UNIVERSE SIMULATORS

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ABSTRACT

Whether they seek to verify theories of the origin and evolution of the large-scale structure of the Universe, understand more about its past or make predictions for its future, scientists rely on supercomputers to model and create cosmological simulations. In the areas of physics and astrophysics, with nowadays computational resources it is feasible to simulate complex physical systems with an accuracy which is useful. The article presents two different approaches for simulating universes – the hydrodynamic cosmological simulations and N-body cosmological simulations and their corresponding state-of-the-art implementations.

KEYWORDS: *astrophysics, cosmology, smoothed-particle hydrodynamics, N-body simulation*

1. INTRODUCTION

Computational astrophysics involves the use of computers and numerical methods for solving problems identified by astrophysics researches, when the mathematical models, which describe astrophysical systems, are impossible to be calculated analytically [1][2]. Even if the results generated by such methods do not represent the exact solution, these approximations are far more valuable than precise solutions of approximate equations that can be determined analytically.

Notable results by computation in astrophysics were obtained in the following areas of activity:

- Stellar structure and evolution
- Radiation transfer and stellar atmospheres
- Astrophysical fluid dynamics
- Planetary, stellar, and galactic dynamics

Since about 95% of the Universe consists of “darkness” – 72% dark energy and 23% dark matter, solving the mystery of the dark energy’s nature can only be achieved through indirect observation [3]. Future space surveys will capture the light of billions of galaxies and astronomers will evaluate the subtle distortions, caused by light, deflected of these background galaxies by a foreground but invisible distribution of mass – the dark matter.

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The primary tools for researching cosmic structure formation are simulations [4], which astrophysicists use to study how matter clusters in the Universe by gravitational aggregations. Due to advancements, simulations now include the visible, baryonic matter as well as non-baryonic cold dark matter.

The process of a cosmological simulation is comprised of two parts [5]: the first part requires the generation of initial conditions as stated by the structure formation model to be investigated – these conditions will be used as input. In the following step, algorithms simulate the evolution of particles by tracking their trajectories under their mutual gravity. Put it simply, cosmological simulations are just tools used to investigate how millions of particles evolve, since the particles try to sample the matter density field as precisely as possible. In the end, cosmologists study the output of these simulations to check if it matches the data gathered by space surveys, and to judge and understand any found discrepancies. The Figure 1 sketches the evolution of the Universe and the gap between observations gathered from the Cosmic Microwave Background (which describe the early Universe), and current observations, which these simulations are trying to cover.

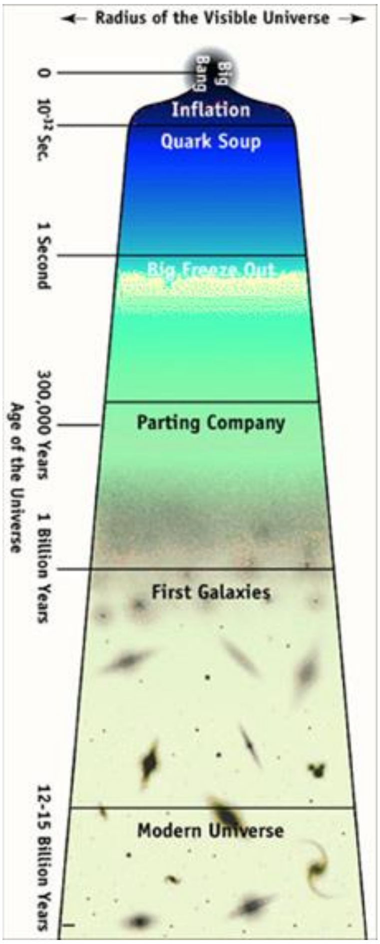

Figure 1. Cosmic Timeline [5]

During the past decade, very accurate Cosmic Microwave Background (CMB) experiments such as WMAP [6] and Planck [7] brought us to the era of high precision cosmology.

