DEVELOPMENT OF APPLE WORKGROUP CLUSTER AND PARALLEL COMPUTING FOR PHASE FIELD MODEL OF MAGNETIC MATERIALS

A Thesis

by

YONGXIN HUANG

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

May 2009

Major Subject: Aerospace Engineering

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Approved by:

Chair of Committee,	Yongmei Jin
Committee Members,	Raymundo Arroyave
	Zoubeida Ounaies
Head of Department,	Dimitris Lagoudas

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ABSTRACT

Development of Apple Workgroup Cluster and Parallel Computing

for Phase Field Model of Magnetic Materials. (May 2009)

Yongxin Huang, B.S., University of Science and Technology of China

Chair of Advisory Committee: Dr. Yongmei Jin

Micromagnetic modeling numerically solves magnetization evolution equation to process magnetic domain analysis, which helps to understand the macroscopic magnetic properties of ferromagnets. To apply this method in simulation of magnetostrictive ferromagnets, there exist two main challenges: the complicated micro-elasticity due to the magnetostrictive strain, and very expensive computation mainly caused by the calculation of long-range magnetostatic and elastic interactions. A parallel computing for phase field model based on computer cluster is then developed as a promising tool for domain analysis in magnetostrictive ferromagnetic materials.

We have successfully built an 8-node Apple workgroup cluster, deploying the hardware system and configuring the software environment, as a platform for parallel computation of phase field model of magnetic materials. Several testing programs have been implemented to evaluate the performance of the cluster system, especially for the application of parallel computation using MPI. The results show the cluster system can

simultaneously support up to 32 processes for MPI program with high performance of interprocess communication.

The parallel computations of phase field model of magnetic materials implemented by a MPI program have been performed on the developed cluster system. The simulated results of a single domain rotation in Terfenol-D crystals agree well with the theoretical prediction. A further simulation including magnetic and elastic interaction among multiple domains shows that we need take into account the interaction effects in order to accurately characterize the magnetization processes in Terfenol-D. These simulation examples suggest that the paralleling computation of the phase field model of magnetic materials based on a powerful cluster system is a promising technology that meets the need of domain analysis.

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I want to thank James Munnerlyn, Computer System Manager with the Aerospace Engineering Department, for helping with the installation and maintenance of our cluster system. I also thank Dr. Srinivasan for answering my questions which helped me start the work on computer cluster.

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1 INTRODUCTION

1.1 Magnetic microstructure analysis

Magnetic phenomenon and magnetic materials, since their discovery, have been used for a very long period of time. Lodestone, the material with a spontaneous magnetic state, has been used in the compass to indicate north and south for almost two thousand years. With today's fast growing technology, magnetic materials find wider applications in many fields. Among various magnetic materials, ferromagnetic materials, like iron, nickel, cobalt, some of rare earths and their alloys, are widely used in permanent magnets, information recording system, and so on. This is because ferromagnetic materials exhibit many unique behaviors. For example, ferromagnetic materials can be significantly magnetized under a relatively small applied magnetic field. Using this property, electromagnets, such as iron core solenoids, can multiple an applied magnetic field by thousand of times to generate large magnetic fields. After removal of the applied magnetic field, ferromagnetic materials tend to keep their magnetized state, leading to history dependent behavior, so called hysteresis. With this hysteretic characteristic, ferromagnetic materials find important applications as information recording media. Another important characteristic of ferromagnetic materials is magnetostriction, a phenomenon of interdependence between magnetization and deformation.

This thesis follows the style of Applied Physics Letters.

Ferromagnetic materials with significant magnetostriction are used in actuators and sensors because they show a measurable mechanical response to the magnetic field and vice versa.

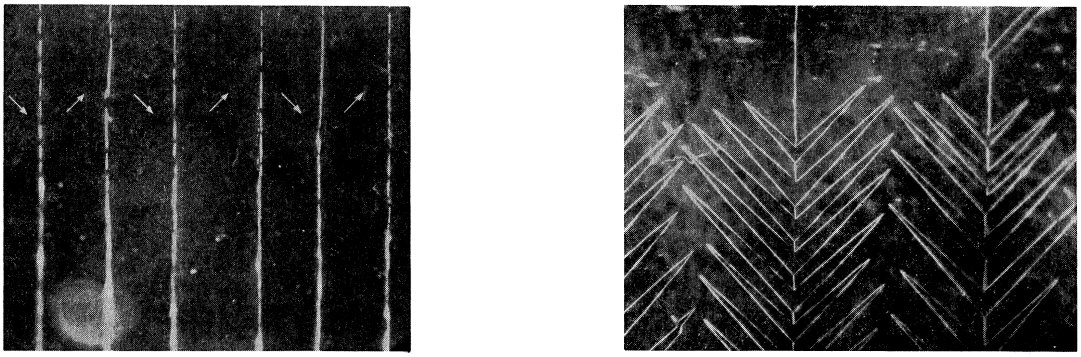
The above-mentioned ferromagnetic characteristics can not be explained without the magnetic domain analysis. Some basic statements from the domain analysis are listed here[1]: (a) Permanent atomic magnetic moments exist in the ferromagnetic materials under Curie temperature. (b) The atomic magnetic moments will align with each other along certain crystallographic direction to form substructures in ferromagnetic materials. A substructure with uniform magnetization direction is called a magnetic domain. (c) In a demagnetized state, the magnetic domains with different magnetization directions will neutralize each other and the material will exhibit no bulk magnetization. (d)When magnetized under a driving magnetic field, the magnetic domain will reorient to align with the applied magnetic field and the material will exhibit macroscopic magnetization and high permeability.

The domain analysis, mainly based on domain theory, gained success in explaining the magnetization process, magnetic hysteresis and so on, in the first several decades of 20th century.[1] At the same time, a growing amount of experimental evidence, confirmed the existence of the magnetic domains (see a magnetic domain observation in Figure 1.1). Domain analysis bridges the magnetic microstructure and the macroscopic magnetic properties of ferromagnetic materials. Today, it has become a necessary tool to

understand macroscopic magnetic properties and to develop new magnetic materials. To process the domain analysis, domain observation and micromagnetic theory are two approaches that complement each other.[2]

Domain observation, such as Bitter patterns, magneto-optical methods, X-ray, and transmission electron microscopy (TEM), can directly or indirectly reveal the magnetic domain pattern based on different mechanisms. Figure 1.1 shows the domain pattern on the surface of Si-Fe single crystal revealed by Bitter patterns.[1] However, experimental observations of domain evolutions under an applied field are time consuming and costly. Moreover, the available observation technologies are limited to external surface while the domain structure inside the bulk sample is not necessarily the same as that of external surfaces. Given this limitation, the domain observation cannot offer enough information to study magnetic domains in many cases.

Micromagnetism is an effective theoretical approach to studying domain structures. The possible domain structures can be obtained based on the principle of total free energy minimization.[3] However, the micromagnetic equations are highly non-linear and non-local. The minimization can be done analytically for very limited simple cases in which a linearization is possible. Moreover, as mentioned previously, domain structures are history dependent, so it is necessary to track the domain evolution in domain analysis. Micromagnetic modeling, where the magnetization evolution equation is numerically solved, offers a powerful simulation tool for domain analysis.[4,5]



(a) (b)

Figure 1.1 Magnetic domain patterns on single crystals of silicon iron (a) single domain structure (b) complex domain structure.[6]

In spite of the big success of the micromagnetic modeling in studying magnetic domain phenomena, it cannot realistically treat magnetostrictive effect which involves heterogeneous magnetostrictive strain coupled to local magnetization distribution. In this thesis, phase field micromagnetic microelastic model is employed to simulate domain microstructure evolution, which combines micromagnetic model and phase field microelastic model as discussed in the next section.

1.2 Phase field model

Phase field method is successfully applied to modeling a wide range of domain phenomena[7], including ferroelectric domain evolution[8-11], spinodal decomposition[12], martensintic (ferroelastic) transformation[13-15] and solidification[16,17]. The phase field

method uses the spacial distribution of field variables to describe the domain microstructures. For example, in decomposition the local concentration is used as the field variable. Therefore, the domain with the homogenous physical property is represented by the region with the homogenous field variables in the computational region. At the domain boundaries, the field variables change continuously forming smooth interfacial regions with finite thickness, i.e., diffused interfaces. For diffused interfaces, there is no need to explicitly track the boundaries, which is a great advantage of the phase field method.

The spacial and temporal evolution of field variables is described by the phase field kinetic equations: Ginzburg-Landau equation for martensitic transformation[18], Cahn-Hilliard equation for decomposition[19], and Landau-Lifshitz equation for magnetic switching[20]. The phase field variables obtained by solving the kinetic equations describe domain microstructure evolution which decreases the system free energy and eventually reaches the energy minimizing equilibrium state under given external condition.

Recently, a phase field micromagnetic microelastic model has been developed to study the magnetic domain microstructure evolution in giant magnetostrictive materials, which combines micromagnetic model of domain switching and phase field microelastic model of martensitic transformation[21,22]. The model is briefly described below.

The evolving magnetic domain structure in a magnetic material is described by magnetization direction field $\mathbf{m}(\mathbf{r})$, whose average value gives the macroscopic magnetization $M_s \langle \mathbf{m}(\mathbf{r}) \rangle$ (M_s being saturation magnetization). The total system free energy for arbitrarily distributed magnetization field is a sum of magnetocrystalline anisotropy energy F^{ani}, exchange energy F^{exch}, magnetostatic self-energy F^{mag}, external magnetic energy $F^{\text{ex-mag}}$, elastic self-energy F^{el}, and external elastic energy $F^{\text{ex-el}}$: [1,21]

$$
\begin{aligned}
F &= F^{\text{ani}} + F^{\text{ex-mag}} + F^{\text{exch}} + F^{\text{mag}} + F^{\text{el}} + F^{\text{ex-el}} \\
&= \int \left[K_1 (m_1^{c2} m_2^{c2} + m_2^{c2} m_3^{c2} + m_3^{c2} m_1^{c2}) + K_2 m_1^{c2} m_2^{c2} m_3^{c2} \right] d^3 r - \mu_0 M_s \int m_i(\mathbf{r}) H_i^{\text{ex}} d^3 r \\
&\quad + \int A \left| grad\, \mathbf{m}(\mathbf{r}) \right|^2 d^3 r + \frac{1}{2} \mu_0 M_s^2 \fint \frac{d^3 k}{(2\pi)^3} \left| \mathbf{n} \cdot \tilde{\mathbf{m}}(\mathbf{k}) \right|^2 \\
&\quad + \frac{1}{2} \fint \frac{d^3 k}{(2\pi)^3} \left[C_{ijkl} - n_p C_{ijpq} \Omega_{qr}(\mathbf{n}) C_{klrs} n_s \right] \tilde{\varepsilon}_{ij}^0(\mathbf{k}) \tilde{\varepsilon}_{kl}^{0*}(\mathbf{k}) - \int \sigma_{ij}^{\text{ex}} \varepsilon_{ij}^0(\mathbf{r})\, d^3 r ,
\end{aligned}
\qquad (1)
$$

where $m_i^c(\mathbf{r}) = Q_{ij}(\mathbf{r}) m_j(\mathbf{r})$, $\mathbf{Q}(\mathbf{r})$ is rotation matrix field describing the grain structure, K_1 and K_2 are material constants characterizing magnetocrystalline anisotropy, A is exchange stiffness constant, $\mathbf{H}^{\text{ex}}$ is external magnetic field, ~ indicates Fourier transform, the integral $\fint$ is evaluated as a principal value excluding the point $\mathbf{k} = \mathbf{0}$, $\mathbf{n} = \mathbf{k}/k$, μ_0 is the vacuum permeability, $\Omega_{ij}(\mathbf{n})$ is Green function tensor inverse to $\Omega_{ij}^{-1}(\mathbf{n}) = C_{ikjl} n_k n_l$, $\boldsymbol{\sigma}^{\text{ex}}$ is the external stress, and magnetostrictive strain field $\boldsymbol{\varepsilon}^0(\mathbf{r})$ is given as

$$
\varepsilon_{ij}^0(\mathbf{r}) = \alpha_{pqrs}^c Q_{pi}(\mathbf{r}) Q_{qj}(\mathbf{r}) Q_{rk}(\mathbf{r}) Q_{sl}(\mathbf{r}) m_k(\mathbf{r}) m_l(\mathbf{r}) \qquad (2)
$$

Under given external conditions, the evolution of magnetization field is described by the Landau-Lifshitz-Gilbert equation:

$$\partial \mathbf{m}/\partial t = \gamma \mathbf{m}(\mathbf{r},t) \times \delta F/\delta \mathbf{m} - \alpha \mathbf{m} \times \left(\mathbf{m} \times \delta F/\delta \mathbf{m}\right), \tag{3}$$

where γ and α are the constants accounting for gyromagnetic process and phenomenological damping.

The simulation of domain microstructure evolution in magnetic materials is performed by numerically solving Eqs. (1)-(3) over discritized computational grids under given initial and external boundary conditions. For such a computation, two major problems arise; they are long computation time and large memory.

It is noted that, for a system of N computational grids, dipole-dipole interactions require $O(N^2)$ number of floating point computation for each time step, which is reduced to $O(N \log N)$ when a Fourier spectral method is adopted.[17] For our simulations, it is usually desirable to consider typical computation size of 512×512 and 256×256×256 for 2D and 3D simulations, respectively. Moreover, the number of time steps is usually as high as one million or even more. Therefore, given current performance of a single processor computer, the total computation time would be unacceptable, especially for three dimensional problems.

Another serious problem for phase field simulations is the large memory requirement. It requires a number of arrays to hold the field variables and related parameters associated with all computational grids. For the typical simulation sizes used in phase field modeling, the required memory size is far beyond the capability of a single processor computer.

