Computational Gravitational Dynamics with Modern Numerical Accelerators

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Abstract—We review the recent optimizations of gravitational \(N\)-body kernels for running them on graphics processing units (GPUs), on single hosts and massive parallel platforms. For each of the two main \(N\)-body techniques, direct summation and tree-codes, we discuss the optimization strategy, which is different for each algorithm. Because both the accuracy as well as the performance characteristics differ, hybridizing the two algorithms is essential when simulating a large \(N\)-body system with high-density structures containing few particles, and with low-density structures containing many particles. We demonstrate how this can be realized by splitting the underlying Hamiltonian, and we subsequently demonstrate the efficiency and accuracy of the hybrid code by simulating a group of 11 merging galaxies with massive black holes in the nuclei.

Keywords—stellar dynamics; galaxy dynamics; supermassive black holes; Tree-code; direct summation; Graphics-processing units; supercomputers.

I. INTRODUCTION

The first recordings of theoretical astronomy date back to the Egyptian 18th dynastic (1550-1292 BC) calculations by pharaoh Hatshepsut’s architect Senmut; part of the murals found in his tomb at Del el-Bahri is exhibited at [http://www.metmuseum.org]. Such calculations enable astronomers to recognize structure and describe patterns in the heavens; a branch of astronomy that is still relevant for classification and charting. Today’s astronomers hardly use clay tablets or stilae, but the instruments with which observations are conducted have been growing gradually.

The size of telescopes has increased from the 1 cm\(^2\) refractor that Lippershey build in 1608, to the \(\sim 110\, \text{m}^2\) collecting area of the Gran Telescopio Canarias. This 20-fold doubling of collecting area has been achieved in the last 400 years. Digital computers were only introduced at the end of the 1940s starting with a computational speed of about 100 modern floating point operations per second (or flops, ENIAC could perform about 360 multiplications in 6 decimal places per second) to about \(3 \cdot 10^{18}\) flops today; a 44-fold doubling in raw performance in only 65 years. Astronomers have therefore grown adiabatically in the improvement of their instruments, whereas computer scientists have experienced an explosive evolution.

This revolution in the availability of digital computers is still ongoing and has led to an entirely new branch of research in which facilities are not on high mountain tops on the Canary islands, but in the room next door. Astronomers realized quickly that they could use computers to archive, process, analyze and mine the copious amounts of data taken by observing campaigns. The biggest impact in the way astronomers pursued their scientific questions however, has been by means of simulation.

The fundamental complexity of astronomical research lends itself ideally for computation, because it is characterized by the enormous temporal and spatial scales, complex non-linear processes and the extremes of space. With the introduction of the digital computer it suddenly became possible to study processes in the intergalactic vacuum, hot plasma’s at stellar surfaces, billion-year time-scale processes and black hole physics; none of which can be studied in Earth-based laboratories.

The largest remaining limitation in studying the universe by means of computation are introduced by the software, and in particular our limited understanding of the algorithms for resolving the wide range of temporal and spatial scales, and for solving coupled fundamental physical processes.

Here we report on our experience in designing new algorithms for solving some of the software-related problems using recent hardware developments of attached accelerators. We limit ourselves to gravitational dynamics, and in particular to the gravitational \(N\)-body problem \(\Box\), because here the developments have been quite pronounced and the application is sufficiently general that the algorithms can be generalized to other research fields.
II. THE SEPARATION OF DIRECT AND HIERARCHICAL METHODS

Gravitational $N$-body dynamics poses an excellent research field for computing, because the physics based on Newton’s law of gravity can be calculated from first principles and has not changed (much) since 1687. The consequences of this long-range energy-conserving force are pronounced and extremely difficult to study analytically, leaving the computer as the only remaining alternative for research.

