High-Level Data Partitioning for Parallel Computing on Heterogeneous Hierarchical HPC Platforms

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Abstract—The current state and foreseeable future of high performance scientific computing (HPC) can be described in three words: heterogeneous, parallel and distributed. These three simple words have a great impact on the architecture and design of HPC platforms and the creation and execution of efficient algorithms and programs designed to run on them. As a result of the inherent heterogeneity, parallelism and distribution which promises to continue to pervade scientific computing in the coming years, the issue of data distribution and therefore data partitioning is unavoidable.

This data distribution and partitioning is due to the inherent parallelism of almost all scientific computing platforms. Cluster computing has become all but ubiquitous with the development of clusters of clusters and grids becoming increasingly popular. Even at a lower level, high performance symmetric multiprocessor (SMP) machines, General Purpose Graphical Processing Unit (GPGPU) computing, and multiprocessor parallel machines play an important role. At a very low level, multicore technology is now widespread, increasing in heterogeneity, and promises to be omnipresent in the near future. The prospect of prevalent many-core architectures will inevitably bring yet more heterogeneity.

Scientific computing is undergoing a paradigm shift like none before. Only a decade ago most high performance scientific architectures were homogeneous in design and heterogeneity was seen as a difficult and somewhat limiting feature of some architectures. However this past decade has seen the rapid development of architectures designed not only to exploit heterogeneity but architectures designed to be heterogeneous. Grid and massively distributed computing has led the way on this front. The current shift is moving from this to architectures that are not heterogeneous by definition, but heterogeneous by necessity. Cloud and exascale computing architectures and platforms are not designed to be heterogeneous as much as they are heterogeneous by definition. Indeed such architectures cannot be homogeneous on any large (and useful) scale. In fact more and more researchers see heterogeneity as the natural state of computing.

Further to hardware advances, scientific problems have become so large that the use of more than one of the above platforms in parallel has become necessary, if not unavoidable. Problems such as climatology and projects including the Large Hadron Collider necessitate the use of extreme-scale parallel platforms, often encompassing more than one geographically central supercomputer or cluster. Even at the core level large amounts of information must be shared efficiently.

One of the greatest difficulties in solving problems on such architectures is the distribution of data between the different components in a way that optimizes runtime. There have been numerous algorithms developed to do so over the years. Most seek to optimize runtime by reducing the total volume of communication between processing entities. Much research has been conducted to do so between distinct processors or nodes, less so between distributed clusters.

This report presents new data partitioning algorithms for matrix and linear algebra operations. These algorithms would in fact work with little or no modification for any application with similar communication patterns. In practice these partitionings distribute data between a small number of computing entities, each of which can have great computational power themselves, and an even greater aggregate power. These partitionings may also be deployed in a hierarchical manner, which allows the flexibility to be employed in a great range of problem domains and computational platforms. These partitionings, in hybrid form, working together with more traditional partitionings, minimize the total volume of communication between entities in a manner proven to be optimal. This is done regardless of the power ratio that exists between the entities, thus minimizing execution time. There is also no restriction on the algorithms or methods employed on the clusters themselves locally, thus maximizing flexibility.

Finally, most heterogeneous algorithms and partitionings are designed by modifying existing homogeneous ones. With this in mind the ultimate contribution of this report is to demonstrate that non-traditional and perhaps unintuitive algorithms and partitionings designed with heterogeneity in mind from the start can result in better, and in many cases optimal, algorithms and partitions for heterogeneous platforms. The importance of this given the current outlook for, and trends in, the future of high performance scientific computing is obvious.

I. INTRODUCTION

Two general areas have provided the motivation for this work—those which are fundamental to this research, and the current state-of-the-art of high performance scientific computing. Areas which fall into the fundamental area include:

- What happens when we want to solve a well-established homogeneous problem on heterogeneous platforms?
- How can the performance of these problems be improved?
- Why have these problems, running on heterogeneous platforms, been largely ignored by research groups?
- Where is scientific computing headed in the future?

Platforms and architectures which are central to the state-of-the-art and future of scientific computing include:

- Super Computing
- Grid Computing
- Cloud Computing
- Cluster Computing
- GPGPU Computing
- Multicore Computing

A. Fundamentals

This work started with a simple question. Take two heterogeneous processing elements—how can they work together to best solve a specific problem? This question immediately raised many more. What happens if we add another element to make three? What about four? Is there something specific about the problems we want to solve that can be exploited to improve performance? How will the data partitioning and distribution impact the communication and execution times? How will the communication network affect the communication times? How will this affect execution times?

Regardless of the answers to these questions, two things are certain. It is desired for these elements to balance the computational load between themselves optimally, and to communicate data necessary for computations optimally. Unfortunately optimality is not always possible. These two tasks often turn out to be surprisingly difficult on heterogeneous platforms. Indeed solutions to problems that prove to be optimal on heterogeneous platforms are rare. Often some of the most simple tasks on homogeneous platforms turn out to be NP-Complete when attempted on heterogeneous ones [1]. Sometimes approximation algorithms are found, often heuristics and problem restrictions are resorted to, and in some cases not even theoretical results exist. In the latter case researchers have deemed it necessary to resort to experimental approaches for reproducibility and comparison studies. Tools to facilitate such have already been developed [2].

To answer our questions we choose as a testbed the problem of matrix matrix multiplication (MMM). Matrices are probably the most widely used mathematical objects in scientific computing and their multiplication (or problems reducible to MMM) appear very frequently in all facets of scientific computing [3]. Indeed, MMM is the prototype of tightly-coupled kernels with a high spatial locality that need to be implemented efficiently on distributed and heterogeneous platforms [4]. Moreover most data partitioning studies mainly deal with matrix partitioning.

Why would we want to extend MMM to heterogeneous platforms? As stated in [4], the future of computing platforms is best described by the keywords distributed and heterogeneous.

Our fundamental motivation stems from two sources. First, there exist many general heterogeneous MMM algorithms which work well for several, dozens, hundreds, or even thousands of nodes, but all currently known algorithms result in simple, perhaps naïve partitionings when applied to the architecture of a small number of interconnected heterogeneous computing entities (two, three, etc.). Examples of these methods are explored in [4]–[8]. As stated earlier we intentionally set out to investigate the particular case of a small number of computing entities to see what is happening in what is sometimes perceived to be a “degenerate” case. We point out that this case is not degenerate. For example, architectures from multicore chips up to grid platforms all regularly deal with small numbers of cores or clusters respectively, and algorithms running on such platforms need to be as efficient as possible. Despite its existence for at least 30 years, parallel MMM research has almost completely ignored this area. Early work is presented in [9], [10], and some early application results in [11]. A full thesis presenting the culmination of these works has recently been completed [12].

Second, we at the Heterogeneous Computing Laboratory\(^1\) are keenly aware of the parallel, distributed and especially the heterogeneous nature of computing platforms which are omnipresent in scientific computing, and that most parallel and distributed algorithms in existence today are designed for, and only work efficiently on homogeneous platforms. After discussing the aforementioned load balancing and communication issues, we will survey modern scientific computing platforms, and where parallelism, distribution and heterogeneity impact them.

1) Load Balancing: The issue of load balancing is well studied and well understood, but not without its challenges. For a detailed study see [13]. Neglecting the obvious such as the nature of the problem itself, failures and fluctuating capability due to other outside influences or factors, the issue can be reduced to a knowledge of the problem and the computing elements themselves. Suppose there is an amount of work \(W\) to do. If element \(A\) is capable of doing a work \(x\) in time \(t_1\) and element \(B\) is capable of doing a work \(y\) in time \(t_2\), the problem can be statically partitioned quite easily. We know that \(A\) works at a speed \(s_1 = \frac{x}{t_1}\) and \(B\) works at a speed \(s_2 = \frac{x}{t_2}\). If we normalize the speeds so that \(s_1 + s_2 = 1\), element \(A\) is to receive an amount of work equal to \(W \times s_1\) and element \(B\) is to receive an amount of work equal to \(W \times s_2\). Theoretically this would result in \(A\) and \(B\) finishing their work partitions in the same time, thus being optimal from a load balancing point of view.

For homogeneous computing elements such a problem scales well. In fact homogeneous systems are a standard platform for many supercomputers today (See Section I-B). Current supercomputers utilize thousands of homogeneous elements.

\(^{1}\text{hcl.ucd.ie}\)
elements (normally nodes or processors) working in parallel. For example, at the time of writing the 11th fastest computer on Earth is “Kraken”, a Cray XT5-HE System Model, with 16,488 AMD x86_64 Opteron Six Core processors running at 2,600 MHz (a total of 98,928 cores) at the National Institute for Computational Sciences/University of Tennessee in Tennessee, USA.2 Kraken is capable of 1,028,851 GFlops. For reference the laptop I am writing on now is an Intel Core Duo T5500 running at 1.66Ghz with 2GB memory, and has a peak performance of around 1Gflop, depending on the benchmark. An embarrassingly parallel problem—that is a problem that can be cut into any number of pieces as small as one wants with little or no communication between processes—could be theoretically balance load by partitioning the problem into 98,928 partitions and have each core solve one of the partitions. This would theoretically solve the whole problem in about one month of the time it would take my laptop. This is of course neglecting an multitude of factors such as data distribution and re-collection times, architectural differences, and vast memory and storage issues.

2) Communication: It is the communication aspects of data partitioning and distribution which make designing such algorithms difficult. Again ignoring faults, other non-related network traffic, etc., does the communication component of data partitioning affect the time it takes to solve the problem? How is it affected? what are these effects? Are there possibilities of deadlocks, race conditions and other parallel communication issues? Most fundamentally, two simple questions arise:

- How does the way we partition the data affect the execution time?
- What is the best way to partition the data so that we minimize the communication time, thus (hopefully) minimizing the execution time?

These questions can be quite difficult to answer—sometimes impossible to answer—but can have a significant effect on the overall execution time.

B. State-of-the-art Scientific Computing

1) The Top500: The website www.top500.org maintains a list of the fastest computers on Earth, updated bi-annually. At the time of writing, the fastest computer on Earth is “K computer”, a SPARC64 VIIIfx with 705,024 cores, 1,410,048 GB of memory and a custom “TOFU” network interconnect, at the RIKEN Advanced Institute for Computational Science (AICS) in Kobe, Japan. K computer has a performance of 10.51 petaflops (quadrillion floating-point operations per second). Most impressively, according to its website, K computer is (as of June 2011) “only half-built”.3

Of particular interest of this report however is the 3rd fastest computer, “Jaguar”, a Cray XT5-HE At Oak Ridge National Laboratory in Tennessee, USA.4 Jaguar is composed of two physical partitions (not to be confused with data partitions). It is these partitions and the fact that is a “small” number of them that are of particular interest in this report for reasons that will

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2www.nics.tennessee.edu/computing-resources/kraken
4www.nccs.gov/computing-resources/jaguar/
is expected to join soon. There is also a connection available which extends to Japan.

Grid’5000 has 1,529 nodes from Altix, Bull, Carri, Dell, HP, IBM and SUN. A total of 2,890 processors with a total of 5,946 cores from both AMD and Intel. Local network connections are Myrinet, Infiniband, and Ethernet. All Grid’5000 sites in France are connected with a 10Gb/s dark fibre link provided by RENATER (The French National Telecommunication Network for Technology Education and Research)\(^6\). Figure 1 Shows the backbones of the Renater Network which connects the sites of Grid’5000. The important aspect of this figure is the architecture of the network connecting the various sites across France, and the connections to sites outside France.

In keeping with the decentralized nature of grid computing, Grid’5000 is funded by INRIA (The French National Institute for Research in Computer Science and Control)\(^7\), CNRS (The French National Centre for Scientific Research)\(^8\), the universities of all sites, and some regional councils. This highlights another advantage of grids—the cost of building and maintaining them can be shared amongst many different bodies easily.

A total of 606 experiments are listed on the Grid’5000 website as completed or in progress. A tiny sample of experiment areas include genetic algorithms, task scheduling, middleware testing, modeling physical phenomena, and linguistic processing. As an example of Grid’5000 performance, the Nancy site has a 92 node Intel Xeon cluster which achieves 7,360 GFlops, and a 120 node Intel Xeon cluster, which achieves 1,536 GFlops. As the Nancy site is average (actually a little lower than average) in size for Grid’5000, we can roughly calculate the power by dividing Nancy’s power by the number of nodes at Nancy then multiplying by the total number of nodes in Grid’5000. This roughly equals 65,000 Gflops, or 36 times slower than Jaguar. This of course is just a rough Gflop count, and does not take any specific parameters into account.

3) Cloud Computing: Cloud computing can have a different definition, depending on the source. Generally it is a form of computing where not only the details of who, what and where a user’s computations are being carried out are hidden from the user, but perhaps even the knowledge and details of how to calculate the computations. The general idea is that a user supplies data to a client program or interface, along with either a full program or program description, and the client program then selects the proper, available servers—which can be anywhere on the globe—and gets the work carried out. When the computation is complete, the results are delivered back to the user. For some applications where there are “canned” solutions available, all the user will have to do is supply the data and specify what solution is desired. In effect all the user needs to do is specify the problem and the solution will be delivered. In most definitions the “cloud” is a metaphor for the Internet, as one could view cloud computing as the computational (number crunching) equivalent of the Internet we know today. All the user knows is to open a web browser, supply information (what they’re looking for) and the results come back. The user doesn’t know from who, or where, and doesn’t care—it just comes.

4) Cluster Computing: In 1982 Sun Microsystems was founded upon the motto “The Network is the Computer”. This philosophy paved the way for the popularization of cluster computing, largely through their software products. At the time computer operating systems were designed only to run on and exploit the power of stand-alone computers. Sun’s operating systems were revolutionary in that they were designed to harness the power of networks of computers.

Two or more such computers working together to achieve a common goal constitute a cluster. The topic itself, and much research focusing specifically on cluster computing as a pure subject is quite old, dating back 30 or more years. In fact such systems first started out as “the poor man’s supercomputer” in academic departments where researchers would leave jobs running perhaps all night instead of purchasing expensive supercomputer time \[^4\].

Cluster Computing has since become the dominant architecture for all scientific computing, including top500 supercomputers. Figure 2 shows the architectures of top500 computers from 1993 to 2010. In 1993 no top500 computers were clusters. They were MPPs, constellations, SMPs, and others—even single processor vector machines. It wasn’t until the late 1990s that the first clusters joined the top500, but

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\(^{6}\)www.renater.fr  
\(^{7}\)www.inria.fr  
\(^{8}\)www.cnrs.fr
their popularity exploded, largely due to low cost and simple maintenance combined with great power. By 2007 about 80% of top500 machines were clusters and the number has grown to the point today where almost all top500 machines are clusters.

Let us demonstrate the prevalence and importance of clusters in the context of this section. Although not comprehensive in terms of state-of-the art scientific computing, this does provide a good overview:

- Top500 - Almost all computers in the top500 are based on cluster platforms
- Grid Computing - All grids are geographically distributed clusters or clusters of clusters.
- Cloud computing - As the name implies, how clusters fit in is slightly “fuzzy” but surely any cloud of even a moderate size would include clusters.
- GPGPU (General-Purpose computing on Graphics Processing Units) is done on clusters of GPU machines.
- Multicore computing physically exists at the processor (single machine) level, but it is clusters of multicore microprocessors that make up many top500 machines and grids.

Thus we have seen quite simply that cluster computing is actually the foundation of all other types of computing discussed here.

5) GPGPU (General-Purpose computing on Graphics Processing Units): Another exciting area of high performance computing in which interest is gathering great pace is using Graphics Processing Units (GPUs) alongside traditional CPUs. Traditionally GPUs are used to take the burden of, and accelerate the performance of, rendering graphics (today often 3D graphics) to a display device. To this end, GPUs have evolved to become in most cases quite specialized in the operations necessary to do so, namely linear algebra operations. This makes them quite unintentionally well suited for many high performance scientific applications, as many of these rely heavily or exclusively on linear algebra operations. Examples of problems which have been explored with this approach include oil exploration, image processing and the pricing of stock options [17].

Beyond the confines of linear algebra, interest has also been gathering in so called General Purpose Computing on Graphics Processing Units or (GPGPU). This seeks to harness the computing power of GPUs to solve increasingly general problems. Recently nVidia and ATI (by far the two largest GPU manufacturers) have joined with Stanford University to build a dedicated GPU-based client for the Folding@home project which is one of the largest distributed computing projects in the world.

Briefly, Folding@home\(^9\) harnesses (mostly) the unused CPU cycles of home computers across the globe to perform protein folding simulations and other molecular dynamics problems. A user downloads a client application and then when the user’s computer is idle, packets of data from a server at Stanford are downloaded, and processed by the client program. Once the data has been processed using the client, the results are sent back to the server and the process repeated. At the time of writing the total number of active CPUs on the project is 286,723 with a total participation of 5,514,891 processing units, 343,843 of which are GPUs, and 1,003,463 are PlayStation 3 consoles running the Cell Processor.\(^10\) The total power of the Folding@home project is estimated to be 2,958,000 Gflops, theoretically 1.27 times faster than Jaguar.

We must keep in mind however that if a problem with the complexity, memory, and data dependencies of those being solved on Jaguar was given to the Folding@home network, it would be incredibly—actually uselessly—slow, and very, very difficult to program.

Nonetheless, Folding@home is an example of extreme heterogeneity. Of course, mixed in those millions of computers are Linux, MAC, and Windows machines as well. The power of such a distributed, heterogeneous “system” can only be effectively harnessed due to the nature of the problems that are being solved. Although extremely large, the problems are embarrassingly parallel. In this case the key is that there are no data dependencies. No user computer needs information from, or needs to send information to, any other user computer. Further, the order in which data is sent back to the server does not matter. As long as all of the results eventually come back, they can be reconstructed back to the original order. If some results don’t come back (which is inevitable), the data necessary to get the results are simply farmed out to another active user. Nonetheless we see a system with the power of a supercomputer, using a heterogeneous hierarchy at every level—client/server, system, processor and core.

For another similar project, see SETI@home\(^11\), which distributes data from the Aricebo radio telescope in Puerto Rico to home users’ computers, which then analyze the data for signs of extra-terrestrial life.

To wrap up the discussion on heterogeneity and GPGPU, nVidia has announced a new configuration using their video cards. Their PhysX physics engine can now be used on two heterogeneous nVidia GPUs in one machine.\(^12\) A physics engine is software that computes and replicates the actual physics of events in real-time to make computer graphics more realistic such as shattering glass, trees bending in the wind.

\(^9\)http://folding.stanford.edu
\(^10\)fah-web.stanford.edu/cgi-bin/main.py?qtype=osstats
\(^11\)setiathome.ssl.berkeley.edu
\(^12\)www.nvidia.com/object/physx\_faq.html\#q4
and flowing water. In this configuration the more powerful GPU renders graphics while the other is completely dedicated to running the PhysX engine.

6) Multicore/Manycore Computing: At a much lower level, multicore technology has become mainstream for most computing platforms from home through high-performance. Multicore processors have more than one core, which is the element of a processor that performs the reading and executing of an instruction. Originally processors were designed with a single core, however a multicore processor can be considered to be a single integrated circuit with more than one core, and can thus execute more than one instruction at any given time. Embarrassingly parallel problems can approach a speedup equal to the number of cores, but a number of limiting factors including the problem itself normally limits such realization. Currently most multicore processors have two, four, six or eight cores. The number of cores possible is limited however, and is generally accepted to be in the dozens. More cores would require more sophisticated communication systems to implement and are referred to as manycore processors.