The phase field micromagnetic microelastic model described above allows all domain-level mechanisms to operate freely, does not impose a priori constraint on the kinetic pathways, accurately treats long-range interactions, and takes into account magnetoelastic coupling due to magnetostriction. Therefore, the model is uniquely capable for domain analysis to help reveal new domain mechanisms and develop new magnetostrictive materials. However, its simulations demand for intensive computation as discussed, and cannot be realized by a single processor computer available today. Parallel computing offers an opportunity here.

1.3 Parallel computing

Parallel computation has been widely used in many fields for large scale scientific simulations for decades, which effectively overcomes the limitations of sequential computation operated by a single processor computer.[23] The general strategy of parallel computation is to make multiple computer resources work simultaneously on one problem that does not fit on single processor computers. A large computational problem is divided into smaller parts to be solved in parallel by multiple processors.

Based on the types of divided or parallelized units in a problem, the parallel computing can be classified into four levels: Bit-level, instruction-level, data-level and task-level. Most scientific parallel computation falls into the category of data parallelism handling huge data but similar operation. “parallelizing loops often leads to similar (not necessarily identical) operation sequences or functions being performed on elements of a large data structure.”[24] This is also true for the simulation of magnetic domains based on the phase field model. In our simulation, the problem of formidable computer time and memory requirement is solved by dividing the data associated with the whole simulated volume into smaller subsets.

For parallel computing, the hardware architecture of the parallel computer is important. Improper hardware architecture may not support the expected parallelism. There are mainly two kinds of hardware architecture: shared memory multiprocessors and distributed memory system. Their main characteristics are briefly explained in the following.

In the shared memory architecture, multiple processors share the same memory, as shown in Figure 1.2. Its advantages include fast memory access by all processors and no need for communications among processors, and easy realization of parallelism for computer programming. With certain programming interfaces, a programmer may easily change the sequential code into shared memory multiprocessing program that

significantly reduces computer running time. However, shared memory multiprocessors system can not scale well, and the number of multiprocessors involved in the parallel computing is limited. It is also constrained by the available amount of the shared memory.

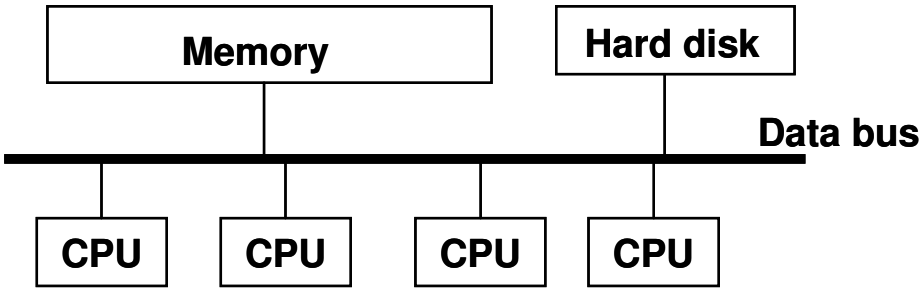


Figure 1.2 The architecture of a shared memory multiprocessors system.

A distributed memory system has multiple independent memories and processors, where a memory can only be directly accessed by the local processor. The architecture, illustrated as Figure 1.3, allows much more memory and processors to be involved in the parallel computation, compared to that of shared memories. Therefore, the problems simultaneously requiring large memory and computation time can be solved through parallelizing the program based on a distributed memory system. But this is not obtained without cost. The complicated communications between processors arise. When a processor needs data in the memory associated with another processor, it requires communiation between the two processors through network, which costs significant

computer time. The true challenge we face here is the computer programming to optimize communications among the processors.

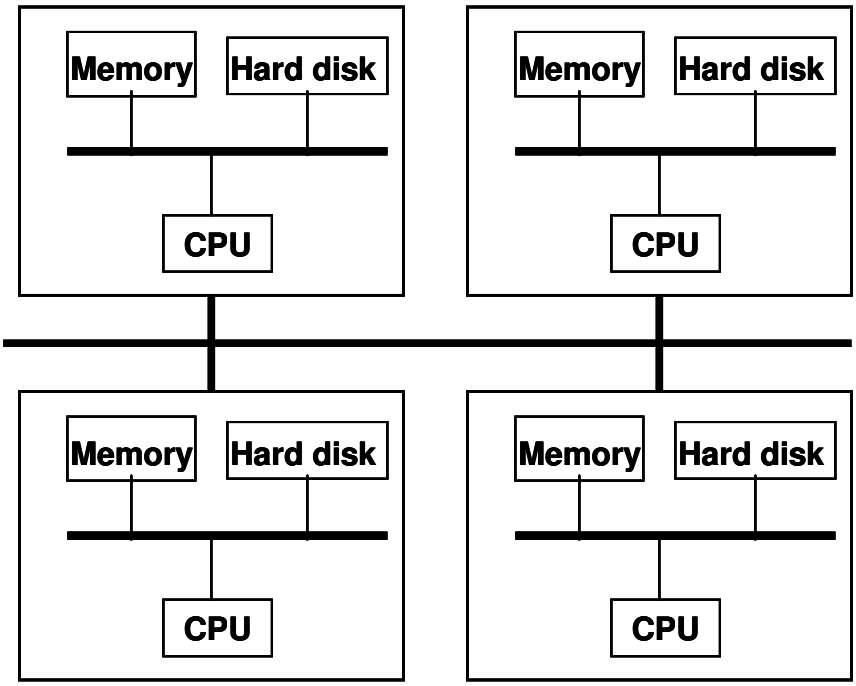


Figure 1.3 The architecture of a distributed memory system.

For the simulations of domain structure evolution using the phase field model as given in section 1.2, the parallel computing on a distributed memory system is a better choice. Therefore, based on the distributed memory architecture, a more specified parallel computing system, computer cluster, is selected as the computational platform. A computer cluster is mainly composed of compute nodes and communication networks. A compute node is similar to a traditional PC with independent processor and memory, and

the network requires high performance with low latency and fast bandwidth speed. The technical details of the computer cluster will be introduced in next section.

1.4 Description of the thesis

This thesis begins with this Introduction. Development of a computer cluster system as platform for parallel computation and the parallel algorithm for phase field model are presented in Section 2 and Section 3, respectively. The performance evaluation of the developed cluster system is introduced in Section 4. In Section 5, the parallel implementation of phase field modeling of magnetization process in Terfenol-D crystals is performed on the developed cluster system. The simulation results is presented and discussed.

2 BUILDING CLUSTER SYSTEM FOR PARALLEL COMPUTATION

2.1 Overview of a computer cluster system

A computer cluster is a high performance computing system consists of a group of computers. The cluster, composed of multiple identical high performance computers (compute nodes) and high performance network, is an ideal platform for scientific parallel computation. Figure 2.1 shows the topology of a general computer cluster. By integrating multiple linked compute nodes into a single cluster under uniform administration, the system performs as a single supercomputer. Computer clusters retain a reasonable price without compromising computation power. Due to these advantages, the computer cluster has become the mainstream of high performance computation and widely used in the field of science, engineering and business. From the TOP500 list of World's Most Powerful Supercomputers of year 2008[25], 80% of supercomputers are computer clusters.

Clusters are divided into two types: custom cluster and commodity cluster. By customizing the compute nodes, networks and operating system, the custom cluster can obtain excellent performance to support parallel computation but at a very high price. In contrast, commodity clusters are mainly composed of commercial off-the-shelf hardware and open source software so that cost can be minimized while performance can be

maximized. Considering the requirement for the computational performance and a limited funding, commodity cluster would be a reasonable high performance computation solution for small research groups. A book[26] for guiding how to build a commodity cluster was provided by Sterling *et al.* as a good handbook for developing a such cluster system

The cluster system mainly consists of compute nodes and networks. Besides being compatible with the given hardware, the software system must meet the needs of administration and management, and support parallel computation. Like developing any other computer system, selecting and deploying hardware system as well as building the software environment are the main tasks when constructing a cluster system.

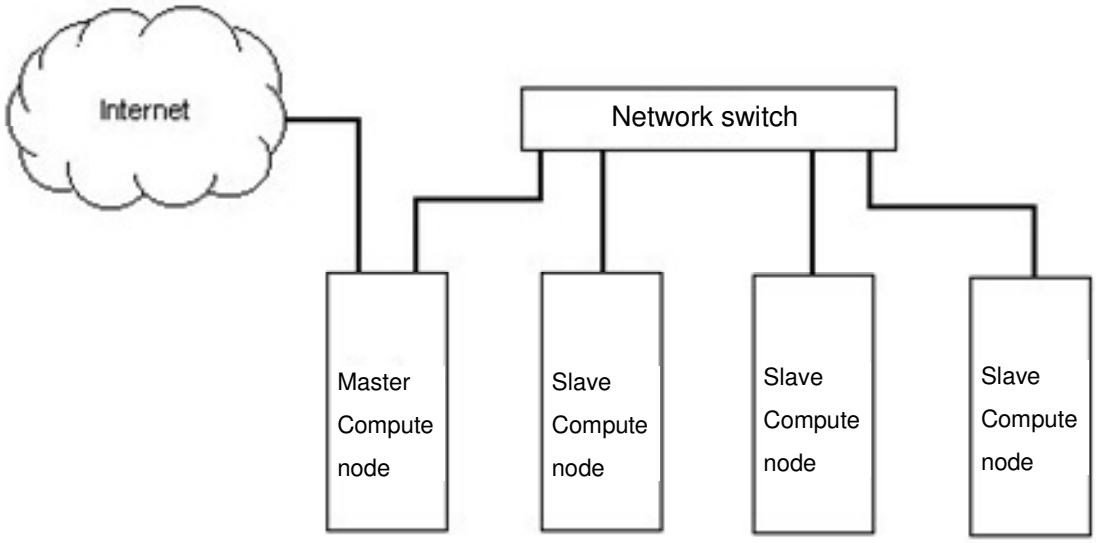


Figure 2.1 Topology of computer cluster.

2.2 Hardware system structure

2.2.1 Compute nodes

The configuration of each individual compute node is one of the most important considerations in the development of a computer cluster. Generally, each individual compute node is an independent computer. The procedure of configuring each individual compute node is similar to the procedure for configuring a conventional PC. Four basic components, the processor, main memory, motherboard, and hard disk, are to be considered and will determine the general performance of the nodes. The space occupied by the compute node must also be considered when many compute nodes are incorporated into the cluster. The commodity cluster may utilize either rack-mounted servers or PCs as its compute nodes. Although the price is higher, the rack-mounted server has a more powerful computational ability. Also, the uniform compact structure of the rack-mounted serve make it easily attachable to the standard enclosure for good organization and great space saving.

There are two kinds of nodes in the cluster though they both are called compute nodes: Master nodes, and slave nodes. Master node will control other nodes to form a uniform system so that the group of nodes would act as a single computer. For small cluster with a limited number of nodes, a single master node would be sufficient for the control and management work of the whole system. Conversely, slave nodes are controlled by a master node to work on assigned job. The master node usually has better performance,

such as larger storing capability and faster processors, to support the management of the whole system. It may or may not directly take part in the parallel computation jobs based on the situation of load balance. For slave nodes, identical configuration is suggested to simplify the cluster system and maintain the load balance for parallel computation.

The number of nodes is another important factor to determine the computation capability of the whole system. More compute nodes included in cluster would involve more processors in the system and naturally increase the computation capability. For example, 1100 Apple Xserve G5 system serve as compute nodes in the System X cluster at Virgin Tech[27], which delivers an incredible computation speed of 12.35 TFlops, was the fastest supercomputer in 2006 all over the world according to the TOP500 list of World's Most Powerful Supercomputers. However, the float operation per seconds can not fully describe the performance of users' practical parallel application on the cluster. Actually, many parallel implementations may run satisfactorily on a computer cluster with no more than 32 processors, due to the scalability of the program and other factors. Therefore, the number of compute nodes must be carefully considered according to the requirement of potential parallel computation.

2.2.2 Communication network

A communication network system connects the compute nodes to form an integrated cluster system. In parallel computation, it is used to transfer data among different compute nodes. The hardware of a general network system includes a switch, an

interface on the compute nodes and cable. Like compute nodes, hardware for the network is also based on commercial commodity. For example, common and economical Ethernet-based networks are most frequently utilized in clusters. But a better performance network with a much higher price is necessary for some parallel computation that involved intense data communication. Therefore, the choice of network hardware is highly dependent on the requirement of potential parallel computation.

In parallel computation, the network is used to deliver information or data among compute nodes. Its performance is described mainly by its bandwidth and latency. Bandwidth is the average rate of information or data delivered via the network. It is usually measured by Bit/s. Higher bandwidth speed will significantly decrease the delivery time, especially for the information with large size. The latency is related to the delay of the information delivered, which is mainly caused by the required responding time between compute nodes to send and receive information. The efficiency of delivering information or data with small size is very sensitive to the latency because the delay time, rather than the direct transferring time, takes the main part in the whole delivering time.

There may be one or two network systems in one computer cluster. The first management network is usually an IP-based Ethernet private network. This network is used for sending and receiving controlling messages. Through this network, master node can reach the whole cluster system by sending instruction to slave nodes, maintain the

operating system, and manage the parallel jobs and so on. Because the management messages delivered are usually relatively small, an Ethernet-based network with moderate performance can satisfy the management requirement. If the computer cluster is used to run some parallel implementation without intense data communication, this management network may also be used to support the data communication among compute nodes in parallel computation. In that case, a single high performance Ethernet-based network will support all communication and no secondary network is needed.

Some parallel application involves intensive interprocess communication to share the data among different nodes. In that case, it is recommended to separate interprocess communication from the management messages through building a secondary high performance network. The computer time consumed by a parallel program consists of two parts: the direct computation time and interprocess communication time. A high performance network with wide bandwidth and low latency would significantly decrease the communication time. Through that, a decreased total computer time and better scalability may be obtained for parallel programs. Due to the critical role played by the network in intensive communication parallel computation, some advanced network technology such as Infinitband and Myrinet, at much higher price, will be used in this secondary high performance network instead of ordinary Ethernet-based system. And if the secondary network is applied, the first management network is only required to have moderate performance to save money.