WMAP

NASA's Explorer mission which launched in June 20101 - **W**ilkinson **M**icrowave **A**nisotropy **P**robe, made fundamental measurements of our Universe, and after WMAP's data stream ended, the analysis of the data collected by it revealed that the mission was in fact, unexpectedly successful. A few of the achievements stated by NASA on **WMA**P's website include [6]:

- determining that baryons make up only 4.6% of the universe
- narrowed down the curvature of space to < 0.4% of "flat" Euclidean
- detected that the amplitude of variations in the density of the Universe is slightly larger on big scales, compared to smaller scales – among other results, this supports the idea of "inflation" and that tiny fluctuations were generated during the expansion and eventually grew to form galaxies
- confirmed predictions of the inflation idea, regarding that the distribution of such fluctuations follows a bell curve with the same properties across the sky, and that the number of hot spots and cold ones on the map is equal

2. RESEARCH STANDARD AND APPROACHES

The standard Lambda Cold Dark Matter (LCDM) model [8], managed to constrain down to a few percent cosmological parameters such as the Hubble constant or the total amount of matter contained by the Universe. For the following decade, future cosmological experiments might potentially change modern physics by clarifying two of the most difficult to find components of the Universe – dark energy and dark matter. This is particularly necessary due to the fact that two of the methods considered to quantify the clustering of matter as a function of time and scale, galaxy clustering and weak lensing rely on predictions of the non-linear dynamics of dark matter as accurate as possible.

As approaches to simulate the universe, two of the most common and successful methods are:

1) Hydrodynamic cosmological simulations – smoothed-particle hydrodynamics (SPH) which works by dividing the fluid into particles, which are in fact a set of discrete elements [9]. A *kernel function* "smoothes" their properties over a special distance - this means that by summing the properties (which are relevant) of all of the "grouped" particles outputs the physical quantity of any particle.
2) *N*-body simulations – the simulation of a dynamical system of particles, influenced by physical forces (e.g. gravity) [10]. For processes of non-linear structure formation, like galaxy halos and galaxy filaments influenced by dark matter, *N*-body simulations can be used for research.

2.1. Bolshoi

Bolshoi [11], and the following work, BigBolshoi [12] (which was a simulation 64 times greater than the initial one), are two of the most accurate cosmological simulations ever made. Ran during 2010-2011 on the NASA's Pleiades supercomputer, the simulation generated the distribution of over 8.6 billion particles of dark matter, across a three-dimensional cube-shaped space of around 1 billion light years on each side. Since the quantum mass is this large it is pointless to attempt to distinguish between dark and baryonic matter. The simulated particles are of dark matter, and the first evolved structures are the dark matter halos which contain the galaxies.

The simulation started about 23 million years after the Big Bang and the initial conditions were generated using the CAMB tools, provided by Wilkinson Microwave Anisotropy Probe website. Because the outputted volume represents an arbitrary portion of the Universe, the comparing its content against observations must be done from a statistical point of view.

Initially, all of the particles were close to being uniformly distributed across the cube. This was the overall setting of the universe after inflation and the first emission of the cosmic background radiation.

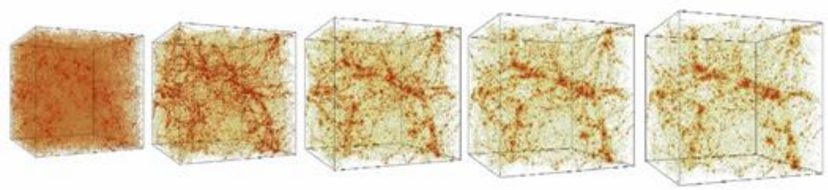

Figure 2. The distribution of particles across the cube, during different evolution stages

The algorithm behind the Bolshoi simulation was an alteration of the one created by Andrey V. Kratsov from the University of Chicago. The first step is to divide the cubical simulation into a grid of smaller cube-shaped cells. Iterative splitting continue until the number of particles contained by a cell drops under a pre-determined threshold. The smallest cell has roughly 4,000 light years for each side, and the mesh is made up of about 16.8 million cells. The simulation used 13,824 processor cores and 13 TB of memory out of NASA's supercomputer based at the Ames Research Center, Pleiades, which was ranked 7th worldwide at the time (end of 2011).

The Bolshoi cosmological simulation, as opposed to the Millenium Run which used cosmological parameters from WMAP1 that became obsolete, used, as parameters, data from WMAP5 that was consistent with WMAP7. Ever since the invention of Cold Dark Matter (1984) and the first CDM *N*-body cosmological simulations which were essential for determining the characteristics of dark matter, these simulations were at the core of calculating predictions on scale where structure has formed.

These large cosmological simulations are now the basis for actual research of the structure and evolution of the Universe, and the clusters of galaxies within. Further studying the generated data could point out the presence and location of satellite galaxies.

