Analysing astronomy algorithms for graphics processing units and beyond

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ABSTRACT
Astronomy depends on ever-increasing computing power. Processor clock rates have plateaued, and increased performance is now appearing in the form of additional processor cores on a single chip. This poses significant challenges to the astronomy software community. Graphics processing units (GPUs), now capable of general-purpose computation, exemplify both the difficult learning curve and the significant speedups exhibited by massively parallel hardware architectures. We present a generalized approach to tackling this paradigm shift, based on the analysis of algorithms. We describe a small collection of foundation algorithms relevant to astronomy and explain how they may be used to ease the transition to massively parallel computing architectures. We demonstrate the effectiveness of our approach by applying it to four well-known astronomy problems: Högbo CLEAN, inverse ray-shooting for gravitational lensing, pulsar dedispersion and volume rendering. Algorithms with well-defined memory access patterns and high arithmetic intensity stand to receive the greatest performance boost from massively parallel architectures, while those that involve a significant amount of decision-making may struggle to take advantage of the available processing power.

Key words: gravitational lensing: micro – methods: data analysis – pulsars: general.

1 INTRODUCTION
Computing resources are a fundamental tool in astronomy: they are used to acquire and reduce observational data, simulate astrophysical processes, and analyse and visualize the results. Advances in the field of astronomy have depended heavily on the increase in computing power that has followed Moore’s law (Moore 1965) since the mid-1960s; indeed, many contemporary astronomy survey projects and astrophysics simulations would simply not be possible without the evolution Moore predicted.

Until recently, increased computing power was delivered in direct proportion to the increase in central processing unit (CPU) clock rates. Astronomy software executed more and more rapidly with each new hardware release, without any further programming work. But around 2005, the advance in clock rates ceased, and manufacturers turned to increasing the instantaneous processing capacity of their CPUs by including additional processing cores in a single silicon chip package. Today’s mainstream multicore CPUs typically have between two and eight processing cores; these are routinely deployed in large-scale compute clusters.

Fig. 1 places the mainstream CPUs from the last ∼20 yr in the clock-rate versus core-count phase space. In this space, the evolution of CPUs turns a ‘corner’ around 2005 when clock rates plateaued and multicore processors emerged. Lying above today’s fastest multicore CPUs in Fig. 1 though are the contemporary graphics processing units (GPUs), boasting hundreds of cores (‘many-core’) and ∼1-GHz clock rates. GPUs are already useful in their own right – providing ∼30 times the raw computation speed of CPUs – but perhaps more interestingly, they represent the likely evolution of CPUs. GPUs demonstrate how computing power can continue to follow Moore’s law in an era of zero (or even negative) growth in clock rates.

The plateau in processor clock rates is problematic for astronomy software composed of sequential codes, wherein instructions are executed one after the other. Such codes derive no direct performance benefit from the presence of multiple processing cores, and their performance will languish for as long as processor clock rates remain steady at ∼3–4 GHz. Astronomy software must be (re-)written to take advantage of many-core processors.

Astronomers are already cognisant of this issue. Shared-and distributed-memory multicore CPU machines have been exploited using the well-known OpenMP and Message Passing Interface (MPI) programming models.1 In addition, a number of researchers have adapted, written and/or re-written classic astronomy codes for the GPU architecture in the last ∼3 yr and gained performance improvements ranging from factors of a few to several hundreds. Some highlights include N-body (e.g. Hamada et al. 2009), radio–telescope signal correlation

1 While the specifics of parallel CPU systems lie outside the scope of this paper, we note that many of the algorithm analysis techniques we describe lend themselves equally well to these architectures.
analysing algorithms for GPUs and beyond

2 A STRATEGIC APPROACH: ALGORITHM ANALYSIS

Algorithm analysis, pioneered by Donald Knuth (see e.g. Knuth 1998), is a fundamental component of computer science – a discipline that is more about how to solve problems than the actual implementation in code. In this work, we are not interested in the specifics (i.e. syntax) of implementing a given astronomy algorithm with a particular programming language or library (e.g. CUDA, OpenCL, Thrust) on a chosen computing architecture [e.g. GPU, Cell, Field Programmable Gate Arrays (FPGAs)]. As Harris (2007) notes, algorithm-level optimizations are much more important with respect to overall performance on many-core hardware (specifically GPUs) than implementation optimizations, and should be made first. We will return to the issue of implementation in future work.

Here we present an approach to tackling the transition to many-core hardware based on the analysis of algorithms. The purpose of this analysis is to determine the potential of a given algorithm for a many-core architecture before any code is written. This provides essential information about the optimal approach as well as the return on investment one might expect for the effort of (re-)implementing a particular algorithm. Our methodology was in part inspired by the work of Harris (2005).

