

Creating future of solid Earth science with high performance computing (HPC): Introduction

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In Japan, high performance computing (HPC) had been driven by computer science community (HPC developer). However, recently, computational science community (HPC user) has been expected to contribute to the planning and development of the next generation HPC showing the scientific and/or social issues to be solved for the next 10-20 years using HPC. In various fields of science using HPC, scientists have started to discuss scientific and/or social issues to be solved in each field. Hence, in this session, we aim to examine such issues in solid Earth science, which HPC can contribute to solve. For social issues, we will focus on earthquake and tsunami disaster mitigation. For scientific issues, we would like to discuss construction of the next generation of solid Earth model based on the big data of seismic waves and crustal deformation obtained by high-density observation networks. We will introduce the contents of the "white paper" of the future plans for computer science in various fields including solid Earth science.

Keywords: HPC, hazard mitigation

The K Computer and Japan Plan for Exascale

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At the end of September 2012, official operation of the Kcomputer has started. Already in many areas we see many great results. Users of K are actually very much impressed having experienced using K. The K is Japanese supercomputer jointly developed by Fujitsu and Riken and everything is made in Japan. The K computer won the top position on TOP500 in 2011 achieving a LINPACK benchmark performance of 10 petaflops - becoming the first supercomputer ever to reach this milestone. The K fell behind China and US machines on the latest TOP500. We believe that the K is still one of the most powerful and user-friendly machine in the world. K demonstrates an extraordinary level of stability. K is capable of sustained performance of 1 PF on real applications in a wide range of science. K is the strong science machine.

Computer simulation is becoming more and more important for contemporary science and engineering. Nobel Prizes 2013 in chemistry and physics show how computing is changing every field of research. Particularly simulations performed on the supercomputer will drive progress in science and technology and play an important role in solving difficult problems that we face as a society. There are very critical issues that need to be solved - global warming, alternative energy, disaster mitigation, new materials, healthcare, security, etc. The role of simulations will become increasingly larger, and the results that they provide will undoubtedly greatly affect society. The new frontiers opened up by the K computer will be presented.

The post K project will be lauced from April 2014. MEXT selected RIKEN AICS to develop a new exascale supercomputer by 2020. The post K is 100 times faster than the current K computer. Architecture is hybrid of general-purpose plus accelerator components. We will push the state of the art in power efficiency, scalability & reliability. Power consumption is limited in the range of 30-40MW.Total project cost is ca. JPY140 billion with about JPY 110 billion coming from the government's budget (JPY 1.2 billion for 2014)

Computer simulation will dramatically increase our ability to understand the world around us. With exascale computing, we are reaching a tipping point in predictive science. Its success will have lasting impact on the planet and people all around the world and for generations into the future. With a planned deployment in 2020, the new system is expected to keep Japan at the leading edge of computing science and technology.

The application of simulation studies using HPC to disaster management: current status and future.

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In Central Disaster Management Council, estimations of damage by anticipated earthquakes have been conducted to plan measures for disaster management(preparedness, emergency response and recovery). Also, when a large earthquake occurs early assessments of the damage have been carried out immediately to grasp the situation of the disaster and to support decision-making for emergency response operations in central government. These estimations and assessments require high accuracy to develop more effective measures and to decide more appropriate operations.

It is indisputable that the sophistication of forecasting techniques of natural phenomena is necessary to mitigate human damage by encouraging residents to evacuate.

In this presentation, we will introduce our approaches described above, and would like to talk about what to expect from the application of simulation studies using High Performance Computing to the disaster management of earthquakes and tsunamis in particular.

