PARALLEL AND DISTRIBUTED COMPUTING
TECHNIQUES IN BIOMEDICAL ENGINEERING

CAO YIQUN

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Declaration

The experiments in this thesis constitute work carried out by the candidate unless otherwise stated. The thesis is less than 30,000 words in length, exclusive of tables, figures, bibliography and appendices, and complies with the stipulations set out for the degree of Master of Engineering by the National University of Singapore.

Cao Yiqun

Department of Electrical and Computer Engineering
National University of Singapore
10 Kent Ridge Crescent, Singapore 119260
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Abstract

Biomedical Engineering, usually known as Bioengineering, is among the fastest growing and most promising interdisciplinary fields today. It connects biology, physics, and electrical engineering, for all of which biological and medical phenomena, computation, and data management play critical roles. Computation methods are widely used in the research of bioengineering. Typical applications range from numerical modelling and computer simulations, to image processing and resource management and sharing. The complex nature of biological process determines that the corresponding computation problems usually have a high complexity and require extraordinary computing capability to solve them.

Parallel and Distributed computing techniques have proved to be effective in tackling the problem with high computational complexity in a wide range of domains, including areas of computational bioengineering. Furthermore, recent development of cluster computing has made low-cost supercomputer built from commodity components not only possible but also very powerful. Development of modern distributed computing technologies now allows aggregating and utilizing idle computing capability of loosely-connected computers or even supercomputers. This means employing parallel and distributed computing techniques to support computational bioengineering is not only feasible but also cost-effective.

In this thesis, we introduce our effort to utilize computer cluster for 2 types of computational bioengineering problems, namely intensive numerical simulations of...
fiber suspension modelling, and multiple-frame laser speckle image processing. Focus has been put on identifying the main obstacles of using low-end computer clusters to meet the application requirements, and techniques to overcome these problems. Efforts have also been made to generate easy and reusable application frameworks and guidelines on which similar bioengineering problems can be systematically formulated and solved without loss of performance.

Our experiments and observations have shown that, computer clusters, and specifically those with high-latency interconnection network, have major performance problem in solving the 2 aforementioned types of computational bioengineering problems, and our techniques can effectively solve these problems and make computer cluster successfully satisfy the application requirements. Our work creates a foundation and can be extended to address many other computationally intensive bioengineering problems. Our experience can also help researchers in relevant areas in dealing with similar problems and in developing efficient parallel programs running on computer clusters.
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Chapter 1 Introduction

The domain of this research is effectively utilizing parallel and distributed computing technologies, especially computer clusters, to support computing demands in biomedical research and practice. Two typical computational problems in bioengineering field are numerical simulation, which is very common in research in computational fluid dynamics; and biomedical image processing, which is increasingly playing an essential role in research in diagnostic and clinical experiments. The complexity of biological systems imposes severe requirements on computing power and latency on both types of problems.

Parallel computing promises to be effective and efficient in tackling these computation problems. However, parallel programming is different from and far more complex than conventional serial programming, and building efficient parallel programs is not an easy task. Furthermore, the fast evolution of parallel computing implies algorithms to be changed accordingly, and the diversity of parallel computing platforms also requires parallel algorithms and implementations to be written with consideration on underlying hardware platform and software environment for research issues in bioengineering.

In this thesis, we investigate how to effectively use the widely-deployed computer cluster to tackle the computational problems in the aforementioned two
types of bioengineering research issues: numerical simulations of fiber suspension modelling, and laser speckle image processing for blood flow monitoring. Computer cluster imposes several challenges in writing efficient parallel programs for those two types of applications, in terms of both coding time and run-time efficiencies. For instance, relatively larger communication latency may hinder the performance of parallel programs running on computer cluster, and it would be desirable if programmers can optimize the communication by hand; however, that extra work would make the programming task less systematic, more complex, and error prone. We introduce several techniques to deal with these general problems of run-time performance, which may widely present in other bioengineering applications. Methods to reduce the programming task and to allow programmers to focus more on computation logic are also proposed.

1.1 Motivation

Fundamental biology has achieved incredibly significant advancement in the past few decades, especially at the molecular, cellular, and genomic levels. This advancement results in dramatic increase in fundamental information and data on mechanistic underpinnings of biological systems and activities. The real challenge is now how to integrate information from as low as genetic levels to high levels of system organization. Achievement of this will help both scientific understanding and development of new biotechnologies. Engineering approaches - based on physics and chemistry and characterized by measurement, modelling, and manipulation - have been playing an important role in the synthesis and integration of information. The
combination of biological science research and engineering discipline has resulted in the fast growing area of biomedical engineering, which is also known as bioengineering.

Of the many methods of engineering principles, computational and numerical methods have been receiving increasing emphasis in recent years. This is mainly because of its physics and chemistry root, as well as the recent advancement of computing technologies, which makes complex computation feasible, cost-efficient and less time-consuming. As a result, computational bioengineering, which employs computational and numerical methods in bioengineering research and industry, has experienced fast adoption and development in the last few years.

The complex nature of biological system contributes to the large computation complexity of these problems. Another important characteristic is the distribution of data and instruments. These together inspire the use of parallel and distributed computing in computational bioengineering. With this computing technique, a single large-scale problem can be solved by dividing into smaller pieces to be handled by several parallel processors, and by taking advantage of distributed specialized computation resources, such as data sources and visualization instruments.

However, there are several challenges involved in using parallel and distributed techniques in computational bioengineering. Firstly, efficient programs utilizing parallel and distributed technique are far from easy development, especially for medical doctors and practitioners whose trainings are not computer programming. This is because programmers of parallel and distributed system, in addition to specifying what values the program computes, usually need to specify how the machine should organize the computation. In other words, programmers need to make
decision on algorithms as well as strategies of parallel execution. There are many aspects to parallel execution of a program: to create threads, to start thread execution on a processor, to control data transfer data among processors, and to synchronize threads. Managing all these aspects properly on top of constructing a correct and efficient algorithm is what makes parallel programming so hard.

When a computer cluster, the most popular and accessible parallel computing facility, is used as the hardware platform, the relatively larger communication latency is a further obstacle in achieving high performance. Practical experience usually shows a threshold of the number of processors, beyond which the performance starts degrading with larger number of processors.

Another important performance criterion, especially for clinical applications, is whether a system is capable of supporting real-time operation. When this is concerned, in addition to computing capacity, latency or lag, defined as the time it takes to get the result after the input is available for the processing system, imposes further performance requirements. When parallel computing is used, the coordination among participating processors, although increases the computing capacity, will result in larger latency.

There is also the challenge from the fact that biomedical engineering is a fast evolving field, with dozens of methods available for each task, and with new methods invented every day. It would be desirable to separate the computational logic from the supporting code, such as thread creation and communication. Parallel processing also complicates this task and computational logic is often tightly coupled with supporting code, making it difficult for non-computer experts to customize the methods to use.
Based on the aforementioned observations, the main research objectives of this thesis are summarized as follows:

- Identify typical performance bottlenecks, especially when common hardware platforms and software environments are used and when typical computational bioengineering applications are concerned;

- Derive methods to solve the above performance problems, without largely complicating the programming task, to introduce complex tools, or to add more overhead;

- Derive methods to achieve real-time processing for specific biomedical application. These methods should be scalable to larger problem size or higher precision of results; and

- Derive methods to achieve core computational logic customizability. This is the best way to reduce programming workload of non-computer medical personnals facing similar programming tasks.

1.2 Thesis Contributions

Our research activities are based on two representative computational bioengineering applications, namely numerical simulations of fiber suspension modelling, and laser speckle image processing for blood flow monitoring. We study how high-performance parallel programs can be built on computer clusters for these applications, with consideration of the special characteristics of this platform.
Fiber suspension simulation is a typical numerical simulation problem similar to N-body problem. Parallel processing technique is used to support larger domain of simulation and thus provides more valid results. With specific problem scale, parallel processing will largely reduce time to acquire simulation result. A computer cluster will be used to perform the computing task. Parallelization is accomplished by spatial decomposition. Each spatial subdomain will be assigned to a parallel process for individual simulation. Neighboring subdomains usually have interactions and need to exchange data frequently. The need for data exchange implies that communication latency will be a significant factor in affecting the overall performance. The idea of using parallel computing to solve this type of problems is not new. However, there is little research done on identifying the bottleneck of performance improvement and optimizing the performance on computer cluster platform. In our research, theoretical analysis, simulations and practical experiments all show that communication latency will increasingly hinder the performance gain when more parallel processors are used. Communication overlap is proved to effectively solve this communication latency problem. This conclusion is supported by both theoretical analysis and realistic experiments.

Laser speckle image processing is chosen as a representative application of biomedical image processing. A large portion of biomedical image processing problems share the important common feature of spatial decomposability, which means the image can be segmented into blocks and processed independently. Although there is little interaction among these blocks, image processing usually requires real-time processing. The second part of the thesis is contributed to the parallel processing of biomedical images using a computer cluster, the most accessible parallel platform. We build a master-worker framework to support this
application family, and build support for real-time processing inside this framework. This framework is simple, highly customizable and portable, and natively supports computer clusters. Potential limitations to real-time processing are analysed and solution is proposed. As a demonstration, real-time laser speckle image processing is implemented. The image processing logic can easily be customized, even in other languages, and this framework for parallel image processing can be easily incorporated into other image processing tasks. Since our framework is portable, it can be used on various types of parallel computers besides the computer cluster, which our implementation is based on.

In summary, we have achieved the following:

- We have found and verified that asynchronism among parallel processes of the same task is a main source of communication latency. This type of communication latency is among the most common types of performance, especially for applications similar to fiber suspension simulation. This latency is independent of communication networking technology used and cannot be reduced by improvement on interconnection networks.

- We have shown why and how communication overlap can help reduce the negative impact of communication latency, including both network-related and asynchronism-related latencies. We have also demonstrated how communication overlap can be implemented with MPICH with p4 device, which does not support real non-blocking data communication. Using this implementation, we have largely improved performance of fiber suspension simulation, and enable more processors to be used without performance degradation.
• We have demonstrated how parallel real-time image processing can be achieved on a computer cluster. The computational logic is also customizable, allowing researchers to use different methods and configuration without rewriting the whole program.

• We have designed a simple, scalable, and portable application framework for real-time image processing tasks similar to laser speckle image processing. Our design effectively separates processing logic from the underlying system details, and enables the application to harness different platforms and probably future parallel computing facilities without program modification.

1.3 Thesis Outline

This paper is divided into four parts, as described in the following paragraphs.

The first part comprises of this introduction, a short introduction to parallel computing, a description of the prototype problems, and the hardware platform and software environment used in this research. This part covers from Chapter 1 to Chapter 3.

The second part, consisting of Chapter 4, focuses on first type of problem, the fiber suspension simulation problem. This is treated as a representative Computational Fluid Dynamics problem, one of the most common problem types in computational bioengineering field. This part describes the common algorithm
skeleton and generic parallel execution strategies, which are optimized for solving this iterative problem on computer clusters.

The third part, consisting of Chapter 5, focuses on another prototype problem, the parallel processing of speckle images. Image processing is another common problem in bioengineering. It usually features large input and output data as well as large computational complexity. The results after processing, including the laser speckle images, would be much more meaningful if they can be obtained in real-time. This need raises even more rigorous performance requirement. This part describes the effort to use computer cluster to tackle this problem. Some properties of this type of problems prevents computer cluster to be an effective platform. Suggestions on how to tackle this difficulty is presented.

In the last part, Chapter 6, a summary is given. Based on the discussion in part 2 and 3, suggestions on interesting future improvement will also be presented.
Parallel and distributed computing is a complex and fast evolving research area. In its short 50-year history, the mainstream parallel computer architecture has evolved from Single Instruction Multiple Data stream (SIMD) to Multiple Instructions Multiple Data stream (MIMD), and further to loosely-coupled computer cluster; now it is about to enter the Computational Grid epoch. The algorithm research has also changed accordingly over the years. However, the basic principles of parallel computing, such as inter-process and inter-processor communication schemes, parallelism methods and performance model, remain the same. In this chapter, a short introduction of parallel and distributed computing will be given, which will cover the definition, motivation, various types of models for abstraction, and recent trend in mainstream parallel computing. At the end of this chapter, the connection between parallel computing and bioengineering will also be established. Materials given in this chapter server as an overview of technology development and will not be discussed in details. Readers will be advised to relevant materials for further information.

2.1 Definition: Distributed and Parallel Computing

Distributed computing is the process of aggregating the power of several computing entities, which are logically distributed and may even be geologically
distributed, to collaboratively run a single computational task in a transparent and coherent way, so that they appear as a single, centralized system.

Parallel computing is the simultaneous execution of the same task on multiple processors in order to obtain faster results. It is widely accepted that parallel computing is a branch of distributed computing, and puts the emphasis on generating large computing power by employing multiple processing entities simultaneously for a single computation task. These multiple processing entities can be a multiprocessor system, which consists of multiple processors in a single machine connected by bus or switch networks, or a multicomputer system, which consists of several independent computers interconnected by telecommunication networks or computer networks.

Besides in parallel computing, distributed computing has also gained significant development in enterprise computing. The main difference between enterprise distributed computing and parallel distributed computing is that the former mainly targets on integration of distributed resources to collaboratively finish some task, while the later targets on utilizing multiple processors simultaneously to finish a task as fast as possible. In this thesis, because we focus on high performance computing using parallel distributed computing, we will not cover enterprise distributed computing, and we will use the term “Parallel Computing”.

2.2 Motivation of Parallel Computing

The main purpose of doing parallel computing is to solve problems faster or to solve larger problems.
Parallel computing is widely used to reduce the computation time for complex tasks. Many industrial and scientific research and practice involve complex large-scale computation, which without parallel computers would take years and even tens of years to compute. It is more than desirable to have the results available as soon as possible, and for many applications, late results often imply useless results. A typical example is weather forecast, which features uncommonly complex computation and large dataset. It also has strict timing requirement, because of its forecast nature.

Parallel computers are also used in many areas to achieve larger problem scale. Take Computational Fluid Dynamics (CFD) for an example. While a serial computer can work on one unit area, a parallel computer with $N$ processors can work on $N$ units of area, or to achieve $N$ times of resolution on the same unit area. In numeric simulation, larger resolution will help reduce errors, which are inevitable in floating point calculation; larger problem domain often means more analogy with realistic experiment and better simulation result.

As predicted by Moore's Law [1], the computing capability of single processor has experienced exponential increase. This has been shown in incredible advancement in microcomputers in the last few decades. Performance of a today desktop PC costing a few hundred dollars can easily surpass that of million-dollar parallel supercomputer built in the 1960s. It might be argued that parallel computer will phase out with this increase of single chip processing capability. However, 3 main factors have been pushing parallel computing technology into further development.

First, although some commentators have speculated that sooner or later serial computers will meet or exceed any conceivable need for computation, this is only true for some problems. There are others where exponential increases in processing power
are matched or exceeded by exponential increases in complexity as the problem size increases. There are also new problems arising to challenge the extreme computing capacity. Parallel computers are still the widely-used and often only solutions to tackle these problems.

Second, at least with current technologies, the exponential increase in serial computer performance cannot continue for ever, because of physical limitations to the integration density of chips. In fact, the foreseeable physical limitations will be reached soon and there is already a sign of slow down in pace of single-chip performance growth. Major microprocessor vendors have run out of room with most of their traditional approaches to boosting CPU performance-driving clock speeds and straight-line instruction throughput higher. Further improvement in performance will rely more on architecture innovation, including parallel processing. Intel and AMD have already incorporated hyperthreading and multicore architectures in their latest offering [2].

Finally, generating the same computing power, single-processor machine will always be much more expensive then parallel computer. The cost of single CPU grows faster than linearly with speed. With recent technology, hardware of parallel computers are easy to build with off-the-shelf components and processors, reducing the development time and cost. Thus parallel computers, especially those built from off-the-shelf components, can have their cost grow linearly with speed. It is also much easier to scale the processing power with parallel computer. Most recent technology even supports to use old computers and shared component to be part of parallel machine and further reduces the cost. With the further decrease in
development cost of parallel computing software, the only impediment to fast adoption of parallel computing will be eliminated.

2.3 Theoretical Model of Parallel Computing

A machine model is an abstract of realistic machines ignoring some trivial issues which usually differ from one machine to another. A proper theoretical model is important for algorithm design and analysis, because a model is a common platform to compare different algorithms and because algorithms can often be shared among many physical machines despite their architectural differences. In the parallel computing context, a model of parallel machine will allow algorithm designers and implementers to ignore issues such as synchronization and communication methods and to focus on exploitation of concurrency.

The widely-used theoretic model of parallel computers is Parallel Random Access Machine (PRAM). A simple PRAM capable of doing add and subtract operation is described in Fortune's paper [3]. A PRAM is an extension to traditional Random Access Machine (RAM) model used to serial computation. It includes a set of processors, each with its own PC counter and a local memory and can perform computation independently. All processors communicate via a shared global memory and processor activation mechanism similar to UNIX process forking. Initially only one processor is active, which will activate other processors; and these new processors will further activate more processors. The execution finishes when the root processor executes a HALT instruction. Readers are advised to read the original paper for a detailed description.
Such a theoretic machine, although far from complete from a practical perspective, provides most details needed for algorithm design and analysis. Each processor has its own local memory for computation, while a global memory is provided for inter-processor communication. Indirect addressing is supported to largely increase the flexibility. Using \texttt{FORK} instruction, a central root processor can recursively activate a hierarchical processor family; each newly created processor starts with a base built by its parent processor. Since each processor is able to read from the input registers, task division can be accomplished. Such a theoretical model inspires many realistic hardware and software systems, such as PVM [4] introduced later in this thesis.

