scientifically defensible inferences about the Universe. To do this, one creates model Universes allowing for different cosmological models and astrophysical effects, mimicking possible observational systematics and even implementing the “clean-up” of observational data from unwanted foregrounds obscuring the signals being searched for. The
The complexity of this task leads inexorably to the use of the world's largest supercomputers.

This requires an end-to-end computational approach, starting from the fundamental theory (Einstein's general relativity and modifications thereof, quantum mechanics), to simulating the formation of large-scale structures in the Universe and creating synthetic maps for the observation of interest, to modeling the instrument, and effects that can bias observations, such as atmospheric turbulence (for a detailed discussion of an end-to-end pipeline for the Large Synoptic Survey Telescope see Ref. [1]). We must understand the observed system as a whole, and determine which physics will have important effects on what scales, where simple modeling suffices, as compared to fully self-consistent simulations, and how uncertainties in modeling and simulations can bias the conclusions. This task is complicated further by the fact that we often cannot directly observe what we desire to study but must draw conclusions from an indirect analysis, as for instance in the use of baryonic tracers (galaxies) of the large-scale structure of the Universe.

In this paper, we focus on describing our current efforts to create synthetic galaxy maps from large-scale simulations for optical surveys, setting aside telescope modeling as a separate problem. In order to build these synthetic maps, we have to simulate the evolution of the mass distribution in large cosmological volumes with exquisite resolution. To demonstrate the scale of this challenge, a quick summary of the relevant scales is as follows. Modern survey depths require covering simulation volumes of order tens of cubic Gpc (1 pc=3.26 light-years); to follow bright galaxies, structures with a minimum mass of $10^{11} M_\odot$ ($M_\odot$=1 solar mass) must be tracked and resolved by at least a hundred simulation particles. The force resolution must be small compared to the size of the objects to be resolved, i.e., $\sim$kpc. This immediately implies a dynamic range (ratio of smallest resolved scale to box size) of a part in $10^6$ ($\sim$Gpc/kpc) everywhere in the entire simulation volume. In terms of the number of simulation particles required, the implied counts range from hundreds of billions to many trillions. This requires access to very large supercomputers and, in today's landscape of diverse supercomputing architectures, a highly scalable and portable N-body code. To this end we have developed HACC (Hardware/Hybrid Accelerated...
Cosmology Code), a high performance code framework targeted at current and future architectures. We will provide a description of HACC in Section 2.

The mass distribution in the Universe is probed indirectly as most of the mass is dark, neither emitting nor absorbing light. Since the presence or absence of light is what we observe, the connection between mass and light is of fundamental importance. To investigate this connection, a major analysis suite has to be created and a seamless workflow must exist to ingest the raw simulation output and produce large-scale maps of galaxies. We have created such an analysis environment, which combines in situ analysis tools with a suite of post-processing steps, described in Section 3. As an example, Figure 1 summarizes the analysis path for the statistics of galaxy surveys. In the article we will focus on describing the different steps on the left side of the image, how to use large-scale supercomputers to create detail maps of our Universe as seen through optical telescopes. The last section will show some concrete examples of our effort.

2. HACC: Enabling Large-Scale Structure Simulations on Modern Supercomputing Platforms

HACC was initially designed for the Roadrunner supercomputer [3,4], the first system to break the Petaflop barrier. With its novel architecture of acceleration via the Cell processor, Roadrunner was by far the most forward looking machine of its generation, providing a glimpse of the current frontier and some illumination of the path to the exascale [5].

The design of a modern high-performance code must begin with an awareness that methods and algorithms should not be developed without an understanding of future programming paradigms and computing and storage architectures. The HACC computational strategy is based on a hybrid representation of physical information on computational grids as well as ‘particles’ that, depending on the context, can be viewed as tracers of mass, or as micro-fluid elements. This hybrid representation is
flexible and can be made to map well to machine architectures as well as to be aligned with multiple programming paradigms. Additionally, it provides a broad choice of methods that can be optimized given architectural, power, and other constraints, and the best combination can be picked for any given platform.

Technically speaking, HACC simulates cosmic structure formation by solving the gravitational Vlasov-Poisson equation in an expanding Universe [6]. The simulation starts from a smooth Gaussian random field that evolves into a ‘cosmic web’ comprised of sheets, filaments, and mass concentrations called halos. An image of the formation of cosmic structures over time is given in Figure 2. The Vlasov-Poisson equation is hopeless to solve as a PDE because of its high dimensionality and the development of nonlinear structure, therefore N-body methods are employed.

