Numerical cosmology on the GPU with Enzo and Ramses

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Abstract.
A number of scientific numerical codes can currently exploit GPUs with remarkable performance. In astrophysics, Enzo and Ramses are prime examples of such applications. The two codes have been ported to GPUs adopting different strategies and programming models, Enzo adopting CUDA and Ramses using OpenACC. We describe here the different solutions used for the GPU implementation of both cases. Performance benchmarks will be presented for Ramses. The results of the usage of the more mature GPU version of Enzo, adopted for a scientific project within the CHRONOS programme, will be summarised.

1. Introduction
The availability of general purpose graphic accelerators (GPUs) has made possible their effective usage for scientific computing. Ultimate High Performance Computing (HPC) systems are increasingly equipped with GPUs employed not just as graphic accelerators but mainly as computational co-processors providing, on suitable classes of algorithms, outstanding performance with power efficiency significantly higher than standard CPUs. Supercomputers are thus increasingly populated with hundreds or thousands of accelerators that can overlap their computing capability with that of CPUs, minimising considerably overall times-to-solution of high-end scientific problems. An efficient exploitation of such hybrid architectures is not a trivial task, often requiring a full re-design and refactoring of the code in order to expose its massively parallel algorithmic components, that can be effectively accelerated by the GPU, and to minimize or hide any latency related to data transfer between the host and the device.

A number of codes for scientific numerical applications have been recently enabled to harness the power of GPUs. In astrophysics the list comprises (but is not limited to) the Bonsai, [1], Cholla [2] and Gamer [3] codes. In this paper, we will focus on the Enzo [4] and the Ramses [5] codes, which are extensively adopted by the computational astrophysics community. Enzo and Ramses are both Adaptive Mesh Refinement multi-species codes, designed to describe the evolution of cosmological structures, galaxies, gas clouds etc. The two codes can run on massive parallel HPC systems thanks to an effective MPI based implementation. An overview of the main features of Enzo and Ramses will be given in section 2.
Enzo and Ramses have been ported to GPUs adopting different strategies and programming models, Enzo exploiting CUDA and Ramses using OpenACC. The different solutions used for the GPU refactoring will be described in the following sections 3 and 4. Note that a CUDA based implementation of the radiative transfer module of Ramses has been developed by [6].

In section 3 we will focus on the re-design and refactoring work performed on Ramses, for which a number of benchmarks comparing the GPU and the CPU versions of the codes will be presented, highlighting the enhancements obtained with the refactoring and pointing out the main factors currently limiting the performance improvements.

The more mature Enzo’s GPU implementation will be introduced in section 4. It is currently used in a project within the CHRONOS\(^1\) programme, supporting high-end computational physics applications. The project aims at studying the origin and evolution of the magnetic field within large-scale structures and exploits the MHD CUDA enabled solver, allowing to overcome the bounds related to memory size, while maintaining the computational time reasonable. An overview of the achieved performance will be presented together with some notable scientific outcomes.

Both Ramses benchmarks and Enzo runs have been performed on the Piz Daint HPC system at ETHZ-CSCS, a Cray XC30 supercomputer accounting for more than 5000 computing nodes, each equipped with an 8-core Intel SandyBridge CPU (Intel Xeon E5-2670) and an NVIDIA Tesla K20X GPU.

Section 5 will summarize the work and draw the main conclusions.

2. Enzo and Ramses Overview

Enzo and Ramses are both Adaptive Mesh Refinement (AMR) codes designed to solve a broad variety of astrophysical problems. The AMR approach is the key feature for the two codes, also in terms of GPU enabling strategy. AMR provides high spatial resolution only where this is actually required, thus ensuring minimal memory usage and computational needs. The codes adopt different AMR solutions, namely Structured AMR (SAMR) by Enzo and Fully Threaded Tree (FTT [7]) by Ramses. With the SAMR approach, the computational domain is represented by a rectangular grid on which a solution of the underlying problem is computed. Regions requiring additional resolution are identified by some suitable criteria and covered by a disjoint union of rectangles (patches), which are then refined by integer factors (usually a factor of two is adopted). The solution is then computed on the superposition of patches. This process is used recursively and refinement are applied in space as well as in time. Similarly, FTT supports local refinements of the spatial domain, but with an unstructured approach, dynamically creating refinements on a cell-by-cell basis, the mesh being able to conform to complex boundaries. Spatial and time refinement criteria are the same as for SAMR.