Work in a similar vein has also been undertaken by Asanovic et al. (2006, 2009) who classified parallel algorithms into 12 groups, referring to them as ‘dwarfs’. While insightful and opportune, these dwarfs consider a wide range of parallel architectures, cover all areas of computation (including several that are not of great relevance to astronomy) and are limited as a resource by the coarse nature of the classification. In contrast, the approach presented here is tailored to the parallelism offered by many-core processor architectures, contains algorithms that appear frequently within astronomy computations and provides a fine-grained level of detail. Furthermore, our approach considers the fundamental concerns raised by many-core architectures at a level of abstraction that avoids dealing with hardware- or software-specific details and terminology. This is in contrast to the work by Che et al. (2008), who presented a useful but highly targeted summary of general-purpose programming on the NVIDIA GPU architecture.

For these reasons, this work will serve as a valuable and practical resource for those wishing to analyse the expected performance of particular astronomy algorithms on current and future many-core architectures.

For a given astronomy problem, our methodology is as follows.

(1) Outline each step in the problem.

(2) Identify steps that resemble known algorithms (see below).

(i) Outlined steps may need to be further decomposed into sub-steps before a known counterpart is recognized. Such composite steps may later be added to the collection of known algorithms.

(3) For each identified algorithm, refer to its pre-existing analysis.

(i) Where a particular step does not appear to match any known algorithm, refer to a relevant analysis methodology to analyse the step as a custom algorithm (see Sections 2.1–2.3). The newly analysed algorithm can then be added to the collection for future reference.

(4) Once analysis results have been obtained for each step, apply a global analysis to the algorithm to obtain a complete picture of its behaviour (see Section 2.4).

Here we present a small collection of foundation algorithms2 that appear in computational astronomy problems. This is motivated by the fact that complex algorithms may be composed from simpler ones. We propose that algorithm composition provides an excellent approach to turning the multicore corner. Here we focus on its application to algorithm analysis; in future work, we will show how it may also be applied to implementation methodologies. The algorithms are described below using a vector data structure. This is a data structure like a FORTRAN or C array representing a contiguous block of memory and providing constant-time random access to

Figure 1. Clock-rate versus core-count phase space of Moore’s law binned every 2 yr for CPUs (circles) and GPUs (diamonds). There is a general trend for performance to increase from bottom left to top right.

(e.g. Wayth, Greenhill & Briggs 2009), adaptive mesh refinement (e.g. Schive, Tsai & Chiueh 2010), galaxy spectral energy distribution (Jonsson & Primack 2010) and gravitational microlensing (Thompson et al. 2010) codes.

Inevitably, a section of the astronomy community will continue with an ad hoc approach to the adaptation of software from single-core to many-core architectures. In this paper, we demonstrate that there is a significant difference between current computing techniques and those required to efficiently utilize new hardware architectures such as many-core processors, as exemplified by GPUs. These techniques will be unfamiliar to most astronomers and will pose a challenge in terms of keeping our discipline at the forefront of computational science. We present a practical, effective and simple methodology for creating astronomy software whose performance scales well to present and future many-core architectures. Our methodology is grounded in the classical computer science field of algorithm analysis.

In Section 2 we introduce the key concepts in algorithm analysis, with particular focus on the context of many-core architectures. We present four foundation algorithms and characterize them as we outline our algorithm analysis methodology. In Section 3 we demonstrate the proposed methodology by applying it to four well-known astronomy problems, which we break down into their constituent foundation algorithms. We validate our analysis of these problems against ad hoc many-core implementations as available in the literature and discuss the implications of our approach for the future of computing in astronomy in Section 4.

2 Note that for these algorithms, we have used naming conventions that are familiar to us but are by no means unique in the literature.
individual elements. We use the notation $v[i]$ to represent the $i$th element of a vector $v$.

**Transform.** Returns a vector containing the result of the application of a specified function to every individual element of an input vector:

$$\text{out}[i] = f(\text{in}[i]).$$

Functions of more than one variable may also be applied to multiple input vectors. Scaling the brightness of an image (defined as a vector of pixels) is an example of a transform operation.

**Reduce.** Returns the sum of every element in a vector:

$$\text{out} = \sum_i \text{in}[i].$$

Reductions may be generalized to use any associative binary operator, e.g. product, min, max, etc. Calculating image noise is a common application of the reduce algorithm.

**Gather.** Retrieves values from an input vector according to a specified index mapping and writes them to an output vector:

$$\text{out}[i] = \text{in}[^{\text{map}}[i]].$$

Reading a shifted or transformed subregion of an image is a common example of a gather operation.

**Interact.** For each element $i$ of an input vector, $\text{in}_1$, sums the interaction between $i$ and each element $j$ in a second input vector, $\text{in}_2$:

$$\text{out}[i] = \sum_j f(\text{in}_1[i], \text{in}_2[j]),$$

where $f$ is a given interaction function. The best-known application of this algorithm in astronomy is the computation of forces in a direct $N$-body simulation, where both input vectors represent the system’s particles and the interaction function calculates the gravitational force between two particles.