The Cell processor is a joint venture between Sony Corporation, Sony Computer Entertainment, Toshiba, and IBM (STI) and has nine cores. One core is referred to as the “Power Processor Element” or PPE, and acts as the controller of the other eight “Synergistic Processing Elements” or SPEs. See Figure 3 for a basic schematic of the processing elements of the Cell processor. The PPE can execute two instructions per clock cycle due to its multithreading capability. It has a 32KB instruction and 32KB L1 cache, and a 512KB L2 cache. The PPE performance is 6.2 GFlops at 3.2GHz. Each SPE has 256KB embedded SRAM and can support up to 4GB of local memory. Each SPE is capable of a theoretical 20.8 GFlops at 3.2GHz. Recently IBM has shown that the SPEs can reach 98% of their theoretical peak performance using optimized parallel matrix matrix multiplication.\(^\text{13}\) The elements are connected by an Element Interconnect Bus (EIB), with a theoretical peak bandwidth of 204.8GB/s.

The Sony PlayStation 3 is an example of the Cell processor at work. To increase fabrication yields, Sony limited the number of operational SPEs to seven. One of the SPEs is reserved for operating system tasks, leaving the PPE and six SPEs for game programmers to use. Clearly this has utilized the Cell to create a more heterogeneous system. This is exemplary of a truly heterogeneous system in practice—functionality can be arranged as desired, and needed.

The Cell processor is used in the IBM “Roadrunner” supercomputer, which is a hybrid of AMD Opteron and Cell processors and is the third fastest computer on Earth (formerly number 1) at 13,752,776 GFlops. The PlayStation 3 “Gravity Grid” at the University of Massachusetts at Dartmouth Physics Department is a cluster of sixteen Playstation 3 consoles used to perform numerical simulations in the areas of black hole physics such as binary black hole coalescence using perturbation theory.\(^\text{14}\)

Clearly the Cell processor is an example of parallel heterogeneous computing at a very low-level, with very diverse applications, and introduces a hierarchy with the PPE controlling the SPE’s, while also maintaining some number crunching abilities itself.

The future of heterogeneous multicore architectures is expanding rapidly. Recently, a research team at the University of Glasgow has announced what is effectively a 1000 core processor, although it differs from a traditional multicore chip as it is based on FPGA technology, which could easily lend itself to heterogeneous use. Second, the release of the first multicore mobile phones has been announced. The natural need for heterogeneity in such platforms is discussed in [18].

Recently, heterogeneous manycore architectures have proven to be a viable option for the future of HPC [19], and heterogeneous execution models have been devised [20]. As mentioned in the abstract, and discussed in [18], data partitioning on multicore architectures is necessary for the implementation of useful parallel algorithms on these platforms. Most recently, in [21], the authors demonstrate examples of just that.

C. Heterogeneity

We have seen that heterogeneity and hierarchy have infiltrated every aspect of computing from supercomputers to GPUs, Cloud Computing to individual processors and cores. We have also seen that in many, many ways all of these technologies are interwoven and can join to form hybrid entities themselves.

To conclude it is fitting to state that homogeneity (even if explicitly designed) can be very difficult and expensive to maintain, and easy to break [22]. Any distributed memory system will become heterogeneous if it allows several independent users to simultaneously run applications on the same system at the same time. In this case different processors will inevitably have different workloads at any given time and provide different performance levels at different times. The end result would be different performances for different runs of the same application.

Additionally, network usage and load, and therefore communication times will also be varied with the end result being

\(^{13}\)www.ibm.com/developerworks/power/library/pa-cellperf/

\(^{14}\)arxiv.org/abs/1006.0663
different communication times for a given application, further interfering with the delivery of consistent performance for the same application being run more than once.

Component failure, aging, and replacement can all also impact homogeneity. Are identical replacement components available? Are they costly? Do all components deliver uniform and consistent performance with age? Even if these problems are managed, eventually when upgrading or replacement time comes, all upgrades and replacements must be made at the same time to maintain homogeneity.

We see now that heterogeneity is the natural state of parallel and distributed systems. Most interestingly, vendors are now starting to intentionally design and construct systems and platforms for high performance scientific computing which are heterogeneous from the outset. This is perhaps a natural progression as specialized hardware and software aimed at one particular class of problem is desired over more general-purpose approaches that yield poor performance.

D. Objectives

The main goal of this report is to present, validate, and experimentally demonstrate a new partitioning algorithm for high performance scientific computing on parallel hierarchal heterogeneous computing platforms. This partitioning could theoretically be deployed on any heterogeneous architecture including all those discussed in Section I-B. It will also be shown that this partitioning can serve as the basis for other new partitionings. The following is a list of other goals that will and must be realized along the way. First the state-of-the-art will be reviewed, before the underlying mathematical principles of this new partitioning are explored. For the cases in which it applies the partitioning will be discussed and it’s optimality proven. A hybrid algorithm will be discussed which is designed to be optimal in all cases for certain problem domains. The construction of a heterogeneous cluster hand-designed specifically for problems discussed in this report will be detailed. The partitioning will be compared to the state-of-the-art and both its benefits and deficits discussed. The partitioning will be modelled, simulated, and then experimentally verified before being shown to be beneficial to application areas indicative of those widely in use today. Then, future directions of research will be presented.

Finally, as stated, most heterogeneous algorithms and partitionings are designed by modifying existing homogeneous ones. The ultimate goal of this report is to demonstrate the concept that unintuitive, non-traditional algorithms and partitionings, designed with heterogeneity in mind from the start, can result in better—and optimal—algorithms and partitionings for high performance computing on heterogeneous platforms.

E. Outline

Section II: Background and Related Work
In this section existing research in the area of heterogeneous parallel data partitioning and matrix matrix multiplication is explored. The state-of-the-art is clearly described and the benefits and drawbacks of current techniques are detailed.

This section describes the design and construction of a heterogeneous cluster specifically for the simulation and testing of heterogeneous algorithms and partitionings. The cluster is unique in its ability to be configured in network parameters and topology which allows for testing on any number of heterogeneous scenarios.

Section III: Partitioning a Matrix in Two – Geometric Approaches
This section presents work on extending partitionings to more than three and to non-square matrices. The Square-Corner Partitioning is shown to be optimal in most cases, and a hybrid partitioning is proposed which would be optimal in all cases.

Section IV: The Square-Corner Partitioning
This section defines the Square-Corner Partitioning and its application to matrix matrix multiplication. The optimality of the partitioning as well as other benefits such as overlapping computation and communication are explored. Experimental results are presented, first on two processors, then on small groups of clusters, then on two larger clusters.

Section V: The Square-Corner Partitioning on Three Clusters
In this section the Square-Corner Partitioning is extended to three clusters. Both topologies possible (fully-connected and star) are explored. Experimental results are given for simulations on three processors and three clusters. Results of overlapping computation and communication are also explored.

Section VI: Applications: Max-Plus Algebra and Discrete Event Simulation on Parallel Hierarchal Heterogeneous Platforms
This section presents the results of applying the Square-Corner Partitioning on Max-Plus Algebra operations and a Discrete Event Simulation Application.

Section VII: Moving Ahead – Multiple Partitions and Rectangular Matrices
This section presents work on extending partitionings to more than three and to non-square matrices. The Square-Corner Partitioning is shown to be useful for the multiplication of rectangular matrices in particular.

Section VIII: Conclusions and Future Work
In this section overall conclusions of this work are drawn, and indications of exciting areas of future work are detailed.
II. BACKGROUND AND RELATED WORK

In 1997, van de Geijn and Watts noted: “It seems somewhat strange to be writing a paper on parallel matrix multiplication almost two decades after commercial parallel systems first became available. One would think that by now we would be able to manage such an apparently straightforward task with simple, highly efficient implementations. Nonetheless, we appear to have gained a new insight into this problem” [23].

It is now 2011 and researchers across the globe are still working with great ferocity on parallel matrix multiplication algorithms! This section presents a summary of parallel matrix multiplication, first and briefly on homogeneous algorithms, then heterogeneous algorithms. We start with the homogeneous case because most heterogeneous algorithms are modifications of their homogeneous counterparts. We will of course end with the current state-of-the-art in heterogeneous parallel MMM algorithms.

In order to discuss these algorithms however, we must discuss data distribution and therefore data partitioning, which is the focus of this report. The partitioning of data directly affects the communication between processing elements. These communications may be over a super-fast bus between cores or long-distance copper or fibre networks, but either way it is typically communications that are an order of magnitude or more slower than processing speed and therefore the most significant bottleneck in parallel and distributed algorithms.

There is a common thread ran through the motivation in Section I-B, from cloud computing with theoretically millions or more machines at work, through supercomputers with hundreds of thousands of processors, down to multicore chips on single machines. This thread is heterogeneity. In fact there was another common thread, distribution, which is due to necessary physical separation of computing elements. Be they two computers on opposite sides of the Earth, or two cores separated by hundredths of a centimeter, computing elements need to be physically separated and therefore must communicate to work together.

This brings up an interesting question—Why must processing elements be physically separated? There are many answers to this question, the main reasons being:

(i) **Heat.** Too many processing elements in too small a space creates too much heat which increases cooling costs in the best case, and in the worst case leads to component failure.

(ii) **Cost.** Along with cooling cost, communication hardware costs are perhaps the largest cost factors. The ultrafast communication buses between cores and processors and main-memory are simply too expensive to scale up. In fact such devices only barely scale out of the micro and into the macro scales. It is much, much cheaper to connect machines with commodity, off-the-shelf communication hardware, than two processors with an ultra-fast motherboard bus that is metres or more long.

(iii) **Convenience.** For economical, social and other reasons, it makes sense to distribute computing resources geographically. In the case of the Folding@home project introduced in the motivation, the utilized resources were already geographically distributed, and then exploited. We also saw that there are computing resources, particularly grids (for example Grid’5000 [16]), that are intentionally built to be geographically distributed. This is not done due to pure physical necessity, but to make cost, maintenance, upgrading and logistics more convenient.

(iv) **Modularity and Reliability.** Closely related to convenience is the modularity and reliability of the system itself. If a supercomputer was just a single, massive processor (if physically feasible), what would happen if it or a crucial component failed? Everything would grind to a halt. What happens if a chip, node, or even an entire cluster or even in the extreme an entire site in Grid’5000 goes down? All other processors, nodes, clusters, and sites go merrily on with their business. This gets even better if the middleware can handle fault tolerance. The user may not realize that a component failed, other than a possibly longer execution time, but not necessarily, and what counts most is the results will still be correct.

(v) “**That’s just the way it is**” or “**That’s just the way things evolve**”. Everything from beings with exoskeletons to animals with internal skeletons, from dinghies to the most massive cargo ships, from subatomic particles to the most massive of stars have a physical size limit per entity. At some point the only way to generate more beings, carrying capacity, or energy, is to make more of them. More things means more space, which necessitates physical distribution.

There are certainly more parameters, especially when individual cases are examined. Perhaps one more question could be asked, particularly in reference to (i) and (ii) above. Why can’t a chip be manufactured which is just one big chip? Let’s ignore heat, cost, reliability and other obvious answers and instead of answering the question directly just render the question itself a moot point. If it were possible to do so we would still be dealing with communications. Communications between individual registers or even in the extreme, transistors on the chip itself, still need to be done optimally or at least efficiently. Again, as in Section I-A we see that communication between different entities is an inherent fact of computing, no matter what scale we are dealing with and no matter how we look at or abstract the issue.

A. Parallel Computing for Matrix Matrix Multiplication

Currently parallel computing is undergoing a paradigm shift. It is spreading from supercomputer centers which have been established utilizing specialized, often custom-built and terribly expensive computers which are used and programmed by highly trained and specialized people to clusters of off-the-shelf commodity workstations that (with the proper libraries and some skill) can be used by “ordinary” people. Here, ordinary is taken to mean people whose primary profession need not be programming supercomputers. Such clusters have already pervaded academia and industry, but promise to do so further, and are now becoming accessible to and “toys” of home users, who desire to use them. Indeed these clusters remain the poor man’s supercomputer [24] as discussed in the
motivation. Cloud Computing promises to carry this concept even further, with additional abstraction, and less expertise needed by the user.

From this point forward we will not consider heterogeneity (or homogeneity for that matter) and communication to be exclusive. From one follows the other. Any parallel architecture (homogeneous or heterogeneous) without some communication somewhere is useless. For this reason we will focus discussion on parallel computing in general at first. We will start with the more simple (and restricted) case, homogeneous parallel computing.

This report exclusively addresses the linear algebra kernel of Matrix-Matrix Multiplication (MMM) as the prototype problem for High Performance Parallel Computing on Heterogeneous Networks (with the exception of some application areas explored later in Section VI). This is a common and justifiable decision as matrices are probably the most widely used mathematical objects in scientific computing [8]. Further to that, MMM is the prototype for a group of tightly coupled kernels with a high special locality that should be implemented efficiently on parallel platforms [both homogeneous and heterogeneous] [4]. Throughout this report, if only one matrix is being discussed, it may be thought of as the product $C$ of two other matrices $A$ and $B$, such that $C = A \times B$. In these cases, $A$ and $B$ are partitioned identically to $C$. This has become a standard in the field.

B. Data Partitioning for Matrix Matrix Multiplication on Homogeneous Networks

The problem of matrix partitioning on homogeneous networks has been well studied. It has perhaps been studied to exhaustion with the exception of the inclusion of application specific issues, or particular hardware/software considerations. In other words the theoretical underpinnings have been established and are very unlikely to undergo a significant change. For more see [25].

Let us start then with homogeneous matrix partitioning for three reasons:

1) Because it is well established

2) Because most heterogeneous algorithms are designed either from, or at least with, their homogeneous counterparts in mind

3) It is often the homogeneous counterparts that heterogeneous algorithms are compared to, particularly to address their effectiveness or lack thereof [26].

When partitioning a matrix for distribution between homogeneous processors\footnote{We begin by talking about partitioning and distribution among individual processors and later will scale this up to individual clusters. Entity will sometimes be used to refer to any unit capable of processing be it a core, processor, cluster, etc.}, the problem of load balancing is easy, as all processors have equal speed, and therefore each partition will have equal area. Thus the issue quickly turns to minimizing communications. The simplest homogeneous partitioning of a matrix is in one dimension, with the matrix partitioned into either rows or columns of equal area as in Figure 4. The other way to accomplish a homogeneous partitioning is to use a two-dimensional partitioning, which results in a grid of partitions as in Figure 5.

Let us start with the two-dimensional case. We have a matrix multiplication $C = A \times B$ and for simplicity we make each a square $n \times n$ matrix. Assume we have $p$ homogeneous processors $P_1, P_2, \ldots, P_p$. Again for simplicity let us assume that the processors are arranged in a grid of size $p_1 \times p_2 = p$ such that $p_1 = p_2$. In this case the processors and the partitions of the matrix overlap each other exactly such that at each step $k$,

- Each processor $P_{i,k}$, $i \in \ldots, p_1$ broadcasts horizontally $a_{i,k}$ to processors $P_{i,*}$
- Each processor $P_{k,j}$, $j \in \ldots, p_2$ broadcasts vertically $b_{k,j}$ to processors $P_{*,j}$

This allows each processor $P_{i,j}$ to update its portion of $C$, using $c_{i,j} = c_{i,j} + a_{i,k} \times b_{k,j}$. In other words, at each step of
the algorithm each processor does the following:

- Each processor broadcasts the part of the pivot column which it owns horizontally to the processors in the same processor row which the processor resides in.
- Each processor broadcasts the part of the pivot row which it owns vertically to the processors in the same processor column which the processor resides in.

This is shown in Figure 6.

The popular SCaLAPACK library uses this technique, but uses a blocked version [27]. In this case, each matrix element (say $C_{i,j}, A_{i,j}$, and $B_{i,j}$) is a square $r \times r$ block. For each processing entity there will be an optimal value of $r$, depending on memory and other architecture-specific details. Usually the number of blocks $\lfloor (n/r) \rfloor \times \lfloor (n/r) \rfloor$ is greater than the number of processors $p_1 \times p_2$. In this case the blocks are distributed in a cyclic fashion so that each processor is responsible for updating several blocks of the $C$ matrix at each step $k$.

It is worth noting at this point that the total volume of communication (TVC) of the calculation described above is proportional to the sum of the half perimeters (SHP) of each partition. This can be viewed rather simply; at each step, each processor responsible for a square of $x \times x$ elements receives $x$ elements from a row-mate and $x$ elements from a column-mate for a total of $2x$ elements. Since the partitions are all equal in size and dimension (if $\sqrt{p}$ evenly divides $n$), the same will be true for all processors. Thus at each step each processor is receiving a number of elements proportional to $2 \times x$, the sum of each partition’s half perimeter.

It is easy to show that the two-dimensional partitioning has a lower TVC than the one-dimensional partitioning. Given a fixed area, the rectangle covering that area and having the smallest perimeter is a rectangle that is square, and the fact that any other partitioning strategy would force at least one partition to be non-square, any other partitioning strategy (including the one-dimensional partitioning described above) would result in a greater SHP, and therefore a greater TVC.

There are other parallel algorithms for MMM, such as:

- Cannon’s algorithm [28]
- DNS [25]
- one-dimensional and two-dimensional Systolic [29]
- Broadcast Multiply Roll [30]
- the Transpose Algorithm [31]
- SUMMA (Scalable Universal Matrix Multiplication Algorithm) [23], which is used in PBLAS (the Parallel Basic Linear Algebra Subprograms) library [32]

Each has its advantages and disadvantages and a discussion of each is beyond the scope of this report. They are mentioned for completeness.

C. Data Partitioning for Matrix Matrix Multiplication on Heterogeneous Networks

Now let us assume a heterogeneous network. We have $p$ heterogeneous processors $P_1, P_2, \ldots, P_p$, each free to run at a speed unique to all other processors. We will express these speeds relatively as $s_1, s_2, \ldots, s_p$. Similar to the homogeneous algorithm above at each time step $k$, there will be a pivot row broadcast vertically and a pivot column broadcast horizontally. These rows and columns can be either made of individual matrix elements or blocks of elements as described above. If we are discussing blocks, they will remain square for efficiency on a processor-local level. We will now see how a modification of the homogeneous algorithm above can lead to heterogeneous ones.

The heterogeneity of processors means that we cannot necessarily partition the matrix into squares. We will generalize and partition the matrix into non-overlapping rectangles. Similar to the homogeneous algorithm, data should be partitioned so that the area of each rectangular partition is proportional to the speed of the processor who owns it. From a load-balancing point of view it is only the area of the rectangles that matter. The dimensions of each rectangle are free for us to choose. Figure 7 shows a heterogeneous partitioning of nine rectangles.

The difficult question is this: What dimensions should each rectangle have to minimize the total inter-partition (and therefore inter-cluster, if each partition were owned by a cluster)
volume of communication? Actually the word difficult turns out to be an understatement. This question (when formally defined) turns out to be NP-complete \[5\]. There is no known polynomial time solution to this question. In other words, for even modestly sized problems, unreasonable (or impossible) lengths of time would be needed to achieve an optimal solution. We must therefore resort to approximation algorithms or heuristics. Generally these begin by imposing a restriction or restrictions on the proposed solution to allow it to run in polynomial time. The next three subsections will explore the state-of-the-art in attempts to do so.