2.4 Architectural Models of Parallel Computer

Despite a single standard theoretical model, there exist a number of architectures for parallel computer. Diversity of models is partially shown in Figure 2-1. This subsection will briefly cover the classification of parallel computers based on their hardware architectures. One classification scheme, based on memory architecture, classifies parallel machines into Shared Memory architecture and Distributed Memory architecture; another famous scheme, based on observation of instruction and data streams, classifies parallel machines according to Flynn's taxonomy.
2.4.1 Shared Memory and Distributed Memory

Shared Memory architecture features a central memory bank, with all processors and this memory bank inter-connected through high-speed network, as shown in Figure 2-2. Shared Memory shares a lot of properties with PRAM model, because of which it was favoured by early algorithm designers and programmers. Furthermore, because the memory organization is the same as in the sequential programming models and the programmers need not deal with data distribution and communication details, shared memory architecture has certain advantage in programmability. However, no realistic shared-memory high-performance machine have been built, because no one has yet designed a scalable shared memory that allows large number of processors to simultaneously access different locations in constant time. Having a centralized memory bank implies that no processor can access it with high speed.
In Distributed Memory architecture, every processor has its own memory component that it can access via very high speed, as shown in Figure 2-3. Accessing memory owned by other processor requires explicit communication with the owner processor. Distributed Memory architecture uses message-passing model for programming. Since it allows programs to be optimized to take advantage of locality, by putting frequently-used data in local memory and reducing remote memory access, programs can often acquire very high performance. However, it imposes a heavy burden on the programmers, who is responsible for managing all details of data distribution and task scheduling, as well as communication between tasks.
To combine the performance advantage of Distributed Memory architecture to the ease of programming of Shared Memory architecture, Virtual Shared Memory, or Distributed Shared Memory (DSM) system, is built on top of Distributed Memory architecture and exposes a Shared Memory programming interface. DSM virtualizes the distributed memory as an integrated shared memory for upper layer applications. Mapping from remote memory access to message passing is done by communication library, and thus programmers are hidden from message communication details underneath. Nevertheless, for the foreseeable future, use of such paradigm is discouraged for efficiency-critical applications. Hiding locality of memory access away from programmers will lead to inefficient access to memory and poor performance until significant improvements have been gained in optimization.

The most common type of parallel computers, computer clusters, belongs to the distributed memory family. With different programming tools, the programmers might be exposed to a distributed memory system or a shared memory system. For example, using message passing programming paradigm, the programmers will have to do inter-process communication explicitly by sending and receiving message, and
are based on the distributed memory architecture; but when a distributed shared memory library such as TreadMarks is used, the distributed memory nature will be hidden from the programmer. As discussed above, we would suggest the use of message passing over distributed shared memory, because communication overhead can be more significant in computer clusters. It is advantageous to allow the programmer to control the details of communication in a message passing system. This will be further discussed in Section 2.7.

2.4.2 Flynn’s Taxonomy

Another classification scheme is based on taxonomy of computer architecture firstly proposed by Michael Flynn [5] in 1966. Flynn differentiated parallel computer architectures with respect to number of data streams and that of instruction streams. According to Flynn, computer architectures can be classified into 4 categories, namely Single Instruction Single Data Stream (SISD), Single Instruction Multiple Data Stream (SIMD), Multiple Instruction Single Data Stream (MISD), and Multiple Instruction Multiple Data Stream (MIMD). This work was later referred to as Flynn's taxonomy.

In Flynn's taxonomy, normal sequential von Neumann architecture machine, which has dominated computing since its inception, is classified as SISD. MISD is a theoretical architecture with no realistic implementation.

SIMD machine consists of a number of identical processors proceeding in a lock step synchronism, executing the same instruction on their own data. SIMD was the major type of parallel computer before 1980s, when the computing capability of a
single processor is very limited. Nowadays, SIMD computing is only seen inside general purpose processors, as an extension to carry out vector computation commonly used, for example, in multimedia applications.

MIMD is the most commonly used parallel computers now, and covers a wide range of interconnection schemes, processor types, and architectures. The basic idea of MIMD is that each processor operates independent of the others, potentially running different programs and asynchronous progresses. MIMD may not necessarily mean writing multiple programs for multiple processors. The Single Program Multiple Data (SPMD) style of parallel computing is widely used in MIMD computers. Using SPMD, a single program is deployed to multiple processors on MIMD computers. Although these processors run the same program, they may not necessarily be synchronized at instruction level; and different environments and different data to work on may possibly result in instruction streams being carried out on different processors. Thus SPMD is simply a easy way to write programs for MIMD computers.

It is obvious that computer cluster is a type of MIMD computer. Most parallel programs on computer cluster are developed in the SPMD style. The same program image is used on each parallel processor, and each processor goes through a different execution path based on its unique processor ID.

A relevant topic is the concept of granularity of parallelism, which describes the size of a computational unit being a single “atom” of work assigned to a processor. In modern MIMD system, the granularity is much coarser, driven by the desire to reduce the relatively expensive communication.
2.5 Performance Models of Parallel Computing Systems

2.5.1 Speedup, Efficiency and Scalability

In order to demonstrate the effectiveness of parallel processing for a problem on some platform, several concepts have been defined. These concepts will be used in later chapters to evaluate the effectiveness of parallel programs. These include speedup, which describes performance improvement in terms of time savings, efficiency, which considers both benefit and cost, and scalability, which represents how well an algorithm or piece of hardware performs as more processors are added.

Speedup is a first-hand performance evaluation. However, it is a controversial concept, which can be defined in a variety of ways. Generally speaking, speedup describes performance achievement by comparing the time needed to solve the problem on \( N \) processors with the time needed on a single processor. This is shown as:

\[
S(n) = \frac{T(1)}{T(n)}; \tag{2-1}
\]

where \( S(n) \) is the speedup achieved with \( n \) processors, \( T(1) \) is the time required on a single processor, and \( T(n) \) is the time required on \( N \) processors. The discrepancies arise as to how the timings should be measured, and what algorithms to be used for different numbers of processors. A widely accepted method is to use optimal algorithms for any number of processors. However, in reality, optimal algorithm is hard to implement; even if it is implemented, the implementation may not perform
optimally because of other machine-dependent and realistic factors, such as cache efficiency inside CPU.

A typical speedup curve for a fixed size problem is shown in Figure 2-4. As the number of processors increases, speedup also increases until a saturation point is reached. Beyond this point, adding more processors will not bring further performance gain. This is the combined result of 1) reduced computation on participating node, and 2) increased duplicate computation and synchronization and communication overhead.

![Typical speedup curve](image)

**Figure 2-4 Typical speedup curve**

The concept of *efficiency* is defined as

\[
E(n) = \frac{S(n)}{n}. \tag{2-2}
\]
It measures how much speedup is brought per additional processor. Based on the
typical speedup curve shown in the figure above, it is evident that typically efficiency
will be decreased upon increase in the number of processors.

The concept of scalability cannot be computed but evaluated. A parallel system is
said to be scalable when the algorithm and/or the hardware can easily incorporate and
take advantage of more processors. This term is viewed as nebulous [6], since it
depends on the target problem, algorithm applied, hardware, current system load, and
numerous other factors. Generally, programs and hardware are said to be scalable
when they can take advantage of hundreds or even thousands of processors.

In practice, the computable speedup and efficiency can be much more complex.
Both values are affected by many factors, which can be algorithmic and practical.
Take superlinear speedup as an example. Superlinear speedup is defined as the
speedup that exceeds the number of processors used. It is proved that superlinear
speedup is not achievable in homogeneous parallel computers. However, when
heterogeneous parallel computers are used, it is possible to achieve it [7]. An example
of practical factors that may lead to superlinear speedup is cache performance: when a
large number of processors are used, problem scale on a single node is largely
reduced, which may result in higher cache hit ratio, fast execution, and finally
probably superlinear speedup even if communication overhead is not negligible.
When the parallel computer is not dedicated to a single parallel computing task, load
difference among the computing nodes will imply heterogeneity and consequently the
possibility of superlinear speedup. That is what we will encounter in later chapters.
2.5.2 Amdahl’s Law

As shown in the previous subsection, efficiency gets reduced as more processors are added. This effect implies the limit of parallel performance: when the number of processors reaches some threshold, adding more processors will no longer generate further performance improvement and will even result in performance degradation, due to decrease in time saving brought by further division of task and increase in overhead of interprocess communication and duplicate computation. Gene Amdahl presents a fairly simple analysis on this [8], which is later referred to as Amdahl’s Law.

Amdahl gave the speedup of a parallel program as:

$$S(n) = \frac{1}{s + \frac{p}{n}} < \frac{1}{s}.$$ \hspace{1cm} (2-8)

where $p$ is the fraction of code that is parallelizable, and $s=1-p$, is that requires serial execution. This inequality implies that superlinear speedup is not achievable and the maximal ideal speedup cannot exceed $\frac{1}{s}$, where $s$ is the ratio of serial code (i.e., the code that requires serial execution) out of the whole program.

Amdahl’s Law is a rough method to evaluate how parallel computing can be effective for a specific problem. Amdahl’s Law has resulted in pessimistic view of parallel processing. For example, if 10% of the task must be computed using serial
computation, the maximal ideal speedup is 10. Since 1967, Amdahl’s Law was used as an argument against massively parallel processing (MPP).

Gustafson’s discovery [9] on loophole of Amdahl’s law has led the parallel computing field out of pessimism and skepticism. Since then, the so-called Gustafson’s Law has been used to justify MPP. Amdahl assumed the problem size to be fixed as the number of processors changes, and thus $s$ and $p$ to be constants. In many scientific applications, problem size is flexible, and when more processors are available, problem size can be increased in order to achieve finer result such as higher resolution or higher precision. To quote Gustafson, “speedup should be measured by scaling the problem to the number of processors, not fixing problem size.” When problem size is changed, $s$ and $p$ are no longer constants, and the limit set by Amdahl’s Law is broken.

According to Gustafson’s observation, the amount of work that can be done in parallel varies linearly with the number of processors and the amount of serial work, mostly vector startup, program loading, serial bottlenecks and I/O, does not grow with problem size. Use $s'$ and $p'$ to represent execution time associated with serial code and parallel code, rather than ratio, spent on the parallel system with $n$ homogeneous processors, then if this task is to be computed on a single processor, the time needed can be represented as:

$$T(1) = s' + np', \tag{2-9}$$

and the scaled speedup can be written as:
\[ s'(n) = \frac{T(1)}{T(n)} = \frac{(s'+np')}{s'+p'} = n - (n-1) \cdot \frac{s'}{s'+p'} = n - (n-1) \cdot s'', \quad (2-10) \]

if \( s'' \) is defined as \( s'/(s'+p') \). \( s'' \) is the ratio of serial code, but has different meaning from the ratio \( s \) in Amdahl’s Law: \( s'' \) is the ratio of serial code with reference to whole program executed on one processor in a parallel execution, while \( s \) is with reference to all code in the whole program for the problem [10]. It must also be noted that \( s \) is a constant that is only relevant to the computation problem, under the precondition that problem scale is fixed; while \( s'' \) is a constant under the precondition of problem scale changes as Gustafson described. Under Gustafson’s Law, the speedup can be linearly increased with the number of processors hired in the computation.

In the context of computational bioengineering, Gustafson’s Law makes more sense than Amdahl’s Law, because with larger computing capability, it is desirable to acquire better result, in terms of resolution in image processing and simulation and in terms of higher precision in many numerical applications. When the problem size is fixed, Amdahl’s Law has told us to reduce the fraction of code that has to be executed in serial. Essentially, we have to reduce the fraction of code whose execution time cannot be reduced by introducing more processors. Since communication code has this feature, we will look into the techniques to optimize inter-processor communication.
2.6 Interconnection Schemes of Parallel Computing Systems

Both Amdahl’s Law and Gustafson’s Law acknowledge the significance of serial code in affecting the parallel computer performance. Another important factor that is closely related to parallel program performance is inter-process communication and synchronization. Especially with modern technology, processing capability of single chip has been tremendously increased; however, inter-process communication has received relatively small improvement, and thus become the bottleneck of overall performance. That also explains the trend of coarser-granularity parallelism. High-performance parallel computers, especially those able to scale to thousands of processors, have been using sophisticated interconnection schemes. Here we cover the major interconnection schemes listed in Figure 2-5 in brief.
Figure 2-5 Illustrations of Simple interconnection schemes

Figure 2-5(A) illustrates the line scheme, which is the simplest connection scheme. In this illustration, circle represents a computing node and line represents direct communication channel between nodes. Computing nodes are arranged on and connected with a single line. Except for the nodes at the two ends, vertex degrees are all 2 and thus the implementation of network interface is simple; routing is simple and the topology can be viewed as recursive. However, communication between any two non-neighbor nodes needs the help of other nodes; the connectivity is only 1 and fault at any node will make the whole system break; and diameter of this corresponding graph is $n-1$, where $n$ is the number of nodes, which implies that the latency could be very high. To summarize, this scheme is simple and low-cost, but will not be able to generate high performance or reliability; and as system scales, the performance degrades rapidly.

Figure 2-5(B) illustrates the ring scheme, which is an enhanced line topology, with an extra connection between the two ends of the line. This increases the
connectivity to 2 and decreases the diameter to half of the corresponding line topology. However, basic characteristics are still the same.

The other extreme is probably the fully-connected topology, in which there is a direct connection between any two computing nodes. Fully-connected topology is shown in Figure 2-5(C). The corresponding graph representation has an edge between any two vertices, and distance between any two vertices is 1. Thus the diameter is 1, and it generates the minimal communication latency, if the physical link implementation is fixed, as well as the maximal connectivity. However, the degree of nodes changes with the number of processors and thus the implementation of network interface must be very complex; and it is hard to be recursive, adding another layer of complexity of implementation and reducing the scalability. To summarize, this scheme will generate the highest performance possible, but due to the complexity and thus cost, it can hardly be scalable: with larger scale, although performance will not degrade at all, complexity will climb very fast at the level of $O(n^2)$.

Similar to fully-connected network, bus network, illustrated in Figure 2-5(E), has direct connection between any two nodes. In fact, bus topology shares the same logical graph representation with fully-connected topology and. Consequently, static characteristics of bus topology are exactly the same as those of fully-connected topology. But connection between any pair of nodes is not dedicated but shared: interconnection is implemented via a shared bus. This reduces the complexity significantly. In fact, its complexity is similar to that of line and ring topology. However, the dynamic characteristics, such as data transfer speed, are more inferior to those of fully-connected counterpart. Although collective communication is now very easy to implement, this single shared bus prevents more than one pair of nodes to
carry out point-to-point communication. As a result, the system does not scale very well.

An intuitive improvement on bus network is to change the bus to eliminate the constraint that only two nodes can communicate at any time. The result is the star network, where a communication switch node is added to replace the shared bus, as shown in Figure 2-5(D). If we treat this switch node as a non-computing node and ignore it in the graph representation, then star network corresponds to the same fully-connected graph as bus network, while the implementation does not have the constraint of bus network; if switch node is viewed as normal computing node, then the corresponding graph has a diameter of 2, supports easy implementation of collective communication with the help of the central switch node, and allows recursive expansion. Except for the switch node, all other nodes have a constant vertex degree of 1. The critical disadvantage is that the connectivity is 1: failure at the switch node will cause the whole system to fail.

For computer clusters, most are built with a star structured interconnection network around a central switch. For better fault tolerance or easier setup, the other interconnection scheme might also be used. Parallel program using message passing might be rewritten to better adapt to different interconnection network.

There are other types of more sophisticated topology schemes, such as tree, mesh, and hypercube, which are widely used in parallel computers with thousands of processors or more. These schemes often scale better to larger scale network with good performance. Readers are advised to [11] for more information about this.
2.7 Programming Models of Parallel Computing Systems

Programming models are high-level abstract views of technologies and applications that hide most architectural details with programmers as the main audience. For MIMD machine like a computer cluster, the most important models include shared-memory model, message passing model, and object oriented model.

In the shared-memory model, multiple tasks run in parallel. These tasks communicate with one another by writing to and reading from a shared memory. Shared-memory programming is comfortable for the programmers, because the memory organization is similar as in the familiar sequential programming models, and programmers need not deal with data distribution or communication details. Popularity of this model was also promoted by its similarity to the theoretical PRAM model. Practice of programming on this model originated from concurrent programming on transparency of data and task placement determines that, besides the simplicity of programming, the performance cannot be predicted or controlled on hardware platform with Non-Uniform Memory Architecture (NUMA) or distributed memory. This performance problem is evident especially on large-scale multiprocessor systems, in which access time to memory at different locations varies significantly and thus memory locality plays critical role in determining overall system performance.

Message passing model is becoming the prevailing programming model for parallel computing system, thanks to the trend to large-scale multiprocessors systems,
including computer clusters. In this model, several processes run in parallel and communicate and synchronize with one another by explicitly sending and receiving message. These processes do not have access to a shared memory or a global address space. Although harder to program compared to previous models, it allows programs to explicitly guide the execution by controlling data and task distribution details. Since everything is under the programmer’s control, the programmer can achieve close to optimum performance if enough effort has been spent on performance tuning. Besides this performance advantage, message passing model is also versatile. Being a relatively low-level model, it is capable of implementing many higher-level models. A typical example is the widely-used SPMD data model, which fits in with many naturally data-parallel scientific applications. Very low-level message passing systems, such as Active Message, are even used to implement shared-memory system by emulating a shared memory. These systems, while allowing easy high-level algorithm design with the help of more friendly high-level models, expose enough low-level details to support and encourage the programmers to manually control and tune the performance. Wide deployment of multicomputers and loosely-coupled computer clusters, which feature expensive communication, promotes the popularity of message passing systems. Message Passing Interface (MPI) [12] and Parallel Virtual Machine (PVM) [4] are the 2 major programming libraries used to build message passing system. MPI is the base of our research and will be covered in detail in the next chapter.

In this chapter, we have reviewed some basic concepts in parallel computing systems. Parallel computing is the simultaneous execution of the same task on
multiple processors in order to obtain faster results. It is used to acquire the results faster and/or to acquire better results, which is useful in many computational bioengineering applications. PRAM is the model of parallel computer to study the algorithm, and in practice, program designers usually have to consider the architectural models of the hardware to better utilize the resources available and to achieve higher performance. In this context, computer cluster belongs to distributed memory MIMD computers. To evaluate the performance, several terms have been defined. Studies on these terms suggest the important role of inter-processor communication. That is why many different interconnection schemes with different levels of complexity have been devised. Computer cluster usually uses the star-structured scheme, but more complex scheme may be employed when the cluster scales to a larger size. We have shown that to have better control on the execution details including inter-processor communication, message passing programming model is suggested.

In the next chapter, we will look into the architecture and programming model used in our research with more details.
Chapter 3 Overview of Hardware Platform and Software Environments for Research in Computational Bioengineering

In this chapter, we will focus on hardware and software platforms we use in our research. As for hardware, 3 types of platforms with message passing architecture are involved in our research, to best take advantage of available resources and to satisfy different requirements. As for software tools, message passing is the main programming paradigm used, and Message Passing Interface (MPI) model and library are used in both research projects. For image processing algorithms that are more suitable for SIMD-style architectures, use of SIMD extension instructions in commodity CPU are also investigated.