These four algorithms were chosen from experience with a number of computational astronomy problems. The transform, reduce and gather operations may be referred to as ‘atoms’ in the sense that they are indivisible operations. While the interact algorithm is technically a composition of transforms and reductions, it will be analysed as if it too was an atom, enabling rapid analysis of problems that use the interact algorithm without the need for further decomposition.

We now describe a number of algorithm analysis techniques that we have found to be relevant to massively parallel architectures. These techniques should be applied to the individual algorithms that comprise a complete problem in order to gain a detailed understanding of their behaviour.

### 2.1 Principal characteristics

Many-core architectures exhibit a number of characteristics that can strongly impact the performance of an algorithm. Here we summarize four of the most important issues that must be considered.

**Massive parallelism.** To fully utilize massively parallel architectures, algorithms must exhibit a high level of parallel granularity; i.e. the number of required operations that may be performed simultaneously must be large and scalable. Data-parallel algorithms, which divide their data between parallel processors rather than (or in addition to) their tasks, exhibit parallelism that scales with the size of their input data, making them ideal candidates for massively parallel architectures. However, performance may suffer when these algorithms are executed on sets of input data that are small relative to the number of processors in a particular many-core architecture.

**Memory access patterns.** Many-core architectures contain very high bandwidth main memory in order 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. neighbouring threads accessing similar locations in memory) is vital to achieving good performance. Fig. 2 illustrates different levels of locality of reference.

Collisions between threads trying to read the same location in memory can also be costly, and write collisions must be treated using expensive atomic operations in order to avoid conflicts between threads.

**Branching.** Current many-core architectures rely on single instruction multiple data (SIMD) hardware. This means that neighbouring threads that wish to execute different instructions must wait for each other to complete the divergent code section before execution can continue in parallel (see Fig. 3). For this reason, algorithms that involve significant branching between different threads

\[100\text{GB/s}.\]

\[\text{GPUs}.\]
may suffer severe performance degradation. Similar to the effects of memory access locality, performance will in general depend on the locality of branching, i.e. the number of different code paths taken by a group of neighbouring threads.

**Arithmetic intensity.** Executing arithmetic instructions is generally much faster than accessing memory on current many-core hardware. Algorithms performing few arithmetic operations per memory access may become memory-bandwidth-bound; i.e. their speed becomes limited by the rate at which memory can be accessed rather than the rate at which arithmetic instructions can be processed. Memory bandwidths in many-core architectures are typically significantly higher than in CPUs, meaning that even bandwidth-bound algorithms may exhibit strong performance; however, they will not be able to take full advantage of the available computing power. In some cases, it may be beneficial to re-work an algorithm entirely in order to increase its arithmetic intensity, even at the cost of performing more numerical work in total.

For the arithmetic intensities presented in this paper, we assume an idealized cache model in which only the first memory read of a particular piece of data is included in the count; subsequent or parallel reads of the same data are assumed to be made from a cache and are not counted. The ability to achieve this behaviour in practice will depend strongly on the memory access pattern (specifically the locality of memory accesses).

### 2.2 Complexity analysis

The complexity of an algorithm is a formal measure of its execution time given a certain size of input. It is often used as a means of comparing the speeds of two different algorithms that compute the same (or a similar) result. Such comparisons are critical to understanding the relative contributions of different parts of a composite algorithm and identifying bottlenecks.

Computational complexity is typically expressed as the total runtime, $T$, of an algorithm as a function of the input size, $N$, using ‘Big O’ notation. Thus, $T(N) = \mathcal{O}(N)$ means a run-time that is proportional to the input size $N$. An algorithm with a complexity of $T(N) = \mathcal{O}(N^2)$ will take four times as long to run after a doubling of its input size.

While the complexity measure is traditionally used for algorithms running on serial processors, it can be generalized to analyse parallel algorithms. One method is to introduce a second parameter: $P$, the number of processors. The run-time is then expressed as a function of both $N$ and $P$. For example, an algorithm with a parallel complexity of $T(N, P) = \mathcal{O}(\frac{N}{P})$ will run $P$ times faster on $P$ processors than on a single processor for a given input size; i.e. it exhibits perfect parallel scaling. More complex algorithms may incur overheads when run in parallel, e.g. those requiring communication between processors. In these cases, the parallel complexity will depend on the specifics of the target hardware architecture.