Shortly after the first $N$-body codes emerged, software development took an interesting direction in simulating more extended systems with more self-gravitating elements (i.e. particles) at the cost of a lower spatial and temporal resolution. This separation was initiated by the development of the tree-algorithm [2], which introduced a collision-less approximation of the former are generally used in combination with high order integrators with individual time stepping [3] whereas the latter are generally combined with phase-space volume-preserving symplectic integrators [4]. (Although there are production codes, in particular for simulating planetary systems, in which direct force evaluations are combined with symplectic integrators.) After this rather strict separation in philosophy we will discuss here how advances in software and hardware have recently led to the reunion of both algorithms. But before we discuss the reunion of algorithms, we discuss the revolution in both field separately.

III. SIMULATING COLLISIONAL SYSTEMS WITH DIRECT FORCE EVALUATION METHODS

Direct $N$-body calculations are generally adopted for studying the dynamical evolution of collisional systems over a relaxation time scale. Areas of research include stability studies of planetary systems, the evolution of star clusters and galactic nuclei with massive black holes.

Enormous advances in software have been achieved by the introduction of individual time-steps, the Ahmad-Cohen neighbor scheme and a rich plethora of regularization techniques. Each of these however, are hard to parallelize. The introduction of block time steps partially solved this problem and opened the way to separate the computational part of the calculation from all-to-all communication, in so called $i$-particle parallelization. The introduction of block-time steps has motivated the development of the GRAPE-family of special purpose computers, and eventual led to to high-performance gravitational $N$-body simulations using attached accelerator hardware, like graphics processing units (GPUs) [5]. See the reviews [6], [1].

The largest simulations conducted using direct $N$-body methods are approaching a million objects. But this is still a small number compared to the Solar system which is composed of one star, 8 planets, 16 moons and several million planetsimals, or the Milky Way Galaxy, which is composed of $\sim 100$ billion stars, each of which may be accompanied by a million-body planetary system.

A. Optimizations for the GPU

For convenience we separate the particles in the stellar system in $j$ particles, which exert a force, and $i$ particles that receive a force. To solve the $N$-body problem the forces exerted by the $j$-particles onto the $i$-particles have to be computed. The particles in subset $j$ can either belong to the same or a completely different set as the $i$-particles. In a worst case the algorithms scale as $N_i N_j \rightarrow N^2$, but because the forces calculated on the $i$-particles are independent the algorithm is embarrassingly parallel for $p = N_i$ cores. However, by design in the individual time step method $N_i \ll N_j$, because only the particles are updated that require a force update at a certain time [6]. [1].

On a GPU the parallelization can be exploited by launching a separate compute thread for each $i$ particle [5]. This is efficient only for $N_i \gtrsim 10^4$ [6]. [1] to warrant the saturation of all compute threads. For a smaller number of $i$ particles the number of active compute threads is not sufficient to hide the memory and instruction latencies. Future devices may require an even larger number of running compute threads to reach peak performance, causing $N_i$ to be even larger before the device is saturated. Adjusting the number of $i$ particles to keep parallel efficiency is not ideal. In an alternative approach, followed by [7], one can parallelize the $j$-particles, while fixing the number of $i$ particles over which we concurrently integrate. We split the $j$-particles in subsets which form the input against which a block of $i$ particles is integrated. The number of $j$-particles per block then increases for smaller $N_i$, making the algorithm efficient even for relatively small $N_i$. This method can fully utilize the GPU performance when the product of $N_i$ and the number of subsets in which the $j$ particles exceed the number of compute threads.

Earlier GPU hardware lacked support for double precision arithmetic, but this did not necessarily pose a problem for most common algorithms, even with a fourth-order Hermite integrator [6]. The largest error in these cases is made in the calculation of the inter-particle distance, but this can be solved by emulating double precision on single-precision hardware. The integration of the orbits of objects with an extreme mass-ratio, like planetesimals around super-massive black holes, remains hard to achieve without IEEE-754 double precision arithmetic. The latest GPUs support double precision and therefore enable such research.

