Advanced Architectures for Astrophysical Supercomputing

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Abstract. Astronomers have come to rely on the increasing performance of computers to reduce, analyze, simulate and visualize their data. In this environment, faster computation can mean more science outcomes or the opening up of new parameter spaces for investigation. If we are to avoid major issues when implementing codes on advanced architectures, it is important that we have a solid understanding of our algorithms. A recent addition to the high-performance computing scene that highlights this point is the graphics processing unit (GPU). The hardware originally designed for speeding-up graphics rendering in video games is now achieving speed-ups of \(O(100\times)\) in general-purpose computation – performance that cannot be ignored. We are using a generalized approach, based on the analysis of astronomy algorithms, to identify the optimal problem-types and techniques for taking advantage of both current GPU hardware and future developments in computing architectures.

1. Introduction

Modern astronomy has come to rely heavily on high-performance computing (HPC). However, all research areas are facing significant challenges as data volumes approach petabyte levels. For instance, the Australian Square Kilometre Array Pathfinder project will produce data at a rate that makes storage in raw form impractical, necessitating on-the-fly reduction and analysis to produce 4GB/s of products. On the modeling front, there is an ongoing desire for larger and more-detailed simulations (e.g., the Aquarius simulation by Springel et al. 2008).

The HPC scene has recently witnessed the bold introduction of the graphics processing unit (GPU) as a viable and powerful general-purpose co-processor to CPUs. GPUs were developed to off-load the computations involved in rendering 3D graphics from the CPU, primarily to benefit video-games. Their continued development has been driven by the $60 billion/year video-game industry. The result of this development can be seen in Figure 1, which plots the clock-rate of a number of CPUs and GPUs against their core-count. GPUs appear toward the top of the plot, exhibiting very high core-counts and performance. Since 2005 (an area on the plot we refer to as the “multi-core corner”), clock-rates in CPUs have plateaued, and manufacturers have instead turned to increasing the number of cores per chip\(^1\). One might therefore consider that CPUs are

\(^1\)This has to do with the difficulty in dissipating the heat produced at higher clock-rates.
now becoming progressively more GPU-like, and that current GPUs provide a picture of future commodity computing architectures.

While CPUs are becoming more GPU-like, the reverse can also be said, with GPUs offering increasingly flexible computing platforms. This flexibility, combined with the availability of general-purpose programming tools, has opened up GPU computation to a wide range of non-graphics-related tasks, notably in the area of HPC.

Both the immediate performance boost provided by GPUs and the expected future of CPU computing provide strong motivation for a thorough analysis of the performance and scalability of our astrophysics algorithms in advanced parallel processing environments. If harnessed correctly, the power of massively-parallel architectures like GPUs could lead to significant speed-ups in computational astronomy and ultimately to new science outcomes.

A number of astronomy algorithms have been implemented on GPUs to date, including direct N-body simulations (e.g., Belleman, Bédorf & Portegies Zwart 2008), the solution of Kepler’s equation (Ford 2008), radio astronomy correlation (e.g., Harris, Haines & Staveley-Smith 2008), phase-space studies of binary black hole inspirals (Herrmann et al. 2009) and gravitational lensing ray-shooting (Thompson et al. 2010). These projects have all reported speed-ups of $O(100)$ over CPU codes\(^2\). However, these algorithms are for the most part “embarrassingly parallel” “low-hanging fruits”, meaning that they can be run on a parallel processing architecture with little or no overhead. This makes them obvious candidates for efficient GPU implementation. The question that remains is: exactly which classes of astronomy algorithms are likely to obtain significant speed-ups by executing on advanced, massively-parallel, architectures?

\(^2\)It is understood that these speed-up measurements are unlikely to have been obtained in a consistent manner; we merely emphasize their order of magnitude.
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2. Our Approach

We propose a generalized approach based around two key ideas:

1. Developing and applying an algorithm analysis methodology relevant to new hardware architectures; and
2. Building and using a taxonomy of astronomy algorithms.

We believe that such an approach will minimize the effort required to turn the “multi-core corner” for computational astronomy and ensure that the solutions found will continue to scale with future advances in technology.

Here we briefly outline a number of “rules of thumb” that may be applied when analyzing astronomy algorithms with respect to their potential on GPUs. Further details will be presented in Barsdell, Fluke & Barnes (in prep.).

