A Grid-Based Bridging Domain Multiple-Scale Method for Computational Nanotechnology

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Abstract. This paper presents an application-level Grid middleware framework to support a bridging domain multi-scale method for numerical modeling and simulation in nanotechnology. The framework considers a multiple-length-scale model by designing specific domain-decomposition and communication algorithms based on Grid computing. The framework is designed to enable researchers to conduct large-scale computing in computational nanotechnology through the use of Grid resources for exploring microscopic physical properties of materials without losing details of nanoscale physical phenomena.

1 Introduction

In the study of nano-materials or nano-devices, a molecular dynamics (MD) model [1] plays an important role. However, many existing MD algorithms have limitations either on length or on time scales due to the lack of enough compute power. Even the most powerful high performance computing (HPC) system is still not powerful enough to perform a complete MD simulation [2]. Therefore, an innovative computational methodology for MD simulations is urgently needed.

Recently-developed concurrent multiscale methods [3] take into consideration of multiple length scales in predicting macroscopic properties. For example, a bridging domain coupling method [4] performs a linkage between the continuum and molecular models. However, if the ratio of mesh size in the continuum domain to the lattice space in the molecular domain is too large, there is a difficult to eliminate a spurious phenomenon in which a nonphysical wave reflection occurs at the interface of different length scales. Therefore, concurrent multiscale methods also require a tremendous computing power. In addition, a small time step (the order of femtosecond) must be selected to meet numerical stability of MD stimulation at the molecular model. Such requirement causes to waste compute time during simulations. A feasible and efficient method is needed to conduct a complete modeling and simulation of large nano systems within long time scales. This requirement stimulates the authors to develop a Grid-based Bridging Domain Multiscale Method (GBDMM).

Grid computing [5-7] enables users to assemble large-scale, geographically-distributed, heterogeneous computational resources together for intensive MD computations. This assemblage is dynamically orchestrated using a set of protocols as well as specialized software referred to as Grid middleware. This coordinated sharing of resources takes place within formal or informal consortia of individuals and/or institutions that are often called Virtual Organizations (VO) [8]. In a similar way, Grid application-specific middleware must be developed for MD related multi-scale methods. We intend to develop a micro/macro coupling method and Grid application middleware for multiscale computation in nano-science and technology.

Section 2 reviews the bridging domain coupling method and describes its extensions in the GBDMM. Section 3 addresses domain-decomposition and communication algorithms for the GBDMM. Section 4 presents the framework of Grid nano-middleware for GBDMM's implementation.

2 Grid-Enhanced Bridging Domain Multiscale Method (GBDMM)

2.1 Bridging Domain Coupling Method

The bridging domain coupling method contains a continuum domain, Ω^C , which is overlapped with a molecular domain, Ω^M , through a bridging domain, Ω^{int} (Fig. 1). The scaling of the molecular and continuum Hamiltonians is performed in the bridging domain. The Lagrange multiplier method is used to conjunct the molecular domain with the continuum domain via constraint condition(s), $\mathbf{u}^C(\mathbf{X}_I, t) - \mathbf{u}_I^M(t) = 0$, where $\mathbf{u}$ is the displacement. The total Hamiltonian of the system can be written as

$$H = \int_{\Omega^C} \beta(\mathbf{X}) (\mathbf{K}^C + \mathbf{U}^C) d\Omega^C + \sum_I (1 - \beta(\mathbf{X}_I)) (\mathbf{K}_I^M + \mathbf{U}_I^M) + \sum_{I \in \Omega^{\text{int}}} \lambda(\mathbf{X}_I) (\mathbf{u}^C(\mathbf{X}_I, t) - \mathbf{u}_I^M(t)) \quad (1)$$

where $\beta(\mathbf{X})$ equals zero in Ω^M and unity in Ω^C except the bridging domain. Within the bridging domain, Ω^{int} , it smoothly varies from zero to one. If an irregular bridging domain is considered, a nonlinear function $\beta(\mathbf{X})$ can be introduced. The function can be derived from a signed distance function, or defined by radial basis functions from a set of points. K and U are the kinetic and potential energies. $\lambda(\mathbf{X})$ is a Lagrange multiplier field that can be obtained from the finite element approximation as shown in Fig. 1. Based on the classical Hamiltonian mechanics, the discrete equations of Equation (1) can be expressed as

