Large Scale Simulations in the Atomic Energy Research

Consortium Representative

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In 2002, the Atomic Energy Society of Japan (AESJ) founded the Division of Computational Science and Technology, which aims for promoting the exchange of broad range of knowledge and experiences of the computational technologies in the atomic energy field. This triggered off the establishment of a research committee on "the Large Scale Simulation" in AESJ, which is also acting as a consortium for the simulation research using the Earth Simulator in the atomic energy field. In the beginning of 2003, the consortium selected nine research topics for applying for the 2003's collaboration projects with the Earth Simulator Center. This report summarizes the research activities of these projects.

1. Consortium for Large Scale Simulations in the Atomic Energy Research Field

In the history of neutron physics, the numerical experiment has played an important role for its advancements. Also, the computational technology has been an indispensable tool for solving various engineering problems in the nuclear industry, such as the reactor core design, thermal hydraulics, safety design, structural design, etc. It is said that "Design by Analysis" and/or "Computer-Aided R&D (CAR&D)" will be the crucial technology for the future developments in this field. With these view, in 2002, the Atomic Energy Society of Japan founded the Division of Computational Science and Technology, which aims for promoting the exchange of broad range of knowledge and experiences of the computational technologies in the atomic energy field. The Division of Computational Science and Technology triggered off the establishment of a research committee on "the Large Scale Simulation" in AESJ, which is also acting as a consortium for the simulation research using the Earth Simulator in the atomic energy field. The activities of the consortium are to discuss the candidate research projects for using the Earth Simulator, exchange the software optimization experiences and mutually evaluate the research outputs, and so on.

In the beginning of 2003, nine research topics were selected by the consortium for applying for the collaboration projects with the Earth Simulator Center, and all of them were approved. In the next section, research activities of these projects are summarized.

2. Summary of research activities

(Name in the bracket is the group representative.)

2.1. Large-Scale Numerical Simulations of Multiphase Flow Behavior in an Advanced Light-Water Reactor Core (Kazuyuki Takase, Japan Atomic Energy Research Institute)

The objective of the research is to establish the thermal design procedure of the reduced-moderation water reactor (RMWR) core with a large-scale simulation, without performing real scale experiments. Large-scale simulations with the Earth Simulator for the flow configuration of water and vapor around each fuel rod surface, which is deeply related to the feasibility and safety of a reactor core, are performed and the two-phase flow structure in the RMWR core is clarified quantitatively. Moreover, since the coolant is strongly influenced of flow disturbance due to the spacer installed in several axial positions, direct numerical simulations are carried out to investigate turbulent structures around each fuel rod surface under the conditions of single-phase flow and Reynolds number of 78,000.

2.2. First Principles Molecular Dynamics Simulation of Solution (Masaru Hirata, Japan Atomic Energy Research Institute)

Preliminary results concerning the water-methanol mixture and the DNA electron/proton transfer using a first principles molecular dynamics method are obtained. In the first case, it is demonstrated that the shear viscosity of the mixture is reproducible roughly from ~100 ps simulations. In the second project, instead, thermal fluctuations are shown to be essential for the spin localization on guanine bases.

2.3. Direct Numerical Simulations of Fundamental Turbulent Flows with the Largest Grid Numbers in the World and its Application of Modeling for Engineering Turbulent Flows (Chuichi Arakawa, University of Tokyo / Japan Atomic Energy Research Institute)

Databases of incompressible turbulence obtained by high-resolution direct numerical simulations (DNSs) with the number of grid points up to 40,963 are systematically analyzed on the Earth Simulator. The DNSs consist of two groups; one is with $K_{max}\eta = 1$ and the Taylor micro scale Reynolds number $R_\lambda = 167–1131$, while the other is with $K_{max}\eta = 2$ and $R_\lambda = 94–675$, where K_{max} is the maximum wave number and η the Kolmogorov length scale. Reynolds number dependence of various turbulence statistics, which include higher-order moments of velocity derivatives, the energy spectra in the near-dissipation wavenumber range, pressure spectra, are investigated. An engineering application is also studied. The physical mechanisms associated with broadband tip vortex noise caused by rotating wind turbines are investigated. The flow and acoustic field around a wind turbine blade is simulated using compressible Large Eddy simulation and direct noise simulation, with emphasis on the blade tip region. The far field aerodynamic noise is modeled using acoustic analogy. Aerodynamic performance and acoustic emissions are predicted for the actual tip shape and an ogee type tip shape. For frequencies above 4 kHz a decrease in sound pressure level by 5 dB is observed for the ogee type tip shape. It is hoped that the simulation results will contribute towards designing new wind turbine blades for reduced noise emission.

2.4. Research on Structure Formation of Plasmas Dominated by Multiple Hierarchical Dynamics (Yasuaki Kishimoto, Japan Atomic Energy Research Institute)

Large scale simulations with high resolutions for two major subjects are performed, i.e. (1) micro-scale electron temperature gradient (ETG) driven turbulence simulations in tokamak plasma using GT3D, a gyro-kinetic toroidal particle code, (2) lightning simulations for high pressure neon gas that is suffered from constant electrostatic field using EPIC3D, a new version of 3-dimensional relativistic particle code EM3D-EB which includes complex atomic and relaxation processes. In the turbulent transport simulation, a new prominent turbulent structure due to micro-scale ETG mode in reversed magnetic shear plasmas, which reveals so-called internal transport barriers, is found. In the lightning simulation, streamer and micro-scale sprite formation are successfully reproduced and an underlying physical process, which leads to fast time scale avalanche events, is resolved.