3.1 Hardware Platform

Parallel program based on message passing paradigm can be run on various platforms, ranging from high-end distributed-memory multiprocessor systems with thousands of processors, such as IBM Blue Gene/L [13], the No. 1 supercomputer in the world as of this writing, to multicomputer system with dozens of CPUs, like the
computer cluster we use in our research. Our research projects mainly rely on a computer cluster for computing power. For the biomedical image processing project, we propose to use Computational Grid to integrate our system into other components of whole system. We also look into the possibility to utilize the vast computing power available in thousands of campus workstations connected via high-speed campus network, as well as the SIMD extension available in modern commodity CPU.

### 3.1.1 Computer Cluster

A computer cluster is a group of loosely coupled computers that work together closely so that in many respects it can be viewed as though it were a single computer. Clusters are commonly (but not always) connected through fast local area networks. Comparing to parallel machines with specific-purpose hardware components, computer clusters use commodity general-purpose components and usually have significant cost advantage. This means that with the same amount of budget, building a computer cluster usually will result in higher system performance. With the fast increase in performance of commodity components and improvement of network technology, computer cluster is now the mainstream architecture of modern parallel machines.

The main piece of hardware used in our research is the Hydra II computer cluster system, built and maintained by Singapore MIT Alliance (SMA). This system consists of one dual-processor head node and 34 uni-processor client nodes, connected via a Gigabit Ethernet switch. The head node is equipped with 2 Pentium III processors, both clocked at 1.3GHz, and 2 GB of RAM. Each client node has one 1.3GHz
Pentium III processors attached with 1GB of RAM. LINPACK benchmark shows the system can generate 27GFlops of average computing power.

### 3.1.2 Computational Grid

*Grid computing* is a very young and uncharted field [14]. Various definitions and designs coexist and numbers of implementations based on different designs have been built and deployed in real applications. Out of them, Computational Grid, described by Open Grid Services Architecture (OGSA) [15], standardized by Open Grid Services Infrastructure (OGSI) [16], and implemented and refined in Globus toolkit by Globus Alliance (http://www.globus.org), is widely accepted as the standard form. Computational Grid, named by analogy to electric power grid, is defined as hardware and software infrastructure that provides dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities. It is hoped that inexpensive, reliable and universally accessible computing power brought by Computational Grid will result in revolutionary development of computing devices, like the electric power grid did in the 1910s. To be specific, one of the many present goals is to allow execution of parallel code across more than one supercomputer site or computer cluster.

Computational Grid is designed to integrate distributed computing power to form a single supercomputer, which would be a rather powerful *hypercomputer* to tackle large-scale computation problems. When message passing programming is to be considered, the mainstream *Message Passing Interface* (MPI) implementation, MPICH, has support for Grid-based communication. Unfortunately, in practice there are a lot of problems to be circumvented. For example, for many computer clusters,
only the head node has the public Internet Protocol (IP) address, which makes the direct Grid-based communication between 2 client nodes residing in different computer clusters impossible. When our research is to be considered, the heterogeneous nature and hierarchical structure of Gird are further barriers to efficient deployment of our flat-structured MPI program.

We use Grid mainly to take advantage of its capability to integrate different types of resources. For many computational bioengineering applications, various types of resources are involved. Take biomedical imaging as a typical example: special-purpose imaging equipment is used to acquire the images possibly in the form of video; a powerful computer is needed to process this image information, preferably in real-time; another computer may present to perform more complex image processing in a non-real-time manner; and a storage device with large capacity may be used for data storage and enquiry. Rather than building a machine consisting of all these components, Grid can help to glue these distributed components together, some of which may already exist. Being able to reuse existing components not only means cost reduction, but also means more scalable system with more desirable functions. For example, imagine the scenario that developers have implemented a good feature in an image processing program based on a hardware platform that best suits this program. Without using Grid, when it is time to build a new system with new image capturing facility, for example, there is usually the need to migrate to a new image processing program that may not suit the application, or to rewrite the existing program on a new platform that may not suit the program. Grid can help integrate this system into a new system without the need to rewrite the program or to migrate to a new hardware platform, and best save the development effort while preserving the functionality.
In our research on parallel biomedical image processing, we look at the option of integrating speckle image processing program with image acquiring facilities using Computational Grid techniques.

### 3.1.3 Network of Workstations

A *Network of Workstations* (NOW) is a computer network which connects several computer workstations together, and by using specific software it allows to use the network as a cluster. Different from nodes of a computer cluster, workstations of NOW is often loosely-coupled, and although they are continuously connected to the network, every workstation is not dedicated to the NOW tasks and some of them will accept tasks from normal interactive user sessions. One of the many goals of NOW is to utilize idle CPU cycles [17]. When a node is overloaded with tasks from interactive user session and is no longer idle, task distribution system of NOW will be removed from this node and be migrated to another node or simply be suspended. Since the progress of subtask is unpredictable, the NOW system is more suitable for problems that can be divided into independent subproblems. Master-worker programming model is an example of suitable models.

The first NOW system was developed at UC Berkeley [18]. As of April 1997, it was listed in the 200 fastest machines in the world, thanks to its 10 GFLOPS performance in LINPACK benchmark. In our university, workstations connected via campus network provide desirable environment to build NOW system. This is because a large portion of CPU cycles are wasted with no user task at all or with tasks requiring little CPU power; besides, all workstations are constantly connected to
high-bandwidth network; furthermore, there are also a lot of research applications suitable to run on NOW system.

Image processing is one of such applications. Non-real-time image processing that employs complex algorithms and thus requires large computing power can take advantage of this computing platform, if the algorithm allows subtasks with little interaction. Such prerequisite holds true for most image processing algorithms, which divide a large image into subimages and process them independently.

In our parallel image processing project, master-worker programming model is used, which implies that NOW system can be used to run the program. In the implementation, the design of portable communication layer allows the program to be ported to use many hardware and software platforms. We suggest future research to implement a BSD socket-based communication layer, which allows the program to run on NOW systems. If other higher-level NOW communication systems are used, such as Active Message [19], it would also be possible and easy to port onto it. Details about the design of portable communication layer will be given in Chapter 5 and relevant suggestion for future research is given in Section 6.5.

3.1.4 Vector processing in commodity CPU and GPU

Major commodity microprocessor vendors have included SIMD instruction extensions in their CPU offerings. For example, Intel has added SIMD instructions since its Pentium MMX offering, and has enhanced this design through Streaming SIMD Extensions (SSE), SSE2, and SSE3, appearing respectively in Pentium III, Pentium 4, and Pentium 4 Prescott revision; the PowerPC vendors has also integrated
its floating point and integer SIMD instruction set, known as AltiVec, in both G4 and G5 CPU families. Utilizing this vector processing capability properly will largely increase the performance of some applications such as image processing.

Graphic Processing Unit (GPU), a common component available in almost every computer, is another source of vector computing power which recently starts to gain a lot of attention. There is a trend of using the GPU rather than CPU to perform computation. This technique is known as General-Purpose computation on Graphics Processing Units (GPGPU) [20] [21]. With graphics and image processing applications being the main consumer of this technique, many non-graphics areas, including cryptography, signal processing, are also benefiting from instinctive powerful vector processing capability of modern GPU.

SIMD extension and GPGPU may largely improve the performance of image processing programs, since many algorithms in this area are SIMD computation and vector processing by nature. Due to time constraint and availability of hardware and software, this technique is not covered in our research. However, it is receiving much research attention recently and may be studied in future research.

3.2 Software Environments for Parallel Programming

As stated in the previous chapter, parallel programming is a complex task. In order to reduce this complexity, different programming models are abstracted, with each providing tools such as special-purpose compilers, libraries and frameworks to simplify programming task. These tools hide many details about parallel execution, such as message transfer and routing, task allocation and migration, and platform
differences. Higher-level programming model will even have commonly-used algorithms pre-implemented in the bounded libraries. As an example, Fluent, a high-level programming system to develop CFD programs with parallel processing capabilities, have built in many CFD-specific functions such as dynamic meshing and acoustics modeling, which makes more like a program than a programming system. Our research is based on message passing programming model and specifically on Message Passing Interface (MPI) standards and MPICH library.

3.2.1 Message Passing Interface and MPICH

Message Passing Interface, or MPI, is the most widely-used message passing standard. The basic functions are defined by the MPI standard [12], and with many implementations targeting almost all distributed memory architectures, it is the de facto industrial standard for message passing programming.

Basically, MPI provides two types of communication operations. Point-to-point operations allow any two processes to exchange information via MPI_Send (for sending), MPI_Recv (for receiving) and their variants. Collective operations are provided so that a set of processes, known as a communicator, can share and dispatch data through broadcast and reduction operations.

When an MPI program runs, the user will explicitly specify the number of parallel processes and how the processes are mapped to physical processors. On startup, each processor starts one or more processes to execute the same program body. Each parallel process will be assigned a rank, which serves as the identity of the process, and which will also cause processes to carry out different computation
despite their common program body. During the execution, processes carry their own computation, without synchronization with other processes unless they encounter an explicit synchronization command. Processes communicate with each other using point-to-point or collective communication primitives, using process rank to address the recipient or sender if it is required. The whole parallel program exits when all the parallel processes have finished. Although there is no requirement on how the computation result is generated, in many cases a head process, usually the one with rank 0, will collect the results from participating processes and assemble the final outcome.

Apart from MPI, another well-known standard for inter-process message passing is called Parallel Virtual Machine, or PVM [4]. One major difference between these 2 standards is that PVM provides semantics for dynamic process creation: a parallel process is capable to spawn a new process on some node. This feature resembles the PRAM model, in which a processor can activate another idle processor to join parallel processing. Because of this, PVM provides more flexibility and scalability, and is more suitable for heterogeneous environment than MPI. Unfortunately, due to lack of development effort and support, PVM suffers from performance problem and lack of important features. As MPI becomes the de facto standard and MPI-2 has adopted numbers of excellent features in PVM, PVM itself is fading out from the parallel programming area.

The two major implementations of MPI standards are MPICH [22] developed by Argonne National Laboratory and LAM by Ohio Supercomputing Center and Indiana University. Our research is heavily based on MPICH and its successor MPICH2. Besides a complete and efficient implementation of MPI-1 standard and partial MPI-2
standard, MPICH also targets a portable design. Area of parallel computing features a large number of different architectures, interconnection scheme and technology, and communication protocols. This makes portability and efficiency often conflicting tasks. MPICH separates a vast set of machine independent functions from a machine specific _abstract device interface_ (ADI), which is about lower-level communications. This design simplifies the job of porting MPICH to different architectures and platforms without much sacrifice of performance. When MPICH is to be ported to a new platform, at the beginning stage, only a small number of fundamental subroutines in ADI need to be implemented, and all other subroutines will be based on these fundamental ones and need not be rewritten. After this step, a functional MPICH is built on this platform. When more development power is available, non-fundamental subroutines in ADI can be selectively reimplemented to take advantage of platform features, and thus performance can be gradually improved. Thanks to this portable design, MPICH has been adopted by almost all major vendors, including IBM, HP, SGI, and SUN, all of which has built their own so-called _native_ MPICH implementation which leverages their hardware features. For example, MPI implementation on IBM Blue Gene/L is based on MPICH and utilizes the platform-specific design of dedicated _collective network_ in its ADI implementation to support efficient broadcast and reduction operations [23].

MPICH2 is an all-new implementation of MPI by the MPICH team. In addition to features of its predecessor, including the portability advantage, MPICH2 includes partial implementation of MPI-2 functions, including one-side communication, dynamic process creation, and expand MPI-IO functionality. One important improvement for our research is that MPICH2 has better support for multithreading. This makes it safe to run another thread for computation while the main thread is busy.
with inter-process communication, which is just the idea of communication-computation-overlap covered in Chapter 4.

3.2.2 Vector Processing Software

Intel provides a set of tools to allow programmer to take advantage of its SSE instruction extension. These tools are provided in forms of new assemblers to understand these extended assembly instructions, dedicated C intrinsic functions, and compiler capable of doing automatic vectorization. Although these tools and techniques are not used in our research due to our focus on programming framework and the relatively simple algorithms we choose for image processing, they may be important for other applications using more complex algorithms.

As for GPGPU, because computing capabilities of different GPU chips differ significantly, programs using GPGPU can hardly be portable. Our research will not use this technology. More information about this technology can be found on the GPGPU website [24] and Fernando’s *GPU Gems* [25].
Fiber suspensions simulation is a typical computational biomechanics/biofluid application. There is complex computation involved in updating dynamic status of a large number of particles through numerous time steps. Therefore, intensive computing power is desired to both expedite the computation and to enable finer results. Parallel computing is commonly used to solve this style of applications, and there is a relatively common routine to convert the serial programs into parallel versions for these applications. However, experiences have shown that these parallel programs do not scale very well to large number of processors, and the overall performance gain from using multiple processors is not satisfactory. In this chapter, we will see how significant this performance problem is in the program we study, when computer cluster is used as the hardware platform. Theoretical analysis and simulation will show that synchronous inter-process communication operations among processes with asynchronous progress are the main obstacle of achieving higher performance. A technique to efficiently utilize the computing power of computer cluster for this style of applications will be proposed based on this study. Practical experiment results will be presented and analyzed.
4.1 An Introduction to the Fiber Suspensions Simulation Problem

Fiber suspensions problem is a common problem in searching for fiber reinforced composites that can be found in many applications requiring the high strength, stiffness, toughness, and light weight. Because of the wide ranges of applications, viscoelastic fiber suspensions have been intensively studied in the last decade.

When most methods decouple the problem and solve them individually, the *Dissipative Particle Dynamics* (DPD) technique [26], using a mesoscopic model of hydrodynamics, tackles this problem at micro-structural point of view. The commonly-used numerical method for DPD is *velocity-Verlet algorithm* [27]. Using a time step approach, it recursively updates the particle status from that of previous step.

A lot of numeric simulation problems, especially those in computational fluid dynamics, share these features with velocity-Verlet algorithm: 1) a set of *evolution equations* are used to describe the trend of status change (such as *acceleration* of each particle) in terms of the current status parameters (such as the current position and velocity of each particle); 2) the status of the current time step and these evolution equations are used to compute the status of the next time step; and 3) by recursively repeat of the status update, a time-domain evolution of the status of objects of interest is archived. This style of simulation often implies very intensive computation because 1) evolution equations often correspond to complex floating-point calculations with high-precision requirement; 2) calculation of status of the next time step from that of
the current time step usually involves many instances of computation based on evolution equations, because of complex inter object intervention; and 3) to generate meaningful time-domain evolution, a large number of time steps need to be computed. By studying the fiber suspension simulation problem, we expect to find out a general method that can also improve the performance of parallel programs for other similar applications.

Algorithms for the above problems often use decomposition to get parallelized. For example, the fiber suspension simulation uses spatial decomposition: the spatial domain of a problem is divided into several subdomains, each of which does its own time-domain evolution using the serial algorithm. Because the subdomains are hardly independent, they need to exchange status information at the end of each time step, usually only with their neighboring subdomains. For linear partition, each subdomain has one left neighbor and one right neighbor. Synchronization of all subdomains at the end of each time step might also be required, for example, for the purpose of collecting global statistics. Communication latency is generated when 1) there is time spent on data transfer in communication or synchronization, and 2) some processes involved in communication or synchronization spend time on waiting for some other processes because the later ones are not ready for the communication or synchronization. It is observed that although using more processors will reduce the computation time, it will not reduce the communication time. Since the communication time does not reduce with the increase of the number of processors, communication latency can be seen as part of the serial factor in Amdahl’s Law, which is introduced in Section 2.5.3, and will limit the performance gain from parallel computing. In the next section, we will look into the relationship between
communication latency and the number of processes used, and why it is impossible to solve this problem by utilizing more advanced networking technology.

4.2 Implementing the Parallel Velocity-Verlet Algorithm using Conventional Method

In this section, velocity-Verlet algorithm and its parallelization will be covered in details. As mentioned above, the velocity-Verlet algorithm uses a time-step approach: the algorithm updates the particle status data of the current step, including the position, velocity and acceleration, from those of the previous time step; and by using a tiny time step value and a large number of steps, evolution of particle status over some time internal can be achieved. Stepwise status update is based on calculation of interactive forces among the particles, which are further computed from particle positions of the previous step.

Similar to N-body problem, to calculate the forces exerted on one particle, the algorithm needs to compute interactive forces among this particle and the others in the domain. To reduce the complexity, only particles within a pre-defined cut radius from the target particle are considered. In this way, if the number of particles per unit volume, or particle density, is constant, the number of operations required by each particle is constant and finite. This also facilitates parallelization of the problem with spatial-domain decomposition. Here is how the spatial decomposition works. The spatial domain of interest is divided into several subdomains, each of which is assigned to a parallel process. In each iteration corresponding to a time step, each
process will update particle status of its own subdomain independently using the
original velocity-Verlet algorithm. At the end of each iteration (which is also the
beginning of the next iteration), processes will have to exchange particle status data,
because 1) over the time there are particles moving from one subdomain to another
one, and 2) particles within one subdomain may have interactive forces with those in
another subdomain and thus particle status data have be shared to finish interactive
force computation. Fortunately, the use of this cut radius will largely reduce the
interprocess communication, and hopefully only the processes handling spatially
neighboring subdomains need to exchange information. Only status of particles
positioning a radius from the subdomain boundaries need to be shared between
processes.

Figure 4-1 illustrates the division of a channel into a fluid channel of interest into
subdomains. In light of these observations, the structure of main program is shown in
Figure 4-2, and its skeleton procedures are explained below:
Figure 4-1 Division of a fluid channel into several subdomains

```python
If this_node is root_node
    read_input_data
    distribute_data_to_nodes
else
    receive_data_from_root_node
end if

while loop_count < max_loop_count
do
    update_loop_count
    if need_to_move then
        move_particles_to_neighbors
    end if
    copy_particles_to_neighbors
    velocity_verlet
    collect_GMV
    broadcast_GMV
    compute_need_to_move
end do
```

Figure 4-2 Pseudo code of program skeleton of fiber suspensions simulation

- **velocity_verlet**: This procedure is to update the status of particles within each subdomain. It computes the status data for the \((n+1)^{th}\) time step based on those data of the \(n^{th}\) time step.
• **move_particles_to_neighbors:** This procedure keeps track of the movement of particles from one subdomain to another subdomain, and updates the respective destination computing process with the status data of the transferred particles.

