Accelerating the Rate of Astronomical Discovery with GPU-Powered Clusters

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Abstract. In recent years, the Graphics Processing Unit (GPU) has emerged as a low-cost alternative for high performance computing, enabling impressive speed-ups for a range of scientific computing applications. Early adopters in astronomy are already benefiting in adapting their codes to take advantage of the GPU’s massively parallel processing paradigm. I give an introduction to, and overview of, the use of GPUs in astronomy to date, highlighting the adoption and application trends from the first ∼100 GPU-related publications in astronomy. I discuss the opportunities and challenges of utilising GPU computing clusters, such as the new Australian GPU supercomputer, gSTAR, for accelerating the rate of astronomical discovery.

1. Introduction

For at least four decades from the 1960s, advances in traditional computation on single-core CPUs has been driven by increases in transistor density and clock rate. This is seen through the well-established Moore’s Law (Moore 1965) biennial doubling in the number of transistors per integrated circuit, and a corresponding increase in processing performance. In principle, it was possible to implement a code once, and achieve faster (approximately double) computation simply by purchasing new hardware, at lower cost, every two years. In practice, new generations of CPUs also provided additional benefits (such as increased system memory, improved caching, etc.), resulting in on-going algorithmic improvements and software updates.

In the early 2000s, CPU clock-rates began to plateau – mainly due to manufacturing constraints, such as difficulties in keeping ever-faster CPUs sufficiently cool to work without melting. Further processing improvements, and the continuation of Moore’s Law growth, were achieved by moving to multi-core solutions. Indeed, the likely future of CPUs is that they will become increasingly multi-core: codes or algorithms that can be expressed in parallel form will derive the most benefit from these new architectures. A preview of this highly multi-core future is available now in the guise of the many-core graphics processing unit (GPU). Leveraging advances in hardware that were designed to enhance and improve graphical performance in support of the many-billion dollar international computer gaming industry, GPUs have rapidly become credible alternatives for low-cost, massively parallel scientific computation. Astronomers have been quick to adopt GPUs as a powerful new component of their computational arsenal.

Following early successes at speeding-up codes on single GPU systems and small-scale GPU clusters, a growing number of research institutions are now making major investments in significant high-performance computing (HPC) clusters deriving a sub-
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substantial fraction of their (theoretical) peak processing performance from GPUs. At the
dawn of this exciting new era of GPU-powered HPC clusters, what do astronomers need
to know about GPUs in order to take advantage of new computational opportunities?
What does a potential 10x or 100x processing speed-up mean in terms of accelerating
the rate of astronomical discovery? What lessons can we learn, and what trends can we
identify, from the early adopters of GPUs in astronomy? And now that we have \( O(100) \)
Tflop/s GPU-clusters at our disposal,\(^1\) just what are we going to do with them?

2. GPUs for Scientific Computation

In essence, the GPU acts as a computational co-processor to the CPU, a mode of op-
eration not unfamiliar to computer programmers (and owners) of the 1980s who could
opt to use a maths co-processor or floating point unit (FPU) to accelerate mathematical
operations. While modern GPUs offer a much wider range of programmable capability
than the earlier FPUs, they are not able to completely replace the CPU – nor are
they likely to. In general terms, GPUs achieve their performance at the hardware level
by trading off the large-memory caches and sophisticated control logic of CPUs (ac-
commodating software solutions for activities as diverse as opening a file from a local
disk, serving a web-page in a browser, and numerical processing for an astrophysical
simulation) for circuit-area devoted to fast floating point computations.

As the potential for using the highly-parallel GPU architecture for scientific com-
putation became apparent (Venkatasubramanian 2003), the notion of general purpose
computation on graphics processing units (GPGPU) began to gain momentum. Early
tries to utilise the increased computational performance of GPUs required program-
mapping in shader languages [e.g. NVIDIA’s C for Graphics, Cg, was used by Rosa et al.
(2004) and Portegies Zwart, Belleman, & Geldof (2007)]. For graphics, the hardware
processing pipeline is optimised to calculate red-green-blue (RGB) colours and alpha
(A) channel transparency for pixels, vertices and polygons, achieved through the use
of customised software fragment shader functions. Implementation of a scientific algo-
rithm was only possible if it could be recast as a shader, often requiring storing data in
structures that shared the “four floating point numbers” structure of RGBA.