2.2.3 Other hardware components

Some support components are also necessary for the cluster system. If compacted rack-mounted servers are chosen as compute nodes, a cooling system is critical to prevent system failure by over-heating. It will remove the system heat output, which mostly comes from the compacted rack-mounted servers. Also, a backup power supply is needed to prevent damage due to a power surge. Finally, all of this hardware needs a standard enclosure for storage.

2.3 Software environment for cluster system

2.3.1 Operating system

An operating system of computer cluster works both for the compute node itself, just like an ordinary PC, and also for the whole network system of the cluster. A sophisticated operating system for a cluster is used to manage each node such as configuring all of hardware resources, managing user accounts, managing memory, hosting application program, and so on. Also, the cluster operating system is in charge of administration and management of the whole cluster system, creating a uniform software environment, building the distributed file system, configuring the private communication networks, and so on.

2.3.2 Communication mechanism and implementation

Complex parallel computation requires intense communication for sharing data, synchronizing processes and so on. This communication can be done by “message passing” for distributed memory system or multithread for SMP (share memory multiprocessors). In the distributed memory system, like cluster, through “sending” and “receiving” messages containing needed data or other information, the compute nodes involved in parallel computation can communicate with each other. Therefore, a standard of message-passing become necessary to formalize the communication style. A corresponding software implementation will work with programming language, through that programmers can control the interprocess communication in their programs.

It is noteworthy that this communication mechanism is highly dependent on the architecture of hardware. As mentioned above, “message passing” communication is mainly based on a distributed memory system, but contemporary clusters usually utilize SMP computers as compute nodes. In another word, the whole cluster is a hybrid system; inside of each node, it has the architecture of share memory multiprocessors while among the compute nodes it is a distributed memory system. This complex structure, called a distributed SMP system, makes the interprocess communication more difficult than pure distributed memory system or SMP system. Generally, a mixture of message passing and multithread communication mechanisms would optimize performance in a hybrid system; however, this would greatly complicate the programming. How to build an optimized communication mechanism on this hybrid SMP cluster system is still under

research. Today, a message-passing communication is typically used exclusively in a SMP nodes cluster though it is obviously not the best choice.

2.3.3 Workload management software

The workload management software is used to manage computing resource for the user applications. Usually, there are multiple users served by a cluster system. A usage policy sets the priority to use computing resource for the applications submitted by different users. For example, some users may always have the highest priority to use the computing resource, or, only the parallel application submitted by certain group of users may use more memory or computing nodes. The workload management software will combine the current state of the cluster system and carry out such sets of policy to manage the usage of computing resources. Generally, there are five responsibilities for the workload management software:

1. Queuing

When users want to run any task on a cluster, a job must be submitted to the workload management system with enough information about this task, like user's account, the needed number of CPU, the amount of memory, the file to execute, and the path storing output files. With the information of submitted jobs, the management system will follow the usage policy to rank all of submitted jobs to form a job queue. The jobs will be executed following the sequence of the queue whenever the needed computing resources become available. Through this queuing system, different usage policies can be carried out. The administrator can designate top priority to certain users in order to prevent them from waiting in queue. Also, it may prefer to run small tasks during daytime to serve

more users, but to run tasks which consume substantial computing resources and computer time at night. These kinds of restrictions can be realized by the queuing function of workload management software on the cluster.

2. Scheduling

Usually, the usage policy given by the administrator can not fully define the executed sequence of submitted jobs. A scheduler will also be used to choose the best job to run. The scheduler will consider the usage policy and current available computing resources to run the best job and optimize the usage of computing resources.

3. Monitoring

The monitoring in workload management software will provide information about computing resources. It will check the state of the compute nodes before assigning jobs in order to assure the compute nodes are error free and meet the requirement of assigned jobs; any discrepancies be reported to system.

Another important application of resource monitoring is to report the performance of running jobs. All of important information such as the usage of CPU, memory, network and other resources on a certain job can be viewed through the monitoring function. With this information, users can evaluate and improve their parallel program. For example, if the resource monitor reported more than 90% computer time was consumed by communication, then the data communication strategy within the program need requires substantial improvement.

4. Resource management

Once a job is submitted to the cluster system and determined as the current best job to run, the workload management software will automatically run the job on the corresponding computing resource, and when the job finishes, it will stop the application and clean up for the next job. These processes are called resource management.

5. Accounting

This function will collect the information of resource usage for certain jobs, users, and groups.

2.3.4 Other software

Some support software would also be necessary when running the aforementioned software. For example, the message passing communication would require OpenSSH as the tool for remote logging from master node to slave nodes.

Also, additional commercial software may be required according to the specific application of users. Some commercial software companies already offer the edition applied for cluster and parallel computation; MATLAB introduced a distributed computing toolbox to support parallel computation on clusters. GridMathematica also delivers a parallelized Mathmatica environment for cluster platform. Such commercial software will allow user to simply explore the advantage of cluster as a parallel computation platform without messing up with complex parallel algorithm.

2.4 Deploying an 8-nodes Apple workgroup cluster with high performance networks

Our Apple workgroup cluster selects 8 powerful Xserve/Intel servers as compute nodes. Mac OS X server, the UNIX based operating system is preinstalled on these servers. Xserve/Intel server integrates and optimizes all of hardware needed for computing nodes, such as processors, memories and network interface to deliver powerful computation capability. The Mac OS X server operating system is customized by the same vendor of servers to optimize the performance of single node. This operating system already includes many tools for administration and management of the whole distributed memory system.

2.4.1 Compute nodes

Two 2.66 GHz Dual-core Intel Xeon processors have been selected for every SMP compute node mainly due to two considerations: the first is that this processor one generation behind the cutting edge, usually has best performance/price. Another reason is that previous computation on other clusters has shown that satisfactory speed can be obtained only if the processors have clock rate above 2.0 GHz. Although faster processors are always welcomed by users, overall performance/price is the key for configuring a system. Especially for a platform of intense parallel computation, the performance of networks, not the processors, are usually the bottleneck of computation, so the newest and fastest processors costing much funding are most likely not to greatly improve the overall performance.

The capability of main memory is very important for scientific and engineering simulation. The problem of “out of memory” is fatal, and prevents researchers exploring some problems interesting but too large (e.g. some 3-dimensional simulation). Therefore, a memory requirement for possible largest simulation for phase field model of magnetic domain has been estimated. It shows that the amount of memory, for every compute note with two Dual-core processors, should be about 8 gigabyte. Accordingly, the total memory would be 64 gigabyte.

The capability of hard disk is 80 GB for compute nodes according to the principle that local disk capacity should be ten times the main memory capacity. But a much larger hard disk (750 GB) is selected for master node for the management work and temporally storing users’ data files.

2.4.2 Interconnect networks

The first management network for the cluster is an Ethernet private network mainly based on 3com 24-port baseline switch, which is a highly affordable, unmanaged Gigabit switch. This gigabit switch has 100MBps bandwidth and around 10^2 us latency.

Myrinet is selected as the second interprocess network system for the Apple workgroup cluster. Myrinet, designed by Myricom, is one of the best network solutions for parallel computation with intensive communication. Myrinet has fast bandwidth and low latency. According to Myricom, the latency of this Myrinet-2000 switch network for data communication using Message Passing Interface (MPI), an implementation of parallel

communication, is only 2.6µs–3.2µs, and the MPI unidirectional data rate is 247 MBytes/s. An advantage of Myrinet is that this Myrinet-2000 switch has independent processor and memory so that the data transmission would not take the main processor clock time to interrupt the process. This feature will significantly improve the efficiency of parallel computation.

To build Myrinet high performance network, a 16-port Myrinet-2000 switch and 8 PCI-X NICs as network interface cards have been selected for the 8-node Apple cluster. The switch has 8 ports available for potential update adding more computing nodes into the system.

2.4.3 Other hardware components

According to Apple Company, the thermal output per Xserve/Intel server is about 1100 BTU/h. So a cooling system with capacity removing at least heat output of 11000 BTU/h is required with 20% headroom for eight compute nodes. But considering the potential of adding more compute nodes, a rack air removal unit with much higher cooling power has been equipped.

APC 1000VA Uninterruptibel Power Supply (UPS) has been selected for protecting head node and networks from damage due to power surges.

NetShelter enclosure, a standard enclosure for storage of 19-inch rack –mount hardware, is selected to accommodate all of hardware including eight compute nodes, two sets of networks switches, rack air removal unit, UPS, and so on.

Appendix A. gives the information of hardware to deploy an 8-node Apple workgroup cluster with high performance network. Figure 2.2 shows the eight Apple Xserver computing nodes, and figure 2.3 shows the completed cluster system.

Figure 2.2 Eight Apple Xserver computing nodes.

Figure 2.3 Apple workgroup cluster system.

2.4.4 Mac OS X Serve operating system

The Mac OS X Serve, designed by Apple Corp for Xserve server, is a powerful operating system for administration and management of workgroup cluster. Its convenient and nice-interface management tools make administration of computing resources and users accounts much easier than traditional Unix/Linux system. At the same time, this UNIX based operating system inherits the main advantages of Unix/Linux system, like supporting almost all of open source software for UNIX/Linux system. In fact, Mac OS X already integrates more than 100 open source projects including OpenSSH, X11, GCC, and so on most used tools.

In addition to the basic administration and management function, Mac OS X Serve also has many advantages for scientific computation. It fully supports 64-Bit computing. The 64-bit addressing of the operating system provides the capability of accessing large memory, and what is more excited for high-performance computation, Mac OS X Serve already includes many 64-bit optimized math libraries for the hardware of Xserve servers, such as BLAS, LAPACK, vBigNum (a vector big number library), vBasicOps (a basic algebraic operations library). All of these math libraries can be easily call from C or Fortran program.

2.4.5 MPICH2 for message passing interface in parallel computation

As 2.3.2 mentioned, a message-passing communication mechanism is used globally in a SMP nodes cluster. The message passing process is specified by Message Passing Interface (MPI)[28]. MPI provides a set of standards for message passing communication, and these standards now have been developed as so-called MPI-2. MPICH2[29], developed by Argonne National Lab, is chosen as the implementation of MPI-2. The actually used in the cluster is MPICH2-MX[30], which is a port of MPICH2 on top of MX (a low-level message-passing system for Myrinet networks) developed by Myricom to optimize Myrinet networks performance for MPI application.

3 PARALLEL COMPUTATION FOR PHASE FIELD MODEL

3.1 Domain decomposition

As 1.2 introduces, the magnetic domain structure is described by the spatial distribution of local unit magnetization vector $\mathbf{m}(\mathbf{r})$. Its evolution is then reflected by the evolution of $\mathbf{m}(\mathbf{r})$, which is obtained at every computing grid by solving equations (1)-(3). A number of huge data associated with the computing grids are used to accommodate the intermediate results, the updated unit magnetization vector field, and other information such as free energy density for each cell. How to handle these huge arrays storing the information associated with each grid is the key for the parallel computation applied here.

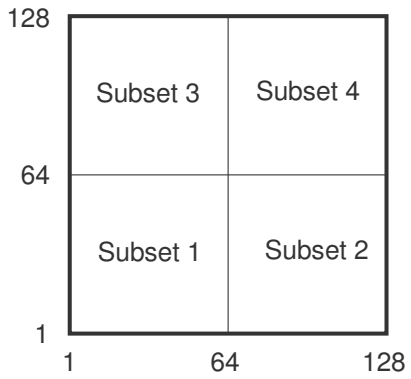
As 1.3 introduced, the parallelism in our simulation is mainly based on the data-level parallel model. In this model, the computational domain of a problem is distributed among compute nodes. Each compute node has certain subset of the data stored on its local memory, and the processor will perform task mainly based on its local data. Figure 3.1 illustrates this method. The computational domain is divided into four subsets with equal size. The data associated with the grid are distributed across four different compute nodes. The processor of each node will perform very similar operation but only on the subset stored on local memory. Through this so-called domain decomposition operation, the huge data array storing large computational domain is easily accommodated by multiple memories on involved compute nodes. This is the very

reason that the data-level parallel computation on distributed memory system can handle the problem of inefficient memory on traditional PC.

In the domain decomposition shown as Figure 3.1, the divided subsets have identical size and geometry. But equally decomposing domain is not the universal solution. The domain decomposition must follow several general rules.

The domain decomposition is directly related with the work load assigned to each compute node. And the load balance is the critical for the efficiency of parallel program. Poor load balance among different compute nodes will seriously break down the program and waste compute resource. The whole parallel program completes only when all of compute nodes complete their subtasks. During this period, the compute nodes cannot be released for new task even if some compute nodes may be idle after completing their own subtasks. The ideal case is that all of compute nodes complete their subtasks at same time. To do so, balance load control is necessary. If the compute nodes have very similar operation on the subsets of data, the operation time is mainly dependent on the size of data. Therefore, the computational domain is naturally decomposed equally, which is just the case of our simulation. But in some complicated situation, the subtasks scale may differ. In those cases, there is no general method to do the domain decomposition. Some advanced method, like monitoring the load balance and real-time adjusting it, may be needed to maintain the parallel performance.

Another important reason to equally decompose computational domain is due to the similar calculation operated by compute nodes. On each node, the equation is solved following almost the same procedures though the data are different. It would be easy for programming loops when the subsets of computational domain have identical size and shape.