• **copy_boundary_particles_to_neighbors:** This procedure copies status data of particles at a radius away from subdomain boundaries to the process(es) that(those) requires them to finish force computation for the next time step. In our implementation, cut radius is always smaller than subdomain width, only processes associated with neighboring subdomains have to exchange particle information, and copy of particle status will cross just one boundary.

• **collect_GMV:** Every subdomain has its own maximum particle velocity. This procedure will collect all the local maximum velocity values and selects the global maximum velocity among the local velocity values.

• **broadcast_GMV:** This procedure broadcasts the global maximum velocity to all the participating computing processes. This GMV is then used to determine whether it is necessary to perform the procedure of move_particles_to_neighbors.

The **velocity Verlet** procedure is the most time-consuming computation. On the other hand, the communication phase consists of move_particles_to_neighbors, copy_boundary_particles_to_neighbors, collect_GMV, and broadcast_GMV. The first 2 procedures are point-to-point
communication while the remaining 2 procedures are collective communication. This algorithm has been successfully implemented using MPICH with FORTRAN binding.

4.3 Performance Study of Conventional Implementation

In this subsection, we study the performance of the conventional implementation of the fiber suspension simulation problem on a computer cluster.

A fiber suspensions simulation program has been built based on the parallel velocity-Verlet algorithm introduced in the previous subsection. The program is successfully deployed and tested on Hydra II computer cluster system introduced in Chapter 3. A standard simulation involves 4 thousand fibers in a channel of size 64x30x30 with nearly 50,000 particles. Simulation is run for 36,000 time steps. As shown in Figure 4-1, each subdomain is assigned to a parallel process, and each process, unless otherwise stated, is assigned to one processor. Processors communicate via interprocessor communication library built on top of Ethernet links to exchange particle status data.

We profile the program using a self-made tool, which precisely records the time spent in crucial parts of the program. These crucial parts include large computation block, and all inter-process communication procedure calls. Our profiling tool is based on counters built in CPU to record the time spent on both communication calls and computation class of interest. This provides the best precision as well as wall clock timing support. We do no use existing profiling tools either because they are incapable of wall clock time profiling (like GNU gprof on x86 platforms) or because they need super-user privilege to install (like PAPI).
Our observations have shown that 1) there is a significant performance improvement with increased number of processors, and 2) when the number of processors passes some value, there is less and less performance improvement obtained through further introduction of more processors. The latter is consistent with Amdahl’s Law, if the communication time is considered as a constant and therefore contributes to the serial fraction of the code. This relationship can be represented as:

$$t(N) = s + \frac{p}{N}$$

$$= s_{comp} + s_{comm} + \frac{p}{N}$$

(4-1)

where $s_{comp}$ is serial computation time and $s_{comm}$ is communication time. When the communication time is larger, according to Amdahl’s Law, the maximum speedup that can be achieved will be smaller. In other words, the limit of maximum performance gets smaller. It can be seen that the communication time plays a significant role in affecting the performance, and it should be kept as small as possible.

Our observations have also shown that when the number of processors further passes some value, the performance starts to degrade. More detailed profiling data shows that communication time will not keep constant but will increase with more processors being used. Table 4-1 shows how the time spent on a typical computation procedure and a typical communication procedure changes when the number of processes varies. From this table we see that although computation gets less
expensive when more processors are used, communication gets more and more time consuming. When the increase in communication time surpasses the decrease in computation time, performance starts to degrade. Since the amount of data being transferred during inter-process communication roughly remains the same, this increase in communication time is brought in by larger communication latency. In the next subsection, theoretical analysis on relationship between communication latency and the number of processes used will be presented. More detailed performance profiling data can be found in subsequent Section 4.5.3, where performance data of conventional implementation and new implementation are compared.

<table>
<thead>
<tr>
<th></th>
<th>2-process</th>
<th>4-process</th>
<th>8-process</th>
<th>16-process</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time spent on a typical communication procedure (in unit)</td>
<td>4372</td>
<td>5126</td>
<td>10836</td>
<td>41270</td>
</tr>
<tr>
<td>Time spent on a typical computation procedure (in unit)</td>
<td>86998</td>
<td>37913</td>
<td>19992</td>
<td>10348</td>
</tr>
</tbody>
</table>

In summary, the fiber suspension simulation problem, as a typical biomechanics problem, can be parallelized using the classic spatial decomposition. However, according to the performance profiling, the parallel program performs unsatisfactory on computer cluster. Analysis shows that with more processors being used, although the computation time of procedures gets smaller, the increased communication latency significantly reduces the performance gain and eventually results in the performance degradation. In the following subsections, we will run a theoretic analysis on communication latency and propose a solution to this problem.
4.4 Communication Latency and the Number of Processes

In this section we will study the relationship between communication latency and the number of processors involved in the computation. In the following text, the term *process* denotes a computing process of a number of parallel processes belonging to the same task. Consider a message passing program running on a homogeneous computer cluster with star-style interconnection scheme; each computing process performs relatively the same amount of computation task and can directly communicate with any other processes. The fiber suspensions simulation problem is solved with velocity-Verlet algorithm and a large number of time steps. A time step corresponds to an iteration of loop in implementation program. In each time step or, in other words, in each loop iteration, the program at each process will do some computation to update its own data; it will then exchange part of these data with other processes before the next step can continue. We notice that with high-performance low-latency networking technology, the latency is now mainly brought by asynchronism between interdependent processes. That is, when one process finishes its computation and is ready for data exchange, the other interdependent processes may still be in computation phase, and therefore the early finished process has to wait. Based on different interdependent relationships, discussion can be divided into two scenarios.
4.4.1 Scenario 1: Barrier Operation in Each Iteration

If a global synchronization operation, such as MPI_Barrier\footnote{MPI_Barrier is an MPI routine which blocks all processes until all have reaches such a routine call} in MPI, is used to synchronize all participating processes, all processes are interdependent with each other. In this scenario, a delay of progress at any one process will cause all the remaining processes to wait. Therefore, the execution time for this iteration will be determined by the process with the slowest progress. Let the execution time on process $n$ for an iteration excluding the time spent on barrier operation be $t_n$. For all processes, execution time for an iteration with the time spent on barrier operation included is $T_N = \max(t_n)\text{, where } n=\text{1, 2, \ldots, } N$. Consider the expectation of the $T_n$, $E(T_n)$. Let $P(\cdot)$ be the probability of an event. When we introduce one more process and assume computation work on each process remains the same, given that $t_n$ for each process is independent,

$$
E(T_{N+1}) = E(\max_{n=1,N+1}(t_n))
= E(\max_{n=1,N}(t_n) \mid \max_{n=1,N}(t_n) \geq t_{N+1}) \cdot P(\max_{n=1,N}(t_n) \geq t_{N+1})
+ E(t_{N+1} \mid \max_{n=1,N}(t_n) < t_{N+1}) \cdot P(\max_{n=1,N}(t_n) < t_{N+1})
\geq E(\max_{n=1,N}(t_n) \mid \max_{n=1,N}(t_n) \geq t_{N+1}) \cdot P(\max_{n=1,N}(t_n) \geq t_{N+1})
+ E(\max_{n=1,N}(t_n) \mid \max_{n=1,N}(t_n) < t_{N+1}) \cdot P(\max_{n=1,N}(t_n) < t_{N+1})
= E(T_N),
$$

(4-2)
where the equality holds if and only if $\prod_{n=1}^{N}(1 - \frac{1}{n}) = 0$, which is not true. This means that when there is a barrier operation in each iteration and the computation complexity in one iteration remains constant, the expectation of execution time for one iteration will be increased if the number of processes is increased. Since the computation does not get complex at any process, this increase in execution time can be attributed to larger communication latency. In other words, when there is a barrier operation in each iteration, the expectation of communication latency will be increased. This conclusion about communication latency will no longer rely on the assumption on constant computation on all processes, because communication latency is independent with computation scale as long as the parallel processes are homogeneous.

This conclusion can also be applied to scenario where barrier operation is not present, but with the presence of an MPI_Reduce\textsuperscript{2} operation followed by an MPI_Bcast\textsuperscript{3} operation. The reduce operation causes the root process to wait until all other processes have reached the same reduce operation, and the broadcast operation causes all the non-root process to wait until the root process has reached the same

\textsuperscript{2} MPI_Reduce is an MPI routine which reduces (or collects) values on all processes to a single value

\textsuperscript{3} MPI_Bcast is an MPI routine which broadcasts a message from a leading process (known as root) to all processes in a process group (known as communicator)
broadcast operation. After the reduce operation, root process has the slowest progress. So root process will be the last to reach broadcast operation, making all the non-root process to wait for the root and then to continue from the broadcast operation simultaneously. The overall effect is that progresses of all processes are now synchronized. The two operations combined produce the same effect as a barrier operation does, and thus the same conclusion can be applied.

4.4.2 Scenario 2: Process Communicating with only Neighboring Processes in Each Iteration

Another common scenario is that at the end of each iteration, each process communicates only with one or more fixed processes. The processes that one process communicates with are called the neighboring processes. When spatial decomposition is used for parallelism, which is the case of velocity-Verlet algorithm used for fiber suspensions simulation, processes working on neighboring spatial subdomains will usually need to communicate with each other and are neighboring processes.

Consider $N$ processes in a line, with $n^{th}$ process communicates with the $(n+1)^{th}$ and $(n-1)^{th}$ process where applicable. When a process reaches the communication phase, it is synchronized with the 2 neighbors (1 if it is a boundary process). For analysis, we define 3 time variables. For process $n$ and iteration $i$, computation time for this iteration is the time from the start of this iteration to the start of communication phase within this iteration, and is denoted as $t_n^{(i)}$; starting from the start of the first iteration, the elapsed time until the start of communication phase within this iteration is denoted as $\tau_n^{(i)}$, and elapsed time until the completion of
communication phase (which is also the completion point of this iteration) is denoted as $T_n^{(i)}$. The following relationship applies:

$$
\tau_n^{(i)} = T_n^{(i-1)} + t_n^{(i)}
$$

$$
T_n^{(i)} = \max(\tau_n^{(i)}, \tau_n^{(i)}, \tau_{n+1}^{(i)})
$$

Figure 4-3 illustrates this relationship. The direct graph in Figure 4-4 can be used to help calculate $T_n^{(i)}$, or the completion time of iteration $i$ at process $n$. This graph grows downwards from top to bottom, with its edges representing the dependency relationship. According to the above equations, each $\tau$ graph vertex depends on a $T$ graph vertex by adding a $t$ value; each $T$ depends on 2 or 3 $\tau$ vertices by selecting the maximum value of these $\tau$ vertices. For example, $T_2^{(2)}$ depends on $\tau_1^{(2)}$, $\tau_2^{(2)}$, and $\tau_3^{(2)}$, and $\tau_3^{(2)}$ further depends on $T_3^{(i)}$. From these recursive dependency relations, it is easy to see that finally all $T_n^{(i)}$ can be represented by the sum of $t$ as:

$$
\sum_{j=\alpha}^{i} t_{\alpha}^{(j)} , \text{ where } j = 1, 2, \ldots, i, \text{ and } 1 \leq \alpha_j \leq N .
$$

(4-4)
Figure 4-3 Relationship between time variables defined for execution time analysis

Figure 4-4 Directed Graph illustrating calculation of execution time
This representation corresponds to a path in the graph. So the execution time of the whole program,

\[ \hat{T} = \max_{i=1}^{N}(T_i^{(W)}) , \]  \hspace{1cm} (4-5)

corresponds to a path \( P \) in the graph, and \( P \) is the \textit{optimal} path to maximize \( \hat{T} \).

Now let us remove a process at the boundary and assume the computation on other processes remains the same. If \( P \) has a vertex corresponding to the removed process, this removal will change \( P \), and reduce the overall execution time, because the new \( P \) is \textit{non-optimal} path in the original graph. If \( P \) does not have a vertex corresponding to the removed process, then the execution time will not change because \( P \) is still the \textit{optimal} path. To summarize, removing a process will not change the execution time or will reduce it; the expectation of the overall execution time will be reduced by this removal, given that the possibility of the event that “\( P \) has a vertex corresponding to the removed process” is not zero. Vice versa, introducing a new process will increase the expectation of the overall execution time. Because the computation at each process does not change, this increase in execution time can be attributed to the increase in communication latency. In short, introducing more processes into parallel computation will increase the expectation of communication latency. Note that this conclusion does not require the assumption that the computation remains constant on each process any more, because communication latency is independent of computation scale as long as the parallel processes are homogeneous.
In the above deduction, the process at boundary is chosen to be removed. This choice is because we do not want to introduce new edges which will complicate the problem. However, as we assume all processes are homogeneous, and \( t_n^{(i)} \) for different \( i \) and \( n \) are of the same distribution, the expectation of overall execution time will only be related to the number of processes we use, and the conclusion drawn above does not lose any generality despite the choice on process to be removed.

A simple MATLAB script is used to simulate this process. \( t_n^{(i)} \) is assumed to come from a normal distribution with a mean of 4 and a standard deviation of 1, and does not change with the number of processes used. This means that the computation scale at each process remains constant. Execution times of 10,000 steps are collected with number of processes ranging from 2 to 8192. The simulation result, in Figure 4-5, shows that the overall execution time grows with the number of processes. This is consistent with theoretical conclusion above.
Figure 4-5 Simulation result: execution time versus number of processes

From Figure 4-5, we also observe that with exponential increase in the number of processes, the increase in execution time gets less and less significant. This is because in the directed graph in Figure 4-4, with more processes, there will be smaller possibility for the event that removing a boundary process will affect path \( P \) and thus reduce the execution time. In other words, with more processes, adding another process will generate less increase in the expectation of overall execution time. Rough deduction shows that if increasing the number of processes from \( N \) to \( 2 \times N \) generates an increase in the expectation of execution time of \( t \), then increasing the number of processes from \( 2 \times N \) to \( 4 \times N \) will generate an increase in the expectation of execution time of the amount \( \frac{t}{2} \).
To summarize these two scenarios, when the computing processes are homogeneous, which means the all computing processes have the same computing capability and are assigned with computation task of relatively the same scale, the expectation of communication latency will increase when more processes are used, if processes use barrier operation to synchronize in each iteration, or if processes communicate with some neighboring processes in each iteration.

4.4.3 Utility of Communication Overlap

Analysis above has shown that, when the overall problem scale is fixed, using more processors and processes will increase the communication latency while reducing the computation time at each process. Therefore, the communication latency will quickly become the bottleneck of further performance improvement. When the increase in communication latency is larger than decrease in computation time, adding more processes will result in negative performance gain.

In the analysis in previous subsections, time spent on real data transfer is ignored, and the communication latency considers only the wait time generated by asynchronous progress among interdependent processes. Consequently, this communication latency cannot be reduced by employing more advanced networking technology. However, communication overlap technique can be used to reduce or even fully hide the impact of this communication latency.

Here is the basic idea of hiding communication latency using communication overlap. For time evolution style algorithms mentioned above in Section 4.1, 4.4.1 and 4.4.2, in iteration $n$ of the main loop, there is computation that is not dependent
on interprocess communication happening at the end of iteration \(n-1\); there is also computation which the communication happening in iteration \(n\) does not depend on. Computation belonging to these 2 types is later referred to as \emph{communication-independent computation}. Similarly, the computation that (probably indirectly) depends on communication happening at the end of previous iteration and the computation that is relied on by the communication happening in the same iteration are referred to as \emph{communication-dependent computation}. If the communication-independent computation can be rescheduled to be carried out when the communication in iteration \(n-1\) or \(n\) is in progress, computation progress and communication progress are overlapped. With this overlap of communication and computation, these 2 program blocks are now executed in parallel rather than in serial, and thus execution time can be shortened.

We now provide analysis on the utility of this technique. We will prove that this technique will reduce the impact of communication latency in long-term running of parallel program even though the main source of this latency, the progress asynchronism among participating processes, is not changed. Similar to the above analysis, communication latency brought by real data transfer is ignored. Consider the two cases shown in Figure 4-6. In this figure, a parallel computation with two participating processes, process 1 and process 2, is considered. Each rectangle represents an iteration of a loop, with unshaded subarea representing \emph{communication-dependent computation}, and shaded subarea representing communication-independent computation, which can overlap with communication in the previous iteration. During the interprocess communication, when one process reaches communication phase before the other one, without communication overlap it may initiates an idle wait for the other one to start the communication, which is the solid subarea in the figure. A
running of 4 iterations is considered. In the first and the third iteration, the 2 participating processes have synchronous progress. In the second iteration, process 1 is delayed; and in the iteration 4, process 2 has a slower progress.

![Diagram showing communication event points](image)

(A)

![Diagram showing communication event points](image)

(B)

**Figure 4-6 (A) non-overlap versus (B) overlap: comparison of latency**

In case (A), in the second iteration, process 1 performs slower than process 2. Therefore, no matter how fast process 2 is, it will has to wait for process 1 to finish before it can do the communication and continue with the next iteration. It appears to process 2 as large communication latency. The overall effect is that execution time of process 2 for this iteration is lengthened. Later, in iteration 4, although process 1 finishes in a shorter time than process 2 does, similar communication latency will now be applied to process 1 and process 1 cannot reclaim it previous delay in iteration.
2. In summary, when no communication overlap is used, at any iteration, delay at progress of one process will be reflected in all interdependent faster processes as larger communication latency, and future faster progress at this very process cannot reclaim this negative effect. Delays will get accumulated over iterations and will increase overall execution time.

   In case (B), the delay of process 1 in iteration 2 does not affect the progress of process 2 because process 2 can continue with its communication-independent computation of iteration 3 without finishing the communication of iteration 2. Later, in iteration 4, process 1 has a faster per-iteration progress and its overall progress catches up with normal progress. The overall effect is that its delay in iteration 2 is reclaimed by its faster progress (like a negative delay) in iteration 4.

   Comparing these 2 cases, the communication overlap technique prevents the delay of progress of one process to affect other processes that interact with this process; it allows the very process to effectively reclaim this delay in the future. In our homogeneous system, the execution times of each iteration at different processes vary around an average value. If the communication overlap technique is not used, a delay, or a positive offset from this average value, will be immediately propagated to neighboring processes and will hopefully affect the overall execution time, while a faster progress, or a negative offset from this average value is hidden by propagation from other neighboring processes. The overall effect is that communication latency gets accumulated over iterations and increases total execution time. To the contrary, if communication overlap is used, a delay will hopefully be reclaimed later by the same process and will not affect the overall progress or the execution time. To summarize, communication overlap technique is effective in reducing the impact of
communication latency brought by asynchronous progress of interdependent processes.