An alternative way to express parallel complexity is using the work, $W$, and depth, $D$, metrics first introduced formally by Blelloch (1996). Here, work measures the total number of computational operations performed by an algorithm (or, equivalently, the run-time on a single processor), while depth measures the longest sequence of sequentially dependent operations (or, equivalently, the run-time on an infinite number of processors). The depth metric is a measure of the amount of inherent parallelism in the algorithm. A perfectly parallel algorithm has a work complexity of $W(N) = \mathcal{O}(N)$ and a depth complexity of $D(N) = \mathcal{O}(1)$, meaning that all but a constant number of operations may be performed in parallel. An algorithm with $W = \mathcal{O}(N)$ and $D = \mathcal{O}(\log N)$ is highly parallel but contains some serial dependencies between operations that scale as a function of the input size. Parallel algorithms with work complexities equal to those of their serial counterparts are said to be ‘work efficient’; those that further exhibit low depth complexities are considered to be efficient parallel algorithms. The benefit of the work/depth metrics over the parallel run-time is that they have no dependence on the particular parallel architecture on which the algorithm is executed, i.e. they measure properties inherent to the algorithm.

A final consideration regarding parallel algorithms is Amdahl’s law (Amdahl 1967), which states that the maximum possible speedup over a serial algorithm is limited by the fraction of the parallel algorithm that cannot be (or simply is not) parallelized. Assuming an infinite number of available processors, the run-time of the parallel part of the algorithm will reduce to a constant, while the serial part will continue to scale with the size of the input. In terms of the work/depth metrics, the depth of the algorithm represents the fraction that cannot be parallelized, and the maximum theoretical speedup is given by $S_{\text{max}} \approx \frac{W}{\alpha}$. Note the implication that the maximum speedup is actually a function of the input size. Increasing the problem size in addition to the number of processors allows the speedup to scale more effectively.

### 2.3 Analysis results

We have applied the techniques discussed in Sections 2.1 and 2.2 to the four foundation algorithms introduced at the beginning of Section 2. We use the following metrics.

(i) **Work and depth.** The complexity metrics as described in Section 2.2.

(ii) **Memory access locality.** The nature of the memory access patterns as discussed in Section 2.1.

(iii) **Arithmetic intensity.** Defined by the triple ratio $r:w:f$ representing the number of read, write and function evaluation operations, respectively, that the algorithm performs (normalized to the input size). The symbol $\alpha$ is used, where applicable, to represent the internal arithmetic intensity of the function given to the algorithm.

The results are presented in Table 1. Note that this analysis is based on the most-efficient known parallel version of each algorithm.

### 2.4 Global analysis

Once local analysis results have been obtained for each step of a problem, it is necessary to put them together and perform a global analysis. Our methodology is as follows.
(i) Determine the components of the algorithm where most of the computational work lies by comparing work complexities. Components with similar work complexities should receive similar attention with respect to parallelization in order to avoid leaving behind bottlenecks as a result of Amdahl’s law.

(ii) Consider the amount of inherent parallelism in each algorithm by observing its theoretical speedup $S_{\text{max}} \approx \frac{W}{M}$.

(iii) Use the theoretical arithmetic intensity of each algorithm to determine the likelihood of it being limited by memory bandwidth rather than instruction throughput. The theoretical global arithmetic intensity may be obtained by comparing the total amount of input and output data to the total amount of arithmetic work to be done in the problem.

(iv) Assess the memory access patterns of each algorithm to identify the potential to achieve peak arithmetic intensity.\(^7\)

(v) If particular components exhibit poor properties, consider alternative algorithms.

(vi) Once a set of component algorithms with good theoretical performance have been obtained, the algorithm decomposition should provide a good starting point for an implementation.

### 3 APPLICATION TO ASTRONOMY ALGORITHMS

We now apply our methodology from Section 2 to four typical astronomy computations. In each case, we demonstrate how to identify the steps in an outline of the problem as foundation algorithms from our collection described at the beginning of Section 2. We then use this knowledge to study the exact nature of the available parallelism and determine the problem’s overall suitability for many-core architectures. We note that we have deliberately chosen simple versions of the problems in order to maximize clarity and brevity in illustrating the principles of our algorithm analysis methodology.

#### 3.1 Inverse ray-shooting gravitational lensing

##### 3.1.1 Introduction

Inverse ray-shooting is a numerical technique used in gravitational microlensing. Light rays are projected backwards (i.e. from the observer) through an ensemble of lenses and on to a source-plane pixel grid. The number of rays that fall into each pixel gives an indication of the magnification at that spatial position relative to the case where there was no microlensing. In cosmological scenarios, the resultant maps are used to study brightness variations in light from an object (e.g. an accretion disc and broad-line emission regions) in the case where there was no microlensing. In cosmological scenarios, the resultant maps are used to study brightness variations in light from an object (e.g. an accretion disc and broad-line emission regions).

The two main approaches to ray-shooting are based on either the direct calculation of the gravitational deflection by each lens (Kayser, Refsdal & Stabell 1986; Schneider & Weiss 1986, 1987) or the use of a tree hierarchy of pseudo-lenses (Wambsganss 1990, 1999). Here, we consider the direct method.

#### 3.1.2 Outline

The ray-shooting algorithm is easily divided into a number of distinct steps, as follows.

(i) Obtain a collection of lenses according to a desired distribution, where each lens has position and mass.

(ii) Generate a collection of rays according to a uniform distribution within a specified 2D region, where each ray is defined by its position.

