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choice of the OpenMP/MPI balance has to be evaluated and decided by the user. Furthermore, I/O strategies have to be developed and tested before the complete system can be used. Using modern parallel I/O libraries is crucial.
Even for hybrid OpenMP/MPI set-ups with a single MPI-task per node, problems arise due to internal limits of the MPI send/receive buffer. This limit is caused by the Integer*4 Byte implementation of the MPI index values. Such problems can be overcome through internal buffering in the applications.

The close interaction between scientists and HPC experts, as well as the thorough preparation by the users and the LRZ, was crucial for the success of this kind of workshop. There are now 25 applications that scale up to the full system size of SuperMUC (147,456 cores of Phase 1 and 86,016 cores of Phase 2, respectively). Two applications showed a sustained performance of more than one PFlop/s for more than 20 hours. The next extreme scale workshop is scheduled for January 2016.

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Visualizing 10^{11} Particles from Cosmological Simulations

Modern cosmological simulations can contain more than 100 billion particles and simulate the evolution of the Universe over several billion years. Besides numerical and statistical analysis of the raw data, visualizations allow cosmologists to literally fly through this simulated Universe to find remarkable structures within the simulation and to study their dynamic behavior. Moreover, such movies allow the general public to gain insights into the structure formation of the Universe. Here, we present the making of a visualization showcase presented at the Supercomputing Conference SC15 in Austin, Texas: a movie of a fly-through a cosmological simulation of 61 billion particles (320 TByte raw data), rendered on 1,280 CPU-cores, using 90,000 core-hours. For the URL of the showcase video and additional information, please see [1]. We also present a new version of the rendering software, realized with GPI-Space, that reduced the time to solution by a factor of 10.

P-Gadget3-XXL

The cosmological simulation code P-Gadget3-XXL is a cosmological, highly optimized and fully OpenMP/MPI parallelized TreePM-MHD-SPH code that enables large-volume, high-resolution cosmological simulations which follow in detail the various physical processes that are needed for a comparison with the experimental data coming from current and forthcoming astronomical surveys and instruments like PLANCK, SPT, DES and eROSITA. For more details, please see [2,3].

The Data-Set

The data-set originates from the Gauss Centre for Supercomputing (GCS) Large-Scale-Project "Magneticum" [1], which was carried out by a collaboration of scientist from the University Observatory Munich (LMU), the Excellence Cluster Origin and Structure of the Universe, and the Leibniz Supercomputing Center (LRZ).

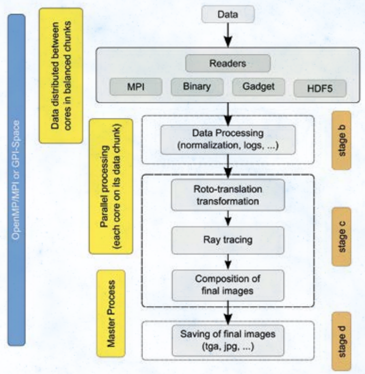

Figure 1: Workflow of the parallelized Splotch algorithm. For more details see [6].

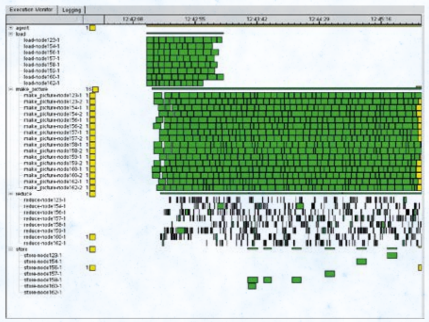

Figure 2: GANTT-chart of GPI-Splotch: Loading of data, rendering and saving the final images are performed in parallel, leading to an overall performance increase of 10x compared to the hybrid OpenMP/MPI version of Splotch (running on 2,048 cores, Intel Westmere).