Before we do it is worth mentioning (again for completeness) that we are and will be discussing static partitionings only. Static partitionings are determined based on input data, and after that the partitioning does not change throughout the course of the program. A dynamic partitioning is one that does (more properly has the ability to) change the initial partitioning or restrictions on the proposed solution to allow it to run in polynomial time. The next three subsections will explore the

D. Restricting the General Approach: A Column Based Partitioning

In \[4\] the authors state the general matrix partitioning problem:

- Given \( p \) computing elements \( P_1, P_2, \ldots, P_p \), the relative speed of which is characterized by a positive constant \( S_i \), where \( \sum_{i=1}^{p} S_i = 1 \)

- Partition a unit square into \( p \) rectangles so that
  - There is a one to one mapping of elements to rectangles
  - The area of the rectangle allocated to element \( P_i \) is equal to \( S_i \) where \( i \in \{1, \ldots, p\} \).
  - The partitioning minimizes \( \sum_{i=1}^{p} (w_i + h_i) \), where \( w_i \) is the width of the rectangle and \( h_i \) is the height of the rectangle assigned to element \( P_i \).

Partitioning the unit square into rectangular partitions with areas proportional to the speed of the processing elements mapped to them is aimed at balancing the load of the work done by each processing element. As a rule there will be more than one partitioning satisfying this condition.

Minimizing the sum of half-perimeters of the partitions, \( \sum_{i=1}^{p} (w_i + h_i) \) is aimed at minimizing the total volume of communication between the elements. This is possible because with the problem of MMM, at each step, each processing element that does not own the pivot row and column receives an amount of data proportional to the half-perimeter of the rectangular partition it owns. Therefore the amount of data communicated at each step between all processing elements will be proportional to the sum of the half-perimeters of all partitions, \( \sum_{i=1}^{p} (w_i + h_i) \), less the sum of the heights of the partitions owning the pivot column, (one in the case of the unit square), and less the sum of the widths of the partitions owning the pivot row (also one for the unit square). Thus at each step the total data communicated will be \( \sum_{i=1}^{p} (w_i + h_i) - 2 \).

Because the total amount of data communicated between the processing elements is the same at each step of the algorithm, the total amount of data communicated during the execution of the algorithm will also be proportional to \( \sum_{i=1}^{p} (w_i + h_i) - 2 \).

Therefore minimization of \( \sum_{i=1}^{p} (w_i + h_i) - 2 \) will minimize the total volume of communication between all partitions. Clearly any solution minimizing \( \sum_{i=1}^{p} (w_i + h_i) \) will also minimize \( \sum_{i=1}^{p} (w_i + h_i) - 2 \).

The authors of \[4\] have shown that this general partitioning problem is NP-Complete and therefore heuristics must be resorted to in order to find optimal solutions. Such a heuristic is presented by \[4\] which restricts the rectangles of the partitioning to forming columns such as in Figure 8. The algorithm follows:

Algorithm 2.1 \[4\]: Optimal column-based partitioning of a unit square between \( p \) heterogeneous processors:

- First, the processing elements are re-indexed in the non-increasing order of their speeds, \( s_1 \geq s_2 \geq \ldots \geq s_p \). The algorithm only considers partitionings where the \( i \)-th rectangle in the linear column-wise order is mapped to processor \( P_i, i \in \{1, \ldots, p\} \).
- The algorithm iteratively builds the optimal \( c \) column partitioning \( \beta(c, q) \) of a rectangle of height 1 and width \( q \), \( \sum_{j=1}^{q} s_j \) for all \( c \in \{1, \ldots, p\} \) and \( q \in \{c, \ldots, p\} \):
  - \( \beta(1, q) \) is trivial.
  - For \( c > 1 \), \( \beta(c, q) \) is built in two steps:
    * First, \( (q - c + 1) \) candidate partitionings \( \{\beta_j(c, q)\}(j \in \{1, \ldots, q-c+1\}) \) are constructed such that \( \beta_j(c, q) \) is obtained by combining the partitioning \( \beta(c-1, q-j) \) with the straightforward partitioning of the last column (the column number \( c \)) of the width \( \sum_{j=1}^{q} s_j \) into \( j \) rectangles of the corresponding areas \( s_{q-j+1} \geq s_{q-j+2} \geq \ldots \geq s_q \).
    * Then, \( \beta(c, q) = \beta_k(c, q) \) where \( \beta_k(c, q) \in \{\beta_j(c, q)\}_{j=1}^{q-c+1} \) and minimizes the sum of the half-perimeters of the rectangles.
- The optimal column-based partitioning will be a partitioning from the set \( \{\beta(c, P)\}_{c=1}^{p} \) that minimizes the sum
of half-perimeters of rectangles.
Algorithm 2.1 runs in $O(p^3)$ time.

E. A More Restricted Column-Based Approach

[33], further restrict the column-based geometrical partitioning by assuming that the processing elements are already arranged in a set of columns (i.e. assuming that the number of columns $c$ in the partitioning and the mappings of rectangles in each column to the processors are given). The algorithm is as follows.

**Algorithm 2.2:** [33]: An optimal partitioning of a unit square between $p$ heterogeneous processors arranged into $c$ columns, each of which is made of $r_j$ processors where $j \in \{1, \ldots, c\}$:
- Let the relative speed of the $i$-th processor from the $j$-th column, $P_{i,j}$ be $s_{i,j}$ where $\sum_{j=1}^{c} \sum_{i=1}^{r_j} s_{i,j} = 1$.
- First, partition the unit square into $c$ vertical rectangular slices so that the width of the $j$-th slice $w_j = \sum_{i=1}^{r_j} s_{i,j}$.
  - This partitioning makes the area of each vertical slice proportional to the sum of speeds of the processors in the corresponding column.
- Second, each vertical slice is partitioned independently into rectangles in proportion to the speeds of the processors in the corresponding column.
Algorithm 2.2 runs in linear time. Figure 9 shows this for a $3 \times 3$ processor grid.

F. A Grid Based Approach

[8] describes a partitioning which imposes a further restriction on the column-based approaches. The restriction is that the partitionings must form a grid as in Figure 10. This can be viewed from another approach. The grid based partitioning is one which partitions the unit square into rectangles so that there exist $p$ and $q$ such that any vertical line crossing the square will intersect exactly $p$ rectangles and any horizontal line crossing the square will intersect exactly $q$ rectangles, regardless of where these lines cross the unit square.

It is proposed and proven in [8] that in the case of a unit square partitioned into a grid of $c$ columns, each of which is partitioned into $r$ rows, the sum of half-perimeters of all partitions will be equal to $(r+c)$. The corollaries which precipitate from this is that the optimal grid based partitioning is one which minimizes $r+c$, and that the sum of half-perimeters of the optimal grid-based partitioning does not depend on the mapping of the processors onto the nodes of the grid. The algorithm for the optimal grid-based partitioning follows.

**Algorithm 2.3:** [8]: Optimal grid-based partitioning of a unit square between $p$ heterogeneous processors:
- Find the optimal shape $r \times c$ of the processor grid such that $p = r \times c$ and $(r+c)$ is minimized.
- Map the processors onto the nodes of the grid.
- Apply Algorithm 2.2 of the optimal partitioning of the unit square to this $r \times c$ arrangement of the $p$ heterogeneous processors.

Step one finds the optimal shape of the processor grid that minimizes the sum of half-perimeters of any grid based partitioning for any mapping of the processors onto the nodes of the grid. Step two simply does the mapping (by any means).
Fig. 11. An optional grid based partitioning returned by Algorithm 2.3. Step three then finds one such partitioning where the area of each rectangle is proportional to the speed of the processor owning it. It is noted that the solution is always column-based due to the nature of Algorithm 2.2. The first step of Algorithm 2.3 is described by Algorithm 2.4.

Algorithm 2.4 [8]: Find \( r \) and \( c \) such that \( p = r \times c \) and \((r + c)\) is minimal:

\[
\begin{align*}
  r &= \lfloor \sqrt{p} \rfloor \\
  \text{while} & \quad (r > 1) \\
  \text{if} & \quad ((p \mod r) == 0) \\
  & \quad \text{goto} \quad \text{stop}; \\
  \text{else} & \\
  r & \quad \text{--} \\
  \text{stop:} & \quad c = p/r 
\end{align*}
\]

Figure 11 shows an optimal grid based partitioning returned by algorithm 2.3.

In [8] the correctness of these algorithms is proven and the complexity of Algorithm 2.4 is shown to be \( O(p^{3/2}) \). Experimental results are also given which demonstrate the effectiveness of the grid based approach.

G. Cartesian Partitionings

The grid-based partitioning strategy is not the most restrictive partitioning problem that has been addressed. A Cartesian partitioning can be obtained from a column-based partitioning by imposing an additional restriction; namely that the rectangular partitionings also make up rows as seen in Figure 12. This results in any given partition having no more than four direct neighbors (up, down, left, right).

Due to the additional restriction imposed by a Cartesian partitioning an optimal partitioning may not be achievable. The load between partitionings may not be perfectly balanced for some combinations of relative computing element speeds. This renders relative speeds unusable and the problem should be reformulated in terms of absolute speeds. The Cartesian partitioning problem can be formulated as follows:

- Given \( p \) processors, the speed of each of which is characterized by a given positive constant, find a Cartesian partitioning of a unit square such that:
  - There is a one to one mapping of partitions to computing elements.
  - The partitioning minimizes \( \max_{i,j} \{ h_i \times w_j \} \), where \( h_i \) is the height of partitions in the \( i \)-th row, \( w_j \) is the width of partitions in the \( j \)-th column, \( s_{i,j} \) is the speed of the computing element owning the \( j \)-th partition in the \( i \)-th row, where \( i \in \{1, \ldots, r\} \), \( j \in \{1, \ldots, c\} \), and \( p = r \times c \).

To the author’s knowledge the Cartesian problem has not been studied as stated above in general form. An algorithm to solve this problem has to find an optimal shape \( r \times c \) of the computing element grid, the mapping of the elements onto the grid, and the size of the partitions allocated to the elements. Simplified versions of the problem have been studied however [6], [34]. If the shape \( r \times c \) of the partitioning is given the problem is proven to be NP-Complete [34]. In addition it is not known if given both the shape \( r \times c \) of the grid and the mapping of computing elements onto the grid are given, there exists a polynomial time solution.

An approximate algorithm of the simplified Cartesian problem where the shape \( r \times c \) is given in Algorithm 2.5.

Algorithm 2.5 [34]: Find a Cartesian partitioning of a unit square between \( p \) processors of the given shape \( p = r \times c \):

- **Step 1.** Arrange the processors so that if linearly ordered row-wise, beginning from the top left corner, they will
go in a nonincreasing order of their speeds.

• **Step 2.** For the processor arrangement, apply a known algorithm to find an approximate solution, \( \{ h_i \}_{i=1}^r, \{ w_j \}_{j=1}^c \).

• **Step 3.** Calculate the areas \( h_i, w_i \) of the rectangles of the partitioning.

• **Step 4.** Rearrange the processors so that \( \forall i, j, k, l : s_{ij} \geq s_{kl} \iff h_i \times w_j \geq h_k \times w_l \).

• **Step 5.** If Step 4 does not change the arrangement of the processors then return the current partitioning and stop the procedure else go to Step2.

### H. Conclusion

In this section we saw that communication is unavoidable in parallel computing. Normally this is thought of in terms of computer networks: wires, switches, routers, etc. However it must be realized that communication occurs even at lower levels than two geographically distributed clusters. It happens between machines in the same rack, and even between cores on a single processor.

We then examined how the partitioning of data, specifically in the case of matrix matrix multiplication, can affect the amount of data that needs to be communicated. After briefly looking at elementary one and two-dimensional partitions, several state-of-the-art methods were explored including general two-dimensional cases, more restricted column-based approaches, even more restricted strategies such as grid based, and finally very restricted two-dimensional approaches in cartesian cases. All of these partitioning strategies have two common threads. They all balance load and they all seek to minimize the sum of communication between partitions, normally through imposing restrictions. However this is not a hard rule, as in some cases relaxing restrictions can lead to better solutions.
III. Partitioning a Matrix in Two: Geometric Approaches

Section II concluded with a continuing thread which was common to a number of partitionings that improved performance by introducing restrictions to the general partitioning problem. It is however possible in some cases to improve performance by relaxing restrictions. In this section we explore one such case. That case is partitioning a matrix in two. The choice of two partitionings is not a restriction however, as future sections will show that this approach is not restricted to just two partitions. It is how the partitions themselves are formed that is the relaxation of restriction.

The initial motivation which led to this work stems from two sources. First, there are many general heterogeneous matrix partitioning algorithms which work well for several, dozens, hundreds, or even thousands of computing entities. We will see that all result in a simple, and non-optimal partitioning when applied to architectures of small numbers of computing entities—in the case of this section, two. As stated earlier we intentionally set out to investigate the case of a small number of computing entities to see what is happening in what is this perceived (by some researchers) “degenerate” case. Despite its existence for at least 30 years, parallel MMM research has almost completely ignored this area. This is perhaps due to a lack of interest in a small number of processors or computers working together. Indeed in these cases the speedup benefits are obviously small. However with modern architectures, particularly cluster-based architectures and grids, small numbers of clusters or sites working together can clearly yield a very attractive benefit. As we will see, perhaps a small number of computing entities is not as “degenerate” as some researchers have believed.

Second, this was borne of a keen awareness of the parallel, distributed and especially the heterogeneous nature of computing platforms which are omnipresent in computing today. In addition, most parallel and distributed algorithms in existence today are designed for and only work well on homogeneous platforms. Finally, most heterogeneous algorithms are based on their homogeneous counterparts. It is now necessary for many new algorithms to be designed with heterogeneous platforms in mind from the start.

A. A Non-Rectangular Matrix Partitioning

All of the state-of-the-art matrix partitioning areas discussed thus far including the specific examples explored, had two common threads—they all balance computational load and they all seek to minimize communication between partitions. Both of these objectives are sought in order to minimize the overall execution time of matrix matrix multiplications.

It is true that there was another design feature common to all. This feature is that they are all rectangular. In all algorithms discussed, the solution sets contained only partitionings which result in nothing but rectangular partitions. Thus, it seems that the partitioning problem itself is somewhat restricted. Most researchers believe that allowing for non-rectangular partitions (relaxing this rectangular restriction) will not significantly improve the performance of the partitioning, and at the same time significantly complicate the solution of the partitioning problem.

This statement seems plausible, however in this section we introduce a non-rectangular partitioning solution that can significantly outperform counterpart rectangular partitionings. In some cases this non-rectangular partitioning can prove to be optimal amongst all partitionings. In addition, it does not significantly add to the complexity of the solution itself.

First we will define exactly what non-rectangular is meant in this context.

B. The Definition of Non-Rectangularity

In Figure 13 there are two partitions, $s_1$ and $s_2$. $s_1$ is non-rectangular and $s_2$ is rectangular. To precisely define what a non-rectangular partition is in context of the general partitioning problem, we start with the definition of a rectangular partitioning.

Definition 3.1 A partitioning of any problem whose solution is to partition the unit square is rectangular if all of the following four rules apply:

1) The unit square is completely tiled by partitions
2) No partitions overlap
3) All partition boundaries are parallel to the boundaries of the unit square
4) All partitions are rectangular

It would seem at first that in order to define a non-rectangular partitioning, all that is needed is to eliminate Definition 3.1, Rule 4. This seems reasonable as non-rectangular partitions would now be allowed, and Definition 3.1, Rule 3 would eliminate circles, triangles, and other exotic partitions.

However, a definition is needed that makes non-rectangular partitionings such as that in Figure 13 and all purely rectangular partitionings mutually exclusive. Eliminating Definition 3.1, Rule 4 would not do so, as purely rectangular partitions would still fit into the new definition of non-rectangular partitions.
The solution is to replace Definition 3.1 Rule 4 with the following—At least one partition is non-rectangular. This gives us the following definition.

**Definition 3.2** A partitioning of any problem whose solution is to partition the unit square is non-rectangular if all of the following four rules apply:

1) The unit square is completely tiled by partitions
2) No partitions overlap
3) All partition boundaries are parallel to the boundaries of the unit square
4) At least one partition is non-rectangular

We are now in a position where rectangular and non-rectangular partitionings are mutually exclusive, and we can differentiate between, and therefore compare, rectangular and non-rectangular partitionings.

**C. A Non-Rectangular Partitioning - Two Partitions**

In Section II-D, the Matrix Partitioning Problem [4] was stated. It is restated more formally as Problem 3.1.

**Problem 3.1:** The Matrix Partitioning Problem

- Given \( p \) computing elements \( P_1, P_2, \ldots, P_p \), the relative speed of which is characterized by a positive constant \( s_i \), where \( \sum_{i=1}^{p} s_i = 1 \)
- Partition a unit square into \( p \) rectangles so that
  - There is a one to one mapping of elements to rectangles.
  - The area of the rectangle allocated to element \( P_i \) is equal to \( s_i \) where \( i \in \{1, \ldots, p\} \).
  - The partitioning minimizes \( \sum_{i=1}^{p} (w_i + h_i) \), where \( w_i \) is the width of the rectangle and \( h_i \) is the height of the rectangle assigned to element \( P_i \).

As Problem 3.1 is restricted to rectangles, we need to reformulate the problem to be more general in order to allow for non-rectangular partitions.

**Problem 3.2:** The General Matrix Partitioning Problem

- Given \( p \) computing elements \( P_1, P_2, \ldots, P_p \), the relative speed of which is characterized by a positive constant \( s_i \), where \( \sum_{i=1}^{p} s_i = 1 \)
- Partition a unit square into \( p \) polygons so that
  - There is a one to one mapping of elements to polygons.
  - The area of the polygon allocated to element \( P_i \) is equal to \( s_i \) where \( i \in \{1, \ldots, p\} \).
  - The partitioning minimizes the sum of half perimeters of all polygons.

In the case of a very small problem size, say \( p = 2 \), every rectangular partitioning of Problem 3.1 or Problem 3.2 will result in one such as that in Figure 14. This is because there is no other way but to partition the unit square into two rectangles but to draw a straight line across the square, while ensuring that each rectangle is of the appropriate area as dictated by Problem 3.1 (or each partition is of the appropriate area as dictated by Problem 3.2).

As Problems 3.1 and 3.2 are equivalent, except that Problem 3.2 relaxes the restriction of rectangular solutions, clearly any rectangular partitioning algorithm can be applied to either, and generate the same solution.

A non-rectangular partitioning however can only be applied to Problem 3.2, but since Problem 3.2 is more general this is not a problem. Such an algorithm follows:

**Algorithm 3.1:** An algorithm to solve Problem 3.2, the General Matrix Partitioning Problem, for \( p = 2 \).

- **Step 1.** Re-index the processing elements \( P_i \) in the non-decreasing order of their speeds, \( s_2 \leq s_1 \).
- **Step 2.** Create a rectangular partition of size \( s_1 \) in the lower right corner of the unit square.
- **Step 3.** Map \( P_2 \) to the rectangular partition of size \( s_2 \), and map \( P_1 \) to the remaining non-rectangular balance of the unit square of size \( 1 - s_2 = s_1 \).

The result of Algorithm 3.1 is of the form in Figure 15. In each case the volume of communication is proportional to the sum of half perimeters of all partitions.