Keywords: disaster managent, damege estimation, HPC

Development of Integrated Earthquake Simulator on K-computer

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Earthquake simulation with high-resolution and high-accuracy could have significant contribution on making rational and effective counter measures against earthquake disaster. Such earthquake simulation must consider whole process from a fault rupture to city responses, since each process has significant effects on the resulting responses. We are now developing such earthquake simulation system on K-computer, which is called Integrated Earthquake Simulator (IES). IES combines spatial data and earthquake simulation with a high-fidelity model to simulate the whole process. The target domain of earthquake simulation is typically very large, making it difficult to prepare sufficient data to construct a high-fidelity model. Even if a high-fidelity model can be constructed, it is difficult to resolve the computational expense due to the discretization of such models. Thus, simplified analyses or analytical methods are typically used in earthquake simulation. However, the construction of high-fidelity models has become popular with recent increases in available spatial data, and a considerable volume of data from high-density observation networks is now available for checking their validity. The realization of analyses using high-fidelity models is desirable. Several examples of analyses using such models can currently be found on the K-class supercomputer, although the resolution is not yet adequate. In this presentation, we discuss the following earthquake simulations (parts of IES) on the K computer, together with problems to be solved: non-linear wave simulation with high resolution, crust deformation analysis with island-scale and the seismic response analysis of soil-structures system.

Keywords: earthquake simulation, high performance computing, high fidelity, high resolution and accuracy

Consideration to the resiliency of protective structures against tsunami by using High Performance Computer

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The Committee for Technical Investigation on Countermeasures for Earthquakes and Tsunami Based on the Lessons Learned from the "Great East Japan Earthquake" (2011) of the Central Disaster Management Council has responded to the Great East Japan Earthquake by proposing that basically, two levels of tsunami must be hypothesized to build future tsunami countermeasures. One is a tsunami hypothesized to build comprehensive disaster prevention countermeasures centered on evacuation of residents. It is set based on a survey of tsunami deposits formed over an ultra-long period and observations of crustal movement, and it is a maximum class tsunami which, although it occurs extremely rarely, causes devastating damage when it does occur. One more is a tsunami which is hypothesized to build coastal protection facilities such as breakwaters and other structures which prevent tsunami from inundating inland regions. It is a tsunami which occurs more often than the maximum class tsunami, and although it is a low type of tsunami, it causes severe damage. At such times, technological development of structures which are capable of resiliently providing effects even under tsunami height which is the object of the design must continue for coastal protection facilities etc. to be improved. So, in this research, the protective effectiveness is considered by using STOC-CADMAS(Arikawa and Tomita, 2005).

Determination of Earth structure using waveform inversion and Spectral-Element Method

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Recent progress in large scale computing by using Spectral-Element Method and the Earth Simulator has demonstrated possibilities to perform full-waveform inversion of three dimensional (3D) seismic velocity structure inside the Earth. Specifically Liu and Tromp (2006) have shown that it becomes feasible to compute finite frequency kernel for seismic velocity structure based on adjoint method. We apply their method to obtain 3D velocity structure beneath East Asia. We take one chunk from global mesh of Spectral-Element Method and compute synthetic seismograms with accuracy of about 10 second. We use GAP-P2 mantle tomography model (Obayashi et al., 2009) as an initial 3D model and try to use as many broadband seismic stations available in this region as possible to perform inversion. We then use the time windows for body waves and surface waves to compute adjoint sources and calculate adjoint kernels for seismic velocity structure. We use the earthquakes, which occurred in East Asia since 2001, with magnitude greater than 5.5 and selected 161 events for this inversion. One iteration of the waveform inversion using 256 cores of massively parallel supercomputer, such as K-computer, requires 0.1 million CPU hours. We have performed several iteration and obtained improved 3D velocity structure beneath East Asia. The result demonstrates that waveform misfits between observed and theoretical seismograms improves with the iteration proceeds and it now becomes feasible to perform waveform inversion within practical computational time. We will use much shorter period in our synthetic waveform computation and will try to obtain seismic velocity structure for basin scale model in our future study.

Acknowledgements: We used F-net seismograms of the National Research Institute for Earth Science and Disaster Prevention. This study was supported by the strategic Programs for Innovative Research "Field 3" Advanced prediction Researches for Natural Disaster Prevention and Reduction.