Applications

All simulations of this project were computed on the SuperMUC system operated at LRZ. The total simulation campaign consumed more than 60 million core-hours of computing time on up to 131,000 cores. It consisted of several medium to large-sized cosmological hydrodynamics simulations, spanning the range from medium to extremely high numerical resolution. Various parameter setups defined in five different types of cosmological boxes were used. The last of these simulations finished in July 2015, data analysis has just started and first scientific publications from this project are expected to be published by the end of 2015. The Magneticum project includes one of the largest cosmological hydrodynamics simulations to date (including sub-resolution models for baryonic matter at galactic scales), evolving 180 billion particles over 100,000 time steps in a box of $(2.7\ Gpc/h)^3$ size with a scientific output of more than 300 TByte, using 25 million core-hours on 86,016 cores of SuperMUC Phase 2 (Intel Haswell). With respect to the number of particles, this simulation is 20 times larger than the previous generation of such simulations and corresponds roughly to a size of about 10% of the visible Universe. Only simulations of this size contain enough statistics to enable the analysis of the properties of the largest structures of the universe. For the movie presented here, a box with smaller size but higher resolution (compared to the largest box mentioned above) was used, as it shows finer details, containing 61 billion particles. Rendering the movie using the Splotch visualization tool ran on 1,280 cores on the fat node island of SuperMUC Phase 1 (Intel Westmere), using 32 TByte of main memory for about 72 hours (i.e. about 90,000 core-hours). The movie had to be rendered several times to find the ideal settings. The movie shows a flight through a small part of the evolving Universe (0.25% of the visible Universe), covering the evolution from redshift z = 9 to z = 0, i.e. a time span from around 560 million years after the Big Bang until today. Besides numerical and statistical analysis of the raw data, these visualizations allow cosmologists to find remarkable structures within the simulations and to study their dynamic behavior. Moreover, such movies allow the general public to gain insights into the structure formation of the Universe.

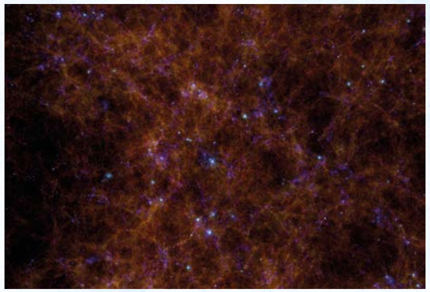

Figure 3: Screenshot from the movie.

The Renderer Splotch

Splotch is a light-weight, fast, and publicly available rendering software for exploration and visual discovery in particle-based datasets coming from astronomical observations or numerical simulations [5]. The rendering algorithm is designed in order to deal with point-like data, optimizing the ray-tracing calculation by ordering the particles as a function of their "depth", defined as a function of one of the coordinates or other associated parameters. Realistic three-dimensional impressions are reached through a composition of the final color in each pixel, properly calculating emission and absorption of individual volume elements. The strengths of the approach are production of high-quality imagery and support for very large-scale data sets through an effective mix of the OpenMP and MPI parallel programming paradigms (a version using GPGPUs is also available). The movie presented here was rendered using the OpenMP/MPI version of Splotch.

The new and improved GPI-Splotch

While creating the visualization showcase presented here, we also tested an integration of Splotch into GPI-Space (called GPI-Splotch). The development of GPI-Splotch was motivated by the observation that the OpenMP/MPI version of Splotch had a parallel efficiency of only 26% on 32 nodes (512 cores) of SuperMUC, which was determined by a timing analysis of OpenMP/MPI-Splotch. The integration into the GPI-Space framework took about three months and was done in order to re-organize the data-flow in Splotch, thus allowing an overlay of the rendering part with the non-parallel parts of the algorithm like file I/O or the aggregation of partial images, as well as introducing a dynamic load balancing scheme (see Fig. 2). GPI-Splotch uses an interface with only three different functions, which can be developed, tested and compiled without GPI-Space, and can then be connected later-on with GPI-Space through a dynamic library. The virtual memory created by GPI-Space to store partial results in memory is based on GPI-2 and profits from the low latencies and high bandwidth that GPI-2 allows [4]. As a small benchmark, we chose a data-set with 5 billion particles (167 GByte) to render 3,425 frames (fly-through the data-set at a fixed time step), generating 161 GByte of picture data. We rendered this benchmark using OpenMP/MPI-Splotch, running on 32 nodes (512 cores). This was the minimal possible number of nodes due to memory requirements. The total rendering time for this benchmark was 14.5 hours. A timing analysis of this benchmark revealed that the compute intensive and parallelizable rendering part took 26% of the total time (20% for rendering, 4% for 3D transformations, and 2% for particle coloring), while the rest was taken by load imbalances and the non-parallel post-processing and writing of the images. Reading the input file was negligible with only 0.3% of the total time. GPI-Splotch needed less memory, which allowed to run the benchmark on 16 nodes, where it already showed a 3.5x performance increase compared to OpenMP/MPI-Splotch on 32 nodes. Moreover, GPI-Splotch scales up to at least 128 nodes (2,048 cores – the largest set-up tested with this small benchmark). On 128 nodes, OpenMP/MPI-Splotch had basically the same runtime as on 32 nodes, whereas GPI-Splotch was 10x faster here. The next target for GPI-Splotch is to re-write the algorithm that interpolates between time-steps, which currently scales as $O((\text{MPI-ranks})^2)$, which currently limits the scalability of Splotch.

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[1] Direct URL to the movie of the visualization showcase: http://www.mpa-garching.mpg.de/HydroSims/Magneticum/Images_Movies/left_hd.avi
More Information and additional videos: http://magneticum.org

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