2.2. PKDGRAV3

Astrophysics researchers from the University of Zurich developed, over three years of work, code designed to maximize the use of modern supercomputing architectures such as the Swiss National Computing Center's "Piz Daint". In the paper [13] recently published by Joachim Stadel, Douglas Potter and Romain Teyssier, the astrophysicists report that in only 80 hours of wall-clock time, the code titled PKDGRAV3. The algorithm generated the successful evolution of over 2 trillion particles, while using more than 4000 GPU-accelerated nodes – from which over 25 billion virtual galaxies were extracted. The same model set another standard in computational astrophysics by simulation 8 trillion particles while running on "Titan" at the Oak Ridge Leadership Computing Facility (OLCF) and exploiting roughly 18,000 GPU-accelerated nodes.

The chosen approach for this particular simulation was to use *N*-body simulations, due to the fact that on such enormous scales, the nature of gravity is non-linear. The dark matter fluid was sampled in a dynamical system where all possible states of the system are represented, by using as many macro-particles as possible. Each of these macro-particles represents a large set of authentic, microscopic particles of dark matter, which evolve without collision while being affected by their mutual gravitational attraction.

The core algorithm – Fast Multipole Method, is a numerical technique which reduced the time to calculate long-range forces in *N*-body systems by using a multipole expansion that allows grouping of nearby sources and treating them as one. This method was introduced by Greengard and Rokhlin in 1987 [14]. PKDGRAV3's version of the FMM algorithm, managed to achieve a peak performance of 10 Pflops.

At the time PKDGRAV3 was benchmarked on Titan, the supercomputer was ranked 2nd fastest supercomputer in the world, scoring a performance of 17.59 Pflops (measured LINPACK performance). Titan's configuration was the following - a Cray XE7 system with 18,688 compute nodes and a Gemini 3-D Torus network, using the AMD Opteron model 6274 with 2.2 GHz clock speed. It also had the largest total system memory – 584 TB (highest across the supercomputer used for simulation, which included Piz Daint and Tödi). The time-to-solution for generating 8×10^{12} particles on this setup was 67 hours. The Table 1 describes the detailed benchmark and scaling results for Titan.

Table 1. PKDGRAV3's performance on Titan

Nodes	N_p	Mpc	TFlops	Time/ Particle
2	1.0×10^9	250	1.2	125 ns
17	8.0×10^9	500	10.3	14.7 ns
136	6.4×10^{10}	1,000	82.2	1.84 ns
266	1.3×10^{11}	1,250	152.5	1.00 ns
2,125	1.0×10^{12}	2,500	1,230.3	0.124 ns
7,172	3.4×10^{12}	3,750	4,130.9	0.0365 ns
11,390	5.4×10^{12}	4,375	6,339.2	0.0236 ns
18,000	8.0×10^{12}	5,000	10,096.2	0.0150 ns

The purpose of the simulation was to model galaxies as little as 1/ 10 of the Milky Way, inside a volume as large the observable Universe. Based on the output of the run, the overall observational strategy was optimized, as well as several adjustments for the experiments, such as minimizing the sources of error, that will take place on the Euclid satellite were made. Its mission to research the nature of dark energy and matter by collecting data will begin in 2020, after the satellite will be launched in space, and last for six years.