- For the rectangular case this is equal to 3.
- For the non-rectangular case in Figure 15 this is equal to Equation 1.

\[
\left( \frac{1 + (1 - y) + (1 - x) + x + y}{2} + x + y \right) = 2 + x + y
\]

(1)

We have left the relative speeds \( s_i \) of the processors \( P_i \) as unknowns (but remember that their sum equals 1), and since both are non-zero, we can make the following observations:

- For the rectangular partitioning, the sum of half perimeters is equal to 3 regardless of the ratio between \( s_1 \) and \( s_2 \).
partitioning has a lower sum of half perimeters than that of rectangular partitioning? The answer is found by answering partitioning’s sum of half perimeters less than that of the rectangular partitioning, and therefore a lower volume of communication. We can then answer the question: Is the non-rectangular partitioning’s sum of half perimeters less than that of the rectangular partitioning? The answer is found by answering

\[ 2 + 2 \times \sqrt{s_2} < 3. \tag{3} \]

Clearly, Inequality 3 is true for all \( \sqrt{s_2} < \frac{1}{2} \). This corresponds to \( s_2 < \frac{1}{4} \), which means that \( s_1 > \frac{3}{4} \). We can therefore conclude that when \( p = 2 \), and \( \frac{s_1}{s_2} > 3 \), the non-rectangular partitioning has a lower sum of half perimeters than that of the rectangular. When \( \frac{s_1}{s_2} = 3 \), the sum of half perimeters of the two partitionings are equal.

In other words as long as the area of the larger partition is greater than three times the smaller, the non-rectangular partitioning will result in a lower sum of half perimeters and therefore a lower volume of communication. We can summarize with the following:

- For ratios \( \rho : 1 \) where \( \rho \in [1,3) \) the rectangular partitioning has a lower total volume of communication.
- For the ratio \( \rho : 1 \) where \( \rho = 3 \) the rectangular and non-rectangular partitionings are equivalent in total volume of communication.

For ratios \( \rho : 1 \) where \( \rho \in (3,\infty) \) the non-rectangular partitioning has a lower total volume of communication. This of course depends on the sum of half perimeters \( \hat{C} \) being proportional to the total volume of communication (TVC) for the non-rectangular solution. This will be explored in Section IV-E. We will then provide a short yet formal proof.

D. Ratio Notation

As in the previous section above, we will be discussing and utilizing the speed (or computational power) ratio between two computing entities (processors, clusters, etc.) often in the coming sections. This ratio will be denoted \( \rho \), where \( \rho = \frac{s_1}{s_2} \), where \( s_1 \) and \( s_2 \) are the relative speeds or processing power of the entities \( s_1 \) and \( s_2 \). For simplicity, these ratios are always normalized so that \( s_2 = 1 \). Therefore the following identities apply:

- in fractional notation, \( \rho = \frac{s_1}{s_2} = \frac{s_1}{1} = \frac{\rho}{1} \Rightarrow \rho = s_1 \)
- and in ratio notation, \( \rho = s_1 : s_2 = s_1 : 1 = \rho : 1 = \rho : s_2 \)

At different times it will be more appropriate to use one over another.

Additionally, because we assume perfect load balancing, \( s_1 \) and \( s_2 \) are proportional to the partition areas assigned to entities \( P_1 \) and \( P_2 \) (or simply just entities 1 and 2) respectively.

E. Optimization

We have seen that for partitioning the unit square into two partitions, a non-rectangular partitioning can have a lower sum of half perimeters than a rectangular one, given the ratio between the two partition areas is \( \rho : 1 \) where \( \rho \in (3,\infty) \).

What can be said about the lower bound of the sum of half perimeters? How close to this lower bound is the non-rectangular partitioning? In [4] the authors give a lower bound for the sum of half perimeters \( \hat{C} \) to be \( LB \) in Equation 4

\[ LB = 2 \times \sum_{i=1}^{p} \sqrt{s_i} \tag{4} \]

where \( p \) is the number of partitions and \( s_i \) is the area of the \( i \)th partition. This is because the half perimeter of any partition is at a minimum when that partition is a square.

We then consider the following case. We have \( p = 2 \), \( s_1 = 1 - \epsilon \) and \( s_2 = \epsilon \) where \( \epsilon \) is some arbitrarily small but positive number. Any rectangular partitioning will require two partitions, formed by drawing a line of length 1 (See Figure 14). This will result in a sum of half perimeters, \( \hat{C} = 3 \), however \( LB \) gets arbitrarily close to 2.

Now we consider the non-rectangular partitioning of Figure 15. As \( \epsilon \to 0 \), the sum of half perimeters \( \hat{C} \to 2 \) and \( LB \to 2 \), which happens to be the half perimeter of the unit square itself, and therefore obviously optimal. Thus the non-rectangular partitioning can be optimal.

In [4], the authors make an experimental comparison of the sum of half perimeters and theoretical lower bound of the column-based rectangular partitioning discussed in Section...
II-D. The comparison between $\hat{C}$ and $LB$ is made in the following manner:

- Two curves are generated for a number of processors (entities) from 1 to 40.
- The first curve reflects the mean value $\frac{C}{LB}$ for 2,000,000 randomly generated partition areas ($s_i$).
- The second curve reflects the minimum value generated for the same.

Clearly the average values give a good idea of how the partitioning performs overall, while the minimum value (with such a large set of randomly generated areas) should reflect on how optimal the partitioning can be for each number of processors (entities). (Note that the number of processors is equal to the number of partitions as there is a one-to-one mapping of processors to partition areas.) Figure 16 shows the results of these experiments (adopted from [4]).

Figure 16 shows a number of interesting characteristics:
- The average values show:
  - By far the worst performance is for $p = 2$, by a factor of approximately 2 over that of the second worst performing case, $p = 6$.
- The minimum values show:
  - “Magic” numbers where the minimum $\frac{C}{LB}$ values are at or near 1, indicating optimal or near optimal solutions. These are numbers where it is theoretically possible to tile the unit square with a grid of $x$ squares of size $(\sqrt{x} \times \sqrt{x})$. Of course these numbers are the perfect squares (1, 4, 9, 16, 25, 36, ...). The average results also show better performance near these numbers.
  - By far the worst performance is for $p = 2$, by a factor of approximately 5, over that of the second worst performing case, $p = 6$. (Note that $p = 3$ just out performs $p = 6$ and is the third worst performing case, as we will discuss this case in Section V.)

It is important to note that in the case of $p = 2$, any and all rectangular partitionings should have the same performance, as they all result in equivalent partitionings in the form of that in Figure 14.

Figure 17 shows the same plot as Figure 16 but with the non-rectangular partitioning data for $p = 2$. In other words for $p = 2$ the non-rectangular partitioning of Figure 15 is used (with $s_2 = \sqrt{s_2} \times \sqrt{s_2}$ but for all other $p$, the partitioning values of Figure 16 have been retained. In addition, for $p = 2$, the restriction $\frac{s_1}{s_2} \geq 3.0$ has been added since it is known that in cases where $\frac{s_1}{s_2} < 3.0$, the rectangular partitioning should be used instead.

Figure 17 shows a number of interesting characteristics:
- The average values show:
  - For the case of $p = 2$, the average value has dropped from 1.105 to 1.054, an improvement of almost 49%.
  - $p = 2$ has gone from the worst average value to third worst, now better than $p = 3$ and $p = 6$.
  - The worst performing average case is now $p = 6$.
- The minimum values show:
  - The worst performing case is now $p = 3$ instead of $p = 2$
  - For the case of $p = 2$ (which was the worst performing case at 1.061), the performance is now optimal (actual value 1.000001). This concludes that $p$ need not be a “magic” number in order for the minimum ratio to be at (or very very near) 1 (optimal).

It is interesting that for the simple case of $p = 2$ a non-rectangular partitioning has out performed a rectangular one in all but a very small practical range of ratios. One more glance at Figures 16 and 17 begs the question, can the non-rectangular partitioning be extended to $p > 2$?

What has been established, is that in the case of $p = 2$, a hybrid partitioning employing any rectangular partitioning for $\frac{s_1}{s_2} < 3.0$, and using the non-rectangular partitioning discussed in this section for all others will give the best theoretical performance known. Further, the only room for improvement lies in the region $\frac{s_1}{s_2} < 3.0$, as above that ratio the non-rectangular partitioning provides an optimal solution to the General Matrix Partitioning Problem (Problem 3.2).

F. Conclusion

This section presented a geometric approach to partitioning a matrix into two partitions. All rectangle-based partitionings
reduce to equivalent partitionings when applied to the General Matrix Partitioning Problem (Problem 3.2), yielding solutions with sum of half perimeters $\hat{C} = 3$, and an accordingly proportional total volume of communication. Despite common belief that a non-rectangular approach would not yield a better result, and significantly complicate the solution [35], a non-rectangular solution was presented which does yield better performance at little-to-no complication. This performance comes in a lower sum of half perimeters than all rectangular partitionings provided the ratio between the areas of the two partitions is greater than $3 : 1$. This non-rectangular solution was shown to be optimal as the sum of half perimeter approaches the theoretically optimal sum of half perimeters $\hat{C} = 2$ as the ratio between partition areas grows. A hybrid algorithm utilizing the non-rectangular algorithm for ratios $\geq 3 : 1$, and any rectangular algorithm for ratios $< 3 : 1$ would yield better overall results compared to all known algorithms.

Further, this section has laid the foundation for Section IV, which will show that an architecture requiring a data partitioning amongst “only” two computing entities is not a degenerate case, as with modern scientific computing platforms each entity/cluster/site/etc. can be of great computational power locally. This concept is extended to more than two processors and useful application areas in Sections V and VI, providing theoretical and experimental proof to show that a partitioning amongst small numbers of computing entities can be quite advantageous.
IV. THE SQUARE-CORNER PARTITIONING

This section introduces the “Square-Corner Partitioning”, whose geometrical version was introduced in Section III. The Square-Corner Partitioning is a top-level, non-rectangular partitioning for matrix multiplication between two clusters or other computing entities. After communication details and theoretical performance are examined, experimental results of simulations using two processors, then experimental results using two different sets of two clusters are presented. The Square-Corner Partitioning is compared to rectangular partitionings in both communication and execution times.

The Square-Corner Partitioning is based on Algorithm 3.1, and accompanying geometrical analysis in Section III. The solution partitioning is similar to Figure 15. Results of experiments on two clusters correlate well with both the simulations presented here and theoretical performances. In the case of two clusters, each of which may have great computational power, this partitioning proves to be an important asset to anyone performing large matrix matrix multiplications, or any problem with a communication schedule similar to MMM.

In Section III a non-rectangular partitioning solving the General Matrix Partitioning Problem (Problem 3.2) for \( p = 2 \) was presented. This partitioning was shown to have a lower sum of half perimeters (SHP) than any rectangular partitioning solving the same problem, provided the ratio between the two was presented. This partitioning was shown to have a lower total volume of communication.\[ \text{TVC} = 2 \times N \times \sqrt{s_2} \]

\[ \text{Theorem 5,}\]

\[ \text{For ratios } \rho : 1 \text{ where } \rho \in [1,3) \text{ the rectangular partitioning has a lower total volume of communication.} \]

\[ \text{For the ratio } \rho : 1 \text{ where } \rho = 3 \text{ the rectangular and non-rectangular partitionings are equivalent in total volume of communication.} \]

\[ \text{For ratios } \rho : 1 \text{ where } \rho \in (3, \infty) \text{ the non-rectangular partitioning has a lower total volume of communication.} \]

This partitioning can be now be more specifically defined as The Square-Corner Partitioning, described by Algorithm 4.1.

Algorithm 4.1: The Square-Corner Partitioning, a solution to the General Matrix Partitioning Problem (Problem 3.2) for \( p = 2 \).

1. **Step 1.** Re-index the processing elements \( P_i \) in the non-decreasing order of their speeds, \( s_2 \leq s_1 \).
2. **Step 2.** Create a square partition of size \( s_2 \) in any corner of the matrix to be partitioned.
3. **Step 3.** Map \( P_2 \) to the square partition of size \( s_2 \), and map \( P_1 \) to the remaining balance of the matrix of size \( s_1 = N^2 - s_2 \), where \( N \) is the size of the matrix.
4. **Step 4.** Do the same for all matrices.

As Figure 18 shows, the rectangular Straight Line Partitioning always results in a TVC equal to \( N^2 \), in two communication steps regardless of the power ratio \( \rho \).

The Square-Corner Partitioning has a TVC equal to Equation 5.

\[ \text{TVC} = 2 \times N \times \sqrt{s_2} \]

where \( N \) is the matrix dimension and \( \sqrt{s_2} \times \sqrt{s_2} \) is the dimension of Cluster 2’s square partitions, shown in Figure 19.

As we have now formally defined the Square-Corner Partitioning, we will formally, yet simply prove that it has a lower TVC than the Straight-Line Partitioning for \( \rho > 3 \).

**Theorem 4.1:** For all power ratios \( \rho \) greater than 3, the Square-Corner Partitioning has a lower TVC than that of the Straight-Line Partitioning, and therefore all known partitionings, when \( p = 2 \).

**Proof:**

\[ TVC_{SCP} < TVC_{SLP} \]

\[ 2 \times N \times \sqrt{s_2} < N^2 \]

\[ \frac{2 \times N^2}{\sqrt{\rho + 1}} < N^2 \]

\[ 2 < \sqrt{\rho + 1} \]

\[ 4 < \rho + 1 \]

\[ 3 < \rho \]

Q.E.D

Similar proofs show that for the power ratio \( \rho = 3 \), the Square-Corner TVC is exactly equal to the Straight-Line TVC, and for ratios \( \rho < 3 \), the Square-Corner TVC exceeds that of the Straight-Line Partitioning.

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**Proof:**

\[ TVC_{SCP} < TVC_{SLP} \]

\[ 2 \times N \times \sqrt{s_2} < N^2 \]

\[ \frac{2 \times N^2}{\sqrt{\rho + 1}} < N^2 \]

\[ 2 < \sqrt{\rho + 1} \]

\[ 4 < \rho + 1 \]

\[ 3 < \rho \]

Q.E.D

Similar proofs show that for the power ratio \( \rho = 3 \), the Square-Corner TVC is exactly equal to the Straight-Line TVC, and for ratios \( \rho < 3 \), the Square-Corner TVC exceeds that of the Straight-Line Partitioning.

We can also simply prove that as defined, the Square-Corner Partitioning minimizes the total volume of communication against variants of the algorithm. Possible variants include assigning non-square partitions to Cluster 2. This means relaxing the \( s_2 \times s_2 \) square partition to become a rectangle of width \( \alpha \), height \( \beta \), and area \( s_2 \). We wish to minimize the total volume of communication, which more generally than Equation 5 can be given by Equation 6.

\[ TVC = \alpha \times N + \beta \times N \]

With the restraints:

\[ \alpha \times \beta = s_2 \], \quad \alpha \leq N \quad \beta \leq N \]

**Theorem 4.2:** The TVC of the Square-Corner Partitioning, \( C \) is minimized only when the Square-Corner Partitioning assigns a square partition to the smaller partition area \( \alpha \times \beta = s_2 \).

**Proof:** The first derivative of \( C \) is set equal to zero and it is shown that this occurs only when \( \alpha = \beta \), and therefore when the partition of area \( s_2 \) is a square. We then see that the second derivative of \( C \) is always positive and therefore any other partition will result in an increase in \( C \).

\[ C = \alpha \times N + \beta \times N \]

\[ dC \]

\[ \frac{dC}{\alpha} = N - \frac{s_2 \times N}{\alpha^2} \]

\[ N - \frac{s_2 \times N}{\alpha^2} = 0 \]

\[ \frac{s_2}{\alpha} = \alpha^2, \quad \vdots \quad \alpha = \beta \]

\[ \frac{d^2C}{\alpha^2} = N + 2 \times \frac{s_2 \times N}{\alpha^3} > 0 \]

Q.E.D

Figure 19 shows the Square-Corner Partitioning and the necessary data movements required to calculate a matrix
product \( C = A \times B \). Clearly the TVC is dependent on the size of the square partition and therefore the ratio \( \rho \) between the two partitions. The communication steps follow:

1) Cluster 1 needs to receive the entire square partition of matrix \( A \) from Cluster 2.
2) Cluster 1 needs to receive the entire square partition of matrix \( B \) from Cluster 2.
3) Cluster 2 needs to receive a set of partial rows of matrix \( A \) from Cluster 1.
4) Cluster 2 needs to receive a set of partial columns of matrix \( B \) from Cluster 1.

It will be shown in Section IV-D, based on Figures 18 and 19, that the Square-Corner Partitioning is not a special case of any Straight-Line Partitioning or vice-versa.

### A. Serial Communications

First we will investigate the case where communication between nodes or clusters is serial—no parallel communication is allowed to occur. In fact it is this scenario that we examined in Section III and so far in this section (because it is in this case that the communication time is proportional to the TVC). This will not be the case if parallel communications are allowed (Section IV-B). This serial communication model is viable and realistic, particularly for grids and other geographically distributed architectures, as physical distance, other traffic and cost may force a serial connection between entities. Indeed for massively distributed projects, such as SETI@home, the number of links that connect computing entities to servers is so great that one of them has a good chance of being serial, and becoming a bottleneck that will limit the whole communication channel to the performance limitations of that bottleneck.

1) Straight-Line Partitioning: For the Straight-Line Partitioning, the TVC is always \( N^2 \), regardless of power ratio, as shown in Figure 18. To be consistent with three more cases that will be examined in this section and Section IV-B we will state this as a limit:

\[
\lim_{\rho \to 0} TVC_{SLP} = N^2
\]

This can be expressed in terms of \( \rho \) as

\[
\lim_{\rho \to \infty} TVC_{SLP} = N^2 \tag{8}
\]

2) Square-Corner Partitioning: The TVC for the Square-Corner Partitioning is given by Equation 5. Additionally, we can see that the Square-Corner Partitioning is optimal if we look at the limit of Equation 5:

\[
TVC_{SCP} = 2 \times N \times \sqrt{\frac{\rho}{2}}
\]

\[
\lim_{\rho \to 0} TVC_{SCP} = 0 \tag{9}
\]

This can be expressed in terms of \( \rho \) as

\[
\lim_{\rho \to \infty} TVC_{SCP} = 0
\]

Figure 20 shows the Square-Corner Partitioning TVC compared to that of the Straight-Line Partitioning with serial communications for power (partition) ratios \( \rho = 1 : 1 \to 25 : 1 \). At a ratio of \( 3 : 1 \) the partitionings are equivalent in TVC, and for \( \rho = 15 : 1 \) the Square-Corner Partitioning’s TVC is one-half that of the Straight-Line Partitioning.

3) Hybrid Square-Corner Partitioning for Serial Communications: Since for ratios \( \rho < 3 : 1 \), the Square-Corner Partitioning has a greater TVC than that of the Straight-Line Partitioning, the two can be combined to create a hybrid algorithm. This Hybrid Square-Corner Partitioning for Serial Communications (HSCP-SC) is equivalent to the Square-Corner Partitioning for \( \rho \geq 3 \), and equivalent to the Straight-Line Partitioning for \( \rho < 3 \).
Figure 21 shows the TVC of the HSCP-SC compared to that of the Straight-Line Partitioning.

Since we know that for $\rho < 3$, the HSCP-SC and SLP are equivalent by definition, we will not compare the HSCP-SC and the SLP experimentally, but will compare the SCP to the SLP experimentally as we have been doing theoretically.

B. Parallel Communications

Next we will investigate the case where communication between nodes or clusters is parallel. In this case, there are two communications happening at the same time: Cluster 1 is transmitting to Cluster 2, and Cluster 2 is transmitting to Cluster 1 as per Figures 18 and 19. This is also a reasonable model, as many network interconnects do allow parallel communications, even over large geographic distance, but at a greater cost than that of serial communication links.