Running high-performance $N$-body simulations on multiple GPUs has become common practice, even though distributing the calculation of several nodes proves less effective due to the limited bandwidth. Latency is not much of a problem because it turns out to be relatively easy to hide most of the latency in other operations. Multi-GPU parallelization is achieved by distributing the $j$ particles over the various GPUs using a round-robin method. This reduces the memory usage, transfer time and the time required to execute the optional prediction step on the $j$ particles. In this scheme the first kernel computes the partial forces of our parallelization over the $j$ particles, and the second kernel sums these.

\footnote{One can read more about symplectic integrators at [http://en.wikipedia.org/wiki/Symplectic_integrator](http://en.wikipedia.org/wiki/Symplectic_integrator)}
The introduction of efficient atomic operators in the latest NVIDIA GPUs made it possible to combine the calculation of the partial forces of the $j$ particles with the actual summation over all forces. This combined operation increases performance and reduces the complexity of maintaining the compute kernels. The above described method is implemented in Sapporo2 (a GPU library for solving the gravitational $N$-body problem) [8] where the amount of work is arbitrarily split up in many independent computation blocks and automatically scale to future architectures. In Fig. 2 we present the performance characteristic of the Sapporo2 library running a single GPU, and four GPUs for $10^3$ to $10^7$ particles.

IV. SIMULATING COLLISIONLESS SYSTEMS WITH HIERARCHICAL DOMAIN-DECOMPOSITION METHODS

The Barnes-Hut tree algorithm [2] turned into a classic shortly after its introduction. In this algorithm the distribution of particles is recursively partitioned into octants until the number of particles in an octant is smaller than a critical value. Once a tree is built and its multipole moments are recursively partitioned into octants until the number of particles is below a certain number are used as a group. However, due to the geometric nature of space partitioning by octrees, the average number of particles in such a group was much smaller than 64, which wastes compute resources. This is solved by sorting the particles into a Peano-Hilbert space filling curve (PH-SFC) [10] and splitting it into groups of 64 particles. The final criterion is to enforce a maximal geometric size of a group: if a group exceeds this size it is recursively split further into smaller groups. An extra benefit of using the PH-SFC is its ability to construct the tree-structure by splitting the SFC in distinct nodes.

B. Parallelization

While accelerators greatly improve the efficiency per node, massive parallel computing with GPUs has become a challenging problem. One crucial bottleneck is the relatively slow communication between the GPU and its host, which directly limits the overall performance. However, due to the long-range nature of Newton’s universal law of gravitation, the computation of mutual forces is by definition an all-to-all operation. Which requires that data has to be exchanged between all the nodes and therefore again requires communication between the CPU and GPU and communication between the different CPUs, which is even slower. 

A. Implementation

In the Barnes-Hut algorithm we can distinguish three fundamental parts: the construction of the tree, computation of quadrupole moments, and the tree-walk in which inter-particle gravitational forces are computed. Traditionally the tree-walk and gravity computation take up the largest part of the computation time. However, if this part would be optimized with the help of accelerators, like the GPU, other parts of the algorithm would become bottlenecks. Either because their relative contribution in the execution time becomes larger or because of the requirement to send data back and forth between the accelerator and the host CPU.

One way to eliminate these bottlenecks and data-transfers is by porting all the computational parts of the tree-code to the GPU. This is the approach taken in Bonsai [9]. In this code the tree-walk and force computations are assimilated into a single GPU kernel which allows for excellent computational efficiency by not wasting GPU bandwidth to store particle interaction lists into memory. Instead, the interaction lists are stored in registers and evaluated on-the-fly during the tree-walk, therefore delivering a performance in excess of 1.7 Tflops on a single K20X [9].

