JST Basic Research Programs

C R E S T

(Core Research for Evolutional Science and Technology)

Annual Report for Research Work in the fiscal year 2005

Research Area :

High Performance Computing for Multi-scale and Multi-physics Phenomena

Research Theme

Hybrid simulations of complex liquid-solid interfaces at nano, meso, and micro range-scales

Name of Research Director, Belonging and Title:

Dr. Shuji OGATA, Nagoya Institute of Technology, Professor

§1. Outline of Research Work

In the present project, we will develop concurrent, hybrid simulation codes for solid-fluid interfacial phenomena at both the nano-to-meso and the micro-to-meso scale-lengths, and will optimize the codes for concurrent usage of the world-wide supercomputers with the grid computation technologies. The hybrid simulation codes will be applied directly to various important phenomena in materials such as the MEMS, the fuel cell, and the catalytic gas-converter.

For the nano-to-meso-scale phenomena, we have developed the simulation code by hybridizing the quantum density-functional theory (DFT) and the classical molecular dynamics (MD) with the buffered-cluster method proposed recently by us. In the hybrid simulation code, an algorithm for adaptive, dynamic selection of the quantum region has been implemented, whose performance has been investigated and improved through simulation runs about the atomic-scale friction of Si-based meso-scale components in MEMS. Also we have compared existing computation schemes for fast computation of atomistic, chemical reactions at complex fluid-solid interfaces, to select a proper scheme to be implemented.

For the micro-to-meso-scale phenomena, we have investigated the proper scale-range to be covered with the lattice Boltzmann method for the fluid dynamics, and have considered algorithms to incorporate atomic-scale material properties at the fluid-solid interface in the lattice Boltzmann method. Those considerations will be utilized in developing hybrid simulation code for the fluid-solid interfaces at the micro-to-meso scales.

Our hybrid DFT-MD simulation code for the nano-to-meso-scale phenomena has been re-implemented with the grid middleware Ninf-G for large-scale, long-time simulation on the world-wide computation grid. The hybrid DFT-MD simulation using several supercomputers in both Japan and USA has been demonstrated successfully.

§2. Content of Research Work

For further advancement of important materials such as the MEMS, the catalytic gas-converter, and the fuel cell, we will develop multi-scale, hybrid simulation codes for complex physicochemical processes near the fluid-solid interfaces. The hybrid simulation codes in the present project will be classified in two types: one type is appropriate to nano-to-meso-scale phenomena and composed of atomistic computation methods, while another type is to micro-to-meso-scale phenomena and composed mainly of coarse-graining methods. The present project has advanced in following points.

1. Approach appropriate to nano-to-meso length-scale

Using the buffered-cluster method proposed by us for the proper mechanical coupling of the classical atomistic region and the quantum electronic region, we have developted concurrent, hybrid quantum-classical simulation code. In the hybrid simulation code, the electronic density-functional theory is adopted for the quantum region, while the molecular dynamics with a semi-empirical inter-atomic potential for the classical region. To minimize the total computation cost, we have proposed and implemented an algorithm to expand and divide the quantum region adaptively as the simulation proceeds. The hybrid simulation code has been applied successfully to study the atomic-scale friction of nano-scaled components of a Si-based material in MEMS, which has clarified the outstanding problems for further sophistication of the hybrid simulation code. The parallel efficiency of the real-space density-functional-theory code has been improved substantially by adaptively varying the boundaries of the data points in real space for the eigenfunctions and the potentials for the valence electrons.

We have analyzed the characteristics and the capabilities of the charge-equilibration-type inter-atomic potential to incorporate chemical reactions in the classical inter-atomic potential that will be used to simulate complex reaction processes at fluid-solid interfaces in inhomogeneous materials with meso-scale structures. We have also investigated possible adaptation of more elementary approaches to incorporate reaction processes at the fluid-solid interfaces.

2. Approach appropriate to micro-to-meso length-scale

The lattice Boltzmann method is suited to describe fluid with dynamic, complex boundary condition since it is controlled with the local scattering terms. The lattice Boltzmann method will therefore play important roles in our project. We have investigated scale-range for proper usage of the lattice Boltzmann method and have considered schemes to incorporate physical properties at the

atomic-scales in the lattice Boltzmann method. Key issues to be solved have been clarified also.

Since the characteristic space-time scales differ significantly between the fluid and the solid descriptions, we have to coarsen the atomistic system in the solid for better scale-match. We have planed to adopt the coarse-grained particles method to obtain the stiffness matrix of the virtual coarse-grained points set in the coarse-graining region in the solid material through the local statistical averages of the atomistic phonons, which will be used to simulate dynamic oscillatory behavior of the solid materials. We have started to implement the coarse-grained particles method. The water generation process in the fuel cell is one of the target physiochemical processes in our project. Considering this, we have started to investigate proper treatment of thermal fluid with vapor-liquid coexistence at complex fluid-solid interfaces.

3. Application of hybrid simulation scheme to grid computation environment

The hybrid simulation codes to be developed in the present project will be composed of computation methods with varying orders of computation operations. Such an inhomogeneity in computation cost is a fundamental characteristic of the multi-scale approach. The hybrid simulation code may be performed efficiently on the computation grid.

We have investigated future fundamental technologies required for robust performance of the hybrid simulation code at large scales. The hybrid quantum-classical simulation code developed originally by the Nagoya Inst. Tech. group has been re-implemented using the grid-middleware Ninf-G developed by the AIST group. We have successfully performed 20days continuous-run of the hybrid simulation code on the Japan-US computation grid constructed with eight supercomputers in total. We have shown that the novel programming style that mixes Grid-Remote-Procedure-Call and MPI enables long-time simulation in the grid computation environment. Our grid-enabled hybrid simulation code has several important features crucial to robust running in the grid environment: dynamic usage of reserved computers, automatic re-allocation of reserved computers at a machine trouble, etc.

§3. Formation of Research Work

Research Director: Prof. Shuji Ogata, Nagoya Institute of Technology

Research Themes:

Development of Hybrid Quantum-Classical Simulation Code for Solid

Development of Hybrid Fluid-Solid Simulation Scheme using Lattice Boltzmann Method

Main Research Collaborator: Dr. Shiaki Hyodo, Toyota Central R&D Labs., Inc.

Research Themes:

Development of Computation Scheme for Complex Fluid-Solid Interfaces

Development of Computation Scheme for Thermal Fluid with Vapor-Liquid Coexistence

Main Research Collaborator: Dr. Yoshio Tanaka, National Institute of Advanced Industrial Science and Technology

Research Theme:

Development of Grid-Enabled Hybrid Quantum-Classical Simulation Code

§4. Publication of Research Results

(4－1) Publication of Thesis (The original Work)

① Number of Publications (0 papers in Domestic journals, 0 papers in International journals)

(4－2) Patent Application

① Cumulative Number

1) Patent Applications in the fiscal year 2005 (Domestic- 0 Cases, Oversea- 0 Cases)

2) Cumulative number of Patent Applications for the research period of CREST (Domestic- 0 Cases, Oversea- 0 Cases)

3) Details for this fiscal year

a) Domestic Application (0 cases)

b) Oversea Application (0 Cases)