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 2006

Research Area :

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

Research Theme:

Hybrid Simulations of Complex Liquid-Solid Interfaces at Nano, Neso, 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 advance elementary simulation codes for large-scale simulation of solid and fluid systems with the conventional hierarchical techniques, and will develop concurrent hybrid codes by coupling them seamlessly to either scale up from nanometer or scale down from micrometer the spatial range of target systems. The target systems include dynamically moving and deforming solid-fluid interfaces with chemical reactions in important engineering materials as the MEMS, the catalytic gas-converter, and the fuel cell.

As for the development of the codes for nano-scale systems, in this fiscal year, we have improved the dynamic re-allocation algorithm for the quantum regions in the hybrid quantum-classical simulation scheme. To demonstrate its performance, we have performed hybrid quantum-classical simulation of the atomic-scale friction of nano-scaled components and the SIMOX processes in the silicon-on-insulator technology. Furthermore, for simulation of the chemical reactions in stressed materials, we have constructed a novel code by combining the hybrid quantum-classical method and the nudged elastic band (NEB) method. The NEB-hybrid quantum-classical code has been applied to calculation of the diffusion barrier of an oxygen atom in stressed Si crystal. Hierarchical, simple modeling of the chemical reactions is essential for long-time simulation of realistic complex interfaces. We have therefore considered applicability of the environment dependent, variable-charge inter-atomic potentials.

As for the development of the codes for micro-to-meso-scale systems, in this fiscal year, we have improved the lattice Boltzmann code by taking into account the hydrophilic/hydrophobic character of the container surface and by introducing an improved scattering function that is useful in situations with relatively high Knudsen numbers, to apply the code to two-phase flows in complex porous media. On the other hand, we have improved the coarse-grained particle method to coarse-grain a multi-component atomistic system to any desired scale in nano- to micro-meter range. For advanced coupling of fluid and solid systems, we have developed a novel algorithm to smooth out a discrete solid-fluid interface. A prototype code that combines the lattice Boltzmann method for fluid and the coarse-grained particle method for solid is constructed.

As for the realization of concurrent hybrid simulation on Grid, in this fiscal year, we have Grid-enabled the NEB-hybrid quantum-classical code with the Grid middleware Ninf-G developed originally in AIST. In addition, we have developed a Grid scheduling module to balance the computation loads of the multiple quantum regions on different compute-sites. Through demonstration runs on a Japan-US supercomputer Grid, we have verified utility of the present code and the module and have clarified the points needs be improved.

§2. Content of Research Work

1. Development of codes for nano-scale systems

1.1 Concurrent hybrid approach

We have developed the hybrid quantum-classical simulation code by coupling the density-functional theory (=quantum) and the molecular dynamics method (=classical), in which a target system is partitioned in real space into regions and either the quantum or the classical method is applied to each region. To develop smart, dynamic re-allocation algorithms of the quantum regions, we have performed hybrid quantum-classical simulation of the atomic-scale friction of nano-scale components (see, Fig. 1) and the high-velocity implantation of oxygen atoms into a Si substrate relating to the SIMOX technology in silicon industries. Understanding the stress dependence of reaction barrier energies is essential for designing advanced nano-devices. We have therefore combined the nudged elastic band (NEB) method and the hybrid quantum-classical method to calculate the minimum energy path and the barrier energy. In the combined code, frequencies of the quantum, the classical, and the NEB calculations are optimized to minimize the total computation time. As a demonstration, we have applied the code to investigate the fundamental issue of calculating the stress dependent oxygen diffusion barrier in Si crystal, to find a rather strong dependence.