The AMR hierarchy management is organized as a tree. In the case of Enzo, each node of the tree represents a patch which is pointed by the coarser father patch, and points to the higher resolution nested son patches. In the case of Ramses, each cell stores information about the parent (at lower resolution), neighbouring (at the same resolution) and children (at higher resolution) cells. In this way, the tree can be quickly traversed during various search operations. Comparing the two approaches, FTT optimizes memory usage and can provide efficient parallel implementations. However, memory access is not as efficient and simple as for the regular patches supported in SAMR.

On the AMR mesh, Enzo and Ramses solve the equations describing the dynamics of the two main matter component in the universe, dark and baryonic matter (DM and BM), driven by the gravitational field, generated by the combined mass distributions. The two codes use a particle-mesh N-body method to follow the dynamics of the collisionless DM component.

\(^1\) http://www.cscs.ch/user_lab/allocation_schemes/chronos_projects/index.html
BM component is represented as an ideal fluid, discretised on the AMR mesh. Its behaviour is described solving the Euler equations through different numerical approaches (e.g. the Piecewise Linear Method, PLM [8], the Piecewise Parabolic Method, PPM [9] or the TVD [10] schema). The gravitational potential is calculated solving the Poisson equation through a multigrid or a combined multigrid plus fast fourier transform approach. A variety of further physical processes is included in the two codes. Standard hydrodynamics is extended to magneto-hydrodynamics (MHD). Sub-grid phenomena, like star formation or supernovae explosions, are modelled. Additional basic physics, like cooling processes or radiative transfer, are supported.

The GPU enabling of the two codes follows distinct strategies, driven by the AMR approach, and programming models, as described in the following two sections.

3. Ramses OpenACC Implementation and Benchmarks

For Ramses, an incremental GPU porting strategy has been defined, extending and optimizing progressively the fraction of the code ported on the accelerator. The hydrodynamics solver has been identified as a primary target for Ramses’ GPU implementation, being among the most computational demanding code’s components and, at the same time, solving a local problem, ideally fitting the accelerators architecture. This first step is being followed by the progressive porting of all the other algorithmic components. This approach ideally fits the OpenACC programming model, which, furthermore, fully supports Fortran 90 and reduces the impact on the source code, minimizing the effort for its management and maintenance. OpenACC has been adopted as the solution for Ramses GPU refactoring.

The main challenge for an effective design of the hydro GPU algorithm is represented by the FTT based data management. The FTT approach allows a prompt identification of sibling and parent cells. However data results scattered in memory and its access, even in the case of neighbouring cells, is often on non contiguous memory locations. This represents a major issue in terms of performance for any processor relying on a cache based memory hierarchy. In order to circumvent this problem, Ramses gathers in a buffer all the data needed for the update of a few cells at a time. The resulting buffer’s size is $N_v \times 6 \times 6 \times 6$ cells, $N_v$ being the number of cells to update set to $N_v \sim 10$, in order to fit the cache memory hierarchy. This solution is not suitable to the GPU, since larger contiguous data chunks are necessary to maximise the GPU occupancy, minimizing at the same time the amount of memory accesses. A simple increase of

