Discrete-Event Simulation Research Team

1. Team members

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2. Research Activities

As computer performance grow, simulation models tend to become the more complex, and models have the more parameters and show complicated behavior. This often increase the number of simulation jobs, and analyses and visualizations of simulation results also become diversified. Each simulation and each analysis will be properly processed by computers if they are specified correctly, but error will easily be introduced by human side. In this sense, supercomputers are demanding not only greater programming skill but also more reliable operation and smarter decision of simulation parameters. To help the latter, the OACIS(**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations), a job management tool for simulations and analyses are designed and developped in the Discrete-Event Simulation Research Team(DESRT). It is coded using Ruby, Ruby-on-rail framework and MongoDB. After installation, users register their applications for simulations and analyses, and their computers from PC to supercomputers like K to the OACIS. Then they can design and order executions of simulations and analyses on its web-browser front end. The ssh connection is used to operate the registered remote computers and Job states are supervised by the OACIS. Current prototype transfers output files of simulations and analysis to the local computer operating the OACIS from remote computers. The results and historical data are preserved in local computer using MongoDB. The first version was released in this year, and cultivation of its user group was started.

Partitioned global address space(PGAS) is an idea to treat memory space managed in each node of massive parallel computer like the K computer as a shared memory computer, which makes programming easier and simpler. A PGAS language named X10[1] is implemented to the K computer. In addition to the C++ version(so-called the native version) of X10 which were available already, Java version(so-callled the managed version) was implemented in this year.

Most simulation models can be formulated as evolutions on certain graphs. For example, particle-dynamics and molecular-dynamics simulations usually update a system configuration using so-called pair lists and neighbor tables, lists of interacting agents, that is, particles or molecules, with each agent[2]. The pair lists define a graph in agents. The graph evolves with motion of agents and agents evolve on the graph, and it is in an opposite extreme of simulation models with so-called a stencil computation algorithm. Stencil computation is on regular lattices, but dynamic and complex graphs are to be a main target of DESRT. Complicated graphs demand additional efforts when we implement on computers: optimization of pipeline, memory and cache, and massive-parallel communications are demanding. So algorithm and coding technology of graph and network simulations and analyses have been studied in DESRT. In this year, automobile traffic which use a graph of road map and treat car agents on it, epidemic propagation which use a graph of human mobility and treat human interactions on it, and graph of social relation were targets.

Accurate observations and high resolution measurements are important to decide simulation parameters, but they are not always available. We can design them appropriately for natural-scientific phenomena, but they are difficult for social-scientific phenomena. All data of human activities in real society do not mean sufficient, but data of many repetitions for various social parameters and systems in various environments with various conditions are necessary in the sense of natural science with Francis Bacon's *"Novum Organum"* style. In this sense, social-scientific models and their simulations are challenging: *Idola* will be everywhere because each of us have one's understandings, interests and perspective about our society. So-called the "Big data" are far-from sufficient, which will intuitively obvious when the data size is compared with natural-scientific data, for example, data flood from modern accelerators and space telescopes. Such situation of data lack, theoretical studies are advantageous, and computer simulations are major driving force of theoretical challenge nowadays. Make models of cloudy target phenomena, examine their behavior precisely, and compare the clear behavior with vague target data to assess the models. This year, a simulation model of automobile traffic flow in Kobe city is analyzed with the standard factor analysis of multivariate statistical analysis. The model is agent-base one simulating motion of each car agent, and only coarse-grained data are adjusted to the real traffic. Estimated factors are reasonably explain what we are experiencing in our daily urban lives.

[1] http://x10-lang.org/

[2] Details of a molecular-dynamics simulation on K-type computers are given in, for example, Hiroshi Watanabe, Masaru Suzuki and Nobuyasu Ito, Computer Physics Communications 184 (2013) 2775, which is available at

http://www.sciencedirect.com/science/article/pii/S187538921400279X.

3. Research Results and Achievements

3.1. The OACIS

First version of the OACIS(**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations)[2] is made open for public use in the beginning of this year on github site[3], and tutorial and user support activities are started[4]. Overview of the OACIS is explained in the Figure 1, and an example of user interface is shown in the Figure 2.

This OACIS version 1.xx.x is for single-user managing up to about millions of jobs operating. Beyond this number of job, job management operations requires too long even for a simple simulator with a few inputs and a few output. Multithreading in parallel machine is now necessary to go beyond this limitation, and an improvement using PGAS language X10 was on schedule. There are two kinds of X10. One is on C++ which is callled the "native version" and the other is on Java called the "managed version". The native version had been available on the K computer and Fujitsu FX10.