The advent of the Compute Unified Device Architecture (CUDA\(^2\)) application pro-
gramming interface (API) from NVIDIA and the open-standard alternative OpenCL,\(^3\)
developed by the Khronos Group, have dramatically changed the usability of the GPU
for general computation.\(^4\) Indeed, certain GPU products from vendors, such as the
Tesla series from NVIDIA, are sold with scientific computing in mind: architecturally
equivalent to consumer graphics hardware, they lack the capacity to output graphics
to a display device, but with increased memory spaces and provision for error correct-
ing memory, which are not required by the home computer gamer. Moreover, while
early generations of GPUs only supported 32-bit (single precision) floating bit compu-

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\(^1\)We use the notation Gflop/s = \(10^9\) floating point operations per second and Tflop/s = \(10^{12}\) flop/s.

\(^2\)http://www.nvidia.com/cuda

\(^3\)http://www.khronos.org/opencl

\(^4\)For more details on GPU programming, see, e.g. Kirk & Hwu (2010) or Sanders & Kandrot (2010).
tion, the higher-end solutions now also provide 64-bit (double precision) support at comparable processing speeds.

3. Early Adopters and Emerging Trends

One of the first astronomical problems adapted to GPU was acceleration of the N-body force problem, through computation of the $O(N^2)$ pair-wise forces between particles. Early GPU implementations were reported by Nyland et al. (2004), using Cg and OpenGL on an NVIDIA GPU, while Elsen et al. (2006) and Elsen et al. (2007) used BrookGPU (Buck et al. 2004) on an ATI X1900XTX card. Both groups found that the high arithmetic intensity of the force calculation was ideally suited to the GPU’s architecture, and simple code optimisations could give speed-ups of more than 20× compared to existing CPU implementations. Moreover, they achieved computational performance comparable to the more expensive, custom GRAPE-6A hardware.

Rosa et al. (2004) examined a real-time problem - recovery of the wave-front phase from a Shack-Hartmann sensor. Reporting on an implementation of the iterative Hudgin algorithm, they found a 10x speed-up for the centroid part of the calculation, but only a 2x speed-up overall compared to a CPU-only implementation. They demonstrated that peak performance on a GPU does require a sufficiently large problem - the CPU out-performs the GPU when there are insufficient processing tasks to keep the GPU pipeline busy.

Schaaf & Overeem (2004) described a Common-Off-The-Shelf (COTS) correlator platform constructed from GPUs, with an eye on future, low-cost solutions scalable to the Square Kilometre Array (SKA). They achieved $\sim 5\times$ better performance (measured as complex multiplications/second) for a 16× larger problem using an NVIDIA GeForce 6800 Ultra GPU, compared with a 2.8 GHZ CPU. The price/Gflop and power usage/Gflop of the GPU were both about 3x better than for CPU.

To examine some of the emerging trends in the adoption of GPUs in astronomy since these early projects, we perform simple bibliometrics using the SAO/NASA Astrophysics Data System Abstract Service. An abstract-only search on various combinations of the terms: GPU(s), graphics processing unit(s), CUDA, and OpenCL resulted in 94 distinct abstracts from 2004-2011 (as of 1 October 2011). There were no relevant abstracts in 2005. An attempt was made to remove duplicate items (e.g. papers that appear separately as an arXiv version and a final published version).

There are, of course, limitations with such an approach. We fail to identify those publications that used GPUs, but did not declare this in the abstract (e.g. Fluke, Barnes, & Hassan 2010), and not all publications on astronomy-related GPU applications appear in ADS [e.g. Hamada & Nitadori (2010); Spurzem, R. and others (2010)]. While additional details on the API and specific hardware used could have been obtained from each of the publications, our intention was to obtain a quick snapshot of the current state of GPU development and the extent of early adoption in astronomy. We can answer questions such as “how are GPUs being used in astronomy?” (Figure 1) and “where are the results being published?” (Figure 2).

Analysis of the abstracts reveals almost 50 unique computational problems in 30 broad application areas, ranging from adaptive optics and algorithm analysis, data

5http://adsabs.harvard.edu
mining and digital signal processing, plasma and protoplanetary disk simulation, to
tree-codes and two-point correlation functions. The vast majority of abstracts present
GPU-based codes or methods (82/94). In this context a “method” relates to a demon-
stration that a particular problem is suited to a GPU, and is often accompanied by a
quoted speed-up (relative to a single-core CPU, or, in a small number cases, a multi-
core CPU implementation) or a peak processing performance [e.g. Hamada & Itaka
(2007); Belleman, Bédorf, & Portegies Zwart (2008); Gaburov, Bédorf, & Portegies
Zwart (2010)]. Of the remaining abstracts, 9 were clearly identifiable as present-
ing new scientific results based on the use of an existing GPU code [e.g. Aubert & Teyssier
(2010); Banerjee, Baumgardt, & Kroupa (2010); Greig, Bolton, & Wyithe (2011)],
and three dealt more generally with the “philosophy” of adopting GPUs for scientific
computing in astronomy [e.g. Barsdell, Barnes, & Fluke (2010)].