Massive Parallelism: Given the large number of processing cores available in GPUs, it is critical that an algorithm be divisible into many fine-grained parallel elements in order to fully utilize the hardware (e.g., an NVIDIA GT200-class GPU may be under-utilized with \( \leq O(10^4) \) threads). Partitioning data, rather than tasks, between parallel threads generally offers a large and scalable quantity of parallelism. This is referred to as the “data-parallel” approach.

Memory Access Locality and Patterns: GPU architectures contain very high bandwidth main memory, \( O(100\text{GB/s}) \), which is necessary to “feed” the large number of parallel processing units. However, high latency (i.e., memory transfer startup) costs mean that performance depends strongly on the pattern in which memory is accessed. In general, maintaining “locality of reference” (i.e., neighboring threads accessing similar locations in memory) is vital to achieving good performance.

Branching: GPUs contain “single instruction multiple data” (SIMD) hardware. This means that neighboring threads that wish to execute different instructions must wait for each other to complete the divergent code section before execution can continue in parallel. For this reason, sections of GPU code that are conditionally executed by only a subset of threads should be minimized.

Arithmetic Intensity: Executing arithmetic instructions is generally much faster than accessing memory on GPU hardware and thus increasing the number of arithmetic operations per memory access can help to hide memory latencies. This is not always possible, and some algorithms will remain bandwidth-limited rather than instruction-limited. However, this is a case where a more drastic re-think of a problem may be required for an efficient solution. For example, the optimal order of a numerical expansion may be different on a GPU architecture than on a CPU architecture.

Host–Device Memory Transfers: GPUs and their host machines (typically) have distinct memory spaces, meaning they must communicate via the PCI-Express bus, which exhibits relatively low bandwidth (currently \( \sim 5\text{GB/s} \)). Transferring data to and from a GPU device can therefore be a significant performance bottle-neck in some situations.

3. Algorithm Classification

Here we present an initial classification, based on application of the “rules of thumb” and reduction to known GPU-efficient algorithms, of a selection of im-
important astronomy problems. High efficiency algorithms correspond to expected $O(100\times)$ speed-ups, while moderate efficiency algorithms are expected to exhibit speed-ups of $O(10\times)$ over traditional CPU implementations:

| Field          | High efficiency                                      | Moderate efficiency                           |
|----------------|------------------------------------------------------|----------------------------------------------|
| Simulation     | • Direct N-body                                       | • Tree-code N-body and SPH                   |
|                | • Fixed-resolution mesh simulations                   | • Halo-finding                               |
|                | • Semi-analytic modelling                            | • Adaptive mesh refinement                   |
|                | • Gravitational lensing ray-shooting                 |                                              |
|                | • Other Monte-Carlo methods                          |                                              |
| Data reduction | • Radio-telescope signal correlation                  | • Pulsar signal processing                   |
|                | • General image processing                           | • Stacking/mosaicing                         |
|                | • Flat-fielding etc.                                 | • CLEAN algorithm                            |
|                | • Source extraction                                  | • Gridding visibilities and single-dish data |
|                | • Convolution and deconvolution                      |                                              |
| Data analysis  | • Machine learning                                   | • Selection via criteria-matching            |
|                | • Fitting/optimisation                               |                                              |
|                | • Numerical integration                              |                                              |
|                | • Volume rendering                                   |                                              |

4. Conclusion

Modern astronomy relies heavily on HPC, and GPUs can provide both significant speed-ups over current GPUs and a glimpse of the probable future of commodity computing architectures. However, their more complex design means algorithms must be considered carefully if they are to run efficiently on these advanced architectures. There is therefore strong motivation to thoroughly analyze and categorize the algorithms of astronomy in order to take full advantage of current and future advanced computing architectures and maximize our science outcomes.

Our preliminary analysis of a broad selection of important astronomy problems leads us to conclude that the data-rich nature of computational astronomy, combined with the efficiency of data-parallel algorithms on current GPU hardware, make for a very promising relationship with current and future massively-parallel architectures. Processors are likely to become even more flexible in the future, potentially improving the efficiency of many astronomy algorithms and opening up new avenues to significant speed-ups.

References

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