The equations for the total volumes of communication so far have been expressed in terms of the area of the smaller, square partition $s_2$. It will be advantageous to express these in terms of the ratio $\rho = \frac{s_1}{s_2} = s_1 : s_2$:

\[
\begin{align*}
\rho &= \frac{s_1}{s_2} \\
\rho &= \frac{s_1}{s_2} \\
\rho &= \frac{1 - s_2}{s_1} \\
\rho &= \frac{1 - s_2}{s_1} \\
\rho &= \frac{1}{\rho} \\
\rho &= \frac{1}{\rho} \\
\rho \times s_2 + s_2 &= 1 \\
\rho \times s_2 + s_2 &= 1 \\
s_2 \times (\rho + 1) &= 1 \\
s_2 \times (\rho + 1) &= 1 \\
s_2 &= \frac{1}{1 + \rho} \\
s_2 &= \frac{1}{1 + \rho}
\end{align*}
\]

1) Straight-Line Partitioning: For the Straight-Line Partitioning, the TVC from Cluster 1 to Cluster 2 ($TVC_{SLP\ 1\rightarrow2}$) is always greater than that from Cluster 2 to Cluster 1 and therefore dominant (except at a 1:1 ratio where $TVC_{SLP\ 1\rightarrow2} = TVC_{SLP\ 2\rightarrow1} = \frac{N^2}{2}$). As per Figure 18:

\[
\begin{align*}
TVC_{SLP\ 1\rightarrow2} &= (1 - s_2) \times N^2 \\
TVC_{SLP\ 1\rightarrow2} &\propto \left(1 - \frac{1}{1 + \rho}\right) \\
TVC_{SLP\ 1\rightarrow2} &\propto \left(\frac{\rho}{1 + \rho}\right) \\
\end{align*}
\]

As with the serial communication case, it can be shown that the Straight-Line Partitioning is not optimal by examining the limit of Equation 11:

\[
\lim_{s_2 \to 0} TVC_{SLP} = (1 - s_2) \times N^2
\]

This can be expressed in terms of $\rho$ as

\[
\lim_{\rho \to \infty} TVC_{SLP} = N^2
\]

Note that Equation 13 is equal to Equation 8, thus the Straight-Line Partitioning performs the same with serial and parallel communications.

2) Square-Corner Partitioning: For the Square-Corner Partitioning, again the volume of communication from Cluster 1 to Cluster 2 ($TVC_{SCP\ 1\rightarrow2}$) is greater and therefore dominant for $\rho > 3 : 1$. For $\rho < 3 : 1$, $TVC_{SCP\ 2\rightarrow1}$ is dominant. At $\rho = 3 : 1$ both TVC values are equivalent. As per Figure 19, we can determine:

\[
\begin{align*}
TVC_{SCP\ 1\rightarrow2} &= 2 \times \sqrt{s_2} \times (1 - \sqrt{s_2}) \times N^2 \\
TVC_{SCP\ 1\rightarrow2} &\propto 2 \times (\sqrt{s_2} - s_2) \\
TVC_{SCP\ 1\rightarrow2} &\propto 2 \times \left(\frac{1}{1 + \rho} - \frac{1}{1 + \rho}\right) \\
TVC_{SCP\ 2\rightarrow1} &= 2 \times s_2 \times N^2 \\
TVC_{SCP\ 2\rightarrow1} &\propto 2 \times s_2 \\
TVC_{SCP\ 2\rightarrow1} &\propto \left(\frac{2}{1 + \rho}\right)
\end{align*}
\]

Where $TVC_{SCP\ 1\rightarrow2}$ is the total volume of communication moving from Cluster 1 to Cluster 2 and $TVC_{SCP\ 2\rightarrow1}$ is the total volume of communication moving from Cluster 2 to Cluster 1.

Therefore the dominant communication for a given ratio $\rho$ for the Square-Corner Partitioning using parallel communications is:

\[
\max(TVC_{SCP\ 1\rightarrow2}, TVC_{SCP\ 2\rightarrow1}) =
\]

\[
\max \left[2 \times \left(\frac{1}{1 + \rho} - \frac{1}{1 + \rho}\right), \left(\frac{2}{1 + \rho}\right)\right]
\]

Figure 22 shows a plot of Equations 12 and 17. This illustrates the Straight-Line and Square-Corner Partitionings with parallel communications for power (partition) ratios $\rho =$
1 : 1 → 25 : 1. Since communications are parallel, only the dominant communication is taken into account. For the SCP this is achieved with the \( \max \) function in Equation 17.

The discontinuity in the TVC of the Square-Corner Partitioning at \( \rho = 3 \) is due to the transition from \( TVC_{SCP} \Rightarrow 2 \rightarrow 1 \) being dominant for \( \rho < 3 \) to \( TVC_{SCP} \Rightarrow 1 \rightarrow 2 \) being dominant for \( \rho > 3 \). (\( TVC_{SCP} \Rightarrow 1 \rightarrow 2 = TVC_{SCP} \Rightarrow 2 \rightarrow 1 \) when \( \rho = 3 \). If we included the non-dominant terms, the curves for both \( TVC_{SCP} \Rightarrow 2 \rightarrow 1 \) and \( TVC_{SCP} \Rightarrow 1 \rightarrow 2 \) are continuous (See Figure 24).

We can also show that for parallel communications the Square-Corner Partitioning is optimal, as is the case for serial communications by examining the limit of Equation 14:

\[
TVC_{SCP} = 2 \times \sqrt{\frac{1}{\rho}} \times (1 - \sqrt{\frac{1}{\rho}}) \times N^2
\]

\[
\lim_{{\rho \to 0}} TVC_{SCP} = 0
\]

This can be expressed in terms of \( \rho \) as

\[
\lim_{{\rho \to \infty}} TVC_{SCP} = 0 \quad (18)
\]

3) Hybrid Square-Corner Partitioning for Parallel Communications: As Figure 22 shows, for ratios less than \( \rho = 2 : 1 \), the Square-Corner Partitioning has a greater TVC than that of the Straight-Line Partitioning when parallel communications are utilized. Thus the two can be combined to create a hybrid algorithm. This Hybrid Square-Corner Partitioning for Parallel Communications (HSCP-PC) is equivalent to the Square-Corner Partitioning for \( \rho \geq 2 \), and equivalent to the Straight-Line Partitioning for \( \rho < 2 \). The HSCP-PC will give the best performance of all known algorithms regardless of \( \rho \). Figure 23 shows the HSCP’s TVC compared to that of the Straight-Line Partitioning.

The TVC of the HSCP-PC is given by:

\[
\min \left[ \frac{\rho}{1 + \rho}, \max \left[ 2 \times \left( \sqrt{\frac{1}{1 + \rho}} - \frac{1}{1 + \rho} \right), \frac{2}{1 + \rho} \right] \right] \quad (19)
\]

As Equation 19 and Figure 24 show, the HSCP-PC is a combination of three functions, as summarized in Table I.

Figure 24 shows the HSCP-PC’s TVC compared to that of the Straight-Line Partitioning and the two components of the Square-Corner Partitioning.

Since we know that for \( \rho < 2 \), the HSCP-PC and SLP are equivalent by definition, we will not compare the HSCP-SC and the SLP experimentally, but will compare the SCP to the SLP experimentally as we have been doing theoretically.
C. Choosing a Corner For the Square Partition

We choose a corner for the position of the square partition for several reasons of convenience as follows. The location does not affect the TVC. Placing the square partition in the corner position of the matrix:

1) Minimizes the number of communication steps necessary, and reduces the complexity of the communication schedule discussed in Section IV-D.
2) Allows the use of the SHP metric as proportional to the TVC as discussed in Section IV-E.
   • In showing that the SHP is proportional to the TVC for the Square-Corner Partitioning (as it is for the rectangular, or Straight-Line Partitioning) we come up with a new metric, the total number of row and column interrupts, $I$. This is explored in Section IV-F.
3) Maximizes an area of the matrix which can allow for the overlapping of communication and computation which will be discussed in Section IV-G.
4) Maximizes the potential size of multiple partitions as will be discussed in Sections V and VII.

D. Minimizing the Number of Communication Steps

Placing the square partition in the corner of the matrix minimizes the number of communication steps necessary to calculate $C = A \times B$. Figure 19 shows that the Square-Corner Partitioning requires a total of four communication steps. Figure 25 shows a partitioning similar to the Square-Corner Partitioning and the necessary data movements required to calculate a matrix product $C = A \times B$ with the square partition adjacent to one of the sides of the matrix.

As Figure 25 shows, the number of communication steps in this case is five. Just as in the case where the square partition is located in one of the corners of the matrix, both square partitions and a number of partial rows and partial columns need to be communicated.

Figure 26 shows a partitioning similar to the Square-Corner Partitioning and the necessary data movements required to calculate a matrix product $C = A \times B$ with the square partition in the center of the matrix, not adjacent to any sides. As Figure 26 shows, the number of communication steps is six. Just as in the case where the square partition is located in one of the corners of the matrix, both square partitions and a number of partial rows and partial columns need to be communicated.

E. Sum of Half Perimeters - A Metric

In Section III we used the sum of half perimeters as a metric which is proportional to the total volume of communication. This is common practice for rectangular partitionings but demands closer inspection for the non-rectangular case.

First let us use two methods to determine the sum of half perimeters for the non-rectangular (Square-Corner) solution on the unit-square.

• Add the entire perimeter of the partitions $s_1$ and $s_2$ and divide the sum by two. Equation 2 gives us $\hat{C} = 2 + 2 \times \sqrt{s_2}$. [5] provides the second way: It is the length of the lines drawn to make the partition(s) plus 2. This also results in $\hat{C} = 2 + 2 \times \sqrt{2}$.

Thus the unit square SHP for the Square-Corner Partitioning is $(2 + 2 \times \sqrt{s_2})$. For a real matrix of size $N$, the SHP is given by Equation 4.2.

$$\hat{C} = 2 \times N + 2 \times \sqrt{s_2}$$

As we have seen in Equations 5 and 20, the TVC and SHP for the Square-Corner Partitioning are expressed in terms of $\sqrt{s_2}$. We can in turn define $\sqrt{s_2}$ in terms of the cluster power ratio, $\rho$ in Equation 21. As always we normalize this ratio so that the power of the slower cluster is equal to 1, so a ratio of $\rho$ is understood to be a ratio of $\rho : 1$.

$$\sqrt{s_2} = \frac{N}{\sqrt{\rho + 1}}$$

To study the proportionality of the SHP and TVC relationship, Table 4.1 lists some actual SHP/TVC ratios for the Square-Corner Partitioning, along with the partitionings in Figures 25 (square partition adjacent to one side) and 26 (square adjacent to no sides). The value of $\sqrt{s_2}$, and therefore
the ratio between the two partitions, is varied. Note that we are working on the unit square.

It is desirable to make a meaningful comparison of the proportionality of the SHP/TVC ratio for the Square-Corner and “Square-Corner-Like” Partitionings and the SHP/TVC ratio for the Straight-Line Partitioning. Initially this proves troublesome, as varying the ratio between only two partitionings for the Straight-Line Partitioning will yield the same ratio regardless of SHP and TVC values, as both are constant. The SHP is always 3, and the TVC is always 1 on the unit square. Table III lists values for the Straight-Line Partitioning SHP/TVC ratios for a varying number of partitions. To keep calculations simple, each partition is given an equal area, and the partition numbers are kept to perfect squares.

Interestingly, plotting the SHP and TVC while varying \( \sqrt{\frac{3}{2}} \) for the Square-Corner and Square-Corner-Like Partitionings (keeping \( p \) constant), but varying the number of partitions \( p \) for the Straight-Line Partitioning, we can see their relative relationships. This is shown in Figure 27.

Figure 27 shows that the Square-Corner Partitioning and Straight-Line Partitionings have equivalent SHP/TVC ratios. Those for the other two Square-Corner-Like Partitionings are also linear, and have the same intercepts as the other lines, only their slope varies.

The intercept for all lines appears to be \((0,2)\). This corresponds to a TVC of 0 (obviously optimal), and a SHP of 2, also optimal (The SHP of the unit-square itself is 2). This however is not the case if we inspect the region below SHP = 3 with greater detail. It is seen that once the SHP reaches 3, the Straight-Line Partitioning cannot proceed towards the optimal \((0,2)\). This is because the SHP cannot be less than 3, and therefore the TVC can never be below 1. However the Square-Corner Partitioning carries no such restriction and does approach, in the limit SHP \( \rightarrow 0 \), the optimal value of TVC = 0. Interestingly, the other two Square-Like Partitionings also approach the optimal value of TVC = 0.

**F. A New TVC Metric - Row and Column Interrupts**

In Section IV-D we saw that for each communication step a number of partial rows and columns had to be communicated. In fact, all communications make up partial rows and columns. Although once all communications have completed it is entire rows and columns that have been communicated in aggregate. This holds for the Straight-Line Partitioning as well. This leads us to conclude that a more general metric, proportional to the TVC, is the number of rows and columns interrupted by partitions boundaries.

For the Square-Corner and Square-Corner-Like Partitionings, the number of rows and columns interrupted is \( \sqrt{\frac{3}{2}} \) rows and \( \sqrt{\frac{3}{2}} \) columns for the square partition, and the same for the polygonal partition for a total of \( 4 \times \sqrt{\frac{3}{2}} \). The TVC is \( 2 \times N \times \sqrt{\frac{3}{2}} \). For the Straight-Line Partitioning, the number of rows interrupted is \( N \) for the first partition and \( N \) for the second for a total of \( 2 \times N \). The TVC is \( N^2 \). From this the following observations can be made:

- For the Square-Corner and Square-Corner-Like Partitionings,
  \[
  \frac{\text{TVC}}{I} = \frac{2 \times N \times \sqrt{\frac{3}{2}}}{4 \times \sqrt{\frac{3}{2}}} = \frac{N}{2}
  \]

- For the Straight-Line Partitioning,
  \[
  \frac{\text{TVC}}{I} = \frac{N^2}{2 \times N} = \frac{N}{2}
  \]

where \( I \) is the total number of rows and columns interrupted by each partition in each partitioning, given by Equation 22.

\[
I = \sum_{i=1}^{p} (r_i + c_i)
\]  
(22)

where \( p \) is the number of partitions, \( r \) is the number of rows interrupted by partition \( i \), and \( c \) is the number of columns interrupted by partition \( i \).
outset. In Section V this will be shown to greatly reduce
with no communication. Cluster S H P while that of C and D are not. At the same time all
partitions have a TVC proportional to their I value, the total
number of row and column interrupts.

We conclude, but do not prove, that Equation 22 is a more
general metric than the SHP for determining the relative TVC
of matrix partitions.

This is due to the fact that the SHP fails to be proportional
to the TVC for polygons whose perimeters are not equal to that
of a bounding rectangle. In Figure 25 the partition owned by
Cluster 1 is a polygon which falls into this category. In Figure
26 the partition owned by Cluster 1 is not even polygonal, but
a polygon with a “hole” cut in it. Nonetheless if one considers
the perimeter of the hole to contribute to the SHP as we did
in Section IV-E, the SHP does behave linearly and converge
on the optimal TVC. Thus the SHP does seem appropriate as
a metric, however the sum of row and column interrupts, I, is
again more appropriate, as it matches exactly the I value of
the other Square-Corner and Square-Corner-Like Partitions,
when their TVC values are equivalent.

The non-rectangular partition in the Square-Corner Parti-
tioning works perfectly with both the SHP and I metrics,
because the SHP is equal to the SHP of the partition’s bounding
rectangle. (Also note that the same is true for all rectangular
partitions.) Figure 28 shows the polygons so far investigated.
A is the non-rectangular partition from the Square-Corner
Partitioning, B is a rectangular partitioning from the Straight-
Line Partitioning. C and D are from the Square-Corner-Like
Partitionings. The TVC of A and B is proportional to the
SHP while that of C and D are not. At the same time all
partitionings A, B, C and D have an I value proportional to
their TVC.

G. Overlapping Communication and Computation

The Square-Corner Partitioning has another advantage over
the Straight-Line Partitioning. There is always a part of the
product matrix C which can be immediately calculated. This
is shown in Figure 29 as the hatched area. The hatched areas
of matrices A and B are those required to calculate area C
with no communication. Cluster 1 owns these areas from the
outset. In Section V this will be shown to greatly reduce
execution times. Placing the square partition in one corner of
the matrix maximizes the area of this immediately calculable
sub-partition, in the corner opposite. We explore this further
in Sections V-D and V-F.

H. HCL Cluster Simulations

To experimentally verify algorithm 4.1, the Square-Corner
Partitioning, we implemented it and the Straight-Line Par-
titioning in Open-MPI [36]. The experiments were carried
out on two identical machines on the HCL Cluster (hcl03
and hcl04). This was done so we could focus solely on the
partitioning method without worrying about any contributions
made by architectural differences. Local matrix computations
utilize ATLAS [37]. The machines were connected with a
switch allowing the bandwidth between the nodes to be
specified, up to 1Gb/s.

1) Serial Communications: Since the HCL switches allow
parallel communications, we simulated a serial communication
link in code. We do this by forcing all communications from
Processor 1 to Processor 2 to complete before the communi-
cations going from Processor 2 to Processor 1 commence.
This is done using MPI_Barrier() calls. Both partitionings
carry out all communications first, then all computations. Thus
preliminarily there is no communication/computation overlap.
All times are averaged over five runs.

The ratio of speeds between the two nodes was varied by
slowing down the CPU of one node relative to the other using
a CPU limiting program as proposed in [2]. This program
supervises a specified processes and using the /proc pseudo-
filesystem, forces the process to sleep when it has used more
than a specified fraction of CPU time. The process is then
woken when enough idle CPU time has elapsed for the process
to resume. Sampled frequently enough, this can provide a fine
level of control over the fraction of CPU time used by the
process. Comparison of the run-times of each node confirmed
that this method results in the desired ratios well within 2%.

a) Comparison of Communication Times: We ran matrix
matrix multiplications using the Square-Corner Partitioning
and the Straight-Line Partitioning for power ratios ranging
from 1:1 to 1:25 and for bandwidth values ranging from
50Mb/s to 1Gb/s. In all cases other than ratios of 1:1, 1:2,
and 1 : 3, the total communication time for the Square-Corner Partitioning was less than that of the Straight-Line Partitioning.

Figure 30 shows the communication times for the Square-Corner and Straight-Line Partitionings for ratios 1 : 1 − 1 : 25 and a network bandwidth of 100Mb/s. The shape of the curves in this figure reflect the TVC relationship between the Square-Corner and Straight-Line Partitionings as theoretically shown in Figure 20.

Figure 31 shows the communication times for the Square-Corner and Straight-Line Partitionings for ratios 1 : 1 − 1 : 25 and a network bandwidth of 500Mb/s. Again the experimental results match the theoretical predictions.

The most important feature of all communication plots is that there is the predicted “crossover” between the Square-Corner Partitioning and Straight-Line Partitioning at a ratio of ρ = 3 : 1, and for all greater ratios the Square-Corner Partitioning has a lower TVC and therefore communication time. In fact the gap between the two partitionings continues to widen with increasing ratio, because \( \lim_{\rho \to \infty} TVC_{SLP} = N^2 \) (Equation 8), and \( \lim_{\rho \to \infty} TVC_{SCP} = 0 \) (Equation 9).

b) Comparison of Total Execution Times: The objective of the Square-Corner Partitioning is to reduce the inter-cluster communication time, resulting in a lower total execution time compared to all other partitionings when the number of partitions, \( p = 2 \). Since the total execution time is dependent on communication and computation time, any savings in total execution time will be dependent on how dominant communication time is in the overall execution time. It can be seen comparing the communication and execution times that the reduction in communication times directly impacts the execution times.