Figure 1. How are GPUs being used in astronomy? An ADS abstract-only search
(1 October 2011) on various combinations of the terms: GPU(s), graphics process-
ing unit(s), CUDA, and OpenCL resulted in 94 publications (there were no relevant
abstracts in 2005). The “other” category combines any application area with 3 or
fewer abstracts. The year 2010 represents the commencement of wider adoption of
GPUs by the astronomical community.

As Figure 1 shows, the year 2010 marked the transition from early exploration of
the capabilities and suitability of GPUs to a restricted number of problems, to one of
widespread adoption across a broad range of application areas in astronomy (62 ab-
stracts across 26 application areas since 2010 – the “other” category combines any ap-
plication area with 3 or fewer abstracts). We anticipate that this trend will continue for at
least the next few years, as the application market is far from being saturated. Amongst
the early applications, Fourier transforms and pair-wise N-body forces were obvious,
“low-hanging fruit”, with straight-forward parallelism. Recent works are tackling more
complex algorithms, such as general relativistic magnetohydrodynamics (Zink 2011).
N-body simulations (and related methods) stand out as being the most popular target for both methods and scientific result abstracts (18/94). The emphasis on scientific computing is clear, with only ten abstracts discussing visualisation/data analysis uses of GPUs – a number comparable with GPU-enabled signal processing for radio astronomy (9/94), adaptive optics (10/94) and hydrodynamics/magnetohydrodynamics (7/94).

Figure 2. Where is GPU-related work being published? Journals include New Astronomy, Monthly Notices of the Royal Astronomical Society, Astrophysical Journal, Astronomy & Astrophysics, Publications of the Astronomical Society of Australia; Conferences include SPIE and ADASS; the arXiv category includes publications that are not clearly identifiable with one of the other categories.

It is interesting to see where GPU-related work is being published – see Figure 2. We identify four categories of publication outlet: journals, arXiv preprints, conference papers and PhD theses. The arXiv category includes papers that have appeared on the arXiv, but are not clearly identifiable with one of the other categories (as of 1 October 2011). The main contributors to the conferences category are SPIE (11/94) – mostly presentations on adaptive optics – and ADASS (6/94). The two main astronomy journals publishing refereed GPU-papers are New Astronomy (13/94) and Monthly Notices of the Royal Astronomical Society (7/94). The important message from this is that journals are prepared to publish GPU methods papers, so get out there and turn your conference papers into more complete publications with details of your algorithms (and kernels), so that others can benefit from your experiences.

Based on abstracts only, other trends were considered. The declared use of particular programming APIs: Cg (2; none since 2007), CUDA (26; since 2008), and OpenCL (7; since 2010). 17 abstracts noted the use of a specific NVIDIA card, with

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*e.g.* papers that are identified as being in-press or accepted to a named journal are counted in the journal category, however, they are still counted towards the year in which they first appeared on the arXiv.
Tesla/Fermi cards increasing in prominence (NVIDIA S1070, C1060, and C2050 cards are identified in six abstracts since 2010). Only two abstracts named ATI cards (Pang, Pen, & Perrone 2010; Elsen et al. 2007). At present, NVIDIA and CUDA do seem to dominate the scientific computing market share, which may be due in part to the more recent appearance of OpenCL as a general-purpose programming API suitable for ATI cards.

Reported speed-ups, relative to CPU-implementations, ranged from 7x [computation of the Fast-Fourier Transform for adaptive optics in Rodríguez-Ramos et al. (2006)] to 600x [solving Kepler’s equations in Ford (2009)], with several projects highlighting one-to-two order of magnitude improvements in performance [radio astronomy signal processing – Harris, Haines, & Staveley-Smith (2008); magnetohydrodynamics – Wong et al. (2009); cosmological lattice computations – Sainio (2010)].

We should treat speed-ups with some caution: achieving performance at the highest end (100x) may be an indication that a less efficient, existing CPU-implementation was being compared with a highly-optimised GPU solution. Moreover, a single precision speed-up is often more impressive than for double (or quadruple – see Ginjupalli & Khanna 2010) precision, so consideration must be made to accuracy over performance. Devoting additional time to optimising existing CPU-codes is possibly not time well spent, particularly if a “simple” GPU code remains faster [see examples in Fluke et al. (2011)], however, an investigation of the potential for parallelisation of an existing single-core CPU code can lead to simple speed-ups through the use of libraries such as OpenMP on multi-core CPU architectures. On the other hand, speed-ups reported even 1-2 years ago against single-core CPUs can comfortably be increased by a factor of a few: while GPU processing rates continue to grow, single-core CPU rates have stalled.