It is considerably more efficient to walk the tree on a GPU by a group of spatially nearby particles rather than by one particle at a time [2]. These nearby particles have similar paths through the tree, and therefore similar interaction lists; by building an interaction list that is valid everywhere within the group, one can reduce the number of tree-walks and make each of them efficient via thread cooperation inside a thread-block. The grouping in [2] is based on the underlying tree-structure, such that tree-cells with the number of particles below a certain number are used as a group. However, due to the geometric nature of space partitioning by octrees, the average number of particles in such a group was much smaller than 64, which wastes compute resources. This is solved by sorting the particles into a Peano-Hilbert space filling curve (PH-SFC) [10] and splitting it into groups of 64 particles. The final criterion is to enforce a maximal geometric size of a group: if a group exceeds this size it is recursively split further into smaller groups. An extra benefit of using the PH-SFC is its ability to construct the tree-structure by splitting the SFC in distinct nodes.

Fig. 2. Wall-clock time as a function of the number of particles in a direct code (upper curves) and a tree code (bottom curves using $\theta = 0.4$).
To maintain single-GPU efficiency when scaled to many GPUs requires both the minimization of the amount of data traffic between different GPUs, and hiding the communication steps behind computations. This is realized by carefully selecting, combining and modifying different well-known parallelization strategies. In the following paragraphs we describe this parallelization strategy.

1) Domain Decomposition: Each GPU computes its local domain boundaries, and the CPUs determine global domain boundaries which are used for mapping particle coordinates into corresponding PH keys [10], the host subsequently gathers a sample of PH-keys from the remote processes and combines these into a global PH-SFC. This SFC is cut into p equal pieces and the beginning and ending PH key determines the sub-domains of the global domain, which are broadcast to all processes. The resulting domain boundaries will not be rectangular but have fractal boundaries, which makes it hard to select particles and nodes that are required on remote nodes. As a consequence, common SFC-based codes [11] generate multiple communication steps during the tree-walk. An alternative method is the Local Essential Tree (LET) method. In this method each process uses the boundaries of the sub-domains to determine which part of its local data will be required by a remote process. This part is called the LET structure. After a process has received all the required LET structures, they are merged into the local tree to compute the gravitational forces.

This LET approach requires the least amount of communication and is therefore preferred in a practical implementation, like in Bonsai. Here the LET method is uniquely combined with the SFC domain decomposition which guarantees that sub-domain boundaries are tree-branches of a hypothetical global octree. This allows for skipping the merging of the imported structures into the local-tree, and process them separately as soon as they arrive, therewith effectively hiding communication behind computations.

2) Computing the gravity: To compute forces on local particles, a target process requires communication with all other processes. In Bonsai this is realized by forcing remote processes to send the required particle and cell data (via the LETs) to the target process. While the GPU on this target process is busy computing forces from the local particles, the other processes to send the required particle and cell data (via the LETs) to the target process. While the GPU on this target process is busy computing forces from the local particles, the other processes prepare particle data for export, as well as sending and receiving data.

The preparation of particle data for export to remote processes is both floating point and memory bandwidth intensive, both must overlap with the communication between the processes. This is achieved by multi-threading, in which each MPI process is split into three thread-groups: one is responsible for communication (the communication thread), one drives the GPU (the driver), and the rest are preparing LET structures. By disconnecting the various pieces of work it is possible to let them overlap and keep force feeding the GPU with computation work while other parts of the CPU take care of handling the relatively slow operations related to inter-node communication.

In order to scale to thousands of compute nodes there is usually the requirement that one needs to have trillions of particles that have to be integrated. The here discussed implementation of Bonsai allows for efficient scaling to thousands of nodes on the Titan supercomputer when using a relatively modest amount of particles.

In Fig.2 we present the performance of the direct N-body and tree-code compute kernels both running on an NVIDIA K20m GPU. The $N^2$ scaling of the direct code is clearly distinguishable from the $N \log(N)$ scaling of the tree-code. Increasing the number of GPUs in the calculations reduces the wall-clock time but does not change the scaling characteristics, but only changes the offset of the duration.