Keywords: Earth structure, Seismic tomography, Synthetic seismogram, Spectral Element Method

Mantle convection simulations on HPC: past, present and future

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In this presentation, we will discuss (a rather personal view of) the possible directions of the advanced numerical studies of mantle dynamics in concert with the progress of high-performance computing in the next era. We will start with a brief overview of the research targets and outcrops of the numerical modelings of mantle convection to date from a viewpoint of geosciences. Then we will discuss the scientific goals which the mantle dynamics researchers are to tackle with in coming years, together with the technical issues in terms of both software and hardware developments.

Keywords: mantle convection, numerical simulation

Cloud Services to Release Techniques of Data Assimilation

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Data assimilation (DA) is a fundamental technique to integrate numerical simulations and observation data in the framework of the Bayesian statistics. The purpose of DA is to provide an assimilation model that enables us to predict the future state and/or to determine parameters in the given simulation model. A sequential Bayesian filter, e.g., Kalman filter and particle filter, alternatively estimates probability density functions of one-step-ahead prediction and filtering, which respectively mean the states conditionally given the past observation data and given both past and present observation data. DA seems to be hard to implement due to complex programming of the procedure and needed numerous computation, which essentially requires High Performance Computing (HPC). Cloud service (CS) can be a solution for this through an implementation of the DA procedure on a parallel computing environment.

We have developed and released several CSs related to DA such as CloCK-TiME (Cloud Computing Kernel for Time-series Modeling Engine) and DA system for seismoacoustic waves. CloCK-TiME enables us to carry out a multivariate time-series analysis using the particle filter through the Internet. Users can, via the user interface, construct observation and system models, and specify optional parameters to control the analysis in detail. DA system for seismoacoustic waves enables us to determine hypocentric parameters through DA based on a numerical simulation related to seismoacoustic wave propagation using the normal model summation and observed infrasound data obtained at Shionomisaki and Sugadaira.

We will discuss the importance and availability of CS for DA researches through introduction of CSs we have developed.

Keywords: cloud computing, data assimilation, time-series analysis, seismoacoustic wave, multivariate analysis

Techniques of Big-Data Processing on the NICT Science Cloud

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This paper is to propose a cloud system for science, which has been developed at NICT (National Institute of Information and Communications Technology), Japan. The NICT science cloud is an open cloud system for scientists who are going to carry out their informatics studies for their own science.

The NICT science cloud is not for simple uses. Many functions are expected to the science cloud; such as data standardization, data collection and crawling, large and distributed data storage system, security and reliability, database and meta-database, data stewardship, long-term data preservation, data rescue and preservation, data mining, parallel processing, data publication and provision, semantic web, 3D and 4D visualization, out-reach and in-reach, and capacity buildings.

In the present study, we examine performance of parallelization of I/O on the NICT Science Cloud system. We examine an I/O performance of data file system; distributed file system (Gfarm). The Gfarm file system shows a tremendous fast I/O, as fast as 23 GB/sec using only 30 servers. We should pay attention to this I/O speed (23GB/sec is 184 Gbps) from the viewpoint of network speed. We also discuss that the distributed file system shows high scalability: Parallelization efficiency in the present examination is higher than 90% in case of parallel file system. We finally discuss high-performance data processing on the NICT Science Cloud. We have already archived several examples using our technique for both Earth and Space observation data and simulation data. The speed up of the data processing is more than 60 times for scientific big-data.

Creating future of solid Earth science with high performance computing (HPC): Discussion

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How the evolution of High Performance Computing (HPC) contributes to progress in earth sciences? We will develop a perspective in the next 10 to 20 years based on comprehensive discussion provided in the session including invited talks. Especially, we will discuss what is necessary for solving the social issues such as improvement of hazard maps, tsunami warning system, long-term forecast, etc. The aim of the concluding discussion is to integrate the opinions of attendees, both speakers and non-speakers, into a proposal for development of next generation HPC as a solution to important problems in terms of scientific breakthrough and social relevance.