The current record holder for a “workstation” GPU (i.e. not a cluster, but still allowing for multiple GPUs within one device) is 1.28 Tflop/s on a Tesla S1070 for computing direct ray-tracing for microlensing (Thompson et al. 2010). As with speed-ups, flop-counts should be treated with caution as there can be a mismatch between operations and clock-cycles when any mathematical operator beyond addition, subtraction or multiplication is used.

4. GPU-Powered Clusters

In terms of theoretical processing power, a single GPU can achieve the same processing performance as a modest CPU cluster – provided the problem can fit in the memory of a single GPU – and a small cluster of GPUs can outperform a O(100)-node CPU-based cluster, with a vast reduction in the amount of inter-node network connectivity required, and at a fraction of the hardware and operating cost. In this context, a GPU cluster is really a hybrid CPU-GPU system, as GPUs cannot manage important tasks like reading data from disks or supporting networks.

A growing number of astronomical institutions are now investing in major GPU-powered HPC clusters, with two of the first being the kolob compute cluster at the

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7http://openmp.org/
8http://kolob.ziti.uni-heidelberg.de/
University of Heidelberg, and the Silk Road facility\(^9\) operated by the National Astronomical Observatories of China (see Spurzem, R. and others 2010).

In 2010, the Australian astronomy community was invited to present expressions of interest to Astronomy Australia Limited (AAL) for new research infrastructure that could be funded by AAL through the Australian Federal Government’s Education Investment Fund. One of the nine successful projects was gSTAR: the GPU Supercomputer for Theoretical Astrophysics Research – a national high-performance computing facility for astronomers. Installation of the gSTAR facility at Swinburne University of Technology commenced in early September 2011.

Phase 1 of gSTAR, with a theoretical peak of \(\sim 130\) Tflop/s (single precision), comprises 51 dual-socket compute nodes each with 2 GPUS (NVIDIA C2070; 6 GB RAM), with an additional 3 high-density GPU compute nodes containing 7 GPUs (M2090: 6GB RAM). In excess of 1 Petabyte of usable disk space, supported by the Lustre file system, is available, and compute nodes are connected via QDR InfiniBand. Phase 2 of gSTAR, scheduled for 2012, will see the addition of further GPUs. Early science on gSTAR is expected to include: high-resolution N-body simulations of star clusters, including incorporation of improved physics; a cosmological microlensing parameter survey; and extensions to the interactive, real-time visualisation framework for terascale datasets (Hassan, Fluke, & Barnes 2011).

As of June 2011, 3 of the top 5 facilities (the National Supercomputing Centers in Tianjin and Shenzhen, and the GSIC Center, Tokyo Institute of Technology) on the TOP500 Supercomputing Sites\(^10\) achieve their benchmark status, in part, through the use of GPUs. These numbers are likely to rise in the next TOP500 list. Consulting the Green500 List,\(^11\) which ranks HPC facilities based on their energy efficiency, 4 of the top 10 use GPUs (ATI Radeon for Nagasaki University and Universitaet Frankfurt; NVIDIA for GSIC Center, Tokyo Institute of Technology and CINECA/SCA - Super-Computing Solution). Moreover, 14 of the Top 20 Green sites are accelerator based, using either GPUs or IBM Cell-based processors – further evidence that GPUs can provide impressive energy efficiency.

Astronomical use of GPU clusters to date has included adaptive-mesh-refinement calculations (e.g. Schive, Tsai, & Chiueh 2010); wavefront correction for adaptive optics (Bouchez et al. 2009); spherical harmonic transforms for Cosmological Microwave Background computations (Szydlarski et al. 2011); further progress on high-resolution, \(N\)-body simulations (Spurzem, R. and others 2010); and real-time, interactive volume rendering of terascale datasets (Hassan et al. 2011).

An innovative approach to gaining very high peak performance was achieved by Hamada & Nitadori (2010) through the use of low-end, commodity graphics cards (576 \(\times\) NVIDIA GT200 cards). A very impressive sustained performance of 190 Tflop/s for a 3 billion-particle, hierarchical \(N\)-body simulation, on a HPC cluster costing just over $400,000 dollars, resulted in an honourable mention for the Gordon Bell Prize at Supercomputing 2010. This raises an interesting comparison between high-end science cards and commodity GPUs - the main difference is double precision performance,

\(^9\)http://silkroad.bao.ac.cn/
\(^10\)http://www.top500.org/
\(^11\)http://www.green500.org (June 2011)
availability of error correcting memory and total memory available. If these are not concerns, then a commodity card may be sufficient.