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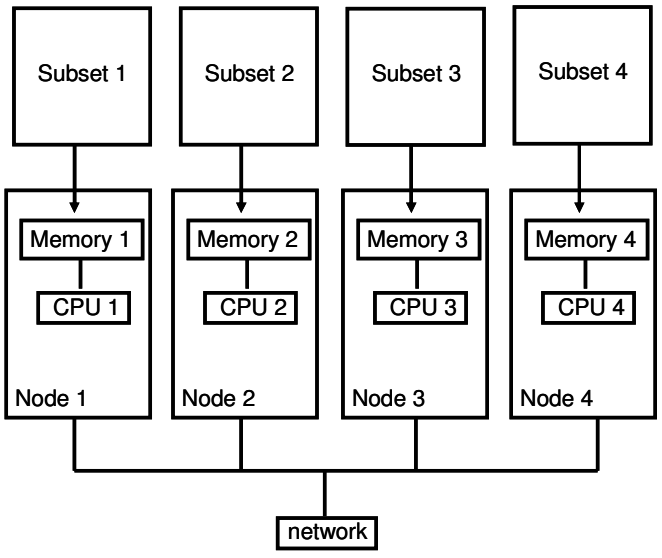


(b)

Figure 3.1 Domain decomposition (a) original computational domain with 128*128 grids. (b) Four subsets of the original computational domain are distributed across four compute nodes.

To decrease data communication among compute nodes is another important consideration when decompose domain. Comparing with traditional sequential programming, complex data communication among compute nodes is the disadvantage for parallel computing based on distributed memory system. The overhead from data communication may greatly increase the computer time, which seriously worsens the performance of parallel computing. Therefore, the domain should be decomposed in a way that the data communication is as little as possible and most of calculation can be supported by local data.

3.2 Data communication based on MPI

Data communication is important in the parallel programming especially on the share memory system. A good data communication control means low overhead and most CPU time is attributed to the data computation rather than communication. MPI (Message Passing Interface) is used in our parallel programming as the communication standard, and MPICH2 is the corresponding implementation applied. The main features of MPI and some important MPI routines are introduced here, followed by the data communication strategy in our program.

3.2.1 Message passing interface

MPI is a communication protocol in parallel computation mainly for distributed memory system while it still can be used for share memory computer. The goal of MPI is “to develop a widely used standard for writing message-passing programs”. It provides the

standards of the process topology, synchronization, point-to-point communication, collective operations, and other operations involving in communication of parallel computation. In MPI, the communicated data is packaged in a message and passed among multiple processors. MPICH2, used by our cluster, is a high-performance implementation of MPI standard. It has a specific set of routines which can be called from Fortran or C language. The implementation of MPI allows programmer manage the data communication by programming.

Unlike the sequential computation, parallel computation based on MPI involves many operations directly controlling the processors and network. We need to understand the architecture of actual used cluster before using MPI control the communication. Globally, there are eight compute nodes connected by network to form the distributed memory system. But for each node, it is a shared memory computer with two CPUs. In each CPU, there are two cores which can perform the instructions independently. A processor or process defined in MPI should be taken as a single core in our cluster. In another word, the Apple 8-node cluster has 32 processors for parallel computation. Based on the knowledge of the architecture of our cluster, we can introduce how MPI works in the data communication.

Firstly, every MPI session needs a communicator to include a group of processes. Here, the process, originally means the set of sequentially executed instructions, always can be taken as the processor. For example, four cores in two dual-core CPU would be included

in a communicator if users require four processes in the parallel computation. There may be more than one communicator in one session to control several groups of processors. In each group, the processors are identified by a unique integer between zero and the number of processors. In our parallel program, only one communicator is used.

Once the communicator is set up, the processors can be identified so that the message can be passed among specific processors. There are two types of data communication applied in our program. The Point-to-Point communication will pass data between two specific processes while collective communication happens among all of processes in the group. The Point-to-Point communication has blocking and non-blocking mechanisms. The blocking communication has some extra operations to assure the process receiving message is ready and waiting for the message. It gains more security but with slower speed compared with non-blocking communication. Both mechanisms have application in our program.

MPICH2 offers routines to manage the data communication operations, like initializing and terminating the MPI process, passing and collecting data among processors. Some important routines used in our fortran program are introduced as follows.

MPI_INIT(ierr)

This routine initializes the MPI execution environment to start a MPI process.

MPI_COMM_SIZE(comm.,size,ierr)

This routine determines the number of processes involved in the group.

MPI_COMM_RANK(comm.,rank,ierr)

This routine determines the rank of the calling process. The parameter “rank” will return a unique integer between 0 to the number of process in the group, which will be used to identify the processor.

MPI_Bcast (buffer,count,datatype,root,coom,ierr)

This routine broadcast a message from one certain process to all other processes involved in the communication group. The message or data address is specified by the parameter buffer, and the process sent message is identified by the parameter root, which is its rank in the group. The parameter count specifies the message size.

MPI_Send (buffer,count,datatype,dest,tag,comm.,ierr) `

This routine sends data located in “buffer” to the process with rank as “dest”. This operation is labeled by the parameter tag.

MPI_Recv(buffer,count,datatype,source,tag,comm.,status,ierr)

This routine receive data sent from process with rank as “source”. The received message is labeled by the parameter tag. This routine always works with MPI_Send to complete the message passing.

MPI_Barrier(comm.,ierr)

This routine makes synchronization in a communication group. Every process will block at the MPI_Barrier routine until all processes in the communication group reach same

MPI_Allreduce(sendbuffer,recvbuffer,count,datatype,op,comm.,ierr)

This routine operates a reduction and writes the results in all process.

From the above description, it shows that the data communication control in the programming is realized by simply setting parameters and calling proper MPI functions. Through that, MPI and its implementation MPICH2 offer a convenient way to directly control hardware such as the processors and network to realize the data communication among independent compute nodes.

3.2.2 Data read and write in parallel computing

Equation (3) is an initial value problem for each grid, so the initial information, like the initial unit magnetization vector on each computing grid must be given to start the Euler scheme. Therefore, program needs to read a huge input file with initial information to start the iteration. In addition, these data associated with the mesh of computing grid must be assigned to different computing nodes as Figure 3.1 shows. The first problem in parallelizing the iteration is how to read the initial data from input files and assigned the data to multiple computing nodes. Accordingly, an opposite problem is how to collect the resulting data from computing nodes and output them to several files in right sequence after the iteration is finished. This parallel reading and writing problem will be discussed here.

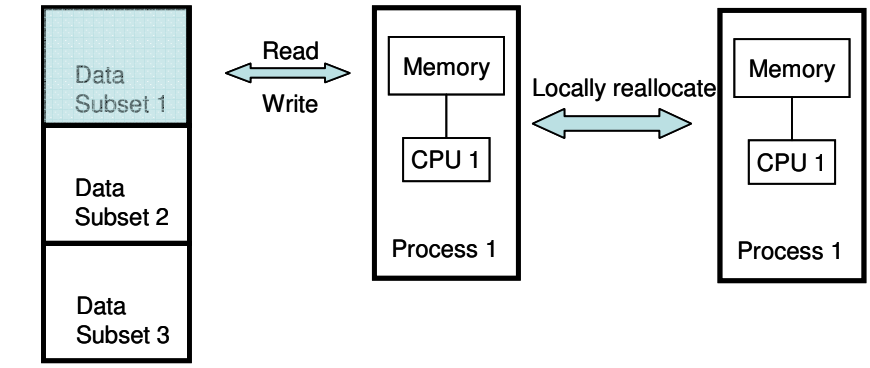
It would be ideal if each computing node can directly read from (or write to) the same file simultaneously. Unfortunately, parallel I/O may induce some serious problem; the output file may be overwrote by the multiple writing operation, the parallel reading may not be supported by ability of the operating system to handle multiple reading operation

at the same time. At current technology a parallel I/O system is still uncertain, some compromise must be made to perform the parallel reading and writing operation.

In our program, sequential rather than parallel reading and writing is applied. There is a process, say the one with rank 1, will handle main operation. The operation includes reading from (or writing to) a single file, distributing input data or collecting resulting data among the local memories of multiple processors in the communication group, and reformatting those data. The actual reading procedure for a parallel implementation is shown as Figure 3.2.

Three processes are assumed to take part in the parallel computation without loss of generality. The process 1 firstly reads the first part of input data and locates them in its local memory. It continues to read the second part of data and uses the MPI routine MPI_Send to send this part of data to process 2. The similar operation follows the second step except that the destination of third part of data is process 3. Accordingly, the process 2 and process 3 will call routine MPI_Recv to receive the data sent from process1 and locate them on their local memory. The opposite operation, writing resulting data to single file, can be figured out in similar way.

It should be pointed out that the MPI sending or receiving operation during above procedure does not have to happen among multiple compute nodes via network. As 2.1 mentioned, the cluster used here is a hybrid system with shared memory computer as



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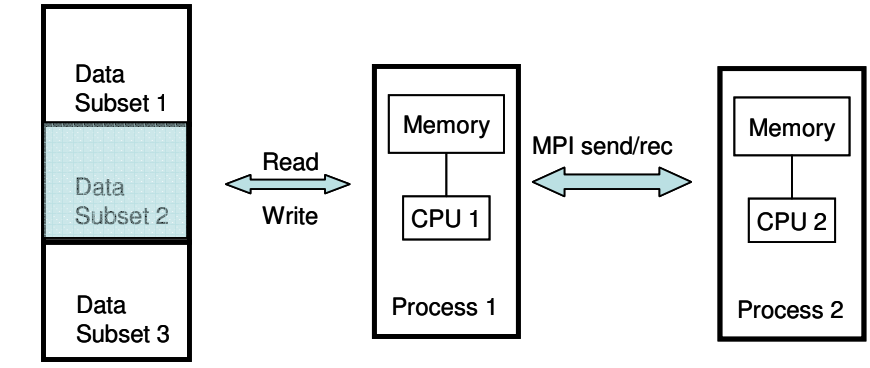

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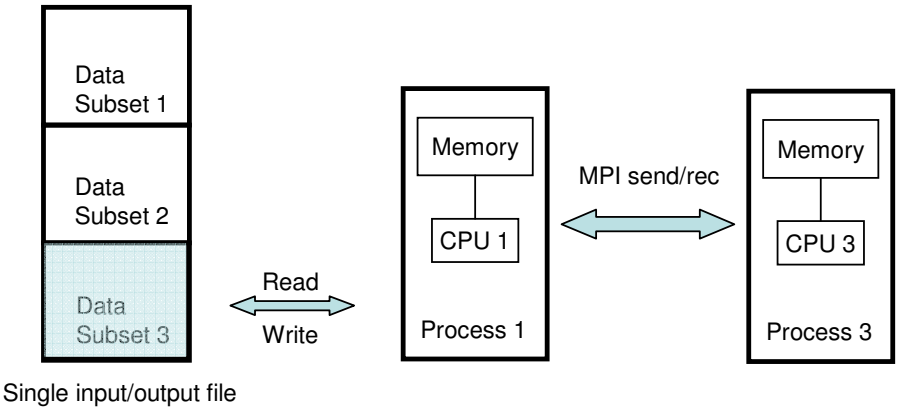


(c)

Figure 3.2 Sequential reading/writing data and distributing data through MPI.

compute node. Therefore, the multiple processors involved in the communication group may belong to the same compute node. As we know, the data communication inside single compute node is much faster than that among multiple compute nodes. It is very important to understand this character to optimize the performance of the parallel implementation on the cluster with hybrid structure.

A similar consideration in above example exists when the first process reads the input data file on the hard drive. Through open directory file system, the common directory accommodates the I/O files and physically locates on the hard drive of the head node in our cluster. Other compute nodes can access the common directory via network, but the access speed is much slower than that accessing local hard drive via data bus. Therefore, if the first process in charge of reading file from hard drive can be assigned to the head node, it will read input file directly from local hard drive through data bus. Especially for the situation involving frequent I/O operation, like intense backup of huge intermediate results, this kind of optimization should be considered.

The sequential reading and writing operation and distributing data through MPI can handle files with moderate size, which is just the case of our current simulation. If the simulation size goes much larger in future, some complex parallel reading and writing technology have to be introduced in our programming. A book by John M. introduces some advanced methods to realize parallel I/O[31].

3.3 Parallel fast Fourier transformation

After the initial data is read and distributed, the iteration based on Euler scheme can start simultaneously on multiple processors in the group. At each step, the main task is to calculate the driving force, $\delta F/\delta \mathbf{m}$, based on current unit magnetization vector field. But the calculation of driving force for each grid is highly dependent on the information related with all other grids in the computational region.

With periodic boundary conditions, fast Fourier transform (FFT) method is often employed to deal with the non-local computation when solving phase field equation[32,33]. The method "converts the integral-differential equations into algebraic equations"[7]. The complexity for the direct computation of interaction between magnetization vectors, $O(N^2)$, will be reduced to $O(N \log N)$ by using fast Fourier transform.

If FFT is implemented in our parallel program, the algorithm of FFT must be parallelized compatible with the parallel program. Because of the wide use of FFT, many references can be found on parallelizing FFT method. However, few parallel FFT codes are publicly available. 2D and 3D parallel FFT subroutines are developed by our group.

4 THE PERFORMANCE EVALUATION OF APPLE WORKGROUP CLUSTER

The performance evaluation includes two parts: test of the software environment to see if the cluster supports general MPI program, and test of data communication performance on the workgroup cluster.

4.1 Verify MPI functions

The developed Apple workgroup cluster is to serve as parallel computing platform for MPI programs. After the software environment is set up, all MPI functions must be carefully tested. The error checking will assure the cluster system can perform as a capable platform of MPI programs.

Some initial tests can be done by directly running the example programs, which come with MPICH2 software. If these programs successfully run on the cluster and return correct results, then a more thorough test is run with the command “make testing” from the top-level of mpich2 directory. It produces a summary of the test results. From the summary, all function related with the MPI functions in fortran program are error free in our cluster system.

4.2 Data communication performance

4.2.1 Benchmarking point-to-point communication

The MPI functions test only can determine if the installed version of MPICH2 is functioning in the current cluster system. But users may be more interested in the performance of their parallel implementation on the cluster system. Besides of the parallel implementation itself, the data communication performance is the most important factor to determine the overall performance of the potential MPI program. Given some performance parameters on the data communication, users may be able to estimate the performance of their MPI programs on the cluster system.