2.5. Development of Fluid Fluid-Structure Interaction program for the Mercury Target (Chuichi Arakawa, University of Tokyo / Japan Atomic Energy Research Institute)

The liquid mercury target, which is a neutron scattering experiment facility, is planed to receive MW class proton pulse beam. Under such condition, high density heat is released and consequently strong pressure wave is generated. Thus the pressure wave propagates through mercury and reflects on the container of target made of hard stainless steel. Then it is anticipated that an erosion of the wall might be caused by the cavitation. A simulation of the interaction between the pressure wave propagation of the liquid mercury and the wall deformation is carried out in order to investigate the possibility of the cavitation in the mercury target. In the project of the year 2003, the fluid-structure interaction program is developed and the fine meshes of the mercury target is generated. Then this large scale model is applied to simulate the interaction between the pressure wave propagation and the wall deformation.

2.6. Large-scale Numerical Simulations for Superconducting Neutron Detector using MgB2 and Half Quantized Vortices in d-dot Array (Masahiko Machida, Japan Atomic Energy Research Institute)

Large-scale numerical simulations for superconducting neutron detector using MgB2 by solving the time-dependent Ginzburg-Landau equation coupled with the Maxwell and the heat diffusion equation are performed. The simulation results revealed that there is a threshold wire width for the neutron detection. On the other hand, by solving the time-dependent Ginzburg-Landau equation considering the coupling between s and d-wave superconductors at the interface, patterns composed of several half quantized vortices seen in d-dot array embedded in the conventional superconductor matrix are investigated. With increasing the d-dot size, it is found that possible patterns of half quantized vortices in a d-dot change from 2 diagonal patterns to 6 patterns including non-diagonal ones. These 6 patterns enable to create novel frustrated systems.

2.7. Electronic and Atomistic Simulations on the Irradiation Induced Property Changes and Fracture in Materials (Hideo Kaburaki, Japan Atomic Energy Research Institute)

Electronic and atomistic simulations are performed to study the fundamental mechanical properties of metals with reference to irradiation, ductile-to-brittle transition, and fracture. For the electronic simulations, the VASP (Vienna ab-initio simulation package) code is tuned on the Earth Simulator and its performance is measured. The purpose of this simulation is to determine the Peierls stress of a screw dislocation in BCC Mo, whose core structures have not yet been clearly determined, and, finally, to understand the hydrogen embrittlement mechanism. For the atomistic simulations, the molecular dynamics code is developed to introduce the layered link cell method to accelerate the vector calculations for the large scale simulations on the Earth Simulator. The purpose of this simulation is to understand the crack-tip microstructures in the fracture process and its interaction processes with the irradiation induced defects and grain boundaries.

2.8. First-principles Molecular Dynamics Simulation of Oxide Layers for Radiation-Tolerant SiC Devices (Atsumi Miyashita, Japan Atomic Energy Research Institute)

Development of the formation technology of the SiO2/SiC interface of high channel mobility and a high dielectric breakdown voltage is indispensable to improve SiC metal-oxide-semiconductor field effects transistors (MOSFETs) performance. Then, the relation between a physical structure and the electric characteristic of an interfacial defect is clarified, and the oxide film growth mechanism on the surface of the SiC crystal is clarified by generating the interfacial defect structure by using a first-principle molecular dynamics method, and calculating an energy level and the electric charge state, etc. When the heating/rapid cooling calculation is done by using the small-scale interface model of about 100 atoms, it is understood that the SiO2 layer becomes amorphous when the heating temperature is 3000 K, heating time 3.0 ps and –1000 K/ps at the speed of rapid cooling. In this condition, the entire free energy has become small most, too. It tends to take the SiO2 layer part apart in a high temperature.

2.9. Large-Scale Simulation of Groundwater Flow and Radioactive Nuclide Transportation (Hiroshi Okuda, University of Tokyo)

Simulation codes for radio nuclide transportation and groundwater flow were optimized on the Earth Simulator and large-scale simulations for more than 10^6 years on the models of real disposal sites are conducted. The results of the simulations will be helpful for making decision of final disposal sites. Also, since in this area of research, there are various kinds of simulation codes, an infrastructure for large-scale simulations, which consists of common and fundamental capabilities, such as parallel I/O for large-scale data sets, parallel visualization and parallel linear solvers, is developed. This infrastructure will be useful for optimization of developing codes and new codes on the Earth Simulator. The VR code, a repository performance assessment code with multiple canister model, is ported and optimized to the Earth Simulator in this year. The VR code is parallelized and vectorized so that vectorization ratio of 95.97%, and parallelization ratio of 99.35% are achieved. The demonstration calculation with one-thousand canister model is performed.