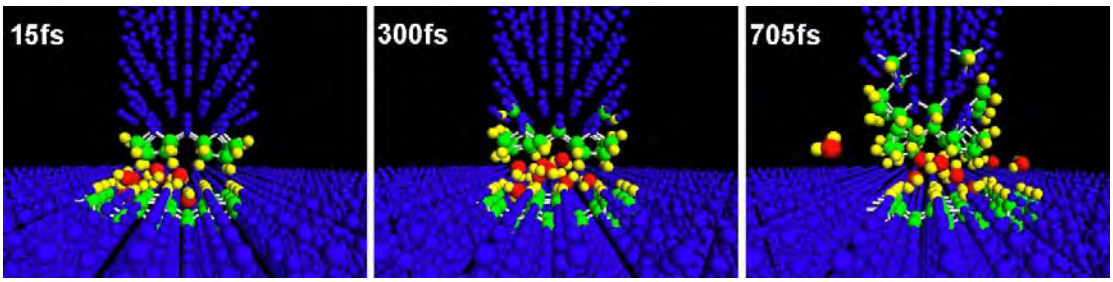

Fig. 1. Hybrid quantum-classical simulation of friction of nano-scale components. A water droplet is adsorbed initially at the Si-tip. Te quantum atoms are highlighted (Si=green, H=yellow, O=red).

1.2 Hierarchical treatment of chemical reactions

Approximate, but fast calculation of the chemical reactions is necessary to perform long-time simulation of realistic, complex solid-fluid interfaces. As one of the promising approaches, we have adopted the environment dependent, variable-charge inter-atomic potential. The γ-alumina is an important material with ionic bonding character, which forms complex porous structures and functions as a support material for a catalyst. To investigate the stress dependence of the atomic diffusion barrier in γ-alumina, we have applied the variable-charge inter-atomic potential to the classical region in the NEB-hybrid quantum-classical method. In addition, we have proposed an accurate time-integration algorithm for interacting classical rigid molecules.

2. Development of codes for micro-to-meso-scale systems

2.1 Advancement of fluid simulation code with hierarchical treatment

We have improved fluid simulation code with the lattice Boltzmann method (LBM) by taking into account the hydrophilic/hydrophobic character of the surface of a container (see, Fig. 2) and by introducing an improved scattering function that is useful in particular for small-scale systems (*i.e.*, Knudsen number ~10), to apply the code to a two-phase flow in a complex porous medium. In addition, we have prepared a prototype code to investigate mutual interaction of the turbulent flow and the small bodies distributed in it.

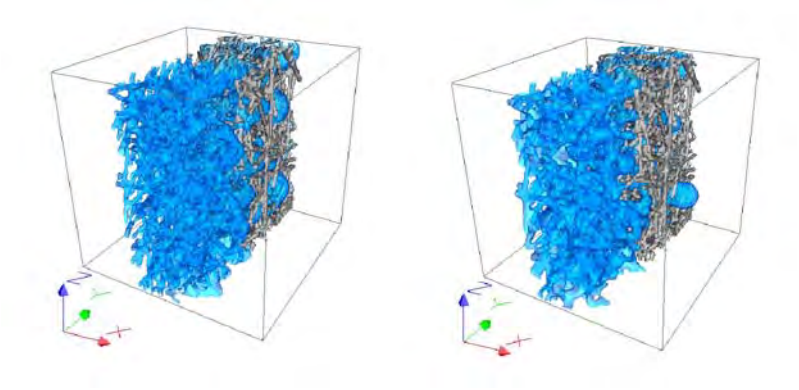

Fig. 2. A two-phase (vapor and liquid) flow in a fibered medium (left, for hydrophilic surface; right, for hydrophobic surface) calculated with LBM.

2.2 Concurrent coupling of fluid and coarse-grained solid

We have improved the coarse-grained particle (CGP) method to coarse-grain an atomistic system in solid phase. The improvements include: extension to multi-component systems and recursive renormalization to any desired scale in nano- to micro-meter range. We have confirmed high accuracies of the CGP method with respect to the elastic moduli, the phonon dispersion relation, and the wave packet propagation.

For accurate coupling of fluid and solid, we have proposed a two-step algorithm to construct a smooth solid-fluid interface from its discrete data by modifying the resetting process in the level-set method. We have confirmed that the LBM combined with the present smoothing method, gives accurate drag coefficients of a solid spherical body due to a flow, even for the case of low-resolution data of the fluid-solid interface.