The program mpptest is a performance test suite. This program is distributed with MPICH2. Once the MPICH2 is installed successfully, the executable, mpptest, is already available. It measures the MPI-based communication performance in several ways to reflect the performance.

By measure some important parameters during the communication, mpptest provides a clear picture both for point-to-point and collective communication performance on our cluster system. In our implementation, block and non-blocking point-to-point communication, and collective communication are operated. Therefore, the mpptest is conducted based on these three types of data communication.

Figure 4.1 and Figure 4.2 show the performance of a single message sent between two processes based on blocking and non-blocking communication, respectively. The bandwidth and latency, two important parameters in communication, are revealed by the tests. The size of messages is automatically chosen in order to reveal the message size where the change of behavior happens.

From Figure 4.1 and Figure 4.2, the latency for small massage is about 4 microseconds, and the maximum bandwidth is about 220MB/sec. The same parameters based on similar hardware, reported by Myrinet, are used to compare with our performance parameters. According to the report from Myrinet, the maximum bandwidth is about 230 MB/sec, and the latency for empty message is about 9 microseconds, which proves that our cluster system have obtained the expected performance in point-to-point communication.

The point-to-point communication tests provide us with certain confidence that the cluster system is functioning properly. Also, the test results show the best bandwidth performance dependent on the message size. From Figure 4.1(b) and Figure 4.2(b), a sudden drop in bandwidth happens when message size is increased to about 32000 bytes. This information may be useful when users try to control the message size to optimize their implementation performance.

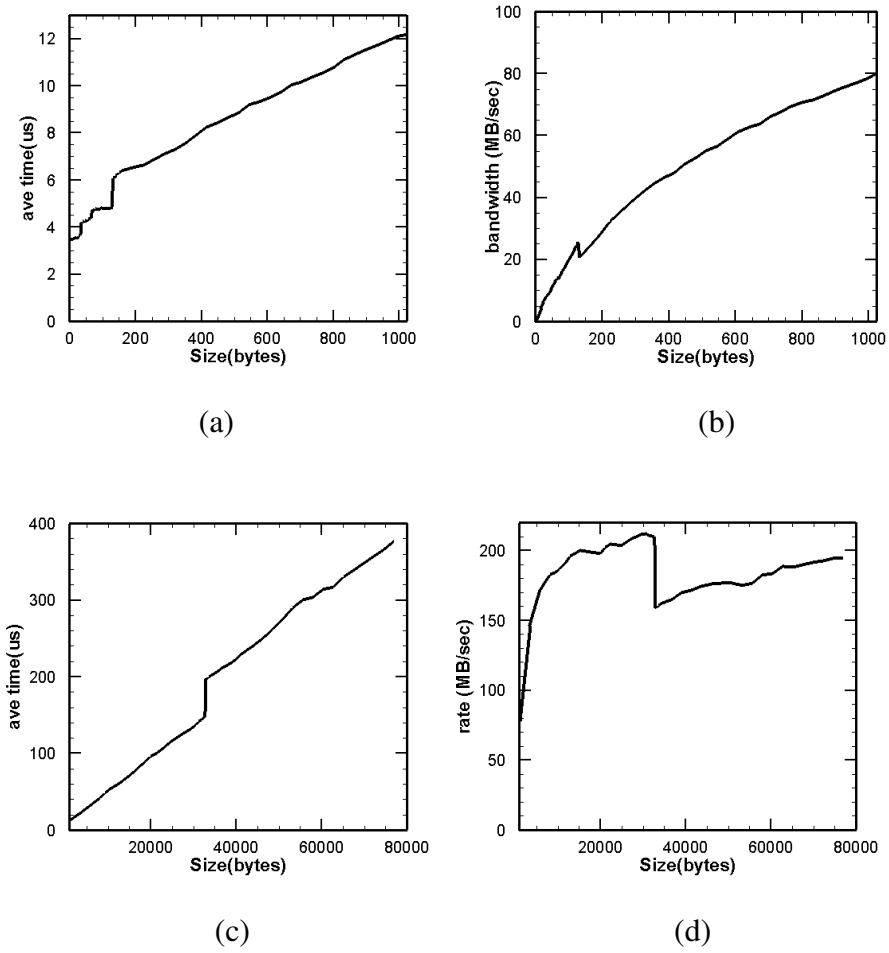


Figure 4.1 Performance of blocking communication based on MPI_send routine.(a)latency for short message (b) bandwidth for short message (c) latency for long message (d) bandwidth for long message.

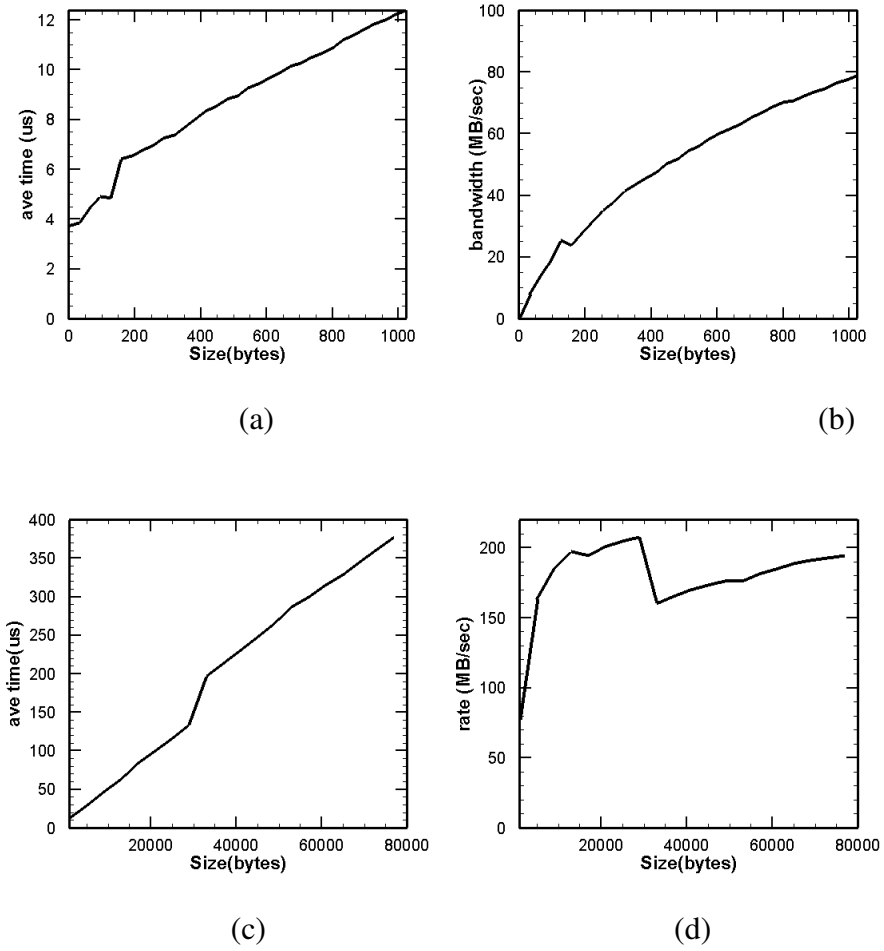


Figure 4.2 Performance of non-blocking communication based on MPI_send routine(a) latency for short message (b) bandwidth for short message (c) latency for long message (d) bandwidth for long message.

Another interesting phenomenon, revealed by the point-to-point communication test, is shown as Figure 4.3.The previous point-to-point communication tests are all conducted between two compute nodes via Myrinet network. However, the developed Apple workgroup cluster is based on shared memory computer nodes. The point-to-point communication can also be operated between two processors within the same compute node. In that situation, the data bus, rather than the Myrinet network, will be in charge of

the communication, and support faster communication speed as Figure 4.3 shows. This communication performance difference may affect the way we distribute parallel tasks among our cluster system.

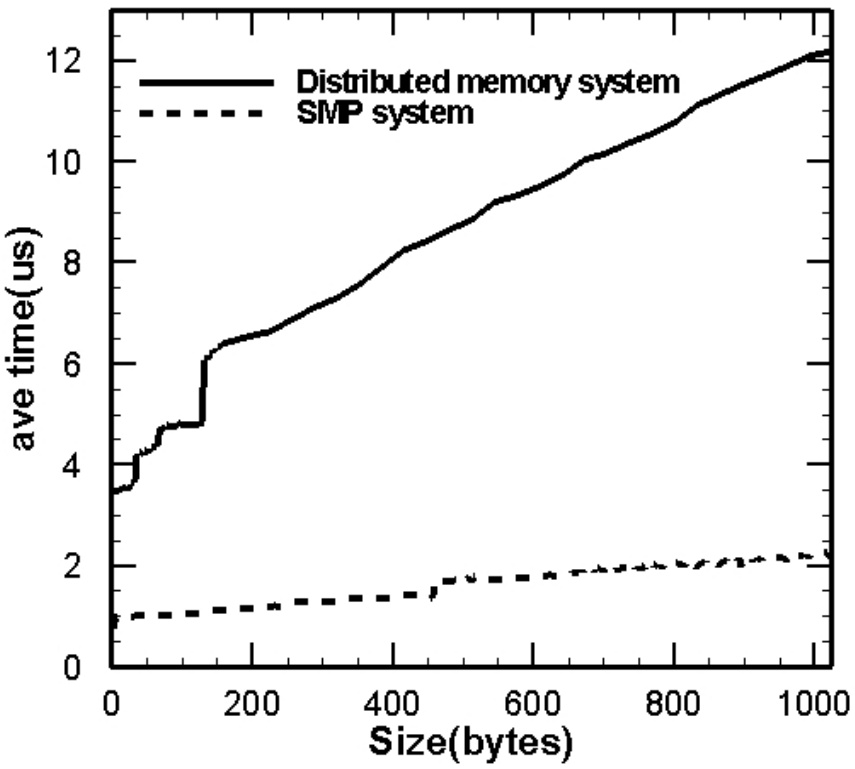


Figure 4.3 Point-to-point communication latency in distributed memory system and shared memory system.

4.2.2 Benchmarking collective communication

Another important data communication type applied in our parallel implementation is collective communication. Mpptest also can measure the communication performance based on this data communication type. The measured communication performance of MPI collective communication routine, MPI_reduce, is showed as Figure 4.4, which

behaves similarly with the one according to the report of Myrinet Company. Like point-to-point communication, a sudden behavior change happens where the message size is increased to 1000 bytes.

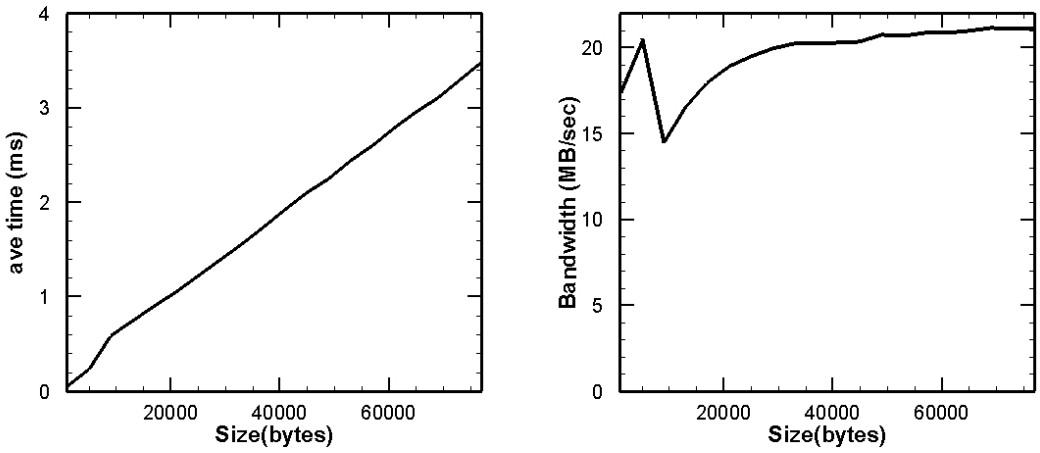


Figure 4.4 Performance of collective communication based on MPI _reduce routine. (a)latency; (b) bandwidth.

Unlike point-to-point communication, collective communication involves multiple processes. As the number of involved processors increases, some MPI routines may induce a latency cost proportional to the number of processors. Therefore, scalability is another important consideration to evaluate a collective communication on our cluster system. Goptest, a MPI benchmarking program distributed with MPICH2, is used to test this property. Goptest will measure the collective communication performance dependent on the number of processors.

Figure 4.5 shows the average time for collective communication dependent on the number of processors. The tested MPI routine is MPI_reduce, and the message size varies from 256 bytes to 1024 bytes. From Figure 4.5, the message passing time does not increase significantly as the number of processors increases. This trend implies that the collective communication will not break down as more processors join in the group.