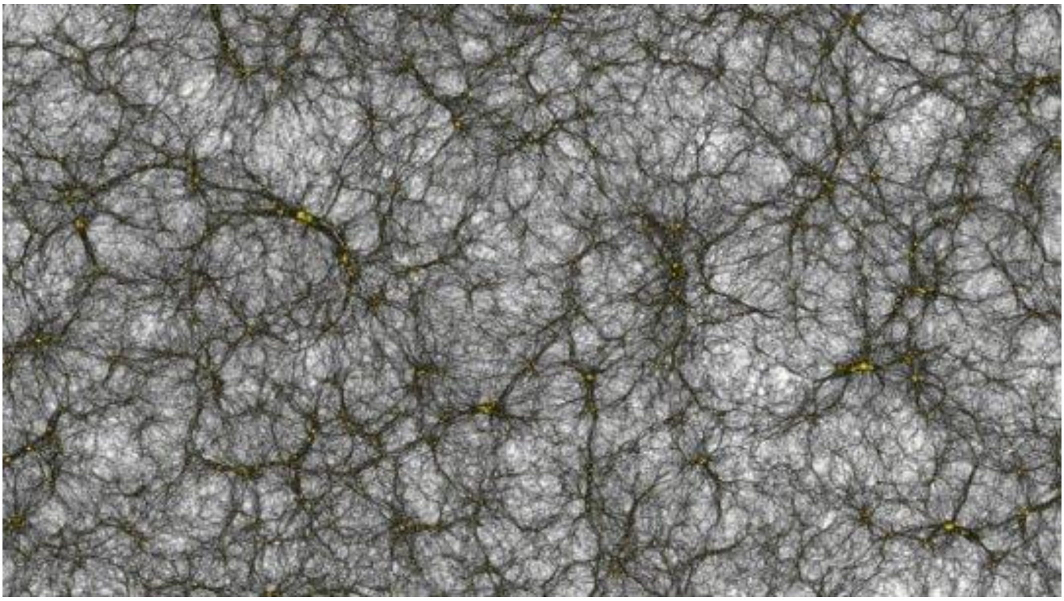

Figure 3. A one billion light years across section of the virtual universe, which displays the distribution of dark matter (*Joachim Stadel, UZH*)

The authors mention that in order to further improve the code, *co-designing* is required, which involves treating algorithmic and computer hardware developments as one design process. They also claim that in the future, simulations will be required to pull fundamental physical parameters from data which will be gathered by surveying, as opposed to using them only for making predictions or understanding effects. Due to the fact that the time-to-solution will continue to decrease as computational speed increases, they also expect similar simulations to run in less than 8 hours within the following decade. Given this, instead of storing raw data and post-process it, tools that analyze data might be attached to the code directly and just change the “instrument” every run.

2.3. Illustris

The Illustris model [15] – created by researchers from several institutions including MIT and Harvard, represents a cube-shaped piece of the universe that is 350 million light-years long on each side and it produces features as small as 1,000 light years. The initial conditions of the model are the parameters of the Universe 12 million years after the Big Bang, and the following 13.8 billion years are simulated by Illustris. The project’s set of large-scale simulations tracks the growth of the Universe, the gravitational pull which matter applies towards itself, the motion of cosmic gas and the emergence of black holes and stars.

The simulation tracks the evolution of more than 12 billion resolution elements in a volume of (106.5 Mpc) 3 which contains 41, 416 galaxies and generated a new degree of fidelity for certain observed features of the universe. Such features include the distribution of the different galaxy shapes and preponderance of specific elements in the Universe.

Establishing a link between the distribution of galaxies made up of normal matter and the observations was achieved by directly accounting for the baryonic component (gas, stars, supermassive black holes, etc.) as well as gravity. Ilustris's set of modeled physical processes is comprised, among others, by galactic winds driven by star-formation and thermal energy injection of black holes. These aspects contribute to achieve a simulated Universe having its modeled galaxies realistically distributed.

In the past, hydrodynamic cosmological simulations were used to study specific problems, due to being very expensive computationally speaking. For the past years, as a result of hardware development, these simulations managed to get enhanced either by increasing volume size and element count, improving the complexity and physical fidelity or by evolving the numerical methods used. Figure 4 describes this evolution over the past decade.

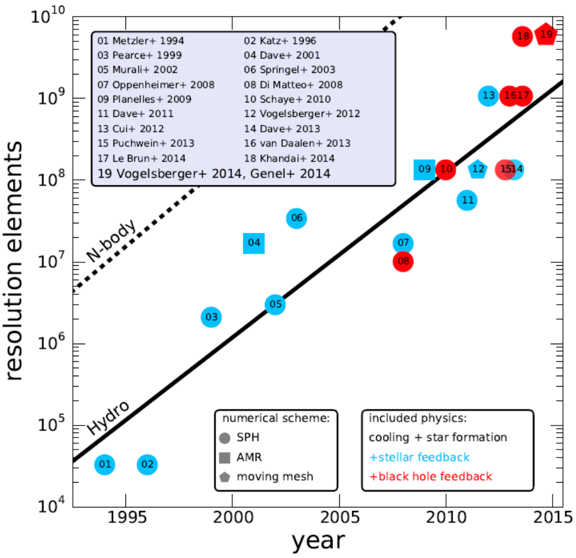

Figure 4. Evolution of hydrodynamical cosmological simulations [15]

Illustris was run across multiple supercomputers such as CURIE at the Alternative Energies and Atomic Energy Commission in France and at the Leibniz Computing Center in Germany, on the SuperMUC computer, but the list includes Harvard's Odyssey, Texas Advanced Computing Center's Stampede and Ranger and also Oak Rridge National Laboratory's Kraken. The largest run took 19 million CPU hours over 8,192 cores.