4.5 Implementing the Parallel Fiber Suspensions Simulation with Communication Overlap

4.5.1 Theoretical Aspects of Communication Overlap

We will now see quantitatively how much communication latency can be hidden. It is possible to overlap communication with computation is because that if we ignore the little CPU involvement in communication phase, communication and computation basically use different types of resources and thus can happen simultaneously instead of successively. (Using normal blocking communication procedures will let communication and computation be executed consecutively.) As mentioned above, in a typical iteration $n$ of the main loop, there are two types of communication-independent computation. Let the time spent of this computation be $t_{\text{comp}}$ and time spent on interprocess communication be $t_{\text{comm}}$. With communication overlap to let these two blocks be executed in parallel, the execution time to finish them will be $\max(t_{\text{comm}}, t_{\text{comp}})$ as opposed to $t_{\text{comm}} + t_{\text{comp}}$ when they are executed in sequence. It can be seen that communication latency can be partially hidden (when $t_{\text{comm}} > t_{\text{comp}}$) or fully hidden (when $t_{\text{comm}} < t_{\text{comp}}$), and the overall execution time will always be reduced.
The challenge of communication overlap technique is how to best reschedule the algorithm to allow the overlap while at the same time preserving the validity of the algorithm. This can be restated as the following scheduling problem: 1) scheduling as much computation as possible to be executed when the communication is being processed; and 2) changing the order of execution during rescheduling should not break the data and control dependences among program blocks. The latter constraint set by dependences usually limits the former. In fact, the existence of communication-dependent computation can also be attributed to this constraint, because this computation and communication has control and/or data dependences. Two methods are used to obtain more opportunity for communication overlap: (A) break large computation blocks which are communication-dependent into small ones, some of which are communication-independent; and (B) conditionally break the data and control dependences to generate more communication-dependent computation while using variable rename and memory copy to preserve the accuracy.

The main loop is the level-1 program block. If we reschedule only inside this level-1 block, most of the operations, which are treated as atomic elements during scheduling, are communication-dependent and cannot be useful for communication overlap. However, if we expand these operations in level-1 block to their implementation, (in the programming language C, function calls are expanded to function implementations,) then with finer-grain scheduling elements there are much more opportunities for communication overlap.

Speculative execution is another technique used to generate more opportunities for communication overlap. Speculative execution is the execution of code whose result may not actually be needed, and is used to circumvent constraints set by control
dependence, for example, to reduce the cost of conditional branch instructions. In such a case, before the condition is computed, which branch is to be executed is unknown. Consequently, code inside the branches cannot be scheduled to be executed prior to the condition gets known. Using speculative execution, one or more of the branches are computed before the condition is available, with variable renames so that speculative execution will not really change variables. Later when the condition gets available, hopefully all or part of speculation execution result can be validated.

Speculative execution is useful in our rescheduling problem because there are conditional branches. One important use is that the procedure move_particles_to_neighbors is conditional, while the condition is need_to_move computed from the global maximum velocity which requires interprocess communication to compute. With speculative execution, some computation of procedure move_particle_to_neighbors can be executed when the interprocess communication is being processed.

Besides this control dependence, there are 3 types of data dependences, namely flow data dependence, anti data dependence, and output data dependence. Both anti and output data dependences can be circumvented via variable rename and memory copy, while flow data dependence cannot be bypassed. An instruction $S_2$ is flow dependent on instruction $S_1$ (or there exists flow data dependence from $S_1$ to $S_2$) when $S_1$ writes to a variable X which is later read by $S_2$. $S_2$ is anti dependent on instruction $S_1$ (or there exists anti data dependence from $S_1$ to $S_2$) when $S_1$ reads from a variable X which is later written to by $S_2$. $S_2$ is output dependent on $S_1$ (or there exists output data dependence from $S_1$ to $S_2$) when $S_1$ writes to a
variable X which is later written to by $S_2$. Both dependences can be circumvented by letting $S_2$ to write another variable $X'$; an instruction to copy $X'$ to $X$ is inserted at the present location of $S_2$. After this scheduling of $S_2$ will not be limited by this dependence. This technique is used to reschedule some particle status update computation to make it execute prior to the particle status is used to compute the forces.

There is also the controversy of maximizing the communication-independent computation blocks and preserving the clearness of algorithm. To best maximize the communication-independent computation blocks, the rescheduling should happen at the instruction or language primitive level. However, that would totally reshuffle the program and leads to complete lose of clarity. Furthermore, the data dependence analysis will be very complex. In fact, fine-grain will not necessarily generate efficient algorithm, given that the rescheduling can only rely on approximation algorithms. Our idea is that a non-optimal time saving in a big program block often generates better result than a large time saving within many tiny program blocks does. The method is that, we do a performance profiling to identify what the time-consuming function calls are in the main loop. Based on the method (A) mentioned above, the communication-dependent time-consuming function calls will be replaced with its implementation and the generated “fat” main loop can have much more communication-independent computation blocks. This is a 1-level expansion. If there is still largely time-consuming function calls after expansion, a further expansion may be done. We will not go any further to do another level of function call expansion, which will largely worsen the clarity of algorithm.
4.5.2 Rescheduling

Our profiling program has helped us to identify critical function calls, which are listed in the algorithm skeleton in Figure 4-2. Some important ones are move_particles_to_neighbors, copy_particles_to_neighbors, and velocity_Verlet. They are extended into their implementations, and the “fat” loop body is listed in Figure 4-7.

```markdown
while loop_count < max_loop_count
    do
        update_loop_count
        particle_status_update_1
        if need_to_move then
            prepare_to_move
            exchange_moved_particles
            clean_particles
        end if
        prepare_to_copy
        exchange_copied_particles
        force_computation
        particle_status_update_2
        collect_GMV
        broadcast_GMV
        compute_need_to_move
    end do

Figure 4-7: Extended pseudo-code showing the structure of main loop
```

There are 2 communication blocks in one loop iteration in our simulation program. The first one, later referred to as communication block 1, is to do particle move and copy (procedure exchange_moved_particles and procedure exchange_copied_particles), and another one, later referred to as communication block 2 (procedure collect_GMV), is to collect the global maximum velocity data. Both computation and communication access and share the same data, which are the particle status information.
There exists control dependence from communication block 2 in iteration \( n-1 \) to move_particles_to_neighbors in iteration \( n \), because the *global maximum velocity* (GMV) collected in procedure collect_GMV determines whether move_particles_to_neighbors needs to be executed for the current iteration. Some computation within move_particles_to_neighbors can be circumvented from this dependence using speculative execution and is scheduled to be executed simultaneously with communication block 2. In the final schedule in Figure 4-8, prepare_to_move is speculatively executed and overlaps with communication block 2.

Anti data dependence exists from collect_GMV of iteration \( n-1 \) to particle_status_update_1 of iteration \( n \). This is because collect_GMV needs to read the particle information, while particle_status_update_1 will write to particle information. However, by letting particle_status_update_1 to output to a backup memory location rather than normal memory storing particle status, it can be overlapped with collect_GMV. Results in the backup memory can be copied back to normal memory location at the original code position of collect_GMV.

Flow data dependence cannot be circumvented, but it largely limits scheduling in our program. The most time-consuming computation, force_computation, is flow data dependent on communication block 1. However, by looking into the force_computation procedure, a large portion of the computation is not data dependent on communication. The force_computation procedure computes forces between all pairs of particles having distance within the cut radius. The particles involved in this computation within one subdomain can be divided into 3 categories, namely moved particles, which are moved from neighboring subdomain in the
previous move_particles_to_neighbors procedure, copied particles, whose status is copied to the current subdomain by copy_particles_to_neighbors, and normal particles, consisting of particles within this subdomain except for those moved particles. Based on this categorization, the interactive forces among particles can be divided into these 6 categories:

1. moved particles versus moved particles,

2. moved particles versus copied particles,

3. moved particles versus normal particles,

4. copied particles versus copied particles,

5. copied particles versus normal particles, and

6. normal particles versus normal particles.

Of these 6 categories, the last one involves only local particles and does not require move_particles_to_neighbors to finish, and thus is not flow dependent on communication block 1. Based on this, force_computation is divided into 2 parts. boundary_force_computation computes forces belonging to category 1 to 5, and non_boundary_force_computation computes forces belonging to category 6. The latter one, which accounts for most of the computation time, can overlap with communication block 1 and can help reduce the impact of communication latency.

The final rescheduling result is shown in Figure 4-8. non_boundary_force_computation overlaps with communication block 1, and speculative particle_status_update_1, prepare_to_move, and
prepare_to_copy overlap with communication block 2. For speculative execution, a complementary procedure is added to validate the result, and for prepare_to_move which uses variable rename to avoid anti data dependence, a complementary procedure is also added to copy the renamed results to original variables.

<table>
<thead>
<tr>
<th>Communication Resources</th>
<th>Computation Resources</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>compute need to move</td>
</tr>
<tr>
<td></td>
<td>particle status update 1 (restore)</td>
</tr>
<tr>
<td></td>
<td>if need_to_move then</td>
</tr>
<tr>
<td></td>
<td>init exchange moved particles</td>
</tr>
<tr>
<td></td>
<td>end if</td>
</tr>
<tr>
<td></td>
<td>init exchange copied particles</td>
</tr>
<tr>
<td>communication block 1</td>
<td>non_boundary_force_computation</td>
</tr>
<tr>
<td>(exchange moved particles, exchange copied particles)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>boundary_force_computation</td>
</tr>
<tr>
<td></td>
<td>particle status update 2</td>
</tr>
<tr>
<td></td>
<td>init collect GMW, broadcast GMW</td>
</tr>
<tr>
<td>communication block 2</td>
<td>; for next iteration:</td>
</tr>
<tr>
<td>(collect GMW, broadcast GMW)</td>
<td>particle status update 1 (with memory rename)</td>
</tr>
<tr>
<td></td>
<td>prepare_to_move (speculative)</td>
</tr>
<tr>
<td></td>
<td>prepare_to_copy</td>
</tr>
</tbody>
</table>

**Figure 4-8 Rescheduling result**

### 4.5.3 Implementation of Communication Overlap

Communication overlap is implemented by using asynchronous (or non-blocking) communication primitive in many programming libraries. Unfortunately, our experiments showed that non-blocking operations in MPICH with p4 device (or MPICH-P4) cannot be used for this purpose. We observed that for message size smaller than 128kB, they perform just like standard send and receive procedures and do not return immediately, and for message size greater than 128kB, although they
return immediately, they do not perform the real data transfer until \texttt{MPI\_Wait} is called, which will block the program anyway. (Note that in the later case, the conclusions in Section 2 still apply. It is like to move the communications down to position of \texttt{MPI\_Wait}.) In other words, the real data transfer always blocks the execution thread and communication and computation cannot happen simultaneously. This is probably because in MPICH-P4 non-blocking MPI operations are implemented with synchronous socket communication, which means it is impossible to make communication and computation happen simultaneously because they are in a single execution thread.

We overlap communication with computation by letting them execute in a separate OS thread. An extra thread is used to regulate computation when the communication is blocking the main thread. At the beginning, the extra thread is blocked in purpose. When the main thread is about to do communication and block, the extra thread will be activated. Upon activated, the extra thread read a status set by main thread, and pick the right computation procedures to start. When the main thread is wakened upon the finish of communication, it checks for extra thread and waits for its completion before it moves on. With careful synchronization between main thread and extra thread, the communication and computation can be scheduled in an overlapped manner. For secure multi-threading, we also move to MPICH2, all-new implementation of MPI by MPICH developers, which has better thread-safe support. Our new implementation based on the schedule above and on the multi-threaded

\footnote{\texttt{MPI\_Wait} is an MPI routine which blocks the process and waits for specified MPI send or receive to complete.}
MPICH2 has improved the performance on computer cluster. The next subsection will list the experiment results.

4.6 Results

Using the experiment configured as listed in Section 4.3, tests are run on 1, 2, 4, 8 and 16 processors, with one process per processor. Wall clock time and CPU time have both been recorded. For comparison purpose, the test is firstly conducted when the system has zero load, and is then conducted when the system has a load of 1. The UNIX program `top` is used to obtain the load information.

4.6.1 CPU Time

CPU Time is a good measurement of computation complexity. When different numbers of processes are used, the overall computation complexity varies and this will result in different CPU times. Table 4-2 shows the overall CPU times for different numbers of processes with and without the communication overlap technique applied. The overall CPU time is computed by adding up the CPU times of the involved processors.

<table>
<thead>
<tr>
<th>Number of processes</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without overlap</td>
<td>53362s</td>
<td>50711s</td>
<td>49382s</td>
<td>50054s</td>
<td>54570s</td>
</tr>
<tr>
<td>With overlap</td>
<td>67914s</td>
<td>60409s</td>
<td>57221s</td>
<td>58129s</td>
<td>62519s</td>
</tr>
</tbody>
</table>

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From Table 4-2, we see that in both experiments with and without overlap applied, the overall CPU times first decrease and then subsequently increase. This is the combined effect of 1) the decrease in complexity of non-optimal algorithms for subproblems as the domain is divided into subdomains - an example of these subproblems is to search for all particle pairs within a radius from a specific particle in velocity-Verlet algorithm; and 2) the increase in the number of duplicated computations of forces associated with particles positioning within a radius away from the boundary of two neighboring subdomains. As the number of processes increases beyond 4, the combined effect is the increase in overall CPU time because the second factor dominates the first.

Table 4-2 also shows that even though the communication overlap technique helps reduce the communication latency, the scheduling adds overhead and results in larger CPU time. An example of overhead is the duplicated needed to separate one program block (or procedure) into two blocks during rescheduling. In the subsequent sections, we will evaluate the performance of applying the communication overlap technique to zero-load system and non-zero load system.

4.6.2 Performance Evaluation using Zero-load System

We first test the program on a zero-load system. This means that our test programs run exclusively on the system with no other programs to compete for the resources, which is the case when the all parallel jobs are submitted to and controlled by a central batch job scheduler. Similar to the CPU time test, only one process is assigned to each processor. We note that due to the non-optimum of the parallel velocity-Verlet algorithm, the computation complexity may decrease with the
increase in the number of processors. Therefore, conventional definition of speedup and efficiency cannot be used. We define observed speedup \( S_o(N) \) and observed efficiency \( E_o(N) \) as:

\[
S_o(N) = \frac{\text{execution time with 1 processor}}{\text{execution time with N processor}},
\]

\[
E_o(N) = \frac{S_o(N)}{N} \times 100%,
\]

and the plots of observed speedup and observed efficiency are shown in Figure 4-9. From this figure, we see that 1) on zero-load system, using communication overlap appears to degrade the observed speedup and observed efficiency and 2) as the number of processes increases, the performance difference between experiment with communication overlap technique applied and that without this technique gets smaller. The overhead introduced by this technique, such as the thread synchronization operations, accounts for the performance degradation. Furthermore, because the system is of zero load, there is little asynchronism among the participating parallel processes and thus small communication latency, leaving small room for this technique to improve performance. However, as the number of processes increases further, as discussed in the previous section, the communication latency is not insignificant any more and the communication overlap technique starts to take effect. This is why the observed efficiency of program having this technique applied decreases slower. When 16 processes are used, program with this technique and the program without this technique demonstrate comparable performances.
A separate test with 32 processes on 16 processors is performed, and performance of the program with the communication overlap technique applied surpasses that of the program without this technique. This behavior demonstrates that the communication overlap technique actually reduces the impact of communication latency as the number of processes gets larger.

In a parallel implementation of an application, the efficiency generally reduces due to the ineffective mapping and increase in communication among processes. In our experiment, the observed efficiency can be larger than 100% because the overall performance benefit outweighs the increased communication overhead. However, this situation is not typical and is influenced by the specific configuration and workload of the system.

Figure 4-9 Observed speedup and observed efficiency on zero-load system

---

5 Because of limitation of usable processors in Hydra II, we could not run 32 processes on 32 processors, but rather 32 processes on 16 processors.
problem size (measured by CPU time) does not remain constant with different numbers of processes. If we compensate the observed efficiency with change of problem size, the new efficiency values will be below 100%. The original efficiency and that after compensation are listed in Table 4-3. Compensation is calculated using the following equation (with $E_p(N)$ being the observed efficiency after compensation):

$$E_p(N) = E_o(N) \times \frac{\text{CPU time of N - process non - overlap program}}{\text{CPU time of 1 - process non - overlap program}} \quad (4-7)$$

<table>
<thead>
<tr>
<th>Number of processes</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>32 (on 16 processes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed speedup when communication overlap is not used</td>
<td>2.04</td>
<td>4.02</td>
<td>7.51</td>
<td>10.27</td>
<td>8.37</td>
</tr>
<tr>
<td>Observed speedup when communication overlap is used</td>
<td>1.69</td>
<td>3.55</td>
<td>6.89</td>
<td>10.10</td>
<td>8.74</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is not used</td>
<td>102%</td>
<td>100%</td>
<td>94%</td>
<td>64%</td>
<td>N/A</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is used</td>
<td>84%</td>
<td>89%</td>
<td>86%</td>
<td>63%</td>
<td>N/A</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is not used, after CPU Time compensation</td>
<td>97%</td>
<td>93%</td>
<td>88%</td>
<td>65%</td>
<td>N/A</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is used, after CPU Time compensation</td>
<td>80%</td>
<td>82%</td>
<td>81%</td>
<td>64%</td>
<td>N/A</td>
</tr>
</tbody>
</table>

In summary, on zero-load system with no other users and with a single process being assigned to each processor, the effect of applying the communication overlap technique is minimal if not undesirable. This is primarily because of the insignificant amount of communication latency. It is also observed that this technique started to show some performance improvement as the number of processes gets larger such as 16 and beyond.

Such zero-load system is idealistic in system with interactive job submission rather than with a global batch job scheduler, because many user processes share the same computer cluster and their processes will actively look for resources. The communication latency will be significant because of the much larger asynchronism among participating parallel processes of a single job. In such a case, communication overlap technique starts to play an important role. In the next section, performance evaluation using non-zero load system is performed to model this scenario with processes competing for resources.