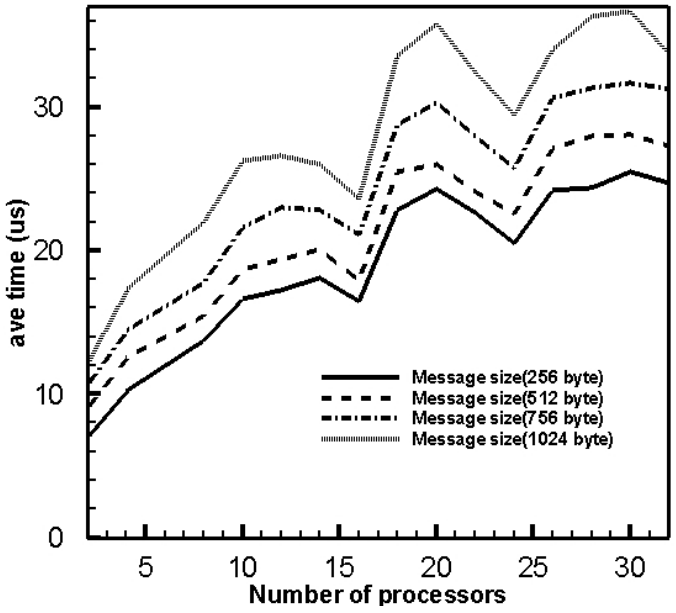
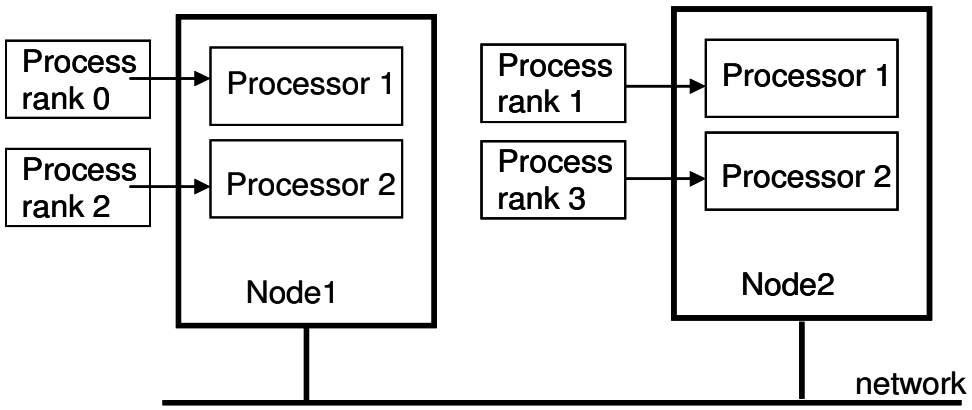


Figure 4.5 Performance of collective communication dependent on number of processors.

An interesting phenomenon related with the hybrid architecture of the Apple workgroup cluster is found in goptest. Before introducing it, a related background about how MPICH2 assigns parallel tasks to processors is given as Figure 4.6 illustrates.



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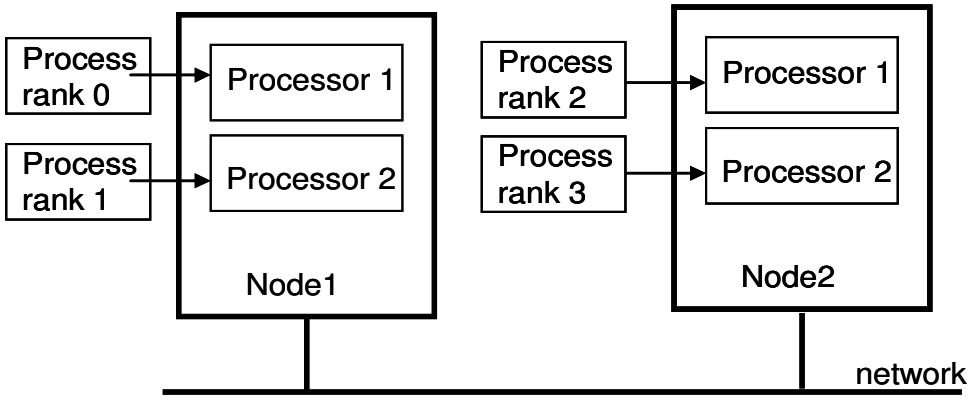


(b)

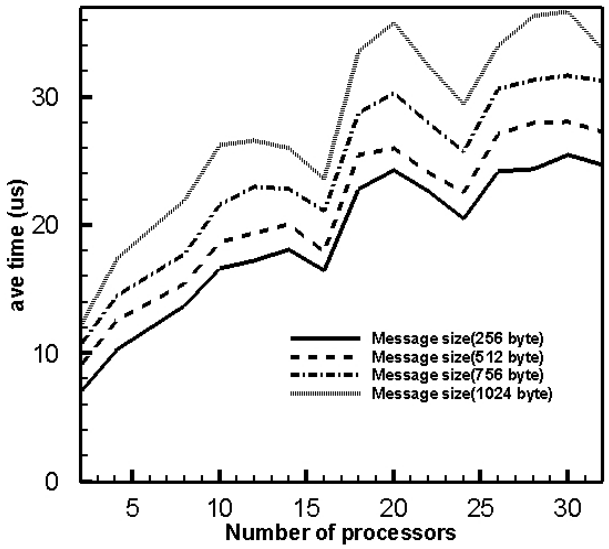
Figure 4.6 The sequence to assign processes among multiple compute nodes. (a) circular way; (b) consecutive way.

When a parallel implementation is started, MPICH2 needs to assign the parallel processes to the involved processors. The computer node in our cluster system has four processors. It can take four processes simultaneously. If a parallel job has four processes working on two compute nodes, the default operation is rank 0 and 2 will be assigned on

first node ,and rank 1 and 3 will be on second node. This circular way is shown in Figure 4.6.a. But MPICH2 does offer option for users to control the process placement explicitly. The user may want to have consecutive ranks on the same node, so that rank 0 and 1 will be on first node and rank 2 and 3 will be on second node. This consecutive way of processes placement is shown in Figure 4.6.b.

The interesting phenomenon in goptest is that the collective communication performance is significantly affected by the way of processes placement. Figure 4.7 shows the average time for message passing dependent on number of processors. Figure 4.7.a is corresponding to the processes placement with circular fashion, and Figure 4.7.b is the results based on the processes placement with consecutive rank within one compute node. Obviously, the performance is greatly improved by assigning consecutive processes within one compute node.

This performance difference induced by the way of processes placement is related with the hybrid architecture of our cluster. Unlike sequential computation, parallel computation is highly dependent on the architecture of the computing platform. Therefore, the optimizing operations for running the parallel implementation are encouraged based on the actual situation of the specified cluster system for the users.



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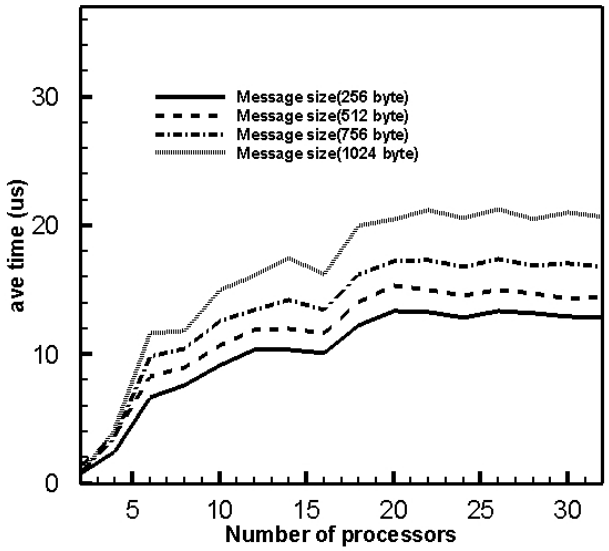

(b)

Figure 4.7 Performance of collective communication. (a) assigning the processes in circular way; (b) assigning the processes in consecutive way.

5 PARALLEL IMPLEMENTATION OF PHASE FIELD MODELING OF MAGNETIZATION PROCESS IN TERFENOL-D CRYSTALS*

Terfenol-D has been the leading magnetostrictive material for magnetomechanical transducers and actuators since its discovery in 1970's.[34] Because of its lower cost, twinned crystals are usually used in technological applications.[35] Twinned crystals are grown along $<11\bar{2}>_c$ direction and composed of alternate crystalline layers of twin relation with $\{111\}_c$ plane whose normal is perpendicular to the $<11\bar{2}>_c$ growth direction.

Growth twinned Terfenol-D crystals have been studied over the past two decades. However, the domain-level mechanisms are still not fully understood. This is because the low magnetocrystalline anisotropy results in magnetization rotation that competes with domain wall motion, and their interplay leads to complex domain-level processes.

Various models have been proposed to explain the magnetomechanical behaviors of Terfenol-D, which are based on different mechanisms. Magnetic domain rotation model assumes no interaction among different domains. The simulation of magnetization

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*Part of this section reprinted with permission from "Phase field modeling of magnetization process in growth twinned Terfenol-D crystals" by Y.Y.Huang and Y.M.Jin, 2008. Applied Physics Letters, **93,** 142504(3pp.). Copyright © 2009 American Institute of Physics.

process is then reduced to the single magnetic domain rotation without considering the domain wall motion. In the single magnetic domain rotation model, the process is

relative simple. The theoretical results are easy to calculate. In this case, the simulated results by the parallel implementation will be compared with the theoretical results to test our cluster and the parallel implementation.

However, the single magnetic domain rotation model is not able to realistically describe the domain evolution in Tefenol-D. In fact, the magnetic and elastic interaction among different domains will greatly affect the magnetic domain evolution. But the computation related with the interaction is very complicated. No previous work has been reported to properly take into account this important interaction. The phase field model of magnetic materials in Section 2.1 can effectively evaluate the interaction effect with the help of parallel computing on our developed workgroup cluster. The simulated magnetization processes in twinned Terfenol-D crystal by our parallel implementation will be presented as a successful application of the parallel computing for phase field model of magnetic materials.

5.1 Simulation of single magnetic domain rotation

Figure 5.1(a) shows the initial spacial distribution of magnetization vectors in a single magnetic domain. All magnetization vectors are oriented along the same easy axis. The crystal structure is assumed to be twinning-free.

The physical properties of Terfenol-D used in our simulation are listed in Table 5.1. The initial horizontal magnetization direction is corresponding to easy axis, $[111]_c$. The vertical direction, along which the magnetic field is applied, is $[\bar{1}\bar{1}2]_c$ in the crystal.

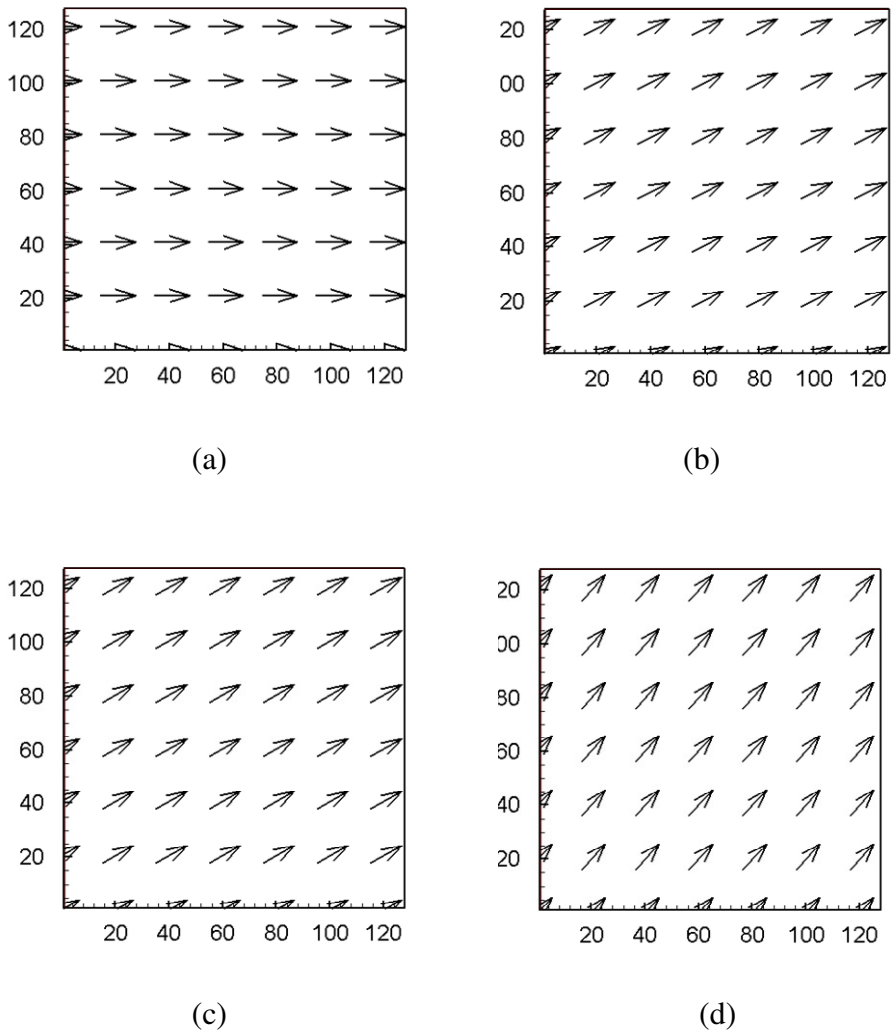

Figure 5.1 The magnetic domain temporal evolution under vertical external magnetic field. (a) time steps=0; (b)time=100; (c) time =500; (d) time =1000.

Table 5.1 The physical properties of Terfenol-D used in the testing simulation

Ms, Saturation Magnetization	$8\times10^{5}\,A/\mathrm{m}$ [36,37]
λ_{100}, Magnetostriction	$90\times10^{-6}\,mm/mm$
λ_{11}	$1640\times10^{-6}\,mm/mm$ [36]
K_1, Magnetocrystalline Anisotropy	$-0.6\times10^{5}\ \mathrm{J/m^3}$ [38]
K_2	$-2.0\times10^{5}\ \mathrm{J/m}$ [38]
E_Y, Yong's modulus	30 Gpa[39,40]
μ, Shear modulus	11.5 Gpa
γ, Possion ratio	0.3[39,40]

When an external magnetic field is applied along vertical direction, the magnetization vectors will homogenously rotate and reorient to the easy axis closer to the direction of external field. This magnetization process driven by the applied field, as the result of minimizing total free energy, has been previously studied by domain theory.

Figure 5.1 shows the simulated results on the temporal evolution of magnetic domain under 2000 Oe applied field along vertical direction. It is shown that the magnetization vectors rotate and reorient to the $[\bar{1}\,\bar{1}\,1]_c$ easy axis, the closest easy axis to the applied field. The simulation results predict same trend of magnetic domain evolution during magnetization process as the theoretical prediction according to domain theory.

Besides the qualitative comparison between our simulation results and theoretical prediction, an analytical solution for this case is also needed to verify the simulation results quantitatively. A simple sequential program can give the correct quantitative results for the magnetization process by tracking the magnetization vector corresponding

to the minimum energy. Following previous work on magnetic domain rotation model[41], the simulation of a single magnetic domain rotation can be reduced to simulate the behavior of a single magnetization vector under an external magnetic field, which is easy to be calculated based on the principle of minimization of free energy. The sequential code to implement this function is included in the Appendix C.