The managed version will be more useful for the extension of OACIS because it has the more powerful library useful for the purpose. In this year, the managed version is now implemented on the K computer and Fujitsu FX10 and extension of the OACIS beyond the limitation of job number will use this X10 managed version.

Implementation of the OACIS may not be easy for users without experience of Ruby and MongoDB. Some users want to implement the OACIS on their Windows machine. Some users committing several projects need to execute several OACIS in one computer. Virtual machine will help to solve these request, and a preliminary version of the OACIS in the Docker container[5] was developped and been testing in this year.

[3] https://github.com/crest-cassia/oacis

[4] https://groups.google.com/forum/#!forum/oacis-users

[5] https://www.docker.com/

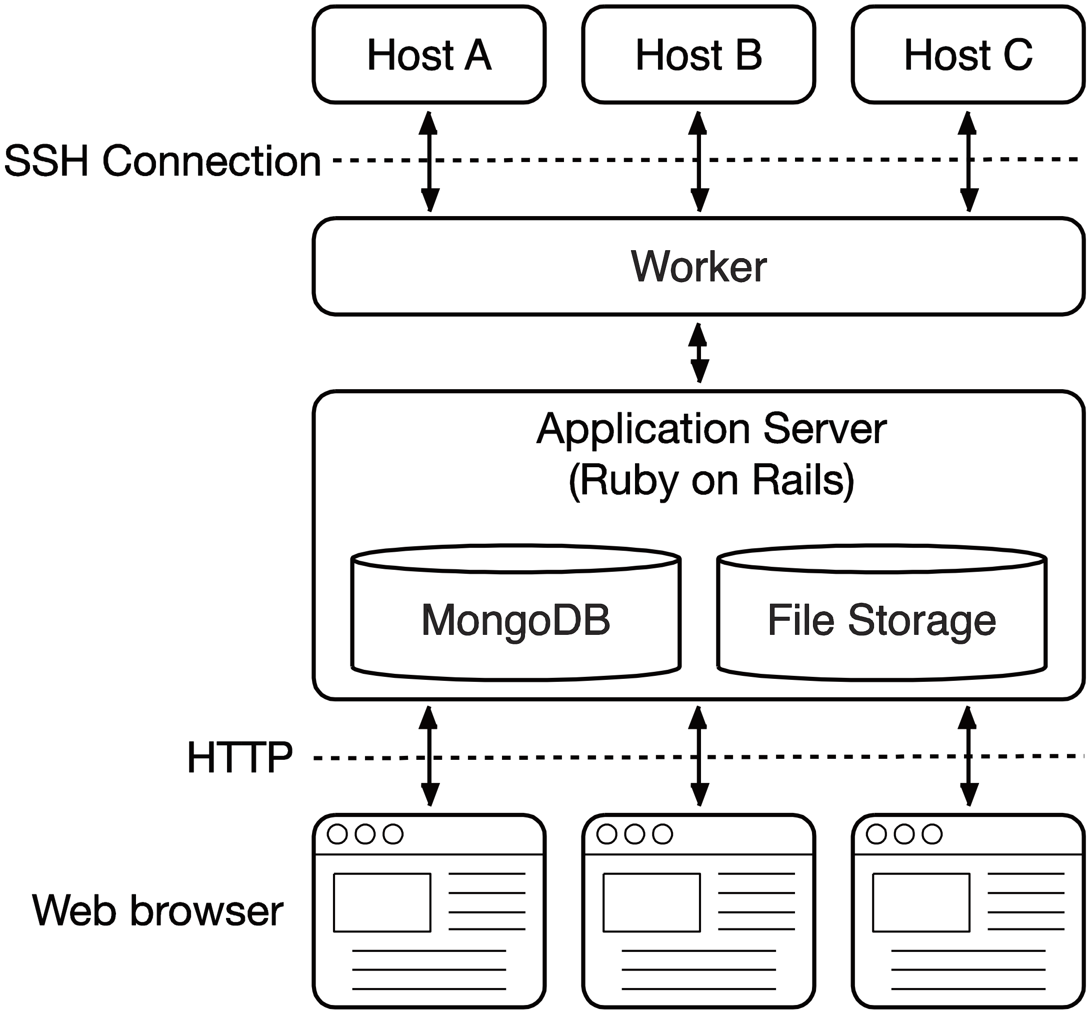
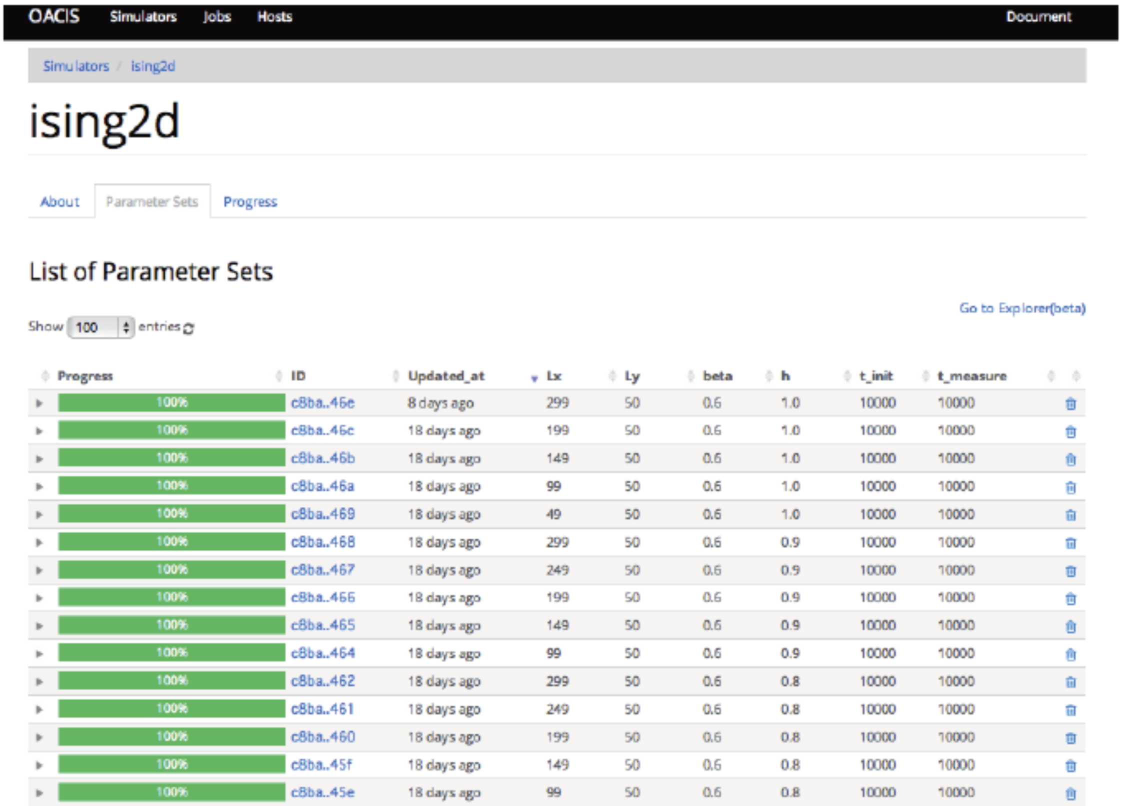