(iii) For each ray, calculate and sum its deflection due to each lens.

(iv) Add each ray’s calculated deflection to its initial position to obtain its deflected position.

(v) Calculate the index of the pixel that each ray falls into.

(vi) Count the number of rays that fall into each pixel.

(vii) Output the list of pixels as the magnification map.

#### 3.1.3 Analysis

To begin the analysis, we interpret Section 3.1.2 as follows.

(i) Steps (i) and (ii) may be considered transform operations that initialize the vectors of lenses and rays.

(ii) Step (iii) is an example of the interact algorithm, where the inputs are the vectors of rays and lenses and the interaction function calculates the deflection of a ray due to the gravitational potential around a lens mass.

(iii) Steps (iv) and (v) apply further transforms to the collection of rays.

(iv) Step (vi) involves the generation of a histogram. As we have not identified this algorithm in Section 2, it will be necessary to analyse this step as a unique algorithm.

According to this analysis, three basic algorithms comprise the complete technique: transform, interact and histogram generation. Referring to Table 1, we see that, in the context of a lensing simulation using $N_{\text{rays}}$ rays and $N_{\text{lenses}}$ lenses, the amount of work performed by the transform and interact algorithms will be $W = O(N_{\text{rays}}) + O(N_{\text{lenses}})$ and $W = O(N_{\text{rays}}, N_{\text{lenses}})$, respectively.

We now analyse the histogram step. Considering first a serial algorithm for generating a histogram, where each point is considered in turn and the count in its corresponding bin is incremented, we find the work complexity to be $W = O(N_{\text{rays}})$. Without further analysis, we compare this to those of the other component algorithms. The serial histogram and the transform operations each perform similar work. The interact algorithm on the other hand must, as we have

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Table 1. Analysis of four foundation algorithms.

| Transform | Reduction | Gather | Interact |
|-----------|-----------|--------|----------|
| $O(N)$    | $O(N)$    | $O(N)$ | $O(NM)$  |
| $O(1)$    | $O(\log N)$ | $O(1)$ | $O(M)$ or $O(\log M)$ |
| Contiguous| Contiguous| Variable| Contiguous |
| $1:1:\alpha$ | $1: \frac{1}{M} \alpha$ | $1:1:0$ | $1: \frac{M}{\alpha} :1:2M\alpha$ |

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\(^7\) Studying the memory access patterns will also help to identify the optimal caching strategy if this level of optimization is desired.
seen, perform work proportional to $N_{\text{rays}} \times N_{\text{lenses}}$. For large $N_{\text{lenses}}$ (e.g. as occurs in cosmological microlensing simulations, where $N_{\text{lenses}} > 10^3$), this step will dominate the total work. Assuming that the number of lenses is scaled with the amount of parallel hardware, the interact step will also dominate the total run-time.

Given the dominance of the interact step, we now choose to ignore the effects of the other steps in the problem. It should be noted, however, that in contrast to cosmological microlensing, planetary microlensing models contain only a few lenses. In this case, the work performed by the interact step will be similar to that of the other steps, and thus the use of a serial histogram algorithm alongside parallel versions of all other steps would result in a severe performance bottleneck. Several parallel histogram algorithms exist, but a discussion of them is beyond the scope of this work.

Returning to the analysis of the interact algorithm, we again refer to Table 1. Its worst-case depth complexity indicates a maximum speedup of $S \approx W = \mathcal{O}(N_{\text{rays}})$, i.e. parallel speedup scaling perfectly up to the number of rays. The arithmetic intensity of the algorithm scales as $N_{\text{lenses}}$ and will thus be very high. Contiguous memory accesses indicate strong potential to achieve this high arithmetic intensity. We conclude that direct inverse ray-shooting for cosmological microlensing is an ideal candidate for an efficient implementation on a many-core architecture.

### 3.2 Hogbom CLEAN

#### 3.2.1 Introduction

Raw (‘dirty’) images produced by radio interferometers exhibit unwanted artefacts as the result of the incomplete sampling of the visibility plane. These artefacts can inhibit image analysis and should ideally be removed by deconvolution. Several different techniques have been developed to ‘clean’ these images. For a review, see Briggs (1995). Here we analyse the image-based algorithm first described by Hogbom (1974). We note that the algorithm by Clark (1980) is now the more popular choice in the astronomy community, but point out that it is essentially an approximation to the Hogbom algorithm that provides increased performance at the cost of reduced accuracy.

The algorithm involves iteratively finding the brightest point in the ‘dirty’ image and subtracting from the dirty image an image of the beam centred on and scaled by this brightest point. The procedure continues until the brightest point in the image falls below a prescribed threshold. While the iterative procedure must be performed sequentially, the computations within each iteration step are performed independently for every pixel of the images, suggesting a substantial level of parallelism. The output of the algorithm is a series of ‘clean components’, which may be used to reconstruct a cleaned image.