AREPO [16], the code behind the simulation, uses an unstructured Voronoi tessellation of the simulation volume, where the mesh-generating points of this tessellation are moved with the gas flow. The adaptive mesh is used to solve the equations of ideal hydrodynamics with a finite volume approach using a second-order unsplit Godunov scheme with an exact Riemann solver.

The authors mention several achievements obtained when comparing the output of the simulation against observations:

- successfully reproducing a wide range of observable properties of galaxies and the relationships between these properties.
- precisely measuring the gas content of the universe, and where it resides
- investigating the number of "satellite" galaxies, their properties, and their connection to cosmology
- study changes in internal structure as galaxy populations evolve in time
- the impact of gas on the structure of dark matter
- “mock” observations

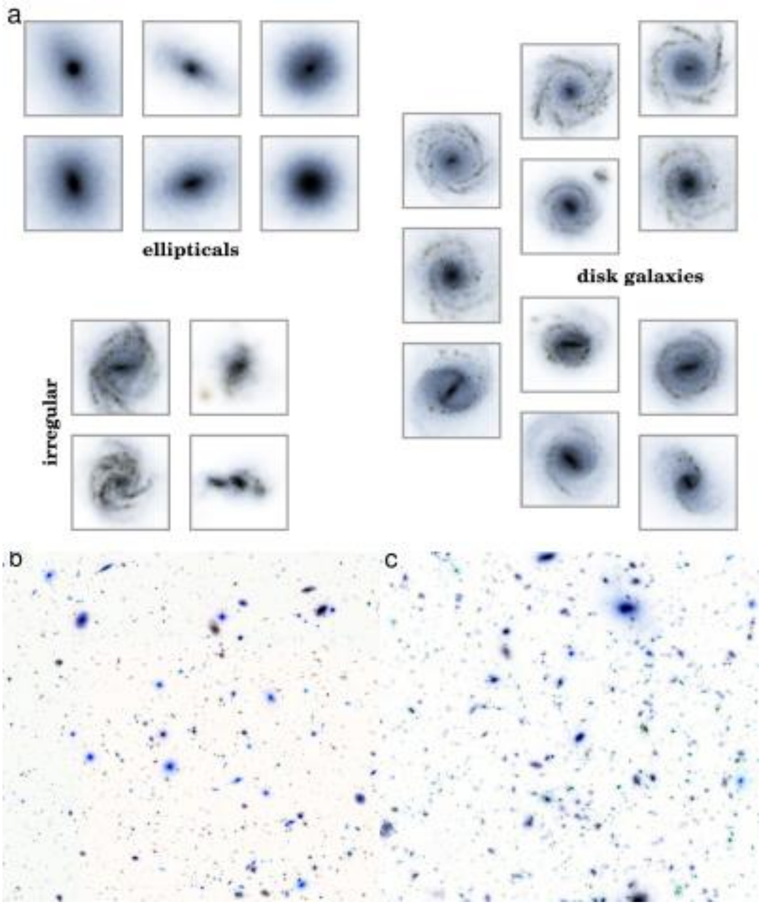

Figure 5. Mock images of the simulated galaxy population [16]

3. ALTERNATIVE APPROACHES

Simulations such as Bolshoi, PKDGRAV3 and Illustris, make a solid statement regarding the "bright future" of computational astrophysics. As projects similar to these 3 will "inevitably" scale up along with hardware developments, and produce larger volumes of higher quality data, another player might join the scene and contribute to explaining the mysteries of dark matter and dark energy.

In their latest work [17], several experimental physicists working for the Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences built a quantum computer with four qubits, controlled by laser pulses. The qubits are in fact calcium ions, trapped electromagnetically.

The quantum computer was used to simulate virtual particles in vacuum, showing that quantum computers can simulate the way particles may behave at extremely high energy levels, hard to generate on Earth. Even though a quantum computer of such small scale might be enough to tackle problems which are otherwise impossible using classical approaches, this particular problem researched could be computed by classical computers as well.

Also, researcher and co-author Peter Zoller mentions that - "We cannot replace the experiments that are done with particle colliders. However, by developing quantum simulators, we may be able to understand these experiments better one day." [18]

In the future, quantum simulations might aid researchers, for example, to mimic the dynamics inside neutron stars.

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