Fig. 1. The bridging domain coupling model for a graphite sheet

Fig. 2. Length scales covered in the BDMM

$$\begin{aligned}\bar{M}_I \ddot{u}_I^C &= \mathbf{f}_I^{\text{ext}C} - \mathbf{f}_I^{\text{int}C} - \mathbf{f}_I^{\text{LC}} & \text{in } \Omega^C, \\ \bar{m}_I \ddot{u}_I^M &= \mathbf{f}_I^{\text{ext}M} - \mathbf{f}_I^{\text{int}M} - \mathbf{f}_I^{\text{LM}} & \text{in } \Omega^M\end{aligned}\quad (2)$$

where $\bar{M}_I$ and $\bar{m}_I$ are the modified nodal and atom masses; $\mathbf{f}_I^{\text{ext}}$ and $\mathbf{f}_I^{\text{int}}$ are the external and internal forces, independently; $\mathbf{f}_I^L$ is the force due to constraints in the bridging domain. During simulation, velocities are obtained independently in the continuum and molecular domains from Equation (2) without the consideration of constraint forces. Constraint conditions are then used to calculate the Lagrange multipliers. Finally, the constraint forces in Equation (2) are used to correct the nodal/atom velocities in the bridging domain, thus eliminating the wave reflection automatically.

2.2 Multiscale Considerations in GBDM

Based on the bridging domain coupling method, we proposed a Bridging Domain Multiscale Method (BDMM), which bridges from nanoscale to microscale to macroscale (Fig. 2). A bridging domain multiscale model contains a macro-scale domain ($\sim 10^{-3}$ m) as a linear elasticity domain in which linear finite element methods (FEM) can be used. The material properties can be obtained from the Representative Volume Element (RVE) technique with molecular dynamics simulation. The BDMM embeds a micro-scale domain ($\sim 10^{-6}$ m) in the macro-scale domain. It models physical behaviors of materials using either nonlinear FEM [9] or extended FEM [10] (if crack propagation is considered at the microscale). Furthermore, a quasi-continuum technique [11] is implemented with the FE methods at the microscale, so that the constitutive equations can be constructed based on the atomic level energy. A sub-domain in a microscale domain can be treated as a nanoscale (molecular) domain ($\sim 10^{-9}$ m) in which molecular dynamics is employed. The BDMM couples various scales without grading down mesh sizes. Such coupling leads to a straightforward implementation of different time steps via a multiple-time-step algorithm.

3 Domain Decomposition and Communication Algorithms

To perform simulations using GBDMM, an efficient algorithm of domain decomposition must be developed. An entire physical domain with multiple length scales specified can be hierarchically divided into multiple sub-domains. The first generation (FG) sub-domains, such as Ω_{01}^M (see Fig3), are generated based on variation in length scales. These sub-domains are allocated on heterogeneous Grid computing resources. Such first-generational domain decomposition is designed to avoid high network latency, and hence produce a loosely-networked computation on Grids.

Each FG sub-domain can further be divided into a number of second generation (SG) sub-domains being parallel-processed on different computational nodes within a Grid resource. A bridging sub-domain is only shared between two SG sub-domains, which belong to two different length scales, respectively. Although one SG sub-domain can be overlapped with two or more SG sub-domains, the bridging sub-domains are not overlapped with each other.

There are two types of communications in the GBDMM (see Fig. 4). The inter-domain communication among the SG sub-domains takes place within an inter-connection within a Grid resource, performing a traditional parallel computation. This computation guarantees the consistency and integrity of SG sub-domains and boundary information for solving the governing equations of atom motions. The procedure for solving equations of atom motion on each Grid cluster is independent. After solving the equations at each time step, communication takes place between two clusters. The bridging coupling techniques are then applied to correct the trial velocities of nodes or atoms in each bridging sub-domain independently.

For example, a simple GBDMM have two sub-domains Ω_A and Ω_B in the molecular domain, allocated to a single Grid resource (often a computing cluster), and Ω_C and Ω_D in the continuum domain, allocated to another Grid resource. The communication between the group of Ω_A and Ω_B , and the group of Ω_C and Ω_D takes place on networks in a Grid environment. Ω_A and Ω_B share an atom E . Bridging domains Ω_A^{int} and Ω_B^{int} perform energy and force calculations. The results from Ω_B^{int} are used to calculate the body potential functions and inter-atomic forces in Ω_A , since Ω_A and Ω_B^{int} share with same atoms. The size of bridging domains depends on the selected potential functions, especially the cutoff distance for Van der Waals potential functions.

The continuum sub-domains, Ω_C and Ω_D share a boundary node F as shown in Fig. 4. F^C and F^D represent the same node F in different sub-domains. Unlike inter-domain communications (which do not require bridging domains), the communication between continuum sub-domains, Ω_C and Ω_D exchange internal forces of boundary nodes through the networks among Grid resources. For instance, the internal force of node F^C , calculated in the sub-domain Ω_C is fetched to the sub-domain Ω_D to form an external force on the node of F^D , but in an opposite direction. A similar procedure is conducted to pass the internal force of node F^D as the negatively external force of node F^C . Therefore, the motions of node F , updated from Ω_C and Ω_D are consistent.