![Figure 1. Ramses’ hydro solver implementation on the GPU: step 1 (left), cells are ordered according to a space filling curve at each level; step 2 (centre), regular rectangular patches are created; step 3 (right), patches are gathered composing large chunks and hydro equations are solved.](image-url)
$N_r$ would not be effective, preserving the number of accesses to main memory. Furthermore, data would be replicated unnecessarily, due to the $6^3$ cubes building process. Hence, for the GPU a specific procedure has been designed and can be summarised as follows (see also Figure 1):

- at a given level of refinement, AMR cells are ordered according to a space filling curve based layout;
- cells are grouped in compact (i.e. with no holes) cubic patches of maximum possible size;
- neighbouring patches are grouped in large chunks collecting all the data necessary for the hydro equations integration, (i.e. inner cells plus boundary cells, properly calculated through interpolation if the patch adjoins cells at a different refinement level;
- hydro equations are solved on the chunk of data
- next chunk of data at the same level starts to be created or, if the level has been solved, calculation on the next coarser level begins.

Data transfers to and from the GPU have been minimised by transferring only necessary data i.e. data belonging the refinement level being updated) are moved to and from the GPU.

| Code version   | Hydro (tot) | Hydro (calc) | Hydro (copy) | Total   |
|---------------|-------------|--------------|--------------|---------|
| CPU (1 core)  | 56218       | 56218        | NA           | 155662  |
| CPU (16 cores)| 2918        | 2918         | NA           | 8775    |
| 1 GPU         | 3009        | 2270         | 739          | 104811  |
| 16 GPUs       | 179         | 115          | 64           | 5718    |

In Table 1 we present some benchmarks performed to compare the CPU and OpenACC versions of the code in a representative cosmological simulation, with a $256^3$ base grid and 8 levels of refinement. The tests were run on a single CPU core, on a full CPU socket (two CPUs sharing a common memory, for a total number of 16 cores), on a single GPU and on 16 GPUs (one GPU per computing node). Column 2 of the Table, compares the timings to run the hydro kernel. On overall, the GPU performs as 16 cores and about 18 times faster than a single core. A fraction of about 75% of the time on the GPU is spent on computation (column 3), while the remaining time is spent on data transfer. Due to the characteristics of the algorithm, this overhead cannot be hidden exploiting asynchronous processes, overlapping computation and data transfer. It will be reduced only porting a larger fraction of the code on the GPU, thus reducing the need for data transfers. The impact of the GPU on the total run time (column 5) is, of course, limited by the fact that only the hydro kernel is running on the accelerator, stressing, once more, the importance of having the majority of the code ported on the GPU. Finally, by comparing the results for 1 and 16 GPUs, we see how, for the case under investigation, the good scalability of the hydro kernel is preserved, despite the work being distributed among 16 distinct nodes, communicating through the network. Again, the copy time is a major source of overhead, the data to be transferred to the device increasing with the number of GPUs relatively to the amount of computation per device.

4. Enzo MHD GPU Simulations

Enzo’s MHD solver, as well as the PLM/PPM hydro solver, have been ported to NVIDIA’s CUDA framework (Wang et al. 2010; The Enzo Collaboration et al. 2013). Data is off-loaded
to the GPU asynchronously on a patch-by-batch basis, effectively overlapping computation and data transfer. All fluxes necessary to update the patch’s cells are computed on the GPU and only fluxes required for flux correction necessary for multilevel, adaptive time-step, calculations are moved back to the CPU, representing the only additional data transfer overhead. The porting onto GPUs replaced many shared temporary arrays of the CPU version into larger temporary arrays that are not shared among loop iterations, and exposed the massive parallelism of the algorithm. The larger memory usage is not a major issue, since updated patches are immediately transferred back to the CPU, freeing the corresponding GPU memory. For further details on the porting onto CUDA, we refer the reader to [11] and [4].

Enzo’s GPU implementation is currently used in a CHRONOS project, aiming at studying the origin of cosmic magnetism in general and the observed distribution of magnetic fields in large scale structures. This is in fact an astrophysical puzzle. On one hand observations provide evidence for magnetic field strengths of up to a few \( \sim \mu G \) in galaxy clusters and galaxies (e.g. [12]), on the other the origin of such strong fields is unclear, given the low upper limits on the primordial magnetic field at the epoch of the Cosmic Microwave Background, and the uncertainty on fields generated by primordial mechanisms is still huge (e.g. [13]).