Figures 33, 34 and 35 show the total execution times for the Square-Corner and Straight-Line Partitionings for ratios 1 : 1 − 1 : 25 and network bandwidths of 100Mb/s, 500Mb/s and 1Gb/s respectively, using serial communications. The crossover at \( \rho = 3 : 1 \) which was predicted theoretically and observed experimentally in the communication times is also present in the execution times. For all ratios \( \rho > 3 : 1 \), the Square-Corner Partitioning out performs the Straight-Line Partitioning.

As bandwidth increases, the ratios where both the Square-Corner and Straight-Line Partitionings are faster than the sequential time (performing the multiplication on the fastest processor only) increase. For the Square-Corner Partitioning, this ratio increases from approximately 17 : 1 to 23 : 1 as the bandwidth increases from 100Mb/s to 1Gb/s.

2) Parallel Communications: In this section we explore the performance of the Square-Corner Partitioning when parallel communications are utilized. All experimental parameters and techniques are the same as Section IV-H1. The only difference is a modified communication schedule, which is described in the following section.

a) Comparison of Communication Times: We ran matrix matrix multiplications using the Square-Corner Partitioning and the Straight-Line Partitioning for power ratios ranging from 1 : 1 to 1 : 25 and for bandwidth values ranging from 50Mb/s to 1Gb/s. In all cases where \( \rho > 2 : 1 \), the total communication time for the Square-Corner Partitioning was less than that of the Straight-Line Partitioning, as predicted.
by theory.

All communications are carried out before computations begin. Non-Blocking MPI_ISend() and MPI_IRecv() communications are used, followed by MPI_Wait() statements. This is done to give control of the communication scheduling to the network layer allowing Ethernet parallelism. The only MPI_Barrier is between the communication and computation code segments.

Figures 36, 37, and 38 show the communication times for the Square-Corner and Straight-Line Partitionings for ratios 1 : 1 − 1 : 25 and network bandwidths of 100Mb/s, 500Mb/s, and 1Gb/s respectively. The shape of the curves in these figures reflect the TVC relationship between the Square-Corner and Straight-Line Partitionings as theoretically shown in Figure 20. Note that with parallel communications this results in a lower communication time when \( \rho > 2 : 1 \).

b) Comparison of Total Execution Times: The objective of the Square-Corner Partitioning is to reduce the inter-cluster communication time, resulting in a lower total execution time compared to all other partitionings when the number of partitions, \( p = 2 \). Since the total execution time is dependent on communication and computation time, any savings in

Fig. 33. Average execution times for the Square-Corner and Straight-Line Partitionings using serial communications. Network bandwidth is 100Mb/s, \( N = 4, 500 \).

Fig. 34. Average execution times for the Square-Corner and Straight-Line Partitionings using serial communications. Network bandwidth is 500Mb/s, \( N = 4, 500 \).

Fig. 35. Average execution times for the Square-Corner and Straight-Line Partitionings using serial communications. Network bandwidth is 1Gb/s, \( N = 4, 500 \).

Fig. 36. Average communication times for the Square-Corner and Straight-Line Partitionings using parallel communications. Network bandwidth is 100Mb/s, \( N = 4, 500 \).

Fig. 37. Average communication times for the Square-Corner and Straight-Line Partitionings using parallel communications. Network bandwidth is 500Mb/s, \( N = 4, 500 \).
total execution time will be dependent on how dominant communication time is in the overall execution time. It can be seen comparing the communication and execution times that the reduction in communication times directly impacts the execution times.

Figures 39, 40 and 41 show the total execution times for the Square-Corner and Straight-Line Partitionings for ratios $1 : 1 - 1 : 25$ and network bandwidths of 100Mb/s, 500Mb/s and 1Gb/s respectively. These figures also show the execution time for the fastest processor executing the multiplication time sequentially on the fastest processor.

As bandwidth increases, the ratio where both the Square-Corner and Straight-Line Partitionings are faster than the sequential time (performing the multiplication on the fastest processor only) increases. For the Square-Corner Partitioning, this ratio increases from approximately $19 : 1$ to $22 : 1$ as the bandwidth increases from 100Mb/s to 1Gb/s.

I. HCL Cluster Experiments

This section presents results of MPI matrix matrix multiplication experiments on a small two cluster configuration of the HCL Cluster. Six machines (hcl03 - hcl08) were used, connected through two switches utilizing the SFP connection between them as shown in Figure 42. Cluster 1 (hcl03, hcl04, hcl05) all have their CPU speeds restricted as in Section IV-H. Thus we have a two cluster architecture which should be well modelled by the simulations in Section IV-H.

1) Comparison of Communication Times: The communication times for this architecture were very close to the simulation using two machines in Section IV-H. Overall the communication times were slightly higher, most likely due to the increased number of machines communicating. Only the bandwidth of the SFP connection was varied as this is the only link between the two clusters.

Figures 43, 44, and 45 show the communication times for the Square-Corner and Straight-Line Partitionings for ratios $1 : 1$ to $1 : 15$ and a network bandwidths of 100Mb/s, 500Mb/s and 1Gb/s respectively. Parallel communications are utilized in all experiments. As with two processors and parallel communications, the Square-Corner Partitioning has a lower communication time for all $\rho > 2 : 1$. $N = 4,500$ for all experiments.
Fig. 42. A two cluster configuration of the HCL Cluster. By bringing up NIC1 and bringing down NIC2 on hcl03 - hcl05, and the opposite for hcl06 - hcl08, and enabling the SFP connection between the switches, two homogeneous connected clusters of three nodes each are formed.

Fig. 43. Average communication times for the Square-Corner and Straight-Line Partitionings utilizing parallel communication. Network bandwidth is 100Mb/s, $N = 4,500$.

Fig. 44. Average communication times for the Square-Corner and Straight-Line Partitionings utilizing parallel communication. Network bandwidth is 500Mb/s, $N = 4,500$.

2) Comparison of Total Execution Times: The overall execution times were again directly influenced by the communication times. Execution times were lower than simulations as expected, due to a three-fold increase in computational power through increased parallelism. It is seen that the increase in bandwidth and corresponding reduction in communication times is the largest factor in reducing the execution times.

Figures 46, 47, and 48 show the total execution times for the Square-Corner and Straight-Line Partitionings for ratios 1 : 1 to 1 : 15 and network bandwidths of 100Mb/s, 500Mb/s and 1Gb/s respectively. As with two processors and parallel communications, the Square-Corner Partitioning has a lower execution time for all $\rho > 2 : 1$.

J. Grid’5000 Experiments

To investigate the scalability of the Square-Corner Partitioning we utilized Grid’5000 (See Section I-B2). Grid’5000 is located across nine sites in France and has 1,529 nodes from Altix, Bull, Carri, Dell, HP, IBM and SUN. There is a total of 2,890 processors with a total of 5,946 cores from both AMD and Intel.
In this section we used two clusters of machines at the Bordeaux site. The first are IBM x4355 dual-processor nodes with AMD Opteron 2218 2.6GHz Dual Core Processors with 2MB L2 Cache and 800MHz Front Side Bus. Each node has 4GB of RAM (2GB per processor, 1GB per core). The second are IBM eServer 325 dual-processor nodes with AMD Opteron 248 2.2GHz single core processors with 1MB L2 Cache. Each node has 2GB of Ram (1GB per processor).

The problem size is $N = 15,000$.

1) Comparison of Communication Times: All communications were 1GB/s Ethernet. Parallel communications are utilized. It can be seen that an effect of keeping the overall computational power constant while increasing the relative power ratio served to flatten out some of the communication curves, particularly those for the Straight-Line Partitioning, where there is a constant amount of communication regardless of the power ratio.

Figure 49 shows the communication times for ratios 1 : 1 to 1 : 8.

2) Comparison of Total Execution Times: Power ratios were varied from 1 : 1 to 1 : 8 by varying the number of CPUs in each cluster while trying to maintain a relatively constant total power. This represents a departure from our simulation and experiment results in Sections IV-H and IV-I, where the overall computational power was not kept constant. All local computations utilized ATLAS.

It can be seen that the reduction in communication time directly impacts the execution time. The expected crossover at power ratio 2:1 is present and for greater power ratios, the Square-Corner Partitioning has a lower execution time.

Both the Square-Corner and Straight-Line Partitionings resulted in lower execution times than the problem being solved on just the fastest cluster, which ran in 198s.

K. Conclusion

This section presented a new data partitioning algorithm, the Square-Corner Partitioning, for matrix matrix multiplication on two heterogeneous interconnected clusters. Compared to more general partitioning algorithms which result in simple “Straight-Line” rectangular partitions on a two-cluster architecture, this new partitioning is proven to reduce the total volume of inter-cluster communication when the power ratio of the two clusters is greater than 3 : 1 when serial
communications are utilized, and greater than $2 : 1$ when parallel communications are utilized. This results in a lower execution time for architectures with these ratios.

This partitioning algorithm can be utilized as the top-level partitioning of a hierarchical algorithm that is to multiply matrices across more than two connected clusters. A tree-like network could deploy this partitioning at each level of the network, allowing individual clusters to handle their computations in any manner locally. When serial communications are utilized, a hybrid algorithm utilizing this new Square-Corner Partitioning for power ratios equal to or greater than $3 : 1$, and the existing Straight-Line Partitioning for ratios of less than $3 : 1$ guarantees that the total volume of communication will be equal to or less than previously existing algorithms for all ratios. When parallel communications are utilized, a hybrid algorithm utilizing this new Square-Corner Partitioning for power ratios equal to or greater than $2 : 1$, and the existing Straight-Line Partitioning for ratios of less than $2 : 1$ guarantees that the total volume of communication will be equal to or less than previously existing algorithms for all ratios.

The Square-Corner Partitioning has several advantages over other Straight-Line Partitionings including the possibility of overlapping communication and computation. This is theoretically and experimentally explored in Section V.
V. THE SQUARE-CORNER PARTITIONING ON THREE CLUSTERS

In this section the Square-Corner Partitioning is extended from an architecture of two clusters to three. We do this because the move from two to three clusters represents a theoretical hurdle, and the three cluster topology is much closer to a $n$ cluster topology than two. A large part of this is due to the fact that a three cluster system introduces a new degree of freedom, in the availability of more than one interconnection topology. Thus we are sacrificing theoretical generality to explore deeper with experimental analysis. We will see in Section VII that generalizing to four or more clusters is a qualitative extension of the three cluster case.

The cases where the Square-Corner Partitioning has a lower total volume of communication than the Straight-Line Partitioning are explored theoretically then experimentally. Topological limitations are also discussed. As in the two cluster case we will start our experiments with three processor simulations before presenting experimental results on Grid’5000. Experimental results correlate well with theory and simulation.

In this research we model three clusters using three processors because a three processor network provides a controllable and tunable environment whose structure is similar to three clusters. In the case of connected clusters, local communications are often an order of magnitude faster than the interconnecting link. Due to physical distance this link is often serialized or of some limited parallelism but depending on architecture parallel links are not ruled out nor considered exotic. Similarly, with three processors local communications (within processor-local registers and memory) are typically fast compared to the inter-processor connection speed. Using an Ethernet switch with a configurable bandwidth allows us to model many different scenarios.

As the case of three clusters brings up a new degree of freedom that was not found in the two cluster case, namely network topology, we explore the impact of this on the partitioning’s effectiveness. In the case of three clusters there are “Star” and “Fully Connected” topologies now available (see Figure 51). We will also explore the case where communications and computations can be overlapped resulting in lower overall execution times.

To our knowledge no research has been conducted to optimize data partitioning techniques for the specific architecture of three connected nodes. The most related work is [4], which introduced a partitioning for matrix matrix multiplication designed for any number of nodes including three. This partitioning exclusively utilizes rectangular partitions, organized in columns, with each rectangle being proportional in area to the speed of the node which is to calculate that partition. This Straight-Line Partitioning in the case of three clusters results in a partitioning as shown in Figure 52.

The Square-Corner Partitioning differs in that the matrix is not partitioned into rectangles. We create three partitions, the first being a square located in one corner of the matrix, the second being a square in the diagonally opposite corner, and the third is polygonal, comprised of the balance of the matrix, as seen in Figure 53. On a star topology where the fastest node is the middle node, this partitioning always results in a lower total volume of communication (see Section V-A). The benefit of a more efficient communication schedule further reduces communication time, which in turn drives down total execution time. On a fully connected topology this minimizes the total volume of communication between clusters for a defined range of power ratios (see Section V-B).

This partitioning also allows for a sub-partition of the matrix product to be calculated without any communications needed. When dealing with hardware that has a dedicated communication sub-system, this can further reduce execution time.

As with the two cluster case in Section IV the total volume of communication of the Square-Corner Partitioning approaches the theoretical lower bound as the power ratio between the nodes grows, unlike existing partitionings which have a TVC bounded by a constant or a function that does not approach the theoretical lower bound.

As discussed in Section III the TVC for a rectangular partitioning is proportional to the sum of the half-perimeters $C$ of all partitions, given by Equation 23 (for a unit square)

$$ C = \sum_{i=1}^{p} (h_i + w_i) $$

where $p$ is the number of nodes, and $h_i$ and $w_i$ are the height and width of the rectangle assigned to node $i$, respectively.

Since the perimeter of any rectangle enclosing a given area is minimized when that rectangle is a square, there is a natural lower bound $LB$ for $C$ given by Equation 24, where $a_i$ is the area of the partition belonging to node $i$. 

\[ \text{Fig. 51. Star and Fully Connected topologies for three clusters.} \]

\[ \text{Fig. 52. A Straight-Line Partitioning for three clusters.} \]
As in the case for two clusters, the lower bound cannot always be met by the Straight-Line Partitioning. However as Figure 53 shows, as \( s_2 \) and \( s_3 \) approach 0, the SHP of the Square-Corner Partitioning approaches 2, which is the perimeter of the unit square itself, and therefore optimal. Figure 54 shows the Straight-Line Partitioning and necessary data movements to carry out \( C = A \times B \) on three heterogeneous nodes or clusters.

\[
\sqrt{s_3}
\]

\[
s_3
\]

\[
N
\]

\[
s_1 = N^2 - s_2 - s_3
\]

\[
\sqrt{s_2}
\]

\[\text{Fig. 53. The Square-Corner Partitioning for three clusters.}\]

\[\text{Cluster 1}\]

\[\text{Cluster 2}\]

\[\text{Cluster 3}\]

\[\text{Fig. 54. A two-dimensional Straight-Line Partitioning and data movements required to carry out } C = A \times B \text{ on three heterogeneous nodes or clusters.}\]

\[LB = 2 \times \sum_{i=1}^{P} \sqrt{a_i}\]  
\[
N^2 + N \times q
\]  
\[
(25)
\]

In order to calculate its partition of \( C \), Cluster 1 needs to receive the respective partitions of \( A \) from Clusters 2 and 3, Cluster 2 needs to receive Cluster 3’s partition of \( B \), and part of Cluster 1’s partition of \( A \), and Cluster 3 needs to receive Cluster 2’s partition of \( B \) and the remaining part of Cluster 1’s partition of \( A \), as shown in Figure 54.

If we define the area of Cluster 2’s partition to be \( s_2 \) and Cluster 3’s partition to be \( s_3 \), Equation 25 can be expressed as Equation 26.

\[N^2 + s_2 + s_3\]  
\[
(26)
\]

When dealing with a star topology where Cluster 1 (the fastest cluster) is the middle topologically, the communications between Clusters 2 and 3 must go through Cluster 1. This has the effect of doubling the total volume of communication between Clusters 2 and 3, as all communications between this pair must first be sent to and received by Cluster 1 before the data can be sent on to the recipient node. This raises the TVC to Equation 27.

\[N^2 + 2 \times (s_2 + s_3)\]  
\[
(27)
\]

The Square-Corner Partitioning differs from the Straight-Line (rectangular) partitioning described above by relaxing the restriction that all partitions must be rectangular. We extend the two node partitioning presented in Section IV by creating two square partitions in diagonally opposite corners of the matrix. Since the total volume of communication is proportional to the sum of half perimeters of the partitions, it is easy to show that the sum of half perimeters is at a minimum when the two slower nodes are assigned square partitions. Therefore, the optimal Square-Corner Partitioning assigns the balance of the matrix to the fastest node. Since a square has the smallest perimeter of any rectangle of a given area we do not consider non-square rectangular corner partitions. Figure 55 shows the partitioning scheme used by the Square-Corner Partitioning and the necessary data movements to calculate \( C = A \times B \).

The total volume of communication of the Square-Corner Partitioning is given by Equation 28, where \( s_2 \) and \( s_3 \) are the areas assigned to Clusters 2 and 3 (the two slower clusters).

\[2 \times N \times (\sqrt{s_2} + \sqrt{s_3})\]  
\[
(28)
\]

As Figure 55 shows, Clusters 2 and 3 do not communicate at all, thus the TVC is equal to Equation 28 for both the fully connected and star topology where Cluster 1 is the middle Cluster topologically.

Other similar (but non-Square-Corner) partitioning methods were also investigated. Examples of two partitionings explored are shown in Figure 56. In the Square-Corner Partitioning, diagonally opposite corners are chosen to minimize the number of communication steps necessary as well as for the reasons discussed in Section IV-C. As shown in Figure 55 the number of communication steps is eight. Placing the squares in corners that are not diagonally opposite as in Figure 56.A requires ten communication steps provided \( \epsilon_1 \neq \epsilon_2 \). If \( \epsilon_1 = \epsilon_2 \) the number...
of steps remains at eight. The total volume of communication is still equal to Equation 28 regardless. If the partitions are nested as in Figure 56.B, the number of communication steps is 12 and a higher TVC results. All other (more exotic) partitioning methods investigated resulted in an increased TVC also.

In the Square-Corner Partitioning, the square partitions cannot overlap. This imposes the following restriction on the relative speeds of the clusters:

\[
\frac{s_2}{s_1} \times \frac{s_3}{s_1} \leq \frac{1}{4}
\]

(29)

where \(s_1 + s_2 + s_3 = 1\) and \(s_1\) is the relative speed of the cluster owning the balance of the matrix (the fastest cluster). A consequence of this is that the possible cluster ratios are somewhat limited. Another way of visualizing this is by noting that the areas of \(s_2\) and \(s_3\) cannot overlap. This eliminates certain ratios such as \(1:1:1\).

A. Comparison of Communications on a Star Topology

Since in the Square-Corner Partitioning Clusters 2 and 3 do not have to communicate at all, the total volume of communication on a star where Cluster 1 is the middle cluster remains equal to Equation 28. The Straight-Line Partitioning has a TVC equal to Equation 27. In terms of cluster speeds, the Square-Corner Partitioning has a lower TVC when Inequality 30 is satisfied.

\[
(\sqrt{s_2} + \sqrt{s_3}) < 1.5 - s_1
\]

(30)

where \(s_1 : s_2 : s_3\) is the ratio representing the node speeds, normalized so that \(s_1 + s_2 + s_3 = 1\), and subject to the restriction of Inequality 29.

In order to see when the Square-Corner Partitioning has a lower total volume of communication than the Straight-Line partitioning, we examined the surface

\[
z = (\sqrt{s_3} + \sqrt{s_2}) - 1.5 + s_1
\]

(31)

which represents the Straight-Line Partitioning’s total volume of communication subtracted from that of the Square-Corner Partitioning. Since \(z < 0\) for all positive values of \(s_1, s_2,\) and \(s_3\), the Square-Corner Partitioning always results in a lower total volume of communication.