Parallel Performance of Particle Method in Many-Core System

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We present a computational performance of the smoothed particle hydrodynamics (SPH) simulation on three types of current shared-memory parallel computer devices: many integrated core (MIC: Intel Xeon Phi) processor, graphics processing units (GPU: Nvidia Geforce GTX Titan), and multi-core Central Processing Unit (CPU: Intel Xeon E5-2680 and Fujitsu SPARC64 processors). We are especially interested in the efficient shared-memory allocation methods with proper data access patterns on each chipset. We first introduce several parallel implementation techniques of SPH code for shared-memory system. Then they are examined on our target architectures to find the best algorithms for each processor unit. In addition, the computing and the power efficiency, which are increasingly important to compare multi device computer systems, are also examined for SPH calculation. In our bench mark test, GPU is found to mark the best arithmetic performance as the standalone device and the most efficient power consumption. The multi-core CPU shows the best computing efficiency. On the other hand, the computational speed by the MIC on Xeon Phi approached to that by two Xeon CPUs. This indicates that using MIC is attractive choice for the existing SPH codes parallelized by OpenMP to gain the computational acceleration by the many many-core processors.

Keywords: high-performance computing, many core, SPH, Parallel Computing, Performance analysis, Shared memory

Numerical investigation of efficient parallelization of large scale quasi-dynamic earthquake generation cycle simulation

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Recently, Ohtani et al. (2011) applied an efficient compression method of full matrix to the problem of earthquake cycles. Since an original full matrix is approximated by a set of sub-matrices with the hierarchical structure, a compressed full matrix is called as H-matrices. By multiplying H-matrices to a column vector, they found that the required floating-point operation reduces to $O(N)$ - $O(N\log N)$ where N means the number of discretization of the model fault, though the original multiplication operation using the full matrix is $O(N^2)$. Owing to H-matrices, required memory and computation time are largely reduced for the problems of M8 earthquake cycles with $N=10^5$ - 10^6 , and it enables us to execute capability computing consisting of many earthquake scenarios using massively parallel computers like the K computer. However, for more realistic simulation with multi-scale earthquakes and their interactions, we must use 100 times larger N at least, and capability computing with massively parallel CPUs will be indispensable.

Following Ohtani et al. (2011), we have implemented MPI parallelization of earthquake cycle simulation with H-matrices. First, we applied a 1D division in the row direction to H-matrices. Then, each MPI process took charge of a divided row band region of H-matrices. Since the original H-matrices have a hierarchical structure consisting of many sub-matrices with large variation in size, it is difficult to divide all sub-matrices into MPI processes without overlapping through the 1D row division. Hence, we arrowed the overlapping sub-matrix to be calculated in both adjacent MPI processes for the simplification of parallelization. Then, through the simulation with $N=3 \times 10^5$, we confirmed a gradual speed-up with the increase of MPI processes up to about 100. However, further increases of MPI processes caused stagnation of speed-up, because the overlapping operation that is not reduced by the increase of MPI processes became dominant.

Accordingly, for more large-scale simulation with many MPI processes, it is necessary to reconsider the parallelization. At first, based on the current 1D division code, we limit the division number in the row direction so as not to increase the ratio of operations with respect to overlapping sub-matrices to the total operations. Then, each row region is divided into further small sub-regions in the column direction, thus we will apply the 2D division of H-matrices. In dividing a particular row region into further sub-regions, we introduce a reference size for the division, B (Block size). The column directional division of H-matrices requires data transfers between sub-matrices. Moreover, depending on the value of B , we also need data transfer inside the large sub-matrix. Though such 2D division increases the data transfers between neighboring MPI processes, the appropriate choices of B and division number in the column direction will realize the equal load balancing among MPI processes in row bands. Accordingly, parallel implementations with 2D division of H-matrices may overcome the overhead due to the increase of data communications.

As tentative results, for $N=1.3 \times 10^6$ problem, we implemented parallel calculations with both 1D and 2D divisions. Though the 1D parallelization cannot reduce the computational time with the increase of MPI processes, 2D parallelization successfully achieves speed-up with the increase of the number of parallelization. For the same number of MPI processes (1024 processes), the 2D implementation is more than two times faster than that of 1D.

In the presentation, we will show the more detail of our parallelization algorithm and its dependencies on the values of N , B , and division numbers.

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Keywords: earthquake cycle, capability computing, parallel computing, H-matrices