HACC uses a combination of grid and particle methods, where the grid methods are used to resolve the large to medium (smooth) length scales and the particle methods are employed to resolve the smaller scales. This split between the long- and short-range solver offers a very convenient organization of the code: the long-range force (in this case an FFT-based solver) exists at the higher level of the code and is essentially architecture-independent. It is implemented in C/C++/MPI and its performance and scaling is dominated by the FFT implementation. We have developed a new pencil-decomposed FFT and demonstrated scaling up to 1,572,864 cores in Sequoia, a 96-rack IBM BG/Q system [7]. The particle-based short-range solver exists at a lower level of the computational hierarchy and is architecture-tunable. It combines MPI with a variety of local programming models (OpenCL, OpenMP, CUDA) to readily adapt to different platforms. To enhance its flexibility, the short-range solver uses a range of algorithms, direct particle-particle interactions, i.e., a \( P^3M \) algorithm [8], as on Roadrunner and Titan, or both tree and particle-particle methods as on the IBM BG/Q (‘PPTreePM’). The grid is responsible for 4 orders of magnitude of dynamic range, while the particle methods handle the critical 2 orders of magnitude at the shortest scales where particle clustering is maximal and the bulk of the time-stepping computation takes place. An in-depth description of the HACC design and implementation, including the long-range solver, the different short-range solvers, the time stepper, and spatial decomposition of the code, as well as its scaling properties, is given in Ref. [9].

HACC’s multi-algorithmic structure attacks several weaknesses of conventional particle codes including limited vectorization, indirection, complex data structures, lack of threading, and short interaction lists. Currently, HACC is implemented on conventional and Cell/GPU-accelerated clusters [3,4,9], on the Blue Gene architecture [7], and is running on prototype Intel Xeon Phi hardware. HACC is the first, and currently the only large-scale cosmology code suite worldwide, that can run at scale on all available supercomputer architectures. HACC achieved outstanding performance on both Sequoia and Titan, reaching almost 14 PFlops
HPC Platform
- Level I Data
- Level II Data
- Realtime Analysis
- Realtime Viz

Analysis Cluster
- Level II + III Data
- Interactive Analysis
- Interactive Viz

Figure 3: Data levels and analysis hierarchy of a cosmological simulation.

(69.2% of peak) on Sequoia, a kernel peak of 20.54 PFlops on 77% of Titan (the full machine was not available for these scaling runs), and 7.9 PFlops of sustained performance on 77% of Titan for the full code. HACC’s outstanding performance and portability has enabled us to carry out some of the challenging simulations needed to advance our understanding of the dark Universe.

3 Analytics Requirements and Tools
Analyzing the data from the large cosmological simulations is as demanding as carrying out the simulations themselves. In fact some of the computational modeling applied to the outputs in post-processing is even more complex than the N-body simulation itself with respect to the physical processes involved. To put the challenge posed by the analysis task into context, a single time snapshot from one of the simulations discussed in Section 4 encompasses 40TB of raw data, and of the order of 100 snapshots have to be analyzed. This amount of data clearly demands a well-thought out analysis strategy, combining in situ and post-processing tools. Another challenge is posed by the fact that the raw data from the simulation is very science-rich. Not only can we generate optical catalogs from the simulation -- the example discussed in the next section -- but also field maps, e.g., the cosmic microwave background temperature, or X-ray flux. It is important to store enough of the already processed data to ensure that new science projects can be carried out at later stages.
In order to design an efficient workflow to tackle these challenges and to decide which analysis tools have to be run in situ and therefore on the HPC system itself (which means that they should scale as well as the main code, a difficult task in and of itself), it is useful to break up the data into three more or less distinct levels: (i) Level I, the raw simulation output, where the particles, densities, etc. live; (ii) Level II, the ‘science’ level, that is, the output rendered as a description useful for further theoretical analysis, including halo and sub-halo information, merger trees, line-of-sight skewers; and (iii) Level III, the ‘galaxy catalog’ level where the data is further reduced to the point that it can be interacted with in real-time. Very roughly speaking, at each higher level, the data size reduces from the previous level by 2 or 3 orders of magnitude.

The data layer plays a crucial role for science applications. Because of the imbalances in the I/O bandwidth relative to peak performance for the computation and the extreme stressing of file systems, it has been apparent for some time that dumping raw data to a storage system for post-analysis is a poor strategy for a problem where intensive analysis of very large datasets is essential. Therefore, we carry out as much of the analysis as possible on the raw Level I data on the HPC system itself, as well as the reduction of Level I data to Level II. The Level II datasets can then be loaded into an analysis cluster and further analyzed. A schematic of the different data levels and analysis hierarchy is shown in Figure 3.