#### 3.2.2 Outline

The algorithm may be divided into the following steps.

(i) Obtain the beam image.
(ii) Obtain the image to be cleaned.
(iii) Find the brightest point, $b$; the standard deviation, $\sigma$; and the mean, $\mu$, of the image.
(iv) If the brightness of $b$ is less than a prescribed threshold (e.g. $|b - \mu| < 3\sigma$), go to step (ix).
(v) Scale the beam image by a fraction (referred to as the ‘loop gain’) of the brightness of $b$.
(vi) Shift the beam image to centre it over $b$.
(vii) Subtract the scaled, shifted beam image from the input image to produce a partially cleaned image.
(viii) Repeat from step (iii).
(ix) Output the ‘clean components’.

### 3.2.3 Analysis

We decompose Section 3.2.2 as follows.

(i) Steps (i) and (ii) are simple data-loading operations and may be thought of as transforms.
(ii) Step (iii) involves a number of reduce operations over the pixels in the dirty image.
(iii) Step (v) is a transform operation, where each pixel in the beam is multiplied by a scale factor.
(iv) Step (vi) may be achieved in two ways, either by directly reading an offset subset of the beam pixels or by switching to the Fourier domain and exploiting the shift theorem. Here we will only consider the former option, which we identify as a gather operation.
(v) Step (vii) is a transform operation over pixels in the dirty image.

We thus identify three basic algorithms in Hogbom $\text{clean}$: transform, reduce and gather. Table 1 shows that the work performed by each of these algorithms will be comparable (assuming that the input and beam images are of similar pixel resolutions). This suggests that any acceleration should be applied equally to all of the steps in order to avoid the creation of bottlenecks.

The depth complexities of each algorithm indicate a limiting speedup of $S_{\text{max}} \approx \mathcal{O}(N_{\text{rays}} / \log N_{\text{rays}})$ during the reduce operations. While not quite ideal, this is still a good result. Further, the algorithms do not exhibit high arithmetic intensity (the calculations involving only a few subtractions and multiplies) and are thus likely to be bandwidth-bound. This will dominate any effect the limiting speedup may have.

The efficiency with which the algorithm will use the available memory bandwidth will depend on the memory access patterns. Both the transform and reduce algorithms make contiguous memory accesses and will thus achieve peak bandwidth. The gather operation in step (vi), where the beam image is shifted to centre it on a point in the input image, will access memory in an offset but contiguous 2D block. This 2D locality suggests the potential to achieve near-peak memory throughput.

We conclude that the Hogbom $\text{clean}$ algorithm represents a good candidate for implementation on many-core hardware, but will likely be bound by the available memory bandwidth rather than arithmetic computing performance.

### 3.3 Volume rendering

#### 3.3.1 Introduction

There are a number of sources of volume data in astronomy, including spectral cubes from radio telescopes and integral field units, as well as simulations using adaptive mesh refinement and smoothed particle hydrodynamics techniques. Visualizing these data in physically meaningful ways is important as an analysis tool, but even small volumes (e.g. 256$^3$) require large amounts of computing power to render, particularly when real-time interactivity is desired.

Several methods exist for rendering volume data; here we analyse a direct (or brute-force) ray-casting algorithm (Levoy 1990).
While similarities exist between ray-shooting for microlensing (Section 3.1) and the volume-rendering technique we describe here, they are fundamentally different algorithms.

3.3.2 Outline

The algorithm may be divided into the following steps.

(i) Obtain the input data cube.
(ii) Create a 2D grid of output pixels to be displayed.
(iii) Generate a corresponding grid of rays, where each is defined by a position (initially the centre of the corresponding pixel), a direction (defined by the viewing transformation) and a colour (initially black).
(iv) Project each ray a small distance (the step size) along its direction.
(v) Determine which voxel each ray now resides in.
(vi) Retrieve the colour of the voxel from the data volume.
(vii) Use a specified transfer function to combine the voxel colour with the current ray colour.
(viii) Repeat from step (iv) until all rays exit the data volume.
(ix) Output the final ray colours as the rendered image.

3.3.3 Analysis

We interpret the steps in Section 3.3.2 as follows.

(i) Steps (ii)–(v) and (vii) are all transform operations.
(ii) Step (vi) is a gather operation.

All steps perform work scaling with the number of output pixels, \( N_{\text{pxls}} \), indicating that there are no algorithmic bottlenecks and thus acceleration should be applied to the whole algorithm equally.

Given that the number of output pixels is likely to be large and scalable, we should expect the transforms and the gather, with their \( \mathcal{O}(1) \) depth complexities, to parallelize perfectly on many-core hardware.

The outer loop of the algorithm, which marches rays through the volume until they leave its bounds, involves some branching as different rays traverse thicker or thinner parts of the arbitrarily oriented cube. This will have a negative impact on the performance of the algorithm on an SIMD architecture like a GPU. However, if rays are ordered in such a way as to maintain 2D locality between their positions, neighbouring threads will traverse similar depths through the data cube, resulting in little divergence in their branch paths and thus good performance on SIMD architectures.