### 4.6.3 Performance Evaluation using Non-zero Load System

Most of the time the simulation program cannot exclusively use a computer cluster (except for system requiring job submission via a batch job scheduler, which often means to wait for some time before the job can start). We now run the test on a system whose nodes all have a load of 1, which means there is already another
program taking 100% of the CPU time and keeping the CPU 100% busy. We call this process an *interfering process*. As each node of the computer cluster has to deal with multiple computation-intensive operating system (OS) processes, the asynchronous switches of OS processes will contribute to large asynchronism among parallel computing processes. If the interfering process itself is not perfectly stable, it will further contribute to the asynchronism among parallel computing processes. Large degree of asynchronism will bring large communication latency and therefore harm the overall performance of the parallel program.

Figure 4-10 shows the observed speedup and observed efficiency of our parallel simulation program under non-zero load situation. From this figure we see that only in the 2-process case the experiment with communication overlap technique applied shows worse performance than that without this technique. This is because the overhead of communication overlap surpasses its benefits. For larger number of processes, the communication latency becomes a main obstacle to high performance. When more processes and processors are introduced, there is severe degradation of efficiency, which limits further increase of performance by adding more processors. Table 4-4 summarizes the results. When the number of processes increases from 8 to 16, observed speedup is improved by 65% (or from 7.16 to 11.85), compared to 93% (or from 1.98 to 3.84) when the process number is increased from 2 to 4. The communication overlap technique effectively tackles this problem and prevents the severe decrease in efficiency as the number of processes increases. For example, increasing the number of processes from 8 to 16 brings an improvement of 86% (from 7.79 to 14.50). In fact, if we take into account the effect of change in problem complexity and uses speedup and efficiency compensation, the efficiency after compensation almost remains constant with communication overlap technique.
applied. This is also shown in Table 4-4 in the last 2 rows. Consequently, for large number of processes when there is large communication latency, use of communication overlap technique will result in large performance improvement because the technique will effectively reduce the impact of communication latency. For example, our test showed that for 16-process case, program with the communication overlap technique applied is 22.3% faster than that without this technique in terms of observed speedup.

![Figure 4-10 Observed speedup and observed efficiency on non-zero load system](image)

<table>
<thead>
<tr>
<th>Number of processes</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed speedup when communication overlap is not used</td>
<td>1.98</td>
<td>3.84</td>
<td>7.16</td>
<td>11.85</td>
</tr>
<tr>
<td>Observed speedup when communication overlap is used</td>
<td>1.82</td>
<td>3.96</td>
<td>7.79</td>
<td>14.50</td>
</tr>
</tbody>
</table>

Table 4-4 Performance evaluation results: non-zero load system (original load is 1)
<table>
<thead>
<tr>
<th>Observed efficiency when communication overlap is not used</th>
<th>99% 96% 89% 74%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observed efficiency when communication overlap is used</td>
<td>91% 99% 97% 91%</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is not used, after CPU time compensation</td>
<td>94% 89% 84% 75%</td>
</tr>
<tr>
<td>Observed efficiency when communication overlap is used, after CPU time compensation</td>
<td>86% 92% 91% 92%</td>
</tr>
</tbody>
</table>

In summary, the effectiveness of the communication overlap technique has become significant when the communication latency is not trivial and especially when the parallel machine has several active computation tasks. This is the case when the number of processors involved in the computation is large and/or the computer cluster is not dedicated to a single computation task. Communication overlap technique and our implementation on MPICH2 have successfully reduced the impact of large communication latency, and significantly improved the measurable performance. As demonstrated in the case of 16 processes, introduction of this technique can increase the efficiency as high as 22.3%.

### 4.7 Conclusion

A large number of computational bioengineering applications employ decomposition to realize parallel computation. Fiber suspension simulation problem, which utilizes spatial decomposition, is a typical example of these applications. A vast majority of these applications suffer from degraded efficiency and even speedup with the increase in the number of processors used, while actually they need more processors to achieve faster computation. In this chapter, we use both experiment and
theoretical analysis to understand a major source of performance bottleneck: asynchronism among participating parallel computing processes. This asynchronism is an important source of communication latency, and the contributed latency grows along with the number of processors. It therefore imposes an increasingly negative impact on performance. Finally when the increase in communication latency brought in by using more processors, together with other overhead, surpasses the benefit, the limit of performance gain from parallel computing is reached.

We propose to use communication overlap technique to reduce the impact of communication latency on performance, which is theoretically proved to be effective, even for communication latency brought in by asynchronism among parallel processes. Multi-threading is used to implement this technique, and block-level rescheduling is performed to generate enough opportunities to allow communication to overlap with computation. Experiments have shown significant improvement under practical conditions on computer clusters. For example, in the experiment with 16 non-dedicated processors, our implementation increases the efficiency as high as 22.3%.

As mentioned above, the fiber suspension simulation problem belongs to a family of similar computational bioengineering applications, and a vast majority of applications in this family suffers from the same performance problem, especially when the program is run on computer clusters. Our work helps to understand a major source of performance bottleneck. We suggest incorporating communication overlap technique into parallel programs for these applications, probably via the same implementation as ours, to reduce the impact of communication latency and to improve the overall parallel execution performance.
Chapter 5 Parallel Image Processing for Laser Speckle Images

Laser speckle, a random interference effect that gives a grainy appearance to objects illuminated by laser light, is widely used as a flow monitoring. It is used in clinical applications as a non-contact, two-dimensional, full-field measurement of retinal microcirculation. Laser Speckle Contrast Analysis (LASCA) is an important technique in this application, which uses CCD camera for image capturing and software digital image processing. When this is used for real-time clinical applications, it imposes severe requirements on computing capacity. We propose to use parallel computers for this task.

5.1 Introduction to Laser Speckle Imaging Technique

5.1.1 Laser Speckle Images

Laser speckle is a random interference effect that gives a grainy appearance to objects illuminated by laser light. When a rough surface is illustrated by laser light, light scattered from different parts of the surface within a resolution cell of the detector (an eye or camera, for example) traverses different paths to reach the image.
plane. At any given point, the interference of light will result in random intensity. The overall effect is high-contrast grainy in appearance, with light and dark “speckles” caused by constructive and destructive interference, respectively, of scattered laser light. In brief, laser speckle is an interference pattern produced by light reflected or scattered from different parts of the illuminated surface. It is a random phenomenon and can only be described in statistical method.

In 1970s, Goodman [28] developed a theory of speckle images using statistical methods. In his theory, ideal conditions for producing a speckle pattern have been assumed, which mean single-frequency laser light and a perfectly diffusing surface with a Gaussian distribution of surface height fluctuations. Goodman showed that under these conditions, the standard deviation of the intensity variations in the speckle image pattern is equal to the mean of intensity. In practice when idea conditions are not met, speckle patterns often have a standard deviation that is less than the mean intensity, and thus a reduction in contrast is observed. Speckle contrast, quantifying this reduction of contrast, is defined as the ratio of the standard deviation to the mean intensity:

\[
K = \frac{\sigma}{<I>} \leq 1
\] (5-1)

This concept of speckle contrast is lately widely used as the most important spatial statistics of speckle images.
5.1.2 Time-varying Laser Speckle Image

When the illuminated object moves slowly as a whole solid object, the speckles move with the object and remain correlated. When the object performs large motion or when the object itself consists of individual moving scatterers (such as blood cells), the speckles decorrelate and the speckle pattern fluctuates. This type of time-varying speckle is frequently observed when biological samples are observed under laser light, because of the flow of fluid inside biological components or even the motion of particles within the cells. These fluctuations encode information about the velocity distribution of the scatterers, such as the particles within the cells of biological systems.

Several methods have been proposed to extract velocity information about the particles from these fluctuations. These methods are whether based on time-integrated speckle technique or time-differentiated speckle technique, both of which are explained below.

The time-integrated speckle technique [29] treats acquired speckle image as temporal integration of speckle fluctuations and uses spatial statistics to translate acquired image pattern into velocity map. It is based on the fact that, in practice, it is impossible to achieve instantaneous measurement of the speckle intensity due to the finite integration time of the detector. Therefore, the obtained speckle image is always integration of speckle fluctuations in the time domain. By measuring the depth of modulation and/or integration time, estimation of particle velocity can be obtained. Single-exposure speckle photography [30], as well as the derived Laser Speckle Contrast Analysis (LASCA) [31] described in the Section 5.1.4, is based on time-
integrated technique and relates the spatial statistics (essentially the contrast) of the time-integrated speckle pattern to the scatterer velocity.

A different approach is the time-differentiated speckle, which captures successive speckle intensity images through continuous scanning and performs temporal statistical analysis. Takai et al [32] used frequency analysis, while Fercher [33] used speckle contrast and largely simplified the analysis. Ruth [34] [35] also used differentiation of the speckle intensity and showed that the velocity is proportional to the mean frequency of the fluctuations, and that this in turn is proportional to the root mean square of the time-differentiated intensity.

5.1.3 Laser Speckle Imaging Systems

Using the techniques above, various Laser Speckle Imaging (LSI) systems have been widely built and deployed in many engineering and especially medical applications. One of the most important potential applications, first recognized by Stern [36], aroused when the fluctuations were caused by the flow of blood; this discovery was later developed into various non-contact and noninvasive blood flow measurement techniques.

Early researchers used the temporal statistics of time-varying laser speckle. This method can only measure the blood velocity at a point. When a map of blood velocity distribution is required, either a mechanical scanning or the successive analysis of the intensity fluctuations at different pixels in a CCD array is needed. The consequence is large delay and non real-time operation.
Single-exposure speckle photography is a technique that removes the need for scanning and offers a true full-field velocity map. It is essentially a photography technique and uses an exposure time that is long enough to allow the faster fluctuating speckles to blur out. The resulting photo is a time-integrated speckle pattern. It then utilizes mathematical models to relate spatial statistics of this time-integrated speckle pattern to the velocity of scatterers. This technique was successfully developed for measurement of a retina blood flow [37].

The disadvantage of single-exposure speckle photography technique is that, although it removes the need for scanning, it suffers from the disadvantage of being a two-stage process that precludes real-time operation. This is because chemical processing is required to develop the film before it can be used for spatial filtering.

5.1.4 Laser Speckle Contrast Analysis

Laser Speckle Contrast Analysis (LASCA) is a digital version of single-exposure speckle photography. By replacing conventional camera with a CCD camera and a frame grabber, the need for photographic stage is eliminated and facilitates digital processing of the resulting photographs. Since the exposure is as short as 20 milliseconds, if the digital processing time is short enough, this technique can support effectively real-time operation.

As shown in Figure 5-1, a LASCA LSI system basically consists of a laser light source, a high-resolution CCD camera, a frame grabber, and a computer equipped with specially developed software that computes the local speckle contrast and converts it to a false-color map of contrast (and hence of velocity). The frame grabber
may also be a specialized software component built for the camera. It is important to select a laser with suitable wavelength. For example, in a blood flow measurement setting, laser wavelength should be selected based on the tissue under observation, as it is necessary to achieve some tissue surface penetration with the laser light for blood flow mapping.

![Figure 5-1 Basic setup of LSI with LASCA](image)

The sample, or area of interest, is illuminated with laser light while the computer acquires a series of images at high speed with the frame grabber and CCD camera. Each acquired image will display a slightly different speckle pattern, caused by the change of position of moving scatterers in the area of interest. Every single frame generated by the frame grabber is a time-integrated speckle pattern. Speckle patterns are then sent to PC for statistical analysis. By assembling a series of frames, a real-time video of velocity map can be achieved.

The principal of LASCA is similar to other time-integrated speckle techniques. LASCA translates reduction of contrast to scatterers velocity. It is clear that the higher are the scatterers velocities, the faster are the fluctuations of speckles and the
more blurring occurs in a given integrated time. It has been shown [30] that given certain conditions, spatial statistics of time-integrated speckle patterns can be linked to temporal statistics of the fluctuations in the following way:

$$\sigma_s^2(T) = \frac{1}{T} \int_0^T C_s(\tau) d\tau,$$  \hspace{1cm} (5-2)

where $\sigma_s^2(T)$ is spatial variance of the time-integrated speckle pattern, $T$ is the integration time, and $C_s(\tau)$ is the autocovariance of the temporal functions at time $t$, defined as

$$C_s(\tau) = \langle \{I(t) - \langle I \rangle\}, \{I(t + \tau) - \langle I \rangle\} \rangle_t.$$  \hspace{1cm} (5-3)

It is now established that spatial statistics used in LASCA is equivalent to techniques using temporal statistics so far as linking the measurements to actual velocities is concerned. All techniques determine the correlation time $\tau_c$ to estimate velocities, and further assumptions are made to link speckle contrast to $\tau_c$. With assumption of Lozentzian velocity distribution, it is shown that:

$$K = \sqrt{\frac{\tau_c}{2T} \left(1 - e^{-\frac{2\tau}{\tau_c}}\right)}.$$  \hspace{1cm} (5-4)
This is further linked to mean velocity by

\[ v_c = \frac{\lambda}{2\pi r_c}, \tag{5-5} \]

where \( \lambda \) is the wavelength of the laser light.

It must be noted that it would be unwise to take too much account of the quantitative value of the LASCA technique. The system being monitored is extremely complex and there are many indeterminate factors in play. Most assumptions made in the analysis are also inconsistent with practice. What is important from a medical point of view is the ability to monitor the changes and variations. From this perspective, LASCA technique is useful for medical applications. Besides, further simplification will not harm the performance much.

### 5.1.5 Modified LSI

LASCA method uses speckle contrast to indirectly measure flow velocity. In practice, to compute speckle contrast, a 5x5 or 7x7 region of pixels is used. Lower numbers reduce the validity of the statistics, whereas higher numbers limit the spatial resolution of the technique. The software computes the speckle contrast \( K \) for any given square, and assigns this value to the central pixel of the square. The process is then repeated for 5x5 or 7x7 squares centered on each pixel in turn. This results in a
smoothing of the contrast map, but the spatial resolution is lost in averaging over a block of pixels. For example, when the image captured consists of 512×512 pixels and a square of 7×7 is used to compute the spatial statistics for each pixel, the resulting image will have resolution effectively reduced by use of this 7×7 squares to 73×73 (pixel blocks). Cheng et al. [38] realized this problem, and suggested a modified LSI (mLSI) which uses temporally derived speckle contrast.

Temporal statistics of time-integrated speckle patterns was previously used to obtain velocity information of a single point [29]. \( N_t \) is defined as

\[
N_t = \frac{<I^2> - <I>^2}{<I>^2} = K^2, \tag{5-6}
\]

where \( <I> \) and \( <I^2> \) are the mean and mean-square values of time-integrated speckle intensity variations during the time interval \( t \). We can see that \( N_t \) is inversely proportional to the velocity of the scattering particle.

Cheng extended this method to obtain a 2-D distribution of blood flow. In this method, \( m \) frames are used to estimate the mean and mean-square values of time-integrated speckle intensity variations. For the \((i^{th}, j^{th})\) pixel, its \( N_t \) is defined as

\[
N_{i,j} = \frac{<I_{i,j,t}^2> - <I_{i,j,t}>^2}{<I_{i,j,t}>^2}, \tag{5-7}
\]

\[ t = 1..m \]
where $I_{i,j,t}$ is the instantaneous intensity of the $i$’th and $j$’th pixel at the $t$’th frame of raw speckle images, and $\langle I_{i,j} \rangle$ is the average intensity of the $i$’th and $j$’th pixel over the consecutive $m$ frames. The results are given as 2-D grey-scale or false-color coded maps that describe the spatial variation of the velocity distribution in the area examined. Both normalized velocity map and the speckle contrast map can be computed thereafter.

5.2 Previous Work

Various implementations of digital image processing for LASCA and mLSI have been built. When CCD cameras are used for imaging, the image processing procedure becomes the only obstacle to achieve real-time operation.

Briers stated in his original paper about his LASCA implementation [30] that the processing takes around 40 seconds, while the image capture takes only 20 microseconds. If the image processing time can be reduced to tens of microsecond’s level, real-time operation is achieved. Although about 10 years has passed since Briers’ initial work, the LASCA technique has not reached the real-time goal. In Briers’ more recent paper [39], he described his improvements in the software that reduce the processing time to one second.

Dunn et al. [40] have been using speckle contrast imaging to monitor cerebral blood flow. They published their MATLAB scripts for computing speckle contrast on the web. We have tested these short MATLAB scripts on a Pentium 4 2.4GHz
workstation with 256 MB of SDRAM. MATLAB profiler has shown that to generate a speckle contrast image of 640x480, the scripts need 39 seconds to do spatial statistics on 10 raw source images.

Researchers in our research group also implemented software for image processing of mLSI speckle images [41]. To save computation time, binning is used to preprocess the image so that less computation is required. Even with a binning size of 2 to reduce the effective image size from 640x480 to 320x240, generating one speckle contrast map using mLSI method will take this MATLAB program around 20 seconds.

Although it is possible to rewrite the whole program using more performance-aware language such as C to approach real-time operation, that would make programming much more difficult, especially with image processing program heavily based on MATLAB image processing toolbox. There is also a trend of move to higher-level and more user-friendly programming environment, to focus more on programmability and to let system software and underlying hardware improvement worry about the performance. Based on this consideration, we propose to leverage parallel processing facility to approach real-time processing of speckle images. It will not only reduce the processing time, but also support larger image with higher resolution, given enough computing resources.

Speckle image processing is by nature suitable for parallel processing. Whether spatial or temporal statistics is used, there is little dependence between two pixels that are far enough from each other, and especially for temporal statistics every pixel is independent of others. Parallelization requires segmentation of the image into several blocks. When spatial statistics is used, each block will overlap with its neighboring
block; and when temporal statistics is used, blocks are disjoint. In both cases, processing of different blocks is independent, and can be scheduled in parallel without the need of interprocess communication. Based on the discussion in the previous chapter, efficiency will not degrade with more processes (and processors) and performance can be easily doubled by doubling the processes (and processors).

At the time of this writing, we have not found any implementation of parallel processing system for laser speckle images. Although there is intensive research work on parallel image processing and there are dedicated conferences on this topic, such as *Parallel and Distributed Methods for Image Processing*, the research results cannot be applied to laser speckle image processing. Most of the work focuses on parallel algorithms for fine-grain parallel computing, usually based on a theoretical model for algorithm research. A large portion of work relies on data parallelism, such as [42] and [43]. Research on practical parallel image processing is usually based on data parallelism with a special-purpose SIMD processor or VLSI circuit. A typical example is Gealow *et al*’s work on pixel-parallel image processing [44], which is based on large processor-per-pixel arrays. A very interesting and more relevant research is the SKIPEER project [45]. In this research, parallel algorithms are categorized into several general algorithmic skeletons. By describing the parallel problems with a combination of supported skeletons and providing the sequential functions, SKIPPER system is capable to generate efficient parallel program without the programmer to deal with any detail of parallel execution.