Additionally, the fact that Cluster 1 must now relay data from Cluster 2 to Cluster 3 and vice-versa introduces a section of the communication schedule that is necessarily serialized in the Straight-Line Partitioning. The Square-Corner Partitioning has no such section and can therefore exploit in full any existing network parallelism.

For the Straight-Line Partitioning, the total volume of communication becomes dependent on which cluster is the middle node topologically, and in turn on the values of \(s_2\) and \(s_3\). These three topologies and their required communications are shown in Figure 57. In the figure, the following are the volumes of each communication:

\[
a + b = N^2 - s_2 - s_3
c = e = s_2
d = f = s_3
\]

The resultant TVCs are shown in Table IV.

In Table IV the TVC for cases where Clusters 2 and 3 are the center nodes topologically are presented as inequalities because it is impossible to separate \(a\) and \(b\) in a general manner. Only their sum (\(a + b = N^2 - s_2 - s_3\)) can be quantified (see Figure 54). Therefore where (\(a + 2 \times b\)) and (\(2 \times a + b\)) appear, only \((a + b)\) is used, thus giving a conservative value for the TVC in these cases.

Note that in Table IV, the TVC calculated for the case where Cluster 1 is the center cluster is equivalent to Equation 27, the TVC calculated in Section V.

For the Square-Corner Partitioning, the total volume of communication is always less when the most powerful cluster (Cluster 1) is the center node. This is shown in Figure 58. Additionally, when Cluster 1 is not the center node, the communication schedule gets more complicated and one side of the network becomes busier than the other. In the figure, the following are the volumes of each communication:

\[
a = h = \sqrt{s_2} \times (N - \sqrt{s_2})
e = d = \sqrt{s_3} \times (N - \sqrt{s_3})
c = g = s_2
b = f = s_3
\]
The three possible star topologies for three clusters using the Straight-Line Partitioning and associated data movements. Labels refer to data movements in Figure 54. Volumes of communication are shown in Table IV.

![Three possible star topologies for three clusters using the Straight-Line Partitioning](image)

### Table IV

<table>
<thead>
<tr>
<th>Center Cluster</th>
<th>TVC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$a + b + c + d + 2 \times e + 2 \times f$</td>
</tr>
<tr>
<td></td>
<td>$= N^2 + 2 \times s_2 + 2 \times s_3$</td>
</tr>
<tr>
<td>2</td>
<td>$a + 2 \times b + c + 2 \times d + e + f$</td>
</tr>
<tr>
<td></td>
<td>$&gt; N^2 + s_2 + 2 \times s_3$</td>
</tr>
<tr>
<td>3</td>
<td>$2 \times a + b + 2 \times c + d + e + f$</td>
</tr>
<tr>
<td></td>
<td>$&gt; N^2 + 2 \times s_2 + 3$</td>
</tr>
</tbody>
</table>

TVC VALUES FOR THE STRAIGHT-LINE PARTITIONING ON THE THREE POSSIBLE STAR TOPOLOGIES SHOWN IN FIGURE 57. LETTERS A - F REFER TO LABELS IN FIGURE 57.

The resultant TVCs are shown in Table V.

Note that in Table V, the TVC calculated for the case where Cluster 1 is the center cluster is equivalent to Equation 28, the TVC calculated in Section V.

### Table V

<table>
<thead>
<tr>
<th>Center Cluster</th>
<th>TVC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$a + b + c + d + e + f + g + h$</td>
</tr>
<tr>
<td></td>
<td>$= 2 \times N \times (\sqrt{s_2} + \sqrt{s_3})$</td>
</tr>
<tr>
<td>2</td>
<td>$2 \times a + b + 2 \times c + d + e + f + 2 \times g + 2 \times h$</td>
</tr>
<tr>
<td></td>
<td>$= 2 \times N \times (2 \times \sqrt{s_2} + \sqrt{s_3})$</td>
</tr>
<tr>
<td>3</td>
<td>$a + 2 \times b + c + 2 \times d + 2 \times e + 2 \times f + g + h$</td>
</tr>
<tr>
<td></td>
<td>$= 2 \times N \times (\sqrt{s_2} + 2 \times \sqrt{s_3})$</td>
</tr>
</tbody>
</table>

TVC VALUES FOR THE SQUARE-CORNER PARTITIONING ON THE THREE POSSIBLE STAR TOPOLOGIES SHOWN IN FIGURE 58. LETTERS A - H REFER TO LABELS IN FIGURE 58.

B. Comparison of Communications of a Fully Connected Topology

On a fully connected topology the Square-Corner Partitioning has a total volume of communication equal to Equation 28 and the Straight-Line partitioning has a total volume of communication equal to Equation 26. In terms of cluster speeds the Square-Corner Partitioning results in a lower total volume of communication when

$$ (\sqrt{s_2} + \sqrt{s_3}) < 1 - \frac{s_1}{2} $$

is satisfied, where again $s_1 : s_2 : s_3$ is the ratio representing the cluster speeds, normalized so that $s_1 + s_2 + s_3 = 1$, and subject to the restriction of Inequality 29.

This inequality shows that the total volume of communication is dependent on the values of $s_2$ and $s_3$ ($s_2$ can be expressed as $1 - s_2 - s_3$). To investigate what values of $s_2$ and $s_3$ result in a lower total volume of communication compared to the rectangular partitioning, we plotted the surface

$$ z = (\sqrt{s_2} + \sqrt{s_3}) - 1 + \frac{s_1}{2} $$

which is negative when the Square-Corner Partitioning’s total volume of communication is less than that of the Straight-Line Partitioning. Figure 59 shows this surface, and Figure 60 shows a contour plot of this surface at $z = 0$. In Figure 60 only the values of $z < 0$ are shown. It is for these values that the TVC of the Square-Corner Partitioning is less than that of the Straight-Line Partitioning.

C. Comparison with the State-Of-The-Art and the Lower Bound

In Section II-D we summarized the work of [4] for the specific case of two nodes or clusters. The authors present
Fig. 59. The surface defined by Equation 33. The Square-Corner Partitioning has a lower TVC for $z < 0$.

where $0 < q < 1$.

The lower bound of the sum of half-perimeters $LB$ is given by Equation 24, and for the case of three nodes is:

$$LB = 2 \times \sum_{i=1}^{p} \sqrt{s_i} = 2 \times (\sqrt{s_1} + \sqrt{s_2} + \sqrt{s_3})$$  (35)

where $s_i$ is the area of the partition belonging to node $i$.

In the case of three nodes, the Square-Corner Partitioning has a sum of half-perimeters equal to Equation 36:

$$\hat{C} = 2 + \sqrt{s_2} + \sqrt{s_3}.$$  (36)

and therefore

$$\lim_{s_2 + s_3 \to 0} \hat{C} = 2$$  (37)

which is equal to the lower bound that cannot be met by the Straight-Line Partitioning.

To compare the Square-Corner sum of half-perimeters with that of the Straight-Line Partitioning and the lower bound, we adopted the same approach as in [4]. We generated 2,000,000 random values for the partition areas $s_2, s_3$ and $s_1 = 1 - s_2 - s_3$, and calculated values for the sum of half-perimeters $\hat{C}$ and the lower bound $LB$. Since we already know that the total volume of communication for the Square-Corner Partitioning (on a fully connected network) is greater for the cases where Equation 33 is positive, we restrict the random areas $s_1, s_2, s_3$ accordingly.

The average sum of half-perimeter to lower bound ratio for the rectangular partitioning is 1.128, while that of the Square-Corner Partitioning is 1.079. Considering that 1.0 is the optimum value, this is an improvement of 38%. The minimum value for the sum of half-perimeter to lower bound ratio for the rectangular partitioning is 1.0595, while that of the Square-Corner Partitioning is 1.0001, an improvement of well over 99%. This also shows that the Square-Corner Partitioning does approach the lower bound which cannot be met by the rectangular partitioning.

In generating 2,000,000 random areas, there are bound to be many that have very large ratios, making them computationally unrealistic. Surely nobody would use two entities in parallel if one of them is slower than the other by an order of hundreds or thousands or greater. We therefore imposed the tighter but more realistic restriction of $s_{\text{max}} / s_{\text{min}} \leq 100$. Even with these much tighter restrictions, the average sum of half-perimeter to lower bound ratio for the rectangular partitioning is 1.104 while that of Square-Corner Partitioning is 1.062, an improvement of 40%. The minimum is improved from 1.059 to 1.008, an improvement of 86%.

D. Overlapping Communications and Computations

The other primary benefit of the Square-Corner Partitioning is overlapping communications and computations. As seen in Figure 55, and in more detail Figure 61, there is a sub-partition $C_1$ of Cluster 1’s $C$ partition which is immediately calculable—no communications are necessary to compute the product of this sub-partition. On an architecture which has a dedicated communications sub-system this quality can be exploited to overlap some communications and computations.
Clusters 1, 2, 3

Partition Communicating

Time = 0

\[ \text{Cluster 1's partition is } (C_1 \cup C_2 \cup C_3). \text{ The sub-partition } C'1 = A_1 \times B_1 \text{ is immediately calculable—no communications are necessary to compute its product.} \]

Fig. 61

4) Optimizing the overlapping of communication and computation could prove difficult and would be platform dependent, unlike other aspects of the Square-Corner Partitioning.

F. HCL Cluster Simulations
To experimentally verify this new partitioning, we implemented matrix multiplications utilizing the optimal Square-Corner Partitioning and the Straight-Line (rectangular) Partitioning in Open-MPI [36]. Local matrix multiplications utilize ATLAS [37]. Experiments were carried out on three identical machines to eliminate contributions of architectural differences. The machines were connected with a full-duplex Ethernet switch that allows the bandwidth between the nodes to be finely controlled.

The ratio of speeds between the three nodes were varied by slowing down CPUs when required using a CPU limiting program as proposed in [2]. This program supervises a specified processes and using the /proc pseudo-filesystem, forces the process to sleep when it has used more than a specified fraction of CPU time. The process is then woken when enough idle CPU time has elapsed for the process to resume. Sampled frequently enough, this provides a fine level of control over the CPU speed. Comparison of the run-times of each node confirmed that this method results in the desired ratios to within 2%.

For simplicity we present results where the speeds of the slower nodes \((s_2 \text{ and } s_3)\) are equal. We varied this relative value from 5 to 25, where \(s_1 = 100 - s_2 - s_3\). Network bandwidth is 100Mb/s, and \(N = 5,000\).

Fig. 64 shows the communication times for the Square-Corner and Straight-Line Partitionings on a star topology. The Square-Corner Partitioning has a lower communication time than the Straight-Line Partitioning in all cases. On average the Square-Corner Partitioning results in a reduction in communication time of approximately 40%.

Fig. 62. Overlapping Communication and Computation from an execution-time point of view.

\[ \text{Calculating } C_2 \text{ and } C_1 \text{ is immediately calculable—no communications are necessary to compute its product.} \]

\[ s_1 = s_{1A} + s_{1B}. \]
The introduction of overlapping communication and computation significantly influences the performance of the Square-Corner Partitioning. For a ratio of $90:5:5$ it is 38% faster than the rectangular partitioning. As the ratio approaches $50:25:25$, the amount of overlap possible approaches zero, and the execution times of the Square-Corner Partitioning with and without overlap converge.

Figure 66 shows the communication times for the fully connected topology. A notable aspect is that the Straight-Line Partitioning’s communication times decrease despite the fact that it is dealing with increasingly higher communication volumes. The reason for this is that the total volume of communication for this partitioning increases much slower than that of both the Straight-Line Partitioning on the star and the Square-Corner Partitioning. It increases so much slower that the increased benefit of more computational parallelism (as $s_2$ and $s_3$ get closer to $s_1$) outweighs the higher communication burden. Still, for ratios more heterogeneous than about $80:10:10$, the Square-Corner Partitioning has a lower total volume of communication, and therefore lower communication times.

Figure 67 shows the overall execution times for the Square-Corner and Straight-Line Partitionings on a fully connected topology. Again the Square-Corner partitioning is shown with and without overlapping. Again, without overlapping the execution times are directly affected by the communication times. For ratios more heterogeneous than about $80:10:10$, the Square-Corner Partitioning out performs the Straight-Line. The introduction of overlapping again significantly influences the performance of the Square-Corner Partitioning. For a ratio of $90:5:5$ the Square-Corner Partitioning is 30% faster than the rectangular. Additionally, the range of ratios where the Square-Corner Partitioning is faster than the rectangular is broadened from about $80:10:10$ to about $60:20:20$. Similar results were seen at other bandwidths, values of $N$, and power ratios, including where $s_2 \neq s_3$.

### G. Grid’5000 Experiments

To experiment with the Square-Corner Partitioning on a large scale, geographically distributed scientific computing
platform we chose three sites on Grid’5000, arranged in a star. Actually it is not the physical topology but the fact that the Square-Corner Partitioning forces Clusters 2 and 3 to communicate through Cluster 1 that “creates” the star topology.

We chose the sites Orsay, Rennes, and Sophia. Orsay was chosen as the center cluster (Cluster 1) as it has the greatest overall power. The desired power ratios were achieved by varying the number of CPUs and cores used at each site. It was not always possible to achieve perfect ratios but they were achieved within a few percent. To determine relative power ratios, test code consisting of serial matrix matrix multiplications were carried out on each type of machine.

Figure 68 shows the communication times for the Square-Corner and Straight-Line Partitionings. Both curves tend towards higher communication times with higher ratios (and therefore increased parallelism). This is attributed to the increase in the TVC with increased ratios. Instability in the results could be due to shared communication links between sites. In addition, we noticed that in a large multi-user environment, network traffic serves to affect the communication of each partitioning without discrimination, unlike in simulations where only one user is allowed to fully exploit or fully saturate one communication link. In the latter scenario it is clear that the partitioning with a higher TVC will saturate a link before one with a lower TVC.

Figure 69 shows the corresponding execution times. As the power ratio between clusters increases, so does parallelism. It seems that the links between sites are fast enough for the increased parallelism to decrease overall execution time despite a higher TVC. The inter-site bandwidth is 10Gb/s, however this does not take into account links internal to each site running at different speeds which do represent a possible bottleneck.

In all cases the Square-Corner Partitioning had a lower TVC, lower communication time, and lower execution time than the Straight-Line Partitioning.

H. Conclusion

We have extended the Square-Corner Partitioning from the two cluster scenario in Section IV to three interconnected clusters. This partitioning has two advantages over existing partitionings. First it reduces communication time due to a lower total volume of communication and a more efficient communication schedule. The total volume of communication is shown to approach the known lower bound unlike existing partitionings. Second it allows for the overlapping of communication and computation.

To determine the viability of this partitioning we modeled the three cluster topology with three processors performing matrix matrix multiplications. Compared to more general partitionings which result in simple Straight-Line Partitionings, the Square-Corner Partitioning is shown to reduce the total volume of communication in all cases for the star topology and in most cases for a fully connected topology. We experimentally show that this directly translates to lower communication times. In the case of the star topology, we show average reductions in communication time of about 40%.

Further experimentation shows that this reduction in communication time directly translates to a reduction in the overall...
execution time, aided by a more efficient communication schedule. Overlapping communication and computation brings further benefit, in both reducing the execution times significantly, and broadening the ratio range where the Square-Corner Partitioning outperforms the Straight-Line Partitioning on a fully connected topology. MPI experiments demonstrate reductions in execution times of up to 38%.
VI. APPLICATIONS: MAX-PLUS ALGEBRA AND DISCRETE EVENT SIMULATION ON PARALLEL HIERARCHAL HETEROGENEOUS PLATFORMS

In this section we demonstrate possible areas of application for the Square-Corner Partitioning and the theoretical results of this report. We do this by exploring computing max-plus algebra operations and discrete event simulations on parallel hierarchal heterogeneous platforms. When performing such tasks on heterogeneous platforms parameters such as the total volume of communication and the top-level data partitioning strategy must be carefully taken into account. Choice of the partitioning strategy is shown to greatly affect the overall performance of these applications due to different volumes of inter-partition communication that various strategies impart on these operations. Max-plus algebra is regularly used in discrete event simulations and many other important computational applications thus warranting the exploration of and improvement upon the running times of basic max-plus operations on parallel platforms which are inherently hierarchal and heterogeneous in nature. The main goal of this section is to present benefits waiting to be exploited by the use of max-plus algebra operations on these platforms and thus speeding up more complex and quite common computational topic areas such as discrete event simulation.

Here we present results of running fundamental max-plus algebra (MPA) operations and discrete event simulations (DES) on parallel hierarchal heterogeneous platforms. The top-level data partitioning strategy is shown to greatly affect the overall performance of these applications due to different volumes of inter-partition communication that various strategies impart on these operations. The Square-Corner Partitioning in particular is shown to reduce the execution times of these operations more than other, more traditional strategies.

Max-plus algebra is a relatively new field in mathematics, dating back approximately 30 years. It has since been shown to have several application areas such as discrete event simulation, dynamic programming, finite dimensional linear algebra, modeling communication networks, operating systems, combinatorial optimization, solving systems of linear equations, biological sequence comparisons and even problems such as crop rotation [38]–[42]. In many scientific and computational applications the structure of MPA matrix multiplication is an important aspect [43]. Additionally, higher powers of MPA matrices are of significant interest and necessary in many application areas [38], [44].

MPA is based on replacing the “normal” algebraic addition operation with a binary max function, and the “normal” multiplication operation with addition. Formally, if we define \( \epsilon = -\infty \), \( e = 0 \), and denote \( R_{\text{max}} \) to be the set \( \mathbb{R} \cup \{ \epsilon \} \), then for elements \( a, b \in R_{\text{max}} \), the operations \( \oplus \) and \( \otimes \) are defined respectively by the following:

\[
a \oplus b \defeq \max(a, b) \quad \text{and} \quad a \otimes b \defeq a + b \quad (38)
\]

Therefore, \( a \oplus \epsilon = \max(e, a) = a \) and \( a \otimes \epsilon = e + a = e \).

We can now formally define max-plus algebra as

\[
R_{\text{max}} = (R_{\text{max}}, \oplus, \otimes, \epsilon, e) \quad (39)
\]

The basic algebraic rules of max-plus algebra are:

- **Associativity**
  \[
  (A \oplus B) \oplus C = A \oplus (B \oplus C)
  \]
  \[
  (A \otimes B) \otimes C = A \otimes (B \otimes C)
  \]

- **Commutativity**
  \[
  A \oplus B = B \oplus A
  \]

- **Distributivity**
  \[
  (A \oplus B) \otimes C = A \otimes C \oplus B \otimes C
  \]

In general the \( \otimes \) operation has precedence over the \( \oplus \) operation.

MPA matrices are denoted \( R_{\text{max}}^{m \times n} \), where \( m \) and \( n \) are the matrix dimensions. For the MPA matrices \( A \in R_{\text{max}}^{m \times n} \) and,
B. Discrete Event Simulation

Discrete event simulation is a very broad and well-studied field and therefore the purpose of this section is to acquaint the reader with the specific technique utilized in this section. Briefly, DES is a collection of techniques and methods which when applied to the study of a discrete-event dynamical system generates sequences which characterize the system behavior. This includes modeling concepts for abstracting essential features of the system into a set of precedence and mathematical relationships, which can be used to describe the system and more importantly for design, and to predict its behavior, performance, and drawbacks/bottlenecks. For more see any good DES text such as [45].