Fig. 3. Domain decomposition for the GBDMM method

Fig. 4. A demonstration for domain communications

After equations of motion are solved independently on each cluster, bridging-domain communication takes place independently in each bridging sub-domain, such as Ω_{AC}^B and Ω_{BD}^B . For instance, the trial velocities of atoms in Ω_{BD}^B of Ω_B are transferred to Ω_D , while the trial velocities of nodes in Ω_{BD}^B of Ω_D are transferred to Ω_B . The bridging domain coupling technique is then applied to correct the trial velocities of atoms in Ω_{BD}^B of Ω_B as well as in Ω_{BD}^B of Ω_D , respectively on each mater nodes.

4 Framework of Grid Middleware for GBDMM Implementation

An application-level Grid middleware framework is designed (in Fig. 5) to enable a GBDMM implementation. In this framework, middleware manages available computing resources, schedules decomposed domains to appropriate Grid resources (i.e. clusters). It contains (1) a task scheduling advisor (TSA) that takes the result of domain decomposition as input to produce scheduling plans and achieve high-performance simulation through load-balancing; and (2) an information broker (IB) that leverages Grid information services to provide the task scheduling advisor with a resource discovery query functions [12].

The framework is centered on the TSA that is used to schedule sub-domains to an appropriate set of Grid resources discovered to achieve optimal performance: tasks are allocated to balance computations across the available set of resources. The sub-domains are converted to the tasks that are placed in Grid-resource queues. The TSA is designed to achieve high levels of performance by balancing tasks across available resources. It determines the correspondence between tasks and the available Grid resources. Within the TSA, several static scheduling strategies [13] such as Min-min and Max-min have been implemented. The fine granularity of the domain decomposition in GBDMM is designed to achieve high level parallelism. Static scheduling

strategies are developed to assign tasks based on computational intensity information for each sub-domain, as well as the variability in the computing capacity of each Grid resource. The workflow of the nano-middleware enhanced GBDMM with Grid computing is shown as Fig. 6.

Fig. 5. The Grid nano-middleware architecture. Note: Globus is a software project, the purpose of which is to develop protocols and services for computational grids. Condor is a high throughput computing system

Fig. 6. The work flow of GBDMM

TSA is used to schedule sub-domains to an appropriate set of Grid resources discovered to achieve optimal performance: tasks are allocated in a way that balances computations across the available selection of resources. The sub-domains information is converted to the tasks that are placed in Grid-resource queues. The TSA is designed to achieve high levels of performance by balancing tasks across available resources. It determines the correspondence between tasks and the available Grid resources. The TSA deploys both static and dynamic scheduling, planning to operate static and dynamic scheduling on tasks upon the computing recourse available. The TSA dynamically facilitate the swap of tasks between computing resources according to a dynamic performance evaluation. The fine granularity of the domain decomposition in GBDMM is carefully design to achieve high level parallelism. Static scheduling strategies are developed to assign tasks based on computational intensity information for each sub-domain, as well as the variability in the computing capacity of each Grid resource.

Since Grid resources is very a complex set (resources and network complexities), an IB is needed to perform a self-organized-resource discovery. The IB for the nano-middleware is designed based on a self-organized grouping (SOG) method that manages the Grid complexity. Therefore, the IB contains three strategies: 1) to control resource heterogeneity during a certain period of time; 2) to capture resource dynamics through a publishing mechanism and aggregating mechanism that handles resource dynamically; (3) to enable the assemblage of large number of resources for applications across VO boundaries.

The developed information broker is based on a self-organized resource discovery method. It is well known that currently, the Grid represents an extremely complex distributed computing environment for developing applications because: 1) Grid resources (e.g., CPU, network, storage, and special-purpose instrument) are heterogeneous; 2) Grid resources are dynamic, and they tend to have faults that may not be predictable; 3) Grids are often distributed across security domains with large number of resources involved. Due to this complexity, it has been a great challenge for developing efficient methods for Grid resource discovery that refers to the process of locating satisfactory resources based on user requests. Grid resource discovery must handle the search for desirable subsets of large number of accessible resources, the status and availability of which dynamically change.

The workflow of the nano-middleware enhanced GBDMM with Grid computing is shown as Fig. 6. The workflow demonstrates the integration of computational nanotechnology and computer science in this multi-disciplinary project.

5 Conclusion and Future Work

The GBDMM is an extension of the bridging domain coupling method that allows multiple length/time scales to be treated. The GBDMM's domain decomposition and communication are designed to be applicable to distributed Grid resources. The Grid nano-application-middleware includes a task scheduling advisor and an information broker. This middleware enables the GBDM to schedule resources, distribute tasks, and achieve load balancing. Our ongoing work is to implement and apply GBDMM to study mechanical properties of nanostructured materials.

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