When laser speckle image processing is considered, various algorithms used are all relatively simple statistical analysis rather than complex conventional image processing algorithms. The parallelization of these algorithms is relatively simple.
decomposition and does not require complex programming framework or supporting runtime. Computer cluster or network of workstations built from commodity components is chosen as the hardware platform, and data parallelism is not usable. Although SKIPPER is versatile and can support many types of applications, it is too complex for our application.

The programming framework we propose for parallel laser speckle image processing uses a simple master-worker paradigm. Because only laser speckle image processing applications are supported, many logics will be built inside this framework and programmers do not need to handle any parallel execution detail, and performance will also be optimized for this specific application family. Our main goals are customization of processing logic as well as portability to take advantage of many different types of parallel computing resources.

### 5.3 Parallelism of mLSI Algorithm

Temporal statistics-based mLSI algorithm can easily be parallelized with spatial decomposition. For a pixel on source images, the K value computed with mLSI is only relevant to intensity value of this very pixel on several consecutive frames. Because of this, when computing K value is considered, every pixel is independent with the other pixels in the same frame. The extreme decomposition is to assign one pixel to a processor, and none of the processors need to communicate with others in order to compute its corresponding K value. For load balancing purpose, with known number of processors, decomposition of every frame will ensure processors receive relatively the same amount of work load.
When general laser speckle image processing techniques using spatial statistics is considered, the case is more complex. For every pixel in the image, its K value will depend on several neighboring pixels. Because of this, when the image is segmented into several blocks and has each block assigned to a processor, the processors have to exchange pixel values at the segmentation boundaries. To avoid this interprocessor communication, a simple approach is to send all necessary pixels when a block is sent to a processor. In this way, the computation can be performed without the interaction of the working processes. The same programming model as that for mLSI can then be used.

5.4 Master-worker Programming Paradigm

Master-worker paradigm is the main programming paradigm used in parallel speckle image processing program. Master-worker approach is used for task that can be partitioned into several independent subtasks, which can be carried out separately and probably (but not necessarily) in parallel without any inter-subtask communication.
Figure 5-2 Master-worker paradigm

The master-worker paradigm is depicted in Figure 5-2. The master node, usually denoted as node 0, is in charge of farming out work load to workers. Several workers work on work loads assigned by the master node. When a worker finished its current work load, it reports the result back to the master if necessary and triggers the master to send additional work load to the worker. As long as the task can be partitioned into sufficiently small segments, this approach will produce small amounts of idle time for the worker nodes.

Parallel speckle image processing is suitable for master-worker programming paradigm. The master node serves as the feeding point of input image(s), and stores the full speckle image or an array of frames of speckle images. It will segment each image into blocks, based on the number of available workers. In conventional master-work paradigm, subtasks will be maintained by master node in work load poll and wait for a worker to pull them out for further processing. However, for speckle image processing application, because of real-time requirement, indeterminism involved in waiting for processing worker node is unaffordable for any image block. Instead each
block will be determinately assigned to a worker and this worker is expected to finish this subtask in some specific time.

In order to support master-worker program, at least two types of services have to be provided:

- Communication: Portions of computation and results must be passed between master and workers;

- Resource management: System should manage the available computing nodes and preferably their capabilities and loads, and support enquiry of status from program.

Compared to communication, resource management of a master-worker framework can be very complex. For example, it may support resource detection so that master is capable of selecting the most appropriate subtask for the right worker node; it may detect the interconnection scheme used by the computing nodes so that the best routing method can be used to reduce communication latency. As a demonstration work, our research focuses on testing the feasibility of real-time processing with parallel computers, so resource management will be minimized. In fact, a real-time application can hardly depend on an unstable and/or dynamic platform such as that made available by Litzkow et al [17]. A stable environment with static contributing machines, such as a computer cluster, may be a better choice. When a computer cluster is used as the testing platform, the homogeneous environment eliminates the necessity of many resource management functions, because the load is automatically balanced and the worker nodes are static and dedicated. Even if the framework is ported to a heterogeneous environment in the
future, when resource management becomes important, resource management function should also be encapsulated and hidden from application coders. The result is that any expansion to framework will be transparent to application coder and there is no need to modify the application-level code. So the discussion here will not lose any generality.

5.5 Implementation

5.5.1 High-level Architecture

For real-time performance and easy integration into existing medical devices, our new implementation of speckle image processing system will be based on computer cluster systems and Grid technology. The use of computer cluster is to utilize the power of parallel computing to provide central, fast and stable processing of speckle imaging data as well as to take advantage of the homogeneous environment to reduce the system complexity. Since the data capture device is geographically separated from the computing facilities, Grid technology is proposed to be used to integrate all devices together. This also enables central processing of speckle imaging related data for multiple capture devices so that multiple observations of blood flow can be taken at the same time. The top-level system architecture is shown in Figure 5-3. This figure shows that a central processing system is built on a computer cluster, which is integrated with multiple image capture components using the Grid.
At the beginning of a speckle image processing session, the workstation for image capture will negotiate with the central image processing system through the Grid. This negotiation will notify the central image processing system various information about the image stream, such as compression method, frame size, and frame rate. The central image processing system will then allocate enough resources and prepare to work on the new image stream. Upon receiving further acknowledgement from the image processing system, the image capture workstation will start the image capture device and upload image stream to the image processing system; it will also receive corresponding result image or video through the Grid. When the last frame of image has been sent, the workstation will send an End-of-Session command to the image processing system, which will perform post-session work, such as freeing all allocated resource for this image stream and updating load information.
Because the image capture components access the image processing service through the Grid service portal, and does not rely on any information about how the service is built, the image processing service can run on different platforms without any modification to the image capture components. For example, the image processing service can run at a single machine, with Grid service portal also built on this machine; it may later be ported to a computer cluster, with Grid service portal built on the head node which have access to the Grid, and which will further distribute image processing subtasks to slave nodes of the same cluster. Image capture components are unaware of this change and require no change in order to work with the new system.

5.5.2 Master-worker framework implementation details

The image processing service is deployed on a computer cluster, and is built with the master-worker paradigm described in Section 5.4. Figure 5-4 illustrates the structure of the program. A master node gets the input image stream from the Grid service portal. Known as the dispatcher, it will segment every image into several blocks and send each to a worker node. The worker nodes receive the assigned image blocks and apply image processing algorithms. The resulting image will be uploaded to the assembler node, which assembles the output image stream and outputs the result through the Grid service portal. When mLSI technique is used and temporal statistics is based on $M$ frames of input images, output frame rate will be reduced to $1/M$ of the input frame rate, which is shown in the figure.
The system is designed with high-level of customization and portability in mind. It allows the interface and image processing logic to be customized, and support portability to various hardware types and communication libraries by rewriting a small number of underlying communication functions.

Interface controls how the image processing system acquires input images and outputs results. The core of the processing system, consisting of dispatcher, workers and assembler, reads input stream from standard input and outputs to standard output, which means that the interface to outside world can easily be built by wrapping and redirecting the standard input and output. For example, the interface as a Grid service portal is a program that reads input stream through the Grid and writes to the standard input of the core; it also reads from the standard output of the core and writes back to the Grid service consumer.
Considering the many methods, algorithms and parameters to determine in speckle image processing, it is important to separate the processing logic from the supporting code, which deals with initialization, communication, etc. There is also the goal of making the processing logic code independent of the underlying communication method, so that image processing service without any modification can run on any underlying parallel machine which the framework has been ported to. Based on these considerations, a framework called *Abstract Communication Layer* (ACL) has been designed to separate the supporting code out and to serve as a simple general master-worker application framework.

The architecture of ACL is illustrated in Figure 5-5. ACL has built in the main program flow, which will deal with the execution details such as initializing the underlying communication library, determining roles of computing nodes, reading input image stream and outputting result images. The flow control code will call image processing functions in custom logics for master node, worker nodes and assembler node. The custom callback functions in these logics can utilize the master-worker communication functions to handle information exchange between the master and workers and between workers and the assembler.
The flow of the program is shown in Figure 5-6. A session is started after the image capture components have successively finished the negotiation with the image processing system. Based on the provided image stream information as well as the underlying communication configuration, parameters and the environment are initialized. Each computing node will then determine its own role, which is one of master, worker, and assembler. Upon knowing its role, each node will switch to perform its specific role function, which is also illustrated in Figure 5-6.
Figure 5-6 Flowchart of the whole program, master node logic, worker node logic, and assembler node logic.
From the flowchart, it is seen that the custom image processing logic is implemented in the following callback functions:

- **Master init**: This function is called on the master node at the beginning of a session. It can be used to make necessary preparation, such as allocating memory space and calculating parameters. Similar to this function, worker nodes have **Worker init** and assembler node has **Assembler init**.

- **Master work**: This function contains the main processing logic of master node, and will be called for every input image or video frame. Normally, this function implements the segmentation of input image and will call ACL communication functions to feed the segments to worker nodes.

- **Header parse**: This function at master node is used to analyze header information, which is attached before every image. The purpose of the header is to provide extra information to the processing logic. For example, the header may contain information about whether this is the last frame. **Parse extra command** at worker node and that at assembler nodes are for similar purposes; it will extract extra commands from the image segment (for workers) or from the result segment (for the assembler).

- **Worker work**: This function contains the main processing logic of master node and will be called repeatedly until end of session command is detected. Normally this function will read image segment through ACL
communication function and apply image processing algorithms to this segment. When a result image is generated, it will upload the result to assembler node using another ACL communication function.

- **Assembler work**: Similar to Worker work, this function will also be called repeatedly. Normally it will read result image segments from all worker nodes using ACL communication function. These segments will be assembled and post-processed to generate the final resulting image, which can be a K-map or a relative velocity false-color image.

Note that although the framework is written in C, the custom callback function may not necessarily be written in C. Many programming languages provide interfacing capability to C. For example, MATLAB contains a *MATLAB Engine* to allow application to embed MATLAB as the computation engine; it also provides a *MEX file* format to allow MATLAB code to call C functions. Using these two techniques, bidirectional interfacing between framework in C and custom code in MATLAB is accomplished. The framework will call custom code in MATLAB using MATLAB Engine, and the custom code in MATLAB can call ACL communication functions written in MEX file format.

From the above analysis it is clear that the communication between master node and every worker node and that between every worker node and assembler node are based on ACL communication functions. This design prevents the program from being dependent on any specific underlying communication library and hardware. In
order to port to a new platform, only ACL communication functions need to be rewritten. These include the following functions:

- `acl_init`: This is a callback function and will be called upon program start-up. It can be used to initialize underlying communication system.

- `acl_get_rank`: This function returns a unique rank for each participating computing node. This rank (or ID) can be used to perform role determination.

- `acl_get_no_of_processors`: This function returns the total number of participating computing nodes. This is also used for role determination.

- `acl_feed_workers` and `acl_feed_workers_complement`: These two functions together accomplish the communication between the master node and worker nodes. The former is called by the master node with a data structure storing portions of data for each worker node. The latter is called by the worker nodes to receive its portion of data.

- `acl_query_workers` and `acl_query_workers_complement`: These two functions combined accomplish the communication between the assembler node and worker nodes. The former is called by the assembler to collect data from every worker node. The later is called by the slave to submit data to the assembler.
• **acl_stop_workers**: This function provides a means for the master node to terminate work at all worker nodes. Similarly, **acl_stop_assembler** provides a means for a worker node to terminate work at assembler node.

• **acl_finalize**: A callback function that will be called upon the end of the program. ACL can perform necessary resource reclamation work in this function.

By leveraging the underlying communication library, such as MPICH or BSD Socket, implementation of ACL is straightforward. We have finished two versions of MPICH-based ACL implementations, one with data compression and another without, within 350 lines of code. Some functions have their MPICH equivalents and can be implemented by adding a function call wrap. For example, the MPICH subroutine `MPI_Comm_rank` can be directly used for **acl_get_rank**, and `MPI_Comm_size`, also in MPICH, can be used for **acl_get_no_of_processors**. Other functions require more work but remain to be easy. For example, **acl_feed_workers** is implemented by calling `MPI_Send`, the MPI subroutine to send data from one process to another, for each worker node.

### 5.5.3 Special Considerations

1. **acl_stop_workers and acl_stop_assembler**

   Most communication libraries do not provide primitives to terminate a remote process. With MPICH, even if you terminate the node having rank 0, none of the
other node will exit because of the terminating node. In fact, the call to 
*MPI_Finalize* will not return until all participating nodes call that function, which 
means all nodes have to actively terminate themselves. So using MPICH, 
*acl_stop_workers* and *acl_stop_assembler* can only implemented at a higher 
level. For example, a dedicated channel for commands can be used; or a header can be 
added to the beginning of each image segment being transferred.

To avoid overhead of adding the barely-used command channel, 
*acl_stop_workers* and *acl_stop_assembler* are implemented by sending specially 
designed faked image data which in fact contain a text message. The receivers will 
not confuse it with normal images because of its abnormal size.

However, this implementation may not be used to terminate the remote processes 
prematurely or asynchronously. In other words, when the remote processes are busy 
processing normal images, it is impossible to stop them immediately, because the 
terminating command is encoded also in an image, and will not be read until all prior 
images have been successfully processed. To implement asynchronous terminating 
command, a possible solution is to use another supervising process on each node, 
which will monitor the status of the computing process and stop it upon receiving the 
command. This is not implemented in our ACL implementation.

2. **Concerns on Real-time Processing**

Computing capacity and latency is an important issue in real-time applications. 
Computing capacity concerns whether the CPU is fast enough to keep pace with the
input stream, and latency concerns whether the output comes too late after the corresponding input frame.

Computing capacity is easier to be ensured. If the images come in at $N$ fps, there is $1/N$ second for processing at the master node, worker nodes and assembler node, respectively. A typical value of $N$ is 30. In this case, master node, worker nodes and assembler node all have 33 milliseconds of processing time for one frame of image. Normally that is enough time for speckle image processing, especially when the image has been segmented and a sufficient number of processors have been used.

Communication overlap can be used to allow larger communication and computation time. When the input image stream is at the frame rate of $N$ fps, total processing time of one image segment at the worker, including the time to receive the image segment from the master and that to send the result image to the assembler, should be kept below $1/N$ second. Otherwise, it exhibits as there is not enough computing capacity to process image stream at that frame rate. When the communication time is too large and leaves not enough time for image processing, communication overlap technique introduced in the previous chapter can be used to allow the communication and computation happen simultaneously, and thus roughly $1/N$ second can be spent on communication and computation, respectively.

Latency is relatively complex. From the Figure 5-4 it is seen that the image processing system has a pipeline structure and increase in the pipeline depth will imply larger latency. Fortunately, pipeline involved in this application has depth of only 3. Suppose it takes $t_{input}$ for that data to travel from the image capture
components to the image processing interface. Denote the time to dispatch it and pass it to worker is $t_{\text{dispatch}}$. On receiving the block for this frame, the worker will generate output false-color image. Denote the time for worker to process is $t_{\text{worker}}$. Denote the time to pass it to the Assembler and the time to assemble is $t_{\text{assemble}}$. Finally, suppose it takes $t_{\text{output}}$ for the output to reach the visualization device. The total latency can now be represented as:

$$ t = t_{\text{input}} + t_{\text{dispatch}} + t_{\text{worker}} + t_{\text{assemble}} + t_{\text{output}}. $$  \hspace{1cm} (5-8)

Of all the components in the above equation, $t_{\text{input}}$ and $t_{\text{output}}$ are not controlled by the image processing system. Of the remaining three components, $t_{\text{worker}}$, compared to the other two, is easier to control simply by using more processors and thus smaller image segments. But $t_{\text{dispatch}}$ and $t_{\text{assemble}}$ are relatively more significant, because there are communication involved and the image data being transmitted is relatively large. Even if more processors (and thus processes) are used, data involved in the dispatching and assembling remains the same. The result is that, although there is no bottleneck in the pipeline that leads to insufficient processing capacity, the image stays for too long time in the pipeline and therefore the result image is output long after the corresponding source image is inputted.

The solution is to communicate with compressed image data rather than with raw data. Because compression is a computation-intensive task, algorithm should be
chosen carefully for this real-time application. LZO [46] compression library, a block compression library that favors speed over compression ratio, is used for this task.

Specifically for mLSI which uses temporal statistics, the following solution may be used. When $M$ consecutive frames are used to compute one output image, for the number 1 to number $M$-1 frame, they are processed normally as depicted in Figure 5-4. After the number $M$-1 frame is processed, all results are transmitted from workers to the assembler. When the number $M$ frame is available at the master, it is not segmented and sent to workers; instead it is directly sent to assembler, which will perform fast processing with some simplified algorithm. The final result image is obtained by merging this result with those sent by workers and is soon available at the output end. If the dispatcher and assembler reside on the same machine, there is extra time saving by eliminating the need to do communication.

3. MPICH-specific Latency

When MPICH with p4 device is used to build the ACL, there is extra concern about communication latency. Both master and assembler node perform point-to-point communication with all workers. This is later referred to as $1$-to-$N$ communication. Because MPICH communication is by default blocking, and for master and assembler communicates with all workers one after another, a delay at any worker may affect progress of other workers.

The master node will execute a send command for each worker when dispatching the image segments. The series of send commands are issued one after another. For
large data package, a send command will not return until the data have really been transmitted to the receiving end. In other words, the sequence in which the send commands are issued is the sequence in which the real data transmission is performed. Consequently, a delay at one worker, which is at the receiving end, will possibly cause other workers which are later in the transmission sequence to wait for an extra time. So it is importantly to keep the package size small so that send command will return immediately without waiting for the data to be really transmitted; or to use non-blocking send command so that the real data transmission sequence will be independent of the sequence in which the send commands are issued.