Level I analysis requires algorithms for tasks such as halo-finding, determining correlation functions and a host of other statistical measures, building halo merger trees, and carrying out automated sub-sampling of the data. The overall data hierarchy must take the needs of the analysis routines as well as that of the simulation code into account, in order to maintain locality and avoid data movement. Level II data products can be used for science directly or used to produce Level III data products such as mock survey catalogs that include galaxies with realistic colors, luminosities, and morphologies. The computational algorithms we apply to address our science goals include density estimation, anomaly detection, tracking, high-dimensional model fitting, and non-parametric inversion. These techniques are computation and memory intensive and have been developed to work within the raw Level I and Level II data products. To show two concrete examples that will be important for our analysis in the next Section, we now discuss the halo finder, which runs in situ with the simulations and reduces data from Level I to Level II, and the halo merger tree code that acts on Level II data and enables the generation of Level III data.

**Halo Finding:** The ‘halo’ concept plays a very important role within cosmological simulations. Dark matter halos are the hosts of galaxies and by mapping out galaxies we can draw conclusions about the dark matter distribution in the Universe. Halos mark over-densities in the dark matter distribution and can be identified through different algorithms. Most commonly, they are found by either locating density peaks directly and growing spheres out to a characteristic over-density or via
neighbor finding algorithms. Here we will discuss one of the simplest, the so-called friends-of-friends (FOF) algorithm which is used for all of following results. In FOF halo finding, for each particle, every particle within a certain distance, the so-called linking length (usually between 0.15 to 0.2 of the mean inter-particle spacing) is identified as a ‘friend’. The process is then continued for each friend particle, and so on. If the number of particles in such a conglomerate is above a certain threshold (usually approximately ~100 particles) the structure is called a halo. Its center is found by either finding the particles with the most friends (maximum local density) or by determining the potential minimum of the halo, or by finding the average position from all particles in the halo (the center of mass). Naively, the FOF algorithm requires $N^2$ operations, but the algorithm is straightforwardly sped up to $N\log N$ via a tree implementation. In addition, our FOF finder takes full advantage of the already existing overloaded data structure strategy of the main code in order to enable parallel halo finding. Halos can be identified independently on each rank and halos on the edge of a rank are not missed since particle information is available from the neighboring ranks. A final reconciliation step ensures that halos are not counted more than once. For details of the implementation and scaling properties of the algorithm, see Ref. [10].

As mentioned previously, the FOF finder reduces the raw Level I simulation data to Level II data. The halo catalog itself, which contains information about halo properties such as position and velocities, is negligible in size compared to the raw data. In addition to the halo catalog, we store the tags of all particles in halos
(depending on the threshold of what defines a halo, the number of particles in halos is approximately 50% of all particles) and their halo tag (identifying to which halo each particle belongs), which we need to construct halo merger trees, as discussed next. Finally, we store full particle information (positions and velocities) for a subset of particles in halos (usually 1%) to enable placements of galaxies at those positions later on, and all particles in halos above a large mass cut-off. This set of data (halo information and reduced information about particles in halos) defines the set of Level II data connected to the halos and reduces the data volume by a factor of approximately 10. Most of the data is stored in the particle tags of particles that are in halos -- once the halo merger trees are built, this information can be discarded and the data reduction then reaches more than a factor of 100, as stated earlier. Halo finding is carried out for roughly 20% of all global time steps (there are no halos very early in the simulation). Compared to the time stepper itself, the relative cost of the halo finder decreases over time, but is always at a comparable level of time consumption as a single time step. Because of the data size and computation time consumed, it is not feasible to offload this step to a smaller analysis cluster.

**Merger Tree Construction:** The FOF algorithm identifies halos from individual snapshots based on the spatial relationship between particles at a fixed point in time. In order to determine halo temporal evolution, we evaluate the FOF output from the complete sequence of snapshots. Our algorithm compares halos from adjacent snapshots, and constructs a graph for representing evolutionary events. The graph, called a merger tree, represents each halo by a vertex (see Figure 4 for an example), and similar halos in adjacent snapshots with an edge. We define a similarity measure as the fraction of shared particles (i.e., the particle intersection of two halos) to total particles from the earlier of the two halos.

To construct the merger trees between subsequently taken snapshots, it is sufficient to compare the particle membership functions obtained by the FOF finder. However, computing the pairwise similarity matrix for the halos of all the adjacent snapshots requires some efficiency. We implement a technique for determining the intersection cardinality of multiple sets that is linear with respect to the number of particles, after an initial particle sort is performed. We utilize a type of sparse matrix representation for the similarity matrix to reduce the otherwise large memory requirement. The memory reduction is significant due to the large amount of sparsity inherent to the problem, and we have witnessed the computational overhead incurred to be marginal.