The arithmetic intensity of each of the steps will typically be low (common transfer functions can be as simple as taking the average or maximum), while the complete algorithm requires \( \mathcal{O}(N_{\text{pxls}}N_d) \) memory reads, \( \mathcal{O}(N_{\text{pxls}}) \) memory writes and \( \mathcal{O}(N_{\text{pxls}}N_d) \) function evaluations for an input data volume of side length \( N_d \). This global arithmetic intensity of \( N_d1:N_d\alpha \) indicates that the algorithm is likely to remain bandwidth-bound.

The use of bandwidth will depend primarily on the memory access patterns in the gather step (the transform operations perform ideal contiguous memory accesses). During each iteration of the algorithm, the rays will access an arbitrarily oriented plane of voxels within the data volume. Such a pattern exhibits 3D spatial locality, presenting an opportunity to cache the memory reads effectively and thus obtain near-peak bandwidth.

We conclude that the direct ray-casting volume-rendering algorithm is a good candidate for efficient implementation on many-core hardware, although, in the absence of transfer functions with significant arithmetic intensity, the algorithm is likely to remain limited by the available memory bandwidth.

3.4 Pulsar time-series dedispersion

3.4.1 Introduction

Radio telescopes observing pulsars produce time-series data containing the pulse signal. Due to its passage through the interstellar medium, the pulse signature gets delayed as a function of frequency, resulting in a ‘dispersing’ of the data. The signal can be ‘dedispersed’ by assuming a frequency-dependent delay before summing the signals at each frequency. The data are dedispersed using a number of trial dispersion measures (DMs), from which the true DM of the signal is measured.

There are two principal dedispersion algorithms used in the literature: the direct algorithm and the tree algorithm (Taylor 1974). Here we consider the direct method, which simply involves delaying and summing time series for a range of DMs. The calculation for each DM is entirely independent, presenting an immediate opportunity for parallelization. Further, each sample in the time series is operated on individually, hinting at additional fine-grained parallelism.

3.4.2 Outline

Here we describe the key steps of the algorithm.

(i) Obtain a set of input time series, one per frequency channel.
(ii) If necessary, transpose the input data to place it into channel-major order.
(iii) Impose a time delay on each channel by offsetting its starting location by the number of samples corresponding to the delay. The delay introduced into each channel is a quadratic function of its frequency and a linear function of the DM.
(iv) Sum aligned samples across every channel to produce a single accumulated time series.
(v) Output the result and repeat (potentially in parallel) from step (iii) for each desired trial DM.

3.4.3 Analysis

We interpret Section 3.4.2 as follows.

(i) Step (ii) involves transposing the data, which is a form of gather.
(ii) Step (iii) may be considered a set of gather operations that shift the reading location of samples in each channel by an offset.
(iii) Step (iv) involves the summation of many time series. This is a nested operation and may be interpreted as either a transform, where the operation is to sum the time sample in each channel, or a reduce, where the operation is to sum whole time series.

The algorithm therefore involves gather operations in addition to nested transforms and reductions. For data consisting of \( N_s \) samples for each of \( N_c \) channels, each step of the computation operates on all \( \mathcal{O}(N_sN_c) \) total samples. Acceleration should thus be applied equally to all parts of the algorithm.

According to the depth complexity listed in Table 1, the gather operation will parallelize perfectly. The nested transform and reduce calculation may be parallelized in three possible ways: (i) by parallelizing the transform, where \( N_c \) parallel threads each compute the sum of a single time sample over every channel sequentially;
(ii) by parallelizing the reduce, where $N_r$ parallel threads cooperate to sum each time sample in turn; or (iii) by parallelizing both the transform and the reduce, where $N_x \times N_r$ parallel threads cooperate to complete the entire computation in parallel.

Analysing these three options, we see that they have depth complexities of $O(N_x)$, $O(N_x \log N_x)$ and $O(\log N_x)$, respectively. Option (iii) would appear to provide the greatest speedup; however, it relies on using significantly more parallel processors than the other options. It will in fact only be the better choice in the case where the number of available parallel processors is much greater than $N_x$. For hardware with fewer than $N_x$ parallel processors, option (i) will likely prove the better choice, as it is expected to scale perfectly up to $N_x$ parallel threads, as opposed to the less efficient scaling of option (iii). In practice, the number of time samples $N_x$ will generally far exceed the number of parallel processors, and thus the algorithm can be expected to exhibit excellent parallel scaling using option (i).