5. **Accelerating the Rate of Discovery**

There are many reasons why astronomers might be excited about the prospects of adopting GPUs. The most obvious benefits (see also Kirk & Hwu 2010) are the ability to:

- **Run an individual problem faster.** Computing a problem in a few minutes compared to a few days, or a few days compared to a few months; allows real-time solutions to computationally demanding tasks, such as detection of transient radio events [Magro et al. (2011); Barsdell et al. (2012)].

- **Run more problems in the same total wall time.** Permits extensive exploration of parameter space [e.g. black hole inspirals – Herrmann et al. (2010); solving Kepler’s equations – Ford (2009); Lyman-α forest simulations – Greig et al. (2011)]. This promises to be one of the most important new uses of GPU clusters, enabling greater understanding of the effects of initial conditions, and allowing statistical investigations rather than promoting over-analysis of a single simulation result.

- **Solve a bigger problem size in the same wall time as a smaller problem size on a CPU-system.** This permits working at higher/improved resolution or provide greater capacity to explore evolution of systems over more time-steps; handle terascale, and ultimately petascale, image and spectral data cube processing (Fluke et al. 2010), visualisation (Hassan et al. 2011), and data mining (Protopapas 2010). However, if the problem cannot fit within the memory of a single GPU, a great deal of communication may be required between nodes of a GPU cluster. If the bottleneck moves from computation to data transfer, then gains delivered by a processing speed-up may be lost until such time there is a corresponding speed-up in bandwidth (between nodes), an increase in memory bus size (between host and GPU), and a decrease in latency in the interconnect.

- **Solve a more complex computational problem in the same wall time as a simpler problem on a CPU-system.** E.g. use a more accurate solution method, which may exhibit better stability, etc.; enable the inclusion of additional physical properties (e.g. magnetic fields); opportunities to utilise/implement algorithms with improved accuracy rather than an increase in resolution or problem size.

- **Provide much lower price/performance compared to an equivalent CPU-based cluster.** Provides potential for more astronomers to access Tflop/s high performance computing on the desktop, rather than needing to apply/compete for time on national or institution-level HPC supercomputing facilities for all computationally-demanding processing.

The move from traditional CPU systems to GPU-accelerated computation is not without challenges. Identifying, implementing, and optimising relevant algorithms for the highly-parallel GPU architecture can require a greater understanding of computer science fundamentals than many science professional possess: traditional sequential programming skills are arguably easier for "astronomer-programmers" to learn than parallel programming techniques. More importantly, code that has been developed
specifically for single-core CPU will not run on a GPU without substantial modification. In the short term, additional personnel time is required in order to develop GPU codes.

In general, the best results on GPUs are seen for computations that exhibit a large amount of data parallelism (i.e. the same computation performed on many different data values) and high arithmetic intensity (i.e. a high ratio of floating point calculations to memory accesses). Learning to use a GPU effectively means gaining an understanding of a new range of programming tricks, including reducing branching conditions (if/then statements), making judicious use of over-computing (e.g. using zero-mass particles in the pairwise $N$-body force calculation) to keep GPU threads busy, and giving more thought to memory access patterns.

By placing the emphasis on the “total time to science” (Fluke et al. 2011), rather than time spent developing code for GPUs, some of this additional coding work should be made up by the typically $10\times$ (or greater) processing speed-ups. As a growing number of GPU-programming and scripting libraries become available (e.g. PyCuda\textsuperscript{12} and Thrust\textsuperscript{13}), with a goal of improving developer productivity, the short-term need for new code development may be reduced. Interactive data languages such as IDL\textsuperscript{14} can also achieve acceleration through bindings to GPU libraries like GPULib\textsuperscript{15}, bringing the potential for GPU-acceleration to non-C-programming astronomers.

6. Concluding Remarks

At the dawn of the petascale data era, astronomers will be faced with new challenges in data processing and computation. GPU-powered HPC clusters offer a low-cost opportunity to explore new, scalable, massively-parallel algorithms. The processing speed-ups available with GPUs, for the right types of problems, are helping pave the way to new science, through higher-resolution simulations, improved physical modelling, and much greater exploration of parameter spaces. Ultimately, the goal of adopting any new hardware solution in astronomy should be to help improve and enhance our understanding of the Universe. The future of computing for astronomy is here - and it is massively parallel.

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