As mentioned, this approach relies on the result of the FOF algorithm for calculating the halo membership function. Because the clustering algorithm requires halos to have a minimum number of particles, the hard threshold can cause some misidentification of events when halos are near the minimum cutoff value. In order to reduce these misidentifications, we maintain a windowed history of missing halos. The particles from the missing halos are stored for comparison with later snapshots to determine if they re-emerge, and if so, to be treated as coming from some pre-existing halo.
4. The Simulated and the Real Universe

Finally, we show some results from the analysis of recent simulations carried out on Mira at the Argonne Leadership Computing Facility and on Titan at the Oak Ridge Leadership Computing Facility. As mentioned in the Introduction, one important task in the analysis is to transform the mass distribution we obtain from the N-body simulations into actual galaxy catalogs. Simulating galaxies from first principles in a cosmological volume is still far from possible -- the dynamical range is vast and the physics of galaxy formation, inadequately understood. Instead, galaxies can be painted onto the dark matter distributions, using models of different levels of sophistication. The main assumption here is that "light traces mass", meaning that the galaxies trace the density of the mass distribution, which is predominantly dark. This assumption is true only as an approximation; the aim is to develop more complex prescriptions to 'light up' the dark matter distribution with galaxies.

![Graph showing the observed galaxy power spectrum compared to an emulator](image)

*Figure 5: Comparison of a simulated galaxy spectrum to observations from the SDSS-BOSS survey [12]. The power spectrum is the Fourier analog of the two-point correlation function and characterizes the tendency of galaxies to cluster together.*
A simple and powerful approach to this problem uses the so-called Halo Occupation Distribution (HOD) model [10]. In this approach, a number of so-called central and satellite galaxies of a certain type are assigned to a dark matter halo depending on the halo’s mass. The central galaxy lives at the center of the halo and is the brightest galaxy. If the halo is heavy enough to host more galaxies, satellite galaxies are assigned and placed within the halo. The HOD model is described by approximately five parameters that are tuned to match one observable, e.g., the galaxy power spectrum. Once the model is fixed, other observables can be predicted from the galaxy catalog. Recently, we have built synthetic sky maps based on a large Mira simulation evolving 32 billion particles in a \((2.1 \text{ Gpc})^3\) volume and investigated the dependence of the galaxy power spectrum on the five HOD modeling parameters [13]. The best-fit HOD model on top of data from BOSS, the Baryon Oscillation Spectroscopic Survey, is shown in Figure 5. This figure demonstrates how well the results from simulations match the observational data.

While the HOD approach is simple, it has one major shortcoming: it completely neglects the formation history of a halo that surely will carry information about the galaxy population it hosts today. For example, if a halo formed very early and mainly grew through mass accretion, it will not have much star formation today. Or, if the halo underwent a violent merger with another large halo, it will also have a distinct galaxy population. In order to take these effects into account, so-called semi-analytic models (SAMs) have been developed. SAMs follow the evolution of each halo via halo merger trees and solve along the way a set of physics equations that describe galaxy formation in an approximate way. SAMs deliver very detailed descriptions of the galaxies that populate halos, including their colors, positions, and shapes, star formation history, black hole content, etc. The drawback of the SAMs is that they depend on a large number of parameters (two to three hundred) that have to be tuned to observations. In Figure 6 we show an example of our full simulation and analysis pipeline working to create a synthetic galaxy map. The simulation, carried out on Titan, has a mass resolution of \(\sim 10^9 \text{ M}_\odot\) and therefore can capture the smaller halos that host bright galaxies reliably. As the simulation was run, halos were
identified on the fly, and the information of particles resident in halos was stored. From this information, merger trees were constructed to track the evolution of each halo in detail. Finally, a sophisticated semi-analytic model was run on the merger trees, in this case Galacticus [14], to generate a full synthetic galaxy sky.

Our last example shows results from the largest cosmological simulation ever attempted: the Outer Rim simulation. This simulation is currently running on Mira at ALCF and evolves 1.1 trillion particles in a (4225 Mpc)$^3$ volume. As for the Titan run, each particle has a mass of $\sim 10^9$ $M_\odot$ but the volume covered is many times larger. The force resolution in the simulation is $\sim 4.1$ kpc, achieved via a 10240$^3$ PM mesh on the large scales in combination with the tree solver on small scales. To demonstrate the scale of this simulation, we show a slice of the full simulation box in Figure 7 as well as the output from one of the 262,144 ranks the simulation is run on. New science results have been already extracted from the simulation (even though it has not quite yet reached the present epoch) and Figure 8 shows an example of the exciting science results that can be obtained. In this case, a halo at a certain time was extracted, a tessellation-based estimator was used to create its two-dimensional projected density, and a ray-tracing code used to generate a strong gravitational lensing image from a simulated source (see Figure 8 for the workflow). Strong lensing refers to the severe distortion of galaxy images and the generation of multiple images due to the presence of a massive intervening object between the source galaxies and the observer. In our case, the halo from the simulation is the massive object (in the center of the right panel), galaxies are placed behind this lens and the visible arcs are the distorted images as given by a fast ray-tracing algorithm.
The resulting images can then be compared to images taken from, e.g., the Hubble Space Telescope and new clues about the dark Universe can be obtained, such as the properties of the dark matter that makes up the lensing halo.

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