Turning now to the arithmetic intensity, we observe that the computation of a single trial DM involves only an addition for each of the $N_x \times N_c$ total samples. This suggests that the algorithm will be limited by memory bandwidth. However, this does not take into account the fact that we wish to compute many trial DMs. The computation of $N_{DM}$ trial DMs still requires only $O(N_x \times N_c)$ memory reads and writes but performs $N_{DM} \times N_x \times N_c$ addition operations. The theoretical global arithmetic intensity is therefore $1:1:N_{DM}$. Given a typical number of trial DMs of $N_{DM}$, we conclude that the algorithm could, in theory at least, make efficient use of all available arithmetic processing power.

The ability to achieve such a high arithmetic intensity will depend on the ability to keep data in fast memory for the duration of many arithmetic calculations (i.e. the ability to efficiently cache the data). This in turn will depend on the memory access patterns. We note that in general, similar trial DMs will need to access similar areas of memory; i.e. the problem exhibits some locality of reference. The exact memory access pattern is non-trivial though, and a discussion of these details is outside the scope of this work.

We conclude that the pulsar dedispersion algorithm would likely perform to a high efficiency on a many-core architecture. While it is apparent that some locality of reference exists within the algorithm’s memory accesses, optimal arithmetic intensity is unlikely to be observed without a thorough and problem-specific analysis of the memory access patterns.

4 DISCUSSION

The direct inverse ray-shooting method has been implemented on a GPU by Thompson et al. (2010). They simulated systems with up to $10^9$ lenses. Using a single GPU, they parallelized the interaction step of the problem and obtained a speedup of $O(100 \times)$ relative to a single CPU core – a result consistent with the relative peak floating-point performance of the two processing units. These results validate our conclusion that the inverse ray-shooting algorithm is very well suited to many-core architectures like GPUs.

Our conclusions regarding the pulsar dedispersion algorithm are validated by a preliminary GPU implementation we have written. With only a simplistic approach to memory caching, we have recorded a speedup of $15 \times$ over an efficient multicore CPU code. This result is in line with the relative peak memory bandwidth of the two architectures, supporting the conclusions of Section 3.4 that, without a detailed investigation into the memory access patterns, the problem will remain bandwidth-bound.

Some astronomy problems are well suited to a many-core architecture; others are not. It is important to know how to distinguish between these. In the astronomy community, the majority of work with many-core hardware to date has focused on the implementation or porting of specific codes perhaps best classified as ‘low-hanging fruit’. Not surprisingly, these codes have achieved significant speedups, in line with the raw performance benefits offered by their target hardware.

A more generalized use of ‘novel’ computing architectures was undertaken by Brunner, Kindratenko & Myers (2007), who, as a case study, implemented the two-point angular correlation function for cosmological galaxy clustering on two different FPGA architectures. While they successfully communicated the advantages offered by these new technologies, their focus on implementation details for their FPGA hardware inhibits the ability to generalize their findings to other architectures.

It is interesting to note that previous work has in fact identified a number of common concerns with respect to GPU implementations of astronomy algorithms. For example, the issues of optimal use of the memory hierarchy and underuse of available hardware for small particle counts have been discussed in the context of the direct N-body problem (e.g. Bellemar, Bédorf & Portegies Zwart 2008). These concerns essentially correspond to a combination of what we have referred to as memory access patterns, arithmetic intensity and massive parallelism. While originally being discussed as implementation issues specific to particular choices of software and hardware, our abstractions re-cast them at the algorithm level and allow us to consider their impact across a variety of problems and hardware architectures.

Using algorithm analysis techniques, we now have a basis for understanding which astronomy algorithms will benefit most from many-core processors. Those with well-defined memory access patterns and high arithmetic intensity stand to receive the greatest performance boost, while problems that involve a significant amount of decision-making may struggle to take advantage of the available processing power.

For some astronomy problems, it may be important to look beyond the techniques currently in use, as these will have been developed (and optimized) with traditional CPU architectures in mind. Avenues of research could include, for instance, using higher order numerical schemes (Nitadori & Makino 2008) or choosing simplicity over efficiency by using brute-force methods (Bate et al. 2010). Some algorithms, such as histogram generation, do not have a single obvious parallel implementation and may require problem-specific input during the analysis process.

In this work, we have discussed the future of astronomy computation, highlighting the change to many-core processing that is likely to occur in CPUs.

The shift in commodity hardware from serial to parallel processing units will fundamentally change the landscape of computing. While the market is already populated with multicore chips, it is likely that chip designs will undergo further significant changes

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8 We note that Thompson et al. (2010) did not use the CPU’s Streaming SIMD Extensions, which have the potential to provide a speed increase of up to $4 \times$. However, our conclusion regarding the efficiency of the algorithm on the GPU remains unchanged by this fact.

9 FPGAs are another hardware architecture exhibiting significant fine-grained parallelism, but their specific details lie outside the scope of this paper.
in the coming years. We believe that for astronomy, a generalized methodology based on the analysis of algorithms is a prudent approach to confronting these changes – one that will continue to be applicable across the range of hardware architectures likely to appear in the coming years: CPUs, GPUs and beyond.

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