As most DES algorithms are computationally intensive, efforts to parallelize them are numerous. The complexity of most practical DES algorithms however poses numerous obstacles in effective and efficient parallelization. Amongst these are synchronization and timing inconsistencies, synchronous vs. asynchronous simulation, deadlock avoidance and detection, conservative vs. optimistic simulation, recovery strategies, and memory management to name a few [46].

In Section VI-F we present results of the parallelization of a DES modeling technique which although as presented in [42] is sequential, lends itself to parallelization due to a computationally intensive algorithmic core which can be efficiently ported to hierarchal heterogeneous parallel platforms. This core is very similar to a max-plus matrix multiplication, but using logical ‘and’ and ‘or’ operations instead of max-plus operations. We employ this technique—called the Matrix Discrete Event Model (MDEM)—using MPI and utilizing the SCP [9], [10] for the core routine.

C. The Matrix Discrete Event Model

The design, simulation, and analysis of large-scale, complex systems using existing DES techniques such as Petri nets, alphabet-based approaches, perturbation methods, control theoretic techniques, and expert systems design are often difficult to implement and are very labor and time intensive. The MDEM is a hybrid system with logical and algebraic components that seeks to make these processes more efficient. Although the examples in [42] focus on manufacturing systems (see Figure 70), the formulation is also applicable to many DES situations such as travel timetables, operating systems, autonomous guided vehicles, operating systems, and many others. Clearly the number of degrees of freedom, state possibilities, and general complexity of such systems often result in simulations with several thousands (or more) event components.

The MDEM approach is a rule-based model described by four equations: the Model State Equation, Start Equation, Resource Release Equation, and the Product Output Equation: Matrix Discrete Event Model State Equation:

\[
\pi = F_v \times \pi_c + F_r \times \pi_c + F_u \times \pi + F_D \times \pi_D
\]

(40)

Start Equation:

\[
v_s = S_v \times x
\]

(41)

Resource Release Equation:

\[
r_s = S_r \times x
\]

(42)

Product Output Equation:

\[
y = S_y \times x
\]

(43)

Each of these equations are logical, only using or, and, and negation operations. Additionally, all vectors and matrices in these equations are binary. For instance, the vector which is the output of the start equation contains a ‘1’ for each job which is to be started at the given state of the simulation, and a ‘0’ otherwise.

The simulation itself is carried out by first calculating initial conditions from the description of the system. The core of the simulation is carried out by the successive calculation of ‘firing vectors’ which carry the simulation to the next state. This amounts to the repeated calculation of an equation which has the form of a matrix matrix multiplication except that since the approach of the MDEM technique is hybrid—having both algebraic and logical components—the algebraic multiplication and addition operations are replaced with logical ‘or’ and ‘and’ operations respectively. It is this step that constitutes the bulk of the calculation time for the MDEM technique as all other calculations only need to be carried out once.

D. MPI Experiments

In this section we present results of performing MPA matrix matrix multiplications and an MDEM discrete event simulation utilizing both the Square-Corner Partitioning and the Straight-Line Partitioning. Hardware setup is similar to that in Section IV-J, only differing in power ratios.
Communication Time (s)

Fig. 71. Comparison of the total communication times for the square-corner and straight-line partitionings for power ratios ranging from $1 : 1 - 6 : 1$. Max-Plus MMM, $N = 7,000$.

Communication Time (s)

Fig. 72. Comparison of the total execution times for the square-corner and straight-line partitionings for power ratios ranging from $1 : 1 - 6 : 1$. Max-Plus MMM, $N = 7,000$.

worth noting that the execution time is higher than was initially expected but this is due to the lack of an optimizing library for MPA MMM, unlike normal MMM which can benefit from the \texttt{dgemm} routine in the BLAS [47], and ATLAS [37]. It is worth noting that since carrying out a matrix power operation $A^n$ amounts to nothing more than $n$ repeated matrix multiplications, carrying out matrix power operations would also benefit from the above.

\section*{F. The Square-Corner Partitioning for Discrete Event Simulation}

In Section VI-B we outlined the MDEM model for discrete event simulations. We use the same experimental platform as in Section VI-E to demonstrate results on a parallel, heterogeneous platform of the MDEM model. We utilize both the SLP and the SCP for the core routine which is a matrix “and/or” multiplication. We generate the initial conditions so that the core routine involves a large system ($N = 7,000$). All initial calculations and cleanup are carried out on a single processor as these calculations are carried out only once and make up a small percentage of the overall execution time and are not parallelizable.

Figure 73 shows the communication times which are relatively low due to the use of \texttt{char} as the data type (all data is binary). Due to the nature of the MDEM all communications are serialized. The results overall agree with theory, with the $3 : 1$ ratio crossover occurring. Figure 74 shows the execution times for carrying out the described DES using both partitioning techniques. It can be seen that the use of the SCP for the core kernel of the MDEM DES algorithm significantly reduces the execution time for ratios above $3 : 1$, but less so due to the lower communication time compared to the MPA MMM. Again the expected crossover occurs near the ratio of $3 : 1$. The overall shape of the curves are similar to those of Section VI-E as the “and/or” MMM in the MDEM involves a similar computational cost as the max-plus MMM.

\section*{G. Conclusion}

In this section we explored computing max-plus algebra matrix operations and a MDEM discrete event simulation on
parallel hierarchal heterogeneous platforms. We found that the initial top-level data partitioning—particularly the use of the square-corner partitioning—significantly affects overall execution time due to the total volume of inter-cluster communication involved. Notably the square-corner partitioning out performed the straight-line partitioning in all cases where the power ratio between clusters was $\geq 3 : 1$. Future work involves applying similar strategies to speed up more complex routines, perhaps with more complicated and heavyweight communication loads, on parallel hierarchal heterogeneous platforms and experimenting on other parallel hierarchal heterogeneous networks.

Fig. 74. Comparison of the total execution times for the MDEM DES model for both the square-corner and straight-line partitionings, $N = 7,000$. 
VII. MOVING AHEAD – MULTIPLE PARTITIONS AND RECTANGULAR MATRICES

We have seen in Sections III - VI that the Square-Corner Partitioning proves to have a lower total volume of communication and a lower execution time than the Straight-Line Partitioning in many cases for two and three partitions. The question is, can the Square-Corner Partitioning be extended to more than three partitions? We have gained some insight into this question based on the investigation into partition configurations such as those in Figure 75.

Configurations such as those in Figure 75 are not possible extensions of the Square-Corner Partitioning for three partitions. This is due to an increase in the number of communication steps and/or the TVC that violate the definition of the Square-Corner Partitioning. We conclude therefore that similar configurations would not be suitable for a number of partitions greater than three as well. The only configuration we see viable for an extension to four partitions is one such as that in Figure 76.

Moving beyond four partitions, the Square-Corner Partitioning takes on a “diagonal” form such as that in Figure 77. This is because the Square-Corner Partitioning was designed to have as simple a structure as possible, and any other configuration has the possibility of violating the definition of a Square-Corner Partitioning. We conclude therefore that similar configurations would not be suitable for a number of partitions greater than three as well. The only configuration we see viable for an extension to four partitions is one such as that in Figure 76.

Fig. 75. Examples of non-Square-Corner Partitionings investigated.

Fig. 76. An example of a four partition Square-Corner Partitioning

Fig. 77. An example of a multiple partition Square-Corner Partitioning

square partitions completely bisect the matrix being partitioned, in which case the two pieces formed (lower-left and upper-right in Figure 77) will represent one logical partition, as they are owned by the same cluster.

1) Two non-square partitions may be created only in the cases such as that depicted in Figure 77, where

2) No square partitions may communicate with each other. In other words no two square partitions can interrupt the same row or column.

3) Maintain a one-to-one mapping between clusters and (logical) partitions

4) Map (logical) partitions to clusters so that the area of partition $s_i$ is proportional to the speed of cluster $c_i$, where $s_i \in (s_1, s_2, \ldots, s_p)$ where $p$ is the number of partitions and $s_i$ are the areas of the partitions in non-decreasing order, and $c_i \in (c_1, c_2, \ldots, c_p)$ where $c_i$ are the clusters being mapped in non-decreasing order of relative speed.

5) Partition all matrices $A, B, C$ in the same way.

Clearly as the number of clusters (and therefore partitions) increases the number of possible network topologies will increase as well. It is believed that restricting the number and types of topologies will increase the performance of the Square-Corner Partitioning relative to Straight-Line (rectangular) partitionings in many cases.

A. The Square-Corner Partitioning for Partitioning Rectangular Matrices

In order to be as general as possible we are interested in the applicability of the Square-Corner Partitioning to rectangular matrices, not just the restricted case of square matrices. It is believed that the popular test case of the unit square is fitting for rectangular matrices because any partitioning that is optimal on the unit square can be scaled to a rectangle and remain optimal [35].

We will begin in the most general case. We assume only two clusters, each owning one partition. As always each partition has an area proportional to the speed of the cluster which owns it. We then create two partitions, one partition is a rectangle located in any corner of the matrix, and the other partition is polygonal—the rest of the matrix with the area of the first partition removed from it.

To make the case as general as possible we start with a real-valued rectangular area and partition it into two by creating a real-valued rectangular partition within the area. We place three restrictions on this system.
There are two partitions to be created. This necessitates defining only one interior partition, as the other partition will be the area which lies outside the partition defined but inside the rectangular area being partitioned.

- The area to be partitioned and the interior partition are rectangular.
- The area of the two partitions are proportional to the speeds of the clusters owning them.

This gives us a rectangular area of dimension \(x \times y\) and an interior rectangular partition \(\alpha \times \beta\) as in Figure 78.

![Diagram](image)

**Fig. 78.** An example of a rectangular matrix with one rectangular \((\alpha \times \beta)\) partition and one polygonal \((x \times y - \alpha \times \beta)\) partition.

In Section IV we showed that the TVC was minimized when the area equal to the following was minimized:

\[
\text{height of small partition} \times \text{width of matrix} + \text{width of small partition} \times \text{height of matrix}
\]

In Figure 78, this is represented by the shaded area, which equates to \(\Gamma\) below:

\[\Gamma = \alpha \times y + \beta \times x\]  \hspace{1cm} (44)

**Proposition 7.1:** \(\Gamma = \alpha \times y + \beta \times x\) is minimized when the dimensions of the rectangular partition \(\beta \times \alpha\) is scaled to the matrix \(x \times y\) such that \(\frac{\alpha}{\beta} = \frac{y}{x}\).

**Proof:** We will prove Proposition 7.1 by showing that whenever the small partition is not scaled as stated, \(\Gamma\) will always be larger.

Equation 45 describes the state when the rectangular partition is not scaled, i.e. when its height \(\alpha\) is decreased by some quantity \(c < \alpha\), and its width \(\beta\) increased by some other quantity \(c' > \beta\), while maintaining the same area \(\alpha \times \beta\).

\[\alpha \times \beta = (\alpha - c)(\beta + c')\]  \hspace{1cm} (45)

We determine \(c'\) (for simplification later), then we start with the equation for \(\Gamma\), but substitute in the values on the RHS of Equation 45. We then have a function \(S(c)\) which represents the new system, including the non-scaled partition, where \(c\) is the amount that the previously scaled partition has been changed by. Note that a function in terms of only \(c\) is satisfactory as \(c\) is proportional to \(c'\). We show that when \(c = 0\), \(\frac{dS}{dc} = 0\), and that at this point \(\frac{d^2S}{dc^2}\) is positive. It is then shown that any change in \(c\), either positive or negative, will increase \(\Gamma\) (within the definition of the problem), thus concluding the proof.

\[
\begin{align*}
\alpha \times \beta &= \alpha \times \beta + \alpha \times c' - c \times \beta - c \times c' \\
c \times \beta &= \alpha \times c' - c \times c' \\
c \times \beta &= c' (\alpha - c) \\
c' &= \frac{c \times \beta}{\alpha - c} \\
\Gamma &= x \times \beta + y \times \alpha \\
S(c) &= x(\beta + c') + y(\alpha - c) \\
&= x \times \beta + x \times c' + y \times \alpha - y \times c \\
&= x \times \beta + \frac{x \times c \times \beta}{\alpha - c} + y \times \alpha - y \times c
\end{align*}
\]

\[
\frac{dS}{dc} = \frac{x \times \alpha \times \beta}{(\alpha - c)^2} - y
\]

\[
= \frac{x \times \alpha \times \beta}{\alpha^2 - 2 \times \alpha \times c + c^2} - y
\]

\[
= \frac{x \times \alpha \times \beta - y \times \alpha^2 + 2 \times \alpha \times c \times y - y \times c^2}{x}
\]

\[
= \frac{2 \times \alpha \times c \times y - y \times c^2}{x} \quad \text{when } c = 0, \frac{dS}{dc} = 0
\]

\[
\begin{align*}
\frac{d^2S}{dc^2} &= \frac{2 \times \alpha \times y - 2 \times c \times y}{x} \\
&= 2 \times y(\alpha - c)
\end{align*}
\]

\(c \overset{def}{=} \frac{d^2S}{dc^2}\) is positive

It must now be shown that for any \(c > 0\), \(\frac{d^2S}{dc^2}\) is positive, and that for any \(c < 0\), \(\frac{d^2S}{dc^2}\) is negative, to show that the minimum in \(\frac{d^2S}{dc^2}\) when \(c = 0\) is not a local, but a global minimum.

\[
\begin{align*}
\frac{d^2S}{dc^2} &= 2 \times \alpha \times c \times y - y \times c^2 \\
&= c \times y \times (2 \times \alpha - c)
\end{align*}
\]

\(\therefore\) when \(c\) is positive, \(\frac{d^2S}{dc^2}\) is positive

and when \(c\) is negative, \(\frac{d^2S}{dc^2}\) is negative

**Q.E.D.**

Thus we have proven that the area \(\Gamma = \alpha \times y + \beta \times x\) is a minimum when the rectangular partitioning \(\alpha \times \beta\) is scaled so that \(\frac{\alpha}{\beta} = \frac{y}{x}\), but does minimizing \(\Gamma\) minimize the total volume of communication when we are multiplying non-square matrices? The answer is no, as we will see in the next section.

**B. The Square-Corner Partitioning for MMM on Rectangular Matrices**

Figure 79 shows that the TVC is at a minimum when we are dealing with a rectangular matrix matrix multiplication as opposed to partitioning a rectangular matrix

\[\alpha \times n + \beta \times n = n \times (\alpha + \beta)\]  \hspace{1cm} (46)

where \(n\) is one of the three given matrix dimensions, where a \(m \times n\) matrix multiplied by a \(n \times p\) matrix results in a \(m \times p\)
product, and \( \alpha \times \beta \) is the area of the partition placed in the corner of the rectangular matrices.

**Proposition 7.2:** The TVC \( n \times (\alpha + \beta) \) for a multiplication of three rectangular matrices \( C = A \times B \) is minimized when \( \alpha = \beta \), that is when the partition of area \( \alpha \times \beta \) is a square, provided \( \alpha = \beta < m, n, p \) where \( A \) has dimensions \( m \times n \), \( B \) has dimensions \( n \times p \) and \( C \) has dimensions \( m \times p \).

**Proof:** \( n \) is a given constant, therefore the goal is to minimize \( \alpha + \beta \), where \( \alpha \times \beta \) is a constant. Since \( \alpha + \beta \) is proportional to the perimeter of the rectangle with area \( \alpha \times \beta \), and the perimeter of any rectangle of a constant given area is minimized when that rectangle is a square, we conclude that \( \alpha = \beta \).

It is interesting to note that the TVC only depends on one matrix dimension, \( n \), which is the only matrix dimension that does not feature in the product matrix \( C \). (\( n \) only possibly affects the values of the elements of \( C \).) We can conclude that minimizing the SHP on a unit square, then scaling that square to a rectangle does not necessarily minimize the TVC of a matrix matrix multiplication involving that rectangle. This topic area demands further investigation particularly what to do in the case where \( \alpha = \beta \) are \( > m, n \), and/or \( p \).
VIII. CONCLUSIONS AND FUTURE WORK

The current state and foreseeable future of high performance scientific computing can be described in three words: heterogeneous, parallel and distributed. These three simple words have a great impact on the architecture and design of HPC platforms and the creation and execution of algorithms and programs designed to run on them. We have seen that heterogeneity and hierarchy have infiltrated every aspect of computing from supercomputers, GPUs and cloud computing down to individual processors and cores. We have also seen that in many, many ways all of these technologies are interwoven and joined to form hybrid entities themselves. As a result of the inherent heterogeneity, parallelism and distribution which promises to continue to pervade scientific computing in the coming years the issue of data distribution is unavoidable. This, combined with a lack of research into the area of parallel computing on small numbers of (possibly powerful) heterogeneous computing entities provided us with our motivation.

This report presented a new top-level data partitioning algorithm, the Square-Corner Partitioning, for matrix and linear algebra operations. This partitioning was designed from the outset to be parallel and heterogeneous, not relying on homogeneous counterparts as a starting point. In practice this partitioning distributes data between a small number of clusters (each of which can have great computational power in themselves) in a hierarchical manner, which allows it the flexibility to be employed in a great range of problem domains and computational platforms. This partitioning minimizes the total volume of communication between clusters in a manner proven to be optimal for a great range of cluster power ratios, thus minimizing overall execution time. In a hybrid form, working with existing partitionings, the total volume of communication can be minimized regardless of the power ratio that exists between the clusters. It also places no restriction on the algorithms or methods employed on the clusters themselves locally, thus maximizing flexibility.

The Square-Corner Partitioning is shown to have several advantages over more traditional Straight-Line (rectangular) partitionings, not only reducing the total volume of communication in an optimal manner, but allowing the overlapping of communication and computation, and necessitating fewer communication steps.

This partitioning was compared to the state-of-the-art theoretically and experimentally. Both its benefits and deficits were discussed and demonstrated. The Square-Corner Partitioning showed to be beneficial in performing matrix matrix multiplications in several scenarios:

- Two processor MMM
- Small two cluster MMM
- Large two cluster MMM
- Three processor MMM
- Large three cluster MMM

The Square-Corner Partitioning was experimentally shown to be applicable to non-square matrix matrix multiplications and minimizing the total volume of communication in this most general realm of matrix computation. Additionally it is shown to be extendable to more than three clusters.

Most heterogeneous algorithms and partitionings are designed by modifying existing homogeneous ones. With this in mind the last goal of this report was to demonstrate that non-traditional and perhaps unintuitive algorithms and partitionings designed with heterogeneity in mind from the start can result in better, and in cases optimal, algorithms and partitionings for heterogeneous platforms. The importance of this given the current outlook for, and trends in, the future of high performance scientific computing is obvious.

Future work precipitating from the work in this report include the following:

- Experiment with the Square-Corner Partitioning on more platforms and architectures, possibly including Grid Ireland.
- Optimize the overlapping of communication and computations while remaining within the bounds of the Square-Corner definition.
- Experiment with the possible benefits of the Square-Corner Partitioning on low-level architectures such as multi-core processors.
- Apply the Square-Corner Partitioning to more complex linear algebra routines and applications with more complex and heavy weight communication schedules and volumes.
- Experiment with the Square-Corner Partitioning on non-square matrix systems and operations.
- Experiment with more than three partitions to determine what configurations can reduce the TVC and under what conditions this occurs.
- Develop fully the Hybrid Square-Corner Partitioning concept.
- Apply the Square-Corner Partitioning to sparse matrix systems.
- Investigate partitionings for matrix matrix multiplication on non-square matrices as discussed in Section VII-B.
- Explore the role of the Square-Corner Partitioning as well as other novel partitioning algorithms in the domain of cloud computing.
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