We have developed a prototype code that couples the LBM and the CGP method. As a simplest example of the solid system, we have considered a pole (2D) composed of Ar atoms with its bottom fixed, which is immersed in a flow described with the LBM. To bridge the spatiotemporal scale-gap between the fluid and the solid, the pole system is coarse-grained with the CGP method to

the mesh size of the LBM. The Stokes-type drag force on the coarse-grained particle and its reaction to the fluid are used to couple the fluid and the solid systems.

3. Realization of concurrent hybrid simulation on Grid

We have analyzed performance of the large-scale hybrid quantum-classical simulation of the SIMOX process performed on a Japan-US supercomputer Grid (~1000CPU's) at the end of the last fiscal year. Separately, we have Grid-enabled our NEB-hybrid quantum-classical code with the Grid middleware Ninf-G developed originally in AIST (see, Fig. 3). In addition, a Grid scheduling module that balances the computation loads of the multiple quantum regions on different compute-sites is produced. Through demonstration runs on a Japan-US Grid, we have verified utility of the present code and the module and have clarified the points to be improved.

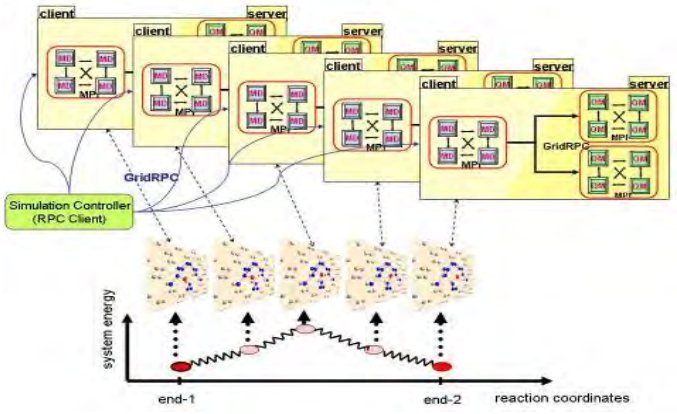

Fig. 3. Schematic view of the NEB-hybrid quantum-classical simulation on Grid.

§3. Formation of Research Work

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

Research Themes:

Development of Hybrid Quantum-Classical Simulation Code

Development of Hybrid Fluid-Solid Simulation Code

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

Research Themes:

Hierarchical Computation Scheme for Complex Fluid-Solid Interfaces

Hierarchical Computation Scheme for Complex Chemical Reactions

Main Research Collaborator: Prof. Kazuhiko Suga, Osaka Prefecture University

Research Themes:

Simulation of Meso-Macro Thermo-Fluid Phenomena in Complex Geometry

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

Research Theme:

Development of Grid-Enabled Hybrid Simulation Codes

§4. Publication of Research Results

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

① Number of Publications (1 times-Domestic, 3 times-International)

② Detailed Information of Thesis

1. Hiroshi Takemiya, Yoshio Tanaka, Hidemoto Nakada, and SatoshiSekiguchi: Implementation of Large-scale Long-run Grid Applications with Varying Problem Size, IPSJ Trans. of Computing Systems, Vol. 47, No. SIG18, pp. 31-43, 2006 (in Japanese).

2. Yoshio Tanaka, Hiroshi Takemiya, Hidemoto Nakada, and Satoshi Sekiguchi: Design and Implementation of Flexible, Robust and Efficient Grid-enabled Hybrid QM/MD Simulation, Computational Methods in Science and Technology, Poznan Supercomputing and Networking Center, Vol. 12, No. 1, pp. 79-87, 2006.

3. Hiroshi Takemiya, Yoshio Tanaka, Satoshi Sekiguchi, Shuji Ogata, Aiichiro Nakano, Rajiv K. Kalia, and Priya Vashishta: Sustainable Adaptive Grid Supercomputing: Multiscale Simulation of Semiconductor Processing Across the Pacific, Proceedings CD-ROM of Supercomputing2006, pp.11, 2006.

4. Shuji Ogata and Takahisa Kouno: Hybrid Simulations for Designing of Nano-Interfacial Structures, Solid State Phenomena, Vol. 127, pp. 57-62, 2007.

（4－2） Patent Application

① Cumulative Number

1) Patent Applications in the fiscal year 2006 (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)