Figure 5.2 shows the comparison of magnetization curves simulated by the parallel implementation of phase field model and a simple sequential program, respectively. The exactly same results suggest that the parallel implementation on our cluster system is functioning properly.

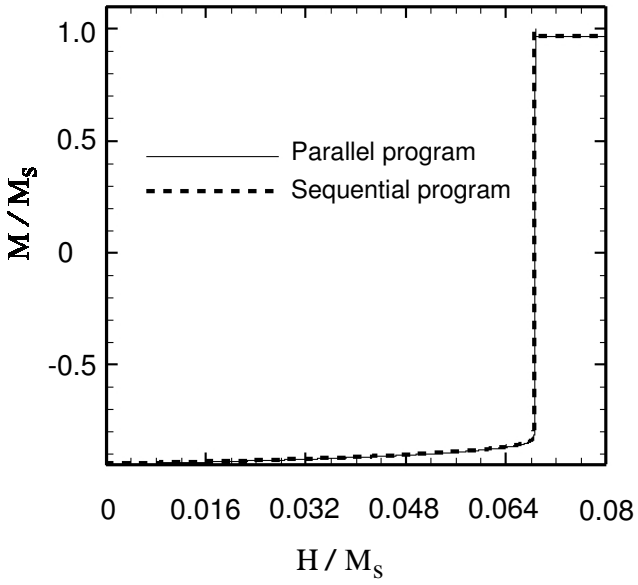

Figure 5.2 Magnetization curve simulated by parallel implementation and a simple sequential program.

5.2 Simulation of magnetization process in twinned single crystal

Most of the previous studies of magnetization processes in Terfenol-D crystal have assumed no interaction among different magnetic domains in Terfenol-D[35,37,41,42]. The magnetic domain rotation without domain wall motion is considered to be the only mechanism during magnetization process, which is against experimental observations. Our parallel computing of the phase field model of magnetic materials will include the magnetic and elastic interaction to quantitatively describe the magnetization processes involving both magnetization rotation and domain wall motion in twinned Terfenol-D crystals.

Figure 5.3 (a) illustrates an energy-minimizing domain configuration in growth twinned Terfenol-D crystal, which is used as initial state of our simulations. The crystal consists of alternate twin-related plate-shaped grains, and magnetization forms continuous 180° domains across twin boundaries covering multiple grains, as shown in Figure 5.3 (a). Figure 5.3 (b) illustrates the crystallographic orientations of a parent layer and its twin layer, as well as the $<111>_c$ easy magnetization axes in respective layers. In the initial state, magnetization vectors are aligned with easy axes throughout the crystal (i.e., V_P1, V_P1' in parent crystal and V_T1, V_T1' in twin crystal), minimizing magnetocrystalline energy. The domain continuity across twin boundaries makes them free of magnetic charge and lattice misfit, minimizing magnetostatic and elastic energies. Such a domain

state is stable and is observed in experiments by applying a compressive stress along the $[11\bar{2}]_c$ growth direction, and is the most desirable initial domain configuration because it

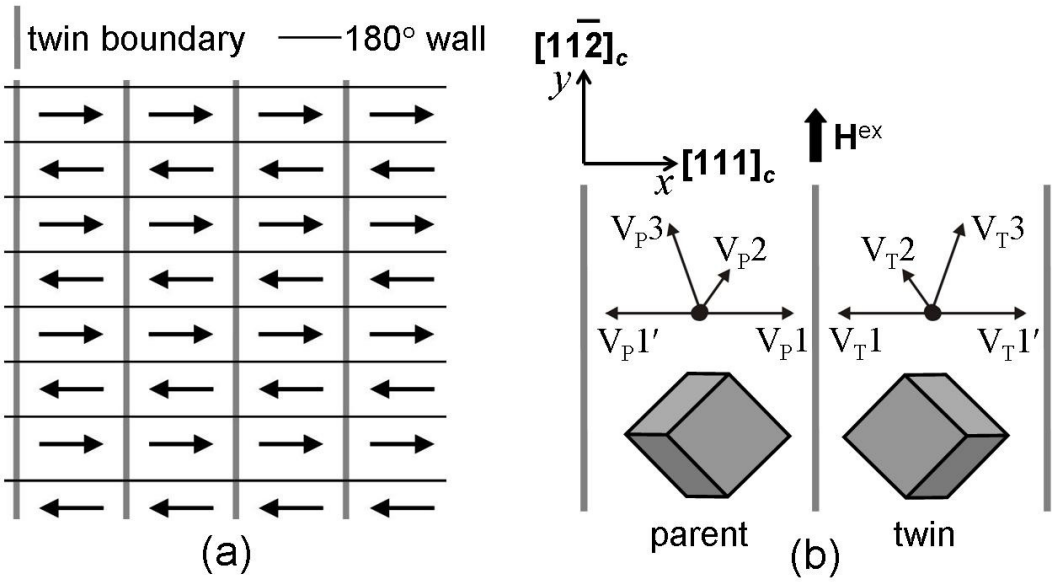

Figure 5.3 (a) Energy-minimizing domain configuration in growth twinned Terfenol-D crystal. Magnetization vectors are aligned perpendicular to (111) growth twin boundaries and form continuous 180° domains. (b) Schematics of crystallographic orientations and magnetization easy axes (projected to the plane of figure) of a pair of twin-related crystals (parent and twin). Only the easy axes whose dot products with applied magnetic field Hex along $[11\bar{2}]_c$ growth direction are non-negative are shown.[43]

generates maximum field-induced deformation under magnetic field along $[11\bar{2}]_c$ growth direction. It is worth noting that, starting from the initial state, complex domain evolution processes take place in response to external magnetic field, where the complexity results from the frustration in magnetic and elastic compatibilities at twin boundaries. With increasing magnetic field applied along $[11\bar{2}]_c$, magnetization vectors tend to reorient to easy axes closer to $[11\bar{2}]_c$, namely, V_P2, V_P3, V_T2, and V_T3. However,

the existence of twin boundaries leads to magnetic charge and lattice misfit there: among the easy axes shown in Figure 5.3(b), besides of the initial state, only V_P2/V_T3 and V_p3/V_T2 are magnetically compatible, but they are elastically incompatible. As a result, significant internal magnetic field and stress field develop, causing strong domain interactions. We simulate the detailed domain evolutions to investigate the important roles played by magnetic and elastic interactions in the magnetization processes. A computation cell of 256×128 with grid size l=10nm and periodic boundary condition is used to describe a representative Terfenol-D volume containing parent and twin grains and initial 180° magnetic domains. The parameter used in the simulation is the same as Table 5.1 lists.

The computer simulations reveal complex domain microstructure evolutions involving both magnetization rotation and domain wall motion, and clarify the underlying domain mechanisms responsible for the experimentally observed jump effect. In order to analyze the respective contributions from magnetostatic interaction and elastic interaction, two different cases are considered: (1) magnetically but not elastically interacting domains with both magnetization rotation and domain wall motion, and (2) taking into account all energy contributions and allowing magnetization to evolve freely. In both cases, magnetic field is applied along $[11\bar{2}]_c$.

The simulated magnetization curves are shown in Figure 5.4. A very large discontinuous change is observed in both cases. This magnetization jump effects have been reported in

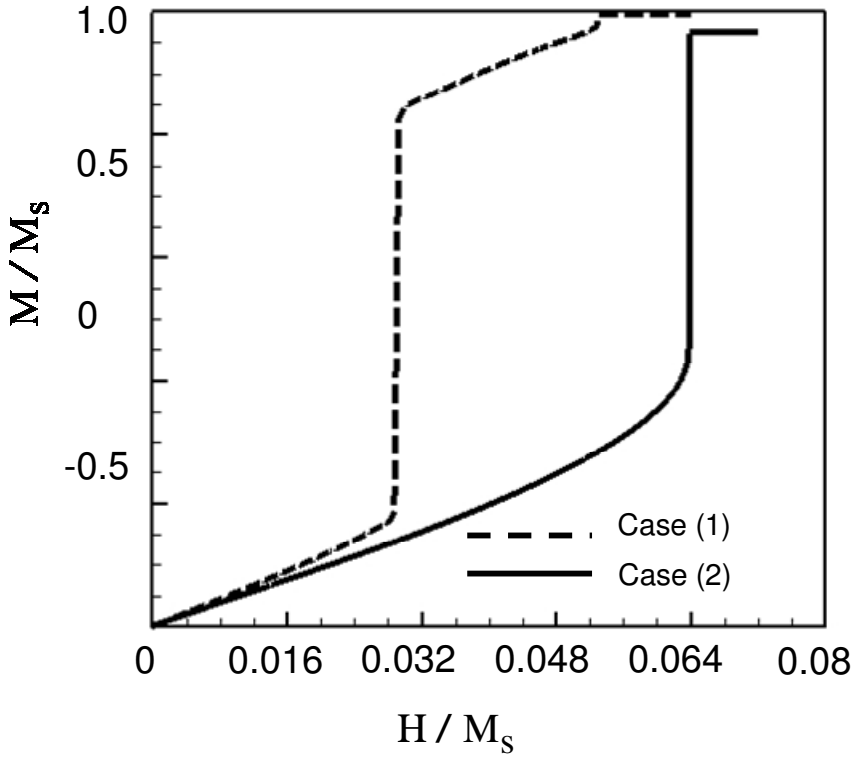

Figure 5.4 Simulated magnetization curve in case (1) and (2).

experimental observation.[38] The magnitude of the applied field corresponding to the jump effect is called critical field. The critical field is an important parameter when describe the magnetization behavior of Terfenol-D.

A detailed magnetic domain evolution during the magnetization process would help to explain the magnetization jump effect. Figure 5.5 and Figure 5.6 show the magnetic domain evolution in response to the applied field in case (1) and case (2), respectively.

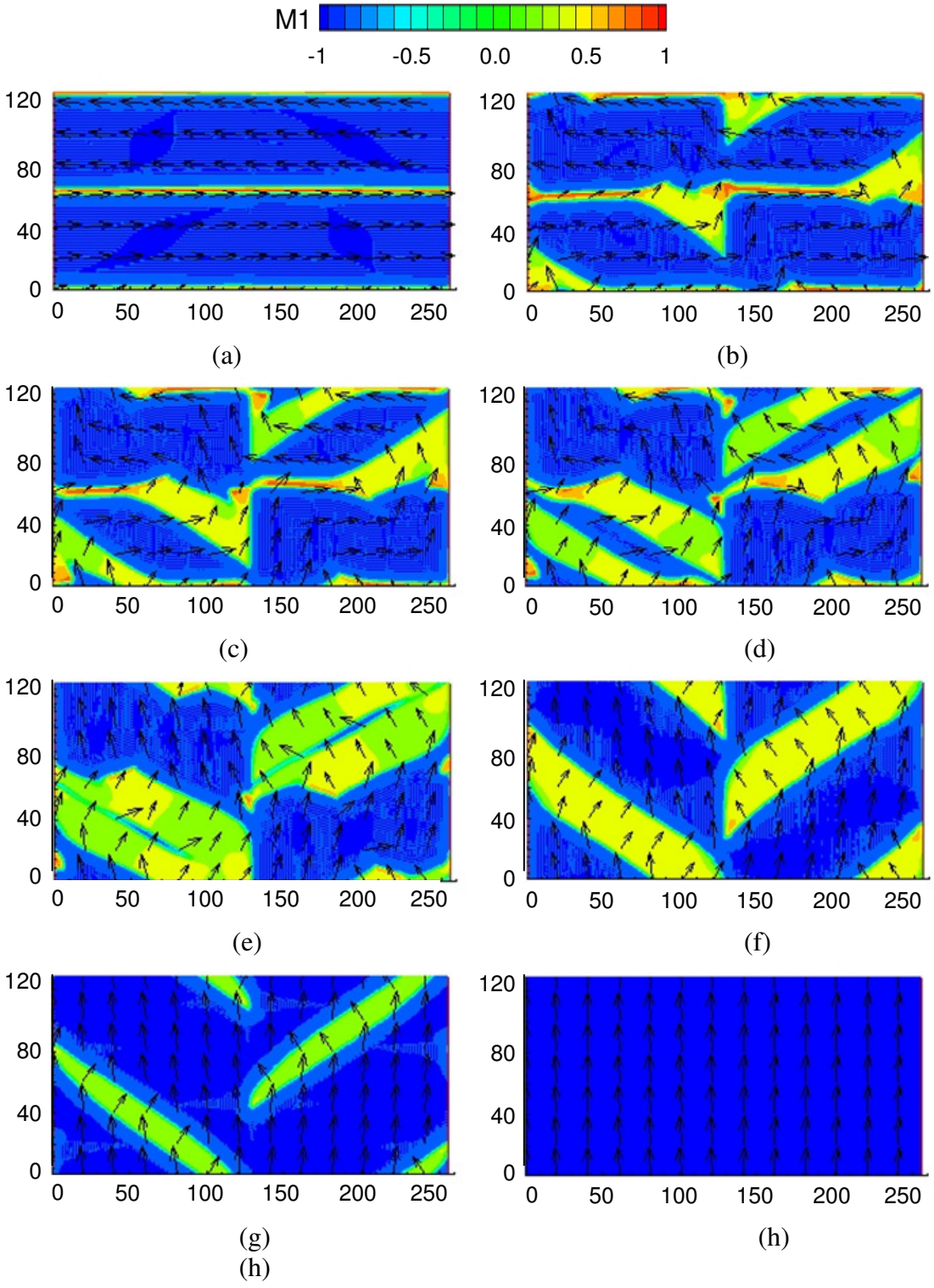

Figure 5.5 Magnetic domain evolution for case (1). The vector plotted is the projection of magnetization vector on the plane. The contour colors represent the magnetization vector component out of the plane.