Cosmological simulations already proved that significant field amplification in galaxy clusters can be achieved by starting from weak cosmological fields and following turbulent small-scale dynamo (e.g. [14] and references therein). However, field amplification in the outer part of clusters and in filaments of the cosmic web is still poorly investigated. Recently, in [15], we tackled this problem. We uses the GPU-ported version of Enzo-MHD to achieve a high-resolution view of magnetic field amplification in the cosmic web. As we were mostly interested in the outer region of clusters and filaments, we primarily used large unigrid simulations, which are less affected by numerical dissipation compared to AMR runs and allow complete surveys of large cosmic volumes.

Running on Piz-Daint on 512 to 2048 computing nodes using, due to memory constraints, one to four tasks per node, we investigated various details of the numerical modelling of cosmic magnetism: from dependence on cluster/filament mass to the convergence with spatial resolution. Furthermore, we explored the role of additional seeding by magnetized jets from active galactic nuclei within clusters. In this project we produced the current largest cosmological MHD simulation to date (2400 \( \times \) cells and dark matter particles), as well as the most complete resolution study to date on the amplification in a cosmic filaments. In particular, the use of the GPU allowed us to complete such large unigrid run in \( \approx 4.5 \times 10^6 \) core hours with 512 nodes, cutting by a factor \( \sim 4 \) the total computational time compared to the CPU version of the code. Figure 2 (left) shows the projected magnetic field strength across a 1200 \( \times \) box simulating (25 Mpc)\(^3\), at the final timestep (redshift \( z = 0 \)). Magnetic fields are advected and amplified where gas matter concentrates, however their intensity never becomes dynamically relevant compared to the gas energy. For the small simulated galaxy clusters/groups, the maximum measured magnetic field is \( \sim 0.1 \mu G \), while the typical strength in filaments is instead \( \sim 0.001 \mu G \). The right panel in Figure 2 shows the potential role played by the additional release of magnetic fields from galaxies inside galaxy clusters. While this can boosts the maximum field inside clusters up to \( \sim 1 \mu G \) (i.e. close to observations), this additional seeding mechanisms does not increase significantly the magnetisation of filaments.

These results suggest that the memory of the seeding event(s) must be kept within filaments, as their evolution is dominated by compression and not by strong turbulence (which would erase any information on the initial seed field, as in galaxy clusters). We are presently working together with radio astronomers involved in the design and testing of the Square Kilometer Array, to assess which crucial information of cosmic magnetic fields will be accessible with the future configurations planned for the SKA, which might be able to give us crucial information of the initial seeding mechanisms of large-scale magnetic fields in the Universe [16].
Figure 2. Projected maps of mass-weighted magnetic field intensity (with overlaid logarithmic contours of projected temperature) for a 1200^3 simulations of a (25 Mpc)^3 volume at z = 0, with a cosmological weak magnetic field initialised at z = 30 (left) or with the additional release of magnetic loops from “galaxies” in the volume at z = 2 (right).

5. Conclusions
This paper has summarised the GPU implementation of the Enzo and Ramses codes. Although only part of both codes is currently implemented to exploit GPU empowered supercomputers, they have already proved the effectiveness of solutions capable of running on hybrid accelerated systems. Enzo has been used to run a number of large MHD simulations overcoming the limitations posed by memory constraints of current CPUs keeping, thanks to the GPU, the computational time acceptable. Ramses, despite the good results obtained for the hydro kernel, is pointing out how the porting of the whole application is often necessary for the full exploitation of the accelerator, minimizing the host-device data transfer overheads. On-going work is finalized to enable the cooling, MHD and gravity modules to the GPU.

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