Similarly, the assembler node will execute a receive command for each worker when assembling the result image segments. These series of receive commands are also issued one after another. Whatever the data package size is, a receive command will not return until the data is really received. So to prevent a delay at one worker to affect others, it is important to use non-blocking receive command. Using this method in this series of point-to-point communication operations, a point-to-point data transfer will happen immediately when the two ends are ready, and will be independent of the sequence in which the receive commands are issued. Therefore, a delay at one worker will not affect progresses of the remaining workers.
5.6 Results and Evaluation

5.6.1 Study of MPICH Blocking and Non-blocking Operations

We first present our study on how the blocking and non-blocking operations of MPICH are performed. The purpose of this experiment is to help determine the design of 1-to-N communication at master node and assembler node.

1. Single Sender with Multiple Receivers

In this case, one sender node will send data to 2 receiver nodes, one after another, with the first receiver delaying 1 second before receiving the data. Tests have been done with different data package sizes and with the 1-second delay enabled and disabled. Result is listed in Table 5-1.

<table>
<thead>
<tr>
<th>Data package size</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>16k bytes</td>
<td>Sender: first send time</td>
<td>0.117 ms</td>
</tr>
<tr>
<td></td>
<td>Sender: second send time</td>
<td>0.065 ms</td>
</tr>
<tr>
<td></td>
<td>Receiver 1: receive time (with 1 second of sleep time)</td>
<td>1004.4 ms</td>
</tr>
<tr>
<td>160k bytes</td>
<td>Sender: first send time</td>
<td>1015 ms</td>
</tr>
<tr>
<td></td>
<td>Sender: second send time</td>
<td>0.014 ms</td>
</tr>
</tbody>
</table>
From Table 5-1 it can be observed that: 1) when the package size is small, the sender will not wait for the corresponding receiving acknowledge from the receiver, therefore, although the first receiver delays for 1 second before receiving data, the second receiver is not affected by this delay. This is because at this data package size, MPICH will transmit the data to receiver even if it has not received a receiving acknowledge from the receiver. 2) When the data package size is large, sender will not return from sending subroutine before the receiver sends the receiving acknowledgement. Consequently, when the first receiver delays for 1 second before receiving data, the second receiver also has its progress delayed. This effect is undesirable for the master node, when the delay at one worker will affect progresses of many other workers.

Now replace the blocking send subroutines with its non-blocking counterparts and redo the above experiments. After all non-blocking communication subroutines have returned, an MPI_WaitAll is added to wait for real data transfer to finish. Times spent on different communication subroutines are listed in Table 5-2.

<table>
<thead>
<tr>
<th>Data package size</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>16k bytes</td>
<td>Sender: first send time</td>
<td>0.134 ms</td>
</tr>
<tr>
<td>Time Type</td>
<td>Time Value</td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>------------</td>
<td></td>
</tr>
<tr>
<td>Sender: second send time</td>
<td>0.066 ms</td>
<td></td>
</tr>
<tr>
<td>Receiver 1: receive time (with 1 second of sleep time)</td>
<td>1003.0 ms</td>
<td></td>
</tr>
<tr>
<td>Receiver 2: receive time</td>
<td>2.8 ms</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time Type</th>
<th>Time Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sender: first send time</td>
<td>0.026 ms</td>
</tr>
<tr>
<td>Sender: second send time</td>
<td>0.007 ms</td>
</tr>
<tr>
<td>Receiver 1: receive time (with 1 second of sleep time)</td>
<td>1018 ms</td>
</tr>
<tr>
<td>Receiver 2: receive time</td>
<td>14.4 ms</td>
</tr>
</tbody>
</table>

From Table 5-2 it is seen that with both small and large data packages, the delay at the first receiver will not affect the second receiver. Detailed analysis shows that 1) at small data package size, the non-blocking send operation performs exactly the same as its blocking counterpart; and 2) at large data package size, the non-blocking send operation returns immediately after the data being transmitted have been copied to the system buffer. This allows the second send command to be executed without being postponed because of the delay in the first receive command.

This result suggests the use of non-blocking operations at the master node, if the package size is large enough. MPICH source code uses 128k bytes as the minimum size of large package.
2. Multiple Senders with 1 Receiver

In this case, 2 senders need to send data to a single receiver node, which uses a loop to receive from these senders one after another. The first sender will delay for 1 second before it sends the data. When blocking receive is used, whatever the package size is, the receiver will not return from the call to receiving subroutine until real data transfer has been accomplished. This implies that receiving from the second sender will definitively be delayed.

We directly test the non-blocking receive without validating property of the blocking receive mentioned above. Similar to non-blocking send, an `MPI_WaitAll` is added to wait for real data transfer to finish. Test result is listed in Table 5-3.

<table>
<thead>
<tr>
<th>Data package size</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>16k bytes</td>
<td>Receiver: first receive time</td>
<td>0.017 ms</td>
</tr>
<tr>
<td></td>
<td>Receiver: second receive time</td>
<td>0.002 ms</td>
</tr>
<tr>
<td></td>
<td>Sender 1: send time (with 1 second of sleep time)</td>
<td>1002.3 ms</td>
</tr>
<tr>
<td></td>
<td>Sender 2: send time</td>
<td>0.137 ms</td>
</tr>
<tr>
<td>160k bytes</td>
<td>Receiver: first receive time</td>
<td>0.018 ms</td>
</tr>
<tr>
<td></td>
<td>Receiver: second receive time</td>
<td>0.001 ms</td>
</tr>
<tr>
<td></td>
<td>Sender 1: send time (with 1 second of sleep time)</td>
<td>1015 ms</td>
</tr>
<tr>
<td></td>
<td>Sender 2: send time</td>
<td>12.3 ms</td>
</tr>
</tbody>
</table>
From Table 5-3, it is seen that with both small and large data package, non-blocking receiving subroutine prevents the second sender to be affected by the delay in the first sender. It is very important to use non-blocking receiving subroutine in assembler, in order to prevent progress delay at one worker to affect other workers.

5.6.2 Experiment Settings and Results

Practical speckle image processing test has been performed. Testing speckle image processing algorithm is based on Cheng’s mLSI [38]. All pixels in the images are processed and 10 consecutive frames are used to generate 1 K map. Images acquired by our colleagues [41] are used to test the program. These images are 696 pixels in width and 520 pixels in height. Every pixel is encoded in 4 bytes, one byte for each of Red, Green and Blue components, and another byte for alpha channel. These color images need to be converted into grey level images, which have intensity encoded in 1 byte. However, to simulate images with higher resolution, these 4 bytes are treated as independent intensity values and the effective pixel number is increased by a factor of 3. In this way, the effective image size is 1392x1040 or 1,447,680 pixels.

Computer cluster mentioned in the previous chapter is used as the testing platform. All image processing job is done at the worker nodes, without using assembler node to compute the last frame of a group of 10 consecutive frames. Communication and computation take place in sequence without communication
overlap technique applied. Based on this setting, time spent on processing every frame of image is recorded and listed in Table 5-4.

<table>
<thead>
<tr>
<th>Setting</th>
<th>Master node: Typical time spent on processing 1 frame of image</th>
<th>Worker node: Typical time spent on processing 1 frame of image</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 processors, no compression used</td>
<td>114 ms</td>
<td>114 ms</td>
</tr>
<tr>
<td>16 processors, no compression used</td>
<td>124 ms</td>
<td>124 ms</td>
</tr>
</tbody>
</table>

From Table 5-4 it is seen that when no compression used, both 8-processor and 16-processor setting cannot handle image processing at real-time at the input frame rate of 33 fps. Detailed analysis shows that the bottleneck is at the master node: the worker nodes spend less than 1 millisecond in computation task, because of the relatively simple mLSI algorithm and the small size of image segment, more than 100 millisecond waiting for the master node to feed it with next frame of data, and another around 10 millisecond in real data transfer from the master node. The master node spends all time in transferring image segments to worker nodes, one after another and one frame after another frame. To accomplish real-time processing, time spent on transferring one frame of image segment must be reduced. Image data compression is used for this purpose.

We now compare two candidate compression libraries, zlib [47] and LZO library [46]. By assuming 10 worker nodes, image segment for each worker node will have
144768 pixels. 144768 bytes of data are used to test different compression methods. The compression result and time using different compression library are listed in Table 5-5. Note that the master node needs to repeat this compression procedure for 10 times for a single frame of input image.

<table>
<thead>
<tr>
<th>Compression method</th>
<th>Size after compression</th>
<th>Compression time</th>
</tr>
</thead>
<tbody>
<tr>
<td>zlib</td>
<td>10.2 Kbytes</td>
<td>21 ms</td>
</tr>
<tr>
<td>LZO</td>
<td>33.3 Kbytes</td>
<td>2 ms</td>
</tr>
<tr>
<td>LZO 2-level compression</td>
<td>25.2 Kbytes</td>
<td>5 ms</td>
</tr>
</tbody>
</table>

From Table 5-5 it is seen that for this image size, machine configuration and frame rate, only LZO compression library can be used to achieve real-time processing. With smaller image size, LZO 2-level compression, which performs another LZO compression on the result of a previous LZO compression, can also be used. For zlib, although it generates desirable compression ratio, the compression is large even for small image size, and can hardly be useful for our application.

With 1 level of LZO compression used, time spent on processing every frame of image is largely reduced and the result is listed in Table 5-6. For both 8-processor and 16-processor settings, time spent on processing one frame of image at the master and worker has fallen under the threshold of 33 milliseconds, and real-time processing is achieved. Currently the processing time excluding time spent on data transmission is
less than 1 millisecond, including the small LZO decompression time, and there is large room to employ better and more complex algorithms or to use higher resolutions. When communication overlap is not used, using 8 processors will allow a worker node to spend around 29 milliseconds in processing 1 frame of image segment, and using 16 processors will allow around 10 milliseconds; when communication overlap is used, both settings allow around 33 milliseconds of image processing with higher image resolutions, if the little time involved in lzo decompression is ignored.

<table>
<thead>
<tr>
<th>Setting</th>
<th>Master node: Typical time spent on processing 1 frame of image</th>
<th>Worker node: Typical time spent on processing 1 frame of image</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 processors, LZO compression used</td>
<td>14 ms</td>
<td>14 ms</td>
</tr>
<tr>
<td>16 processors, LZO compression used</td>
<td>23 ms</td>
<td>23 ms</td>
</tr>
</tbody>
</table>

This result has shown that real-time processing is achieved using our framework. The use of compressed communication channel allows more time to be spent on more complex computation. If the communication overlap technique is used, there is even more time for computation and the use of compression will allow more data to encode the image. That is to say, the system will be able to handle images with higher resolution.
5.7 Conclusion

In this chapter we have described our efforts in building real-time image processing program on parallel platforms, including computer clusters. There is an increasing need for parallel computing for image processing recently, especially in the medical imaging area for the purpose of real-time processing. Laser speckle image processing is a typical example. However, research in parallel image processing usually follows the data parallelism model and uses SIMD or special-purpose platform. Little work is done to leverage the computing power of more accessible computer clusters. We propose and implement a framework for parallel speckle image processing to be run on computer cluster and other type of loosely-coupled multicomputers. It is designed to be simple, utilizing the master-work paradigm. It is also small, portable and scalable: porting the ACL to a new platform only requires reimplementation of less than 10 functions, and the processing logic is separated from underlying hardware platform and software environment. By allowing customization of processing logic and custom code in other language such as MATLAB, programmers can now easily change and extend the function using their favorite languages and relevant libraries. We have studied the requirements of real-time processing, and proposed to compress data using timing-friendly compression library. Experiments have shown that real-time processing is achieved with our chosen image processing algorithm, with further room to accommodate more complex algorithms. If communication overlap is used, it is possible to use more complex algorithms and larger number of processors, and be more tolerant to other overheads. In brief, our
design can be a desirable base to help developers easily build laser speckle processing programs to run efficiently on many different types of parallel computers, to maximally take advantage of the available computing power, and to achieve real-time processing goals.
Chapter 6 Conclusions and Suggestions for Future Work

6.1 Conclusions

Our research is motivated by the need to use computing power to address computation problems in the emerging field of computational bioengineering. This thesis mainly covers several techniques to facilitate use of computer clusters in satisfying computing power for two representative bioengineering research issues.

Fiber suspension simulation is the first, which we choose as a representative for the large number of computational biomechanics applications. These applications use decomposition to exploit parallelism. Our research has pointed out that, for these parallel programs, asynchronism among parallel processes of the same task is an important source of communication latency, especially when they run on computer clusters. We have proposed the use of communication overlap to eliminate impact of communication latency. Our experience of implementing this technique in fiber suspension simulation program is introduced. Realistic experiments on the new
simulation program have shown significant performance gain for both zero-load system, such as computer clusters with a central batch job scheduler, and non-zero load system, such as computer clusters with interactive job submission. For example, in of our test with 16 parallel processes (and processors), program with the communication overlap technique applied was 22.3% faster than that without this technique in terms of observed speedup.

Real-time laser speckle image processing is the second issue, which we choose as an example of many biomedical image processing problems having critical timing requirements. We have found that although there is a lot of research work on parallel image processing, little work is done on utilizing computer cluster for that task, when computer cluster is actually the most accessible parallel computing facility nowadays. Our research has focused on satisfying the timing requirements in real-time laser speckle image processing. We aim at a simple, portable, and highly customizable framework based on the master-worker programming paradigm. Performance profiling shows that it is capable to process laser speckle images in real-time using our chosen algorithm, there is much room to incorporate more complex algorithms. Although our design is centered on the laser speckle image processing problem, the design and the framework can be extended for use in many similar image processing applications.
6.2 Areas for Improvement

There are a lot of areas that we can improve on based on our current research. As for communication overlap technique, especially when it is applied to numerical simulation problems similar to fiber suspension simulation, automation tools can be built to perform high-level control flow rescheduling (Section 6.3). A programming framework with built-in capability of communication overlap used in inter-process communication is also an option (Section 6.4). As for master-worker framework for parallel image processing, an implement of ACL using BSD Socket or WinSock can largely extend the usable computing power in campus environment (Section 6.5). Certain extensions to ACL to facilitate inclusion of MATLAB image processing script can be very useful for bioengineering researchers who are more versed with MATLAB and its powerful image processing toolbox (Section 6.6).

6.3 Automated Control Flow Rescheduling

Automated control flow rescheduling is to automatically reschedule the program at block level to generate more opportunities for communication overlap. The intensive research and great success in instruction scheduling of optimizing compilers is a large impetus to work on automated control flow rescheduling. For high-level control flow rescheduling, it is necessary to ask the programmer to provide necessary information about every reschedulable code block (RCD), such as whether it is communication-relevant or computation-relevant, what shared variables or arrays are
used and how they are used. To make it feasible, the programmer should also follow some programming style, such as to distinguish global (or shared) variables from local variables; they should choose appropriate the granularity of RCD.

The automation tools can build a dependency relationship among RCD from the provided information about RCD. It may first perform a performance profiling through a sample running. Acquired profiling data may help choose the important RCD. If necessary, the user might be prompted to further decompose a RCD because of its significant impact on the performance as well as the complex dependences it involves. After that, dependence relationship graph will be built and rescheduling to generate overlap of communication and computation will be carried out accordingly. All the methods to circumvent data dependence restriction mentioned in Chapter 4 may be used.

Using existing research outcome in the area of instruction scheduling, building the aforementioned automation tools may not face much technical challenge. Such tools may largely promote the use of communication latency in parallel computing for similar numerical simulation problems.
6.4 Programming Framework with Communication Overlap

Communication overlap is very important for decomposition-based parallel programs in computation biomechanics areas, and a framework to prebuild the common details would largely ease the programming tasks. By implementing general logics such as communication latency hiding in the framework, the programmers can focus on writing application-specific code and let the framework writer to worry about the common problems.

A lot of applications in bioengineering share the same features with fiber suspensions simulations. These features include time-step approach, spatial decomposition for parallelization, interprocess communication between neighboring processes in every time step, and (optional) interprocess communication among all processes in every time step. These applications can also share the same high-level control flow but with several customizable application-specific functions.

The programming framework implements the general control flow, with communication overlap applied. It leaves several application-specific functions to be implemented by the users. The framework imposes very strict limitations on how the user code use shared variables. Because the framework has internally used communication overlap and control flow rescheduling, improper use of shared variables will result in invalidation of rescheduling.
6.5 Socket-based ACL Implementation

Considering the almost universal availability of BSD socket on all computer platforms, building a socket-based ACL implementation will allow our ACL-based framework to run on all computers. A Socket-based ACL will allow to take advantage of a large number of high-performance workstations interconnected with high-speed dedicated campus networks and to utilize these otherwise wasted computing resources.

BSD Socket is built in all modern UNIX and Linux workstations and WinSock is in available for every 32-bit Windows PC. With Socket-based ACL, master-worker parallel program based on ACL will be able to utilize almost every workstation and PC in campus as a computing node. Considering the excellent computer network that keeps communication latency low and the large number of machines to choose from, a temporary homogeneous cluster of workstations can always be built at any time. If enough number of dynamic backup machines is also selected, exit of one or more machines from this temporary cluster will not stop or affect progress of ongoing computation.

It is noted that implementing such an ACL version requires a much more complex resource management function. But the computing power it can generate makes it a very interesting area to work on.
6.6 MATLAB extension to ACL

A MATLAB extension to ACL is to allow researchers to write ACL callback functions in MATLAB. Considering the powerful image processing toolbox and a comprehensive mathematical toolset, MATLAB is among the best choice for researchers to try ideas and to write prototype implementations. For production use, most researchers will choose to reimplement MATLAB functions using a more performance-aware language, such as C or C++. However, as the computing power of parallel computer makes slow language less a problem, and as MATLAB itself is getting faster, there is less and less necessity to rewrite MATLAB functions. It is important to support using MATLAB script as the custom logic in our ACL architecture.

The MATLAB extension can allow bidirectional communication between MATLAB and ACL – it will allow ACL to call MATLAB script as the callback functions, and will allow MATLAB script to use ACL communication services. MATLAB provides mechanism to implement both directions. When ACL needs to call a MATLAB script, it can use the MATLAB engine feature. To expose the ACL communication functions to MATLAB script, these functions can be rewritten to follow the MEX file format. After the rewriting, MATLAB script can call these C routines as MATLAB functions.
6.7 Summary

The use of parallel computers in bioengineering research and practice represents a major step in development of bioengineering field. Techniques introduced in this thesis are examples of this development of parallel computing in the subfield of numerical simulations and image processing, with an emphasis of using computer clusters as the supporting platform. Our techniques will benefit computational bioengineering field by effectively powering more intensive simulation with higher precision and better resolution and real-time high-density biomedical image processing.
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