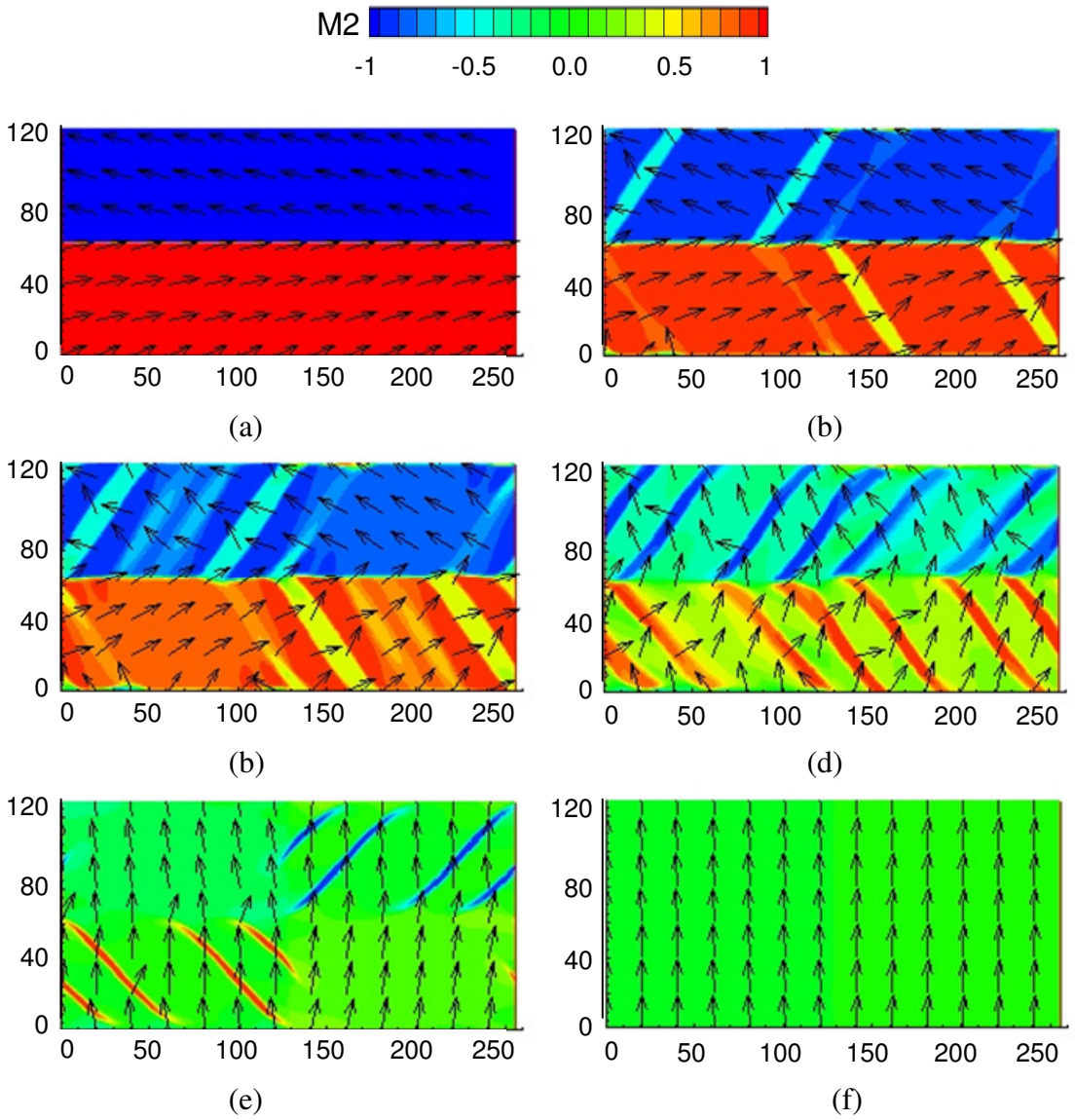

Figure 5.6 Magnetic domain evolution for case (2). The vector plotted is the projection of magnetization vector on the plane. The contour colors represent the magnetization vector component in horizontal direction.

In case (1), the simulation observes nucleation and growth of V_P2, V_P3, V_T2 and V_T3 domains and finds that domain wall motion is the main mechanism producing one-step jump as shown in Figure 5.5. During the magnetization jump, the domains are magnetically compatible both inside grains (forming three-domain configurations

$V_P1/V_P2/V_P3$, $V_T1/V_T2/V_T3$, and two-domain configurations V_P1'/V_P3, V_T1'/V_T3) and across twin boundaries (forming V_P2/V_T3 and V_P3/V_T2 neighboring pairs), which, however, is elastically incompatible. Such domain structure is possible only in a system where elastic interaction energy is significantly smaller than magnetocrystalline anisotropy and magnetostatic interaction energies.

In case (2), the critical field is higher than that in case (1), as Figure 5.6 shows. The higher critical field is due to the additional elastic constraint that necessitates a higher field to activate nucleation and domain wall motion. More complicated domain evolution is also observed in this case. But the phenomenon that domain wall motion follows the initial magnetic domain rotation is observed both in case (1) and case (2).

Comparing the simulated domain evolution in case(1) and (2) with the single magnetic domain rotation model in 5.1, we found that domain interactions through internal magnetic and elastic fields greatly affect the predicted magnetization processes. Thanks to the paralleling computing of phase field model based on our cluster system, we can take into account these complicated interaction effects in order to accurately characterize the magnetization of twinned Terfenol-D crystals, finding the underlying mechanisms involve both domain wall motion and magnetization rotation.

6 CONCLUSIONS AND FUTURE WORK

According to the requirement of the parallel computing for phase field model of magnetic materials, a workgroup cluster system with high performance network was selected as the computation platform to support the parallel implementation. We have successfully deployed the hardware system and configured the software environment to build an 8-node workgroup cluster system, serving as a parallel computing platform for MPI program. The 8-node workgroup cluster can simultaneously support a maximum of 32 processes for a MPI program to speed up the execution. The distributed memory architecture in the cluster system accommodates 64 GB memory to support the parallel computation usually involving huge data. And the high performance Myrinet network greatly improves the performance of data communication among compute nodes.

Several testing programs have been implemented to evaluate the performance of the cluster system, especially for the application of parallel computation using MPI. The tested results show that the cluster system can efficiently execute MPI program with intensive communication.

A simulation of the single magnetic domain rotation in Terfenol-D crystals was performed by our parallel implementation of phase field model of magnetic materials on the cluster system. The simulated results agree well with the theoretical prediction. A further simulation including magnetic and elastic interaction using our parallel implementation shows the important roles of these interaction effects in the

magnetization processes of twinned Terfenol-D crystals. This simulation example proves that the paralleling computing for the phase field model of magnetic materials based on the workgroup cluster system offers a promising tool for realistic domain analysis.

The developed computer cluster and parallel program lay the foundation for our planned future work:

A. Analyze the output of benchmarking implementations to optimize the execution of the MPI program;
B. Perform 3-D simulations of magnetization processes in Terfenol-D single and polycrystals;
C. Simulate domain phenomena in other magnetic materials of interests.

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APPENDIX A. LIST OF HARDWARE IN THE 8-NODE APPLE WORKGROUP CLUSTER

hardware	description
Master node	Xserve Quad Xeon server: Two 2.66GHz Dual-Core Intel Xeon 8GB (8x1GB) memeory 750 GB Serial ATA ADM @ 7200-rpm hard drive 24x Combo (DVD-ROM/CD-RW)
Slave nodes	Xserve Quad Xeon server: Two 2.66GHz Dual-Core Intel Xeon 8GB (8x1GB) memeory 80 GB Serial ATA ADM @ 7200-rpm hard drive 24x Combo (DVD-ROM/CD-RW)
First management network	3Com 24-port Baseline Switch 2824 & cable
Second high performance communication network	16-port Myrinet-2000 switch with Fiber ports and monitoring 8 Myrinet-2000 PCI-X NIC (2MB memory) Myrinet-2000 fiber cable
Back up power supply	APC Smart-UPS 1000VA USB & Serial Rack-Mount 1U 120V
Power supply	APC 14-outlet, 15A, 0U PDU (AP9567)
Cooling system	APC rack air removal unit
Enclosure	APC NetShelter SX 42U Enclosure with Sides

APPENDIX B. INSTALLED SOFTWARE ON THE 8-NODE APPLE WORKGROUP CLUSTER

Software installed	Description
Mac OS X Serve	Operating system, preinstalled by vendor
Apple Remote Desktop	Remote administration tool
Absoft Pro Fortran 10.1 x86-32 OSX	Commercial fortran compiler for Mac OS X system
MX-2G	A low-level message-passing system for Myrinet networks
MPICH2-MX	A port of MPICH2 (an implementation of MPI) on top of MX(ch_mx)
FFTW3	A free C subroutine library for computing the discrete Fourier transform (DFT)

APPENDIX C. SEQUENTIAL PROGRAM OF DOMAIN ROTATION MODEL

```
Program rotation
 implicit none
 integer :: length,H_load_period,Record_period,i,n,j
 real:: k1,k2,time_step,p
 real:: M_initial(3),H_direction(3),H_load_increase(3),tmp,H(3),mh_tmp
 real:: Energy,Force(3),tmp_Force(3),Magnetization(3),Magnetization_sqrt(3)
 real,allocatable:: Energy_record(:),Magnetization_record(:,:),H_record(:,:)
open(unit=11,file="Martensite.dat")
read(11,*)time_step,length,record_period
read(11,*)H_direction
read(11,*)H_load_increase
read(11,*)H_load_period
read(11,*)M_initial
Magnetization=M_initial
read(11,*)k1,k2
read(11,*)H
read(11,*)p
close (11)
allocate(Magnetization_record(3,length/record_period+1),H_record(3,length/record_peri
od+1))
allocate(Energy_record(length/record_period+1))
tmp=sqrt(H_direction(1)**2+H_direction(2)**2+H_direction(3)**2)
H_direction=H_direction/tmp
tmp=sqrt(Magnetization(1)**2+Magnetization(2)**2+Magnetization(3)**2)
Magnetization=Magnetization/tmp
Magnetization_sqrt=Magnetization**2
Energy=k1*(Magnetization_sqrt(1)*Magnetization_sqrt(2)&
               +Magnetization_sqrt(2)*Magnetization_sqrt(3)&
               +Magnetization_sqrt(1)*Magnetization_sqrt(3))&
               +k2*Magnetization_sqrt(1)*Magnetization_sqrt(2)*Magnetization_sqrt(3)&
               -Magnetization(1)*H(1)-Magnetization(2)*H(2)-Magnetization(3)*H(3)
Magnetization_record(:,1)=Magnetization
Energy_record(1)=Energy
do i=1,length
if(mod(i,H_load_period)==0)H=H+H_load_increase
Magnetization_sqrt=Magnetization**2
Force(1)=-2*k1*Magnetization(1)*(Magnetization_sqrt(2)+Magnetization_sqrt(3))&
               -2*k2*Magnetization(1)*Magnetization_sqrt(2)*Magnetization_sqrt(3)&
               +H(1)
Force(2)=-2*k1*Magnetization(2)*(Magnetization_sqrt(1)+Magnetization_sqrt(3))&
               -2*k2*Magnetization(2)*Magnetization_sqrt(1)*Magnetization_sqrt(3)&
```

```
                +H(2)
Force(3)=-2*k1*Magnetization(3)*(Magnetization_sqrt(2)+Magnetization_sqrt(1))&
                -2*k2*Magnetization(3)*Magnetization_sqrt(1)*Magnetization_sqrt(2)&
                +H(3)
tmp_Force=Force
mh_tmp=sum(Magnetization*Force)
Force=Force-mh_tmp*Magnetization
Force(1)=Force(1)+p*(Magnetization(2)*tmp_Force(3)-Magnetization(3)*tmp_Force(2))
Force(2)=Force(2)+p*(Magnetization(3)*tmp_Force(1)-Magnetization(1)*tmp_Force(3))
Force(3)=Force(3)+p*(Magnetization(1)*tmp_Force(2)-Magnetization(2)*tmp_Force(1))
Magnetization=Magnetization+Force*time_step
tmp=sqrt(Magnetization(1)**2+Magnetization(2)**2+Magnetization(3)**2)
Magnetization=Magnetization/tmp
Energy=k1*(Magnetization_sqrt(1)*Magnetization_sqrt(2)&
                +Magnetization_sqrt(2)*Magnetization_sqrt(3)&
                +Magnetization_sqrt(1)*Magnetization_sqrt(3))&
                +k2*Magnetization_sqrt(1)*Magnetization_sqrt(2)*Magnetization_sqrt(3)&
                -Magnetization(1)*H(1)-Magnetization(2)*H(2)-Magnetization(3)*H(3)
if(mod(i,record_period)==0)then
Energy_record(i/record_period+1)=Energy
Magnetization_record(:,i/record_period+1)=Magnetization
H_record(:,i/record_period+1)=H
end if
end do
open(unit=10,file="magnetic.dat")
n=length/Record_period+1
write(10,*)   'VARIABLES= "t", "H1", "H2", "H3", "M1", "M2", "M3" '
do j=1,n
       write(10,*) j,H_record(:,j),Magnetization_record(:,j)
end do
close (10)
open(unit=12,file="Energy.dat")
n=length/Record_period+1
do j=1,n
       write(12,*)j,Energy_record(j)
end do
close (12)
end
```

VITA

Yongxin Huang, was born in Sichuan, China. He obtained his B.S. degree in Modern Mechanics at University of Science and Technology of China in 2006. He came to Texas A&M University to pursue his master degree with Dr. Yongmei Jin in fall 2006. The author can be reached at iamhyx@tamu.edu. His contact address is:

Yongxin Huang

Texas A&M University

Department of Aerospace Engineering

H.R. Bright Building, Rm 701, Ross Street

College Station TX 77840