V. The multi-scale approach

The basis for the gravitational N-body problem is an integrable Hamiltonian. The natural separation in collisional (see §III) and collisionless (see §IV) domains can therefore also be reflected in the Hamiltonian of the form: $H_{\text{regular}} + H_{\text{irregular}}$, which can be solved numerically. This operator splitting approach has been demonstrated to work effectively and efficiently by [12], who adopted the Verlet-leapfrog algorithm to combine two independent gravitational N-body solvers. In this case we can use the direct N-body code (§III) and the tree-code (§IV) for those physical domains for which they are most suited; the direct N-body code for simulating the collisional environment and the tree code for simulating the collisionless system. Such a hybrid numerical solver is ideally suited for simulating planetary systems in a star cluster or the dynamics of supermassive black holes in galactic nuclei. In the next section we will demonstrate the working of this hybrid approach on a problem in which we allow 11 galaxies with black holes in their cores to merge.

In the scheme, the Hamiltonian of the entire system is divided into two parts:

$$H = H_A + H_B,$$

where $H_A$ is the potential energy of the gravitational interactions between galaxy particles and the stars in the sphere of influence of the supermassive black hole in the galactic nuclei ($W_{gc}$):

$$H_A = W_{gc},$$

and $H_B$ is the sum of the total kinetic energy of all particles ($K_g + K_c$) and the potential energy of the galactic nuclei with black hole ($W_c$) and the galaxy ($W_g$)

$$H_B = K_g + W_g + K_c + W_c \equiv H_g + H_c.$$  

The time evolution of any quantity $f$ under this Hamiltonian can be approximated (because we truncated the solution to second-order) as:

$$f'(t + \Delta t) \sim e^{t/\Delta t} e^{A\Delta t} e^{B\Delta t} f(t),$$

which represents a symplectic split in the Hamiltonian. Here the operators $A$ and $B$ are $A_f \equiv \{f, H_A\}$, $B_f \equiv \{f, H_B\}$, and $\{\ldots\}$ denotes the Poisson bracket. The evolution operator $e^{A\Delta t}$ splits into two independent parts because $H_B$ consists of two independent parts without a cross term. This embodies the second-order leapfrog algorithm, the time evolution of which can be implemented as a kick—drift—kick scheme.
VI. SIMULATING GALAXY MERGERS WITH SUPERMASSIVE BLACK HOLES

The hybridization described in §V is of an essence if one is impatient for the results, but cannot afford to have an approximate solution for all orbital integrations. Simulating a one billion particle galaxy-merger simulation easily takes several decennia with an $N^2$ method, but only a few weeks with a tree algorithm, whereas our implementation of the tree algorithm is insufficiently accurate to resolve the intricate dynamical encounters between the black holes (see Fig. 5). We therefore integrate only the few thousand stars near each black hole using the direct $N^2$ algorithm and all the other stars with the tree-code: in this way we benefit from the advantages of both algorithms.

We apply our hybrid numerical scheme running on GPU accelerated clusters using Bonsai [9] for the tree-code and the 4th order Hermite predictor-corrector code called ph4 as the direct $N$-body code. Both codes are incorporated in the Astronomical Multipurpose Software environment, AMUSE [13].

We start with one major galaxy (parent) of mass $M_{\text{parent}} = 2.2 \times 10^{12} \, M_\odot$ using $N = 2.2 \times 10^9$ particles of $10^7 \, M_\odot$, each and one supermassive black hole with a mass of $10^9 \, M_\odot$ in its center. The 10 children are scaled down copies of the parent and distributed according to a Plummer [14] spherical distribution with a virial radius of 500,000 pc (see [15] for details). We ignore the gas content of the Galaxy, stellar evolution and feedback processes. We motivate this limited scope and reduced physics by the assertion that much of the dynamical processes in which we are interested are driven by the gravitational evolution of spiral structure and not by the interstellar gas. The total amount of gas is relatively small $\lesssim 15\%$ compared to the total mass in stars, and it is distributed more homogeneously, and is not expected to drive the global dynamics of the Milky Way. For the local black-hole dynamics however, gas may play an important role, but we consider the galaxies to be dry. In addition, by limiting our scope we are able to run larger simulations and achieve a higher spatial and temporal resolution than otherwise possible. In Fig. 3 we present a rendering of this initial configuration.

In Fig. 4 we present the distance from one of the child’s black holes to that of the parent galaxy’s black hole. The three panels give the result of the same initial realization with a coupling between the tree and direct $N$-body codes and using different precision for each of the simulations (parameterized with the integration time step and the choice of the gravitational softening in the tree code). In the left most, least accurate simulation one would naively conclude that the two black holes coalesce about 6 Gyr after the start of the simulation. With a more precise (smaller softening length and time-step) integration (middle panel) the merger appears to occur at an earlier epoch (at about 2.5 Gyr). With the most accurate calculation (right-most image) we see that the incoming black hole is ejected to large radius after a series of strong encounters between 2 Gyr and 6 Gyr. The closest approaches are not resolved in the figure due to the discrete time-stepping of the output, but the detailed orbital trajectories of the encounter between several of the black holes is presented in Fig. 5. Of the 10 infalling black holes in the most precise calculation 8 were ejected and only 2 merged with the parent black hole, whereas in the least precise calculation all black holes, except one, merged.

In Fig. 5 we present the orbital evolution of 3 of the minor black holes and how they interact with the major black hole. Such complicated orbits cannot be calculated sufficiently accurate with the tree-code to follow the intricacies of the self-gravitating system, but require a high-precision direct $N$-body technique to resolve the subtleties in the chaotic regime, whereas the bulk of the galaxy material (stars and dark matter) are integrated using the hierarchical method. One can even question whether or not a direct method is sufficiently accurate considering the exponential divergence of the solution, but as has been demonstrated in [16], the quasi ergodicity of self-gravitating systems allow for relatively inaccurate calculations to provide statistically meaningful results.
VII. CONCLUSIONS

The use of GPUs has moved high-performance computing to our desktops and elevated scientific calculations in GPU equipped supercomputers to new heights. The self-gravitating systems community, which was already spoiled by the GRAPE family of computers, has been able to quickly benefit from this relatively new technology due to the similarities in architecture. Simulations which 5 years ago could only be performed on expensive special purpose computers or large scale supercomputers can now be performed on a rather ordinary desktop computer.

The enormous advances in hardware development that has been driving the computational gravitational dynamics community has managed to benefit from the use of GPUs by adopting hybrid methods. These have enabled simulations with enormous dynamic range and an unprecedented resolution in mass, and temporal as well as spatial scales.

With these improvements in hardware the pressure on producing efficient and accurate software has increased substantially. Monolithic software cannot cope with the complexities of real life systems, not in terms of scale (temporal and spatial) and not in terms of physics (stellar dynamics, hydrodynamics, etc). Novel numerical techniques are required in order to benefit from the current hardware. This will also allow us to resolve the scales and physics required in astronomical applications.

The hybridization of software in order to achieve these objectives is slowly starting. At the moment the computational astrophysics community is driven by these issues. The Hamiltonian-splitting strategy (see §V) to couple different algorithms is effective but reduces the overall numerical scheme to second order. Higher order coupling strategies are in development, but a self consistent and dynamic coupling between the various scales and physics in the astronomical applications are still far ahead.

In the calculations we presented here we would like to incorporate gravitational radiation in order to study what really happens to the black holes; we still do not know whether or not the black holes are ejected (as indicated in the high-precision simulation) or that general relativistic effects causes them to merge after all.

In a future implementation we consider adding gas via smoothed particles hydrodynamics, which will also be realized using a Hamiltonian splitting technique similar to the one described in section §V. Such a coupling can be realized via the Astronomical Multipurpose Software Environment [13].

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