Figure 1. Overview of the OACIS is shown schematically[1]. The OACIS is between two horizontal broken lines. User in the bottom operates the OACIS through web browsers via HTTP. Host computers registered for job execution in the top are operated by the OACIS via SSH. The OACIS supports job executions on K-computer through K's standard staging, execution, and stage-out scheme.



Progress	ID	Updated_at	Lx	Ly	beta	h	t_init	t_measure
100%	c8ba..46e	8 days ago	299	50	0.6	1.0	10000	10000
100%	c8ba..46c	18 days ago	199	50	0.6	1.0	10000	10000
100%	c8ba..46b	18 days ago	149	50	0.6	1.0	10000	10000
100%	c8ba..46a	18 days ago	99	50	0.6	1.0	10000	10000
100%	c8ba..469	18 days ago	49	50	0.6	1.0	10000	10000
100%	c8ba..468	18 days ago	299	50	0.6	0.9	10000	10000
100%	c8ba..467	18 days ago	249	50	0.6	0.9	10000	10000
100%	c8ba..466	18 days ago	199	50	0.6	0.9	10000	10000
100%	c8ba..465	18 days ago	149	50	0.6	0.9	10000	10000
100%	c8ba..464	18 days ago	99	50	0.6	0.9	10000	10000
100%	c8ba..462	18 days ago	299	50	0.6	0.8	10000	10000
100%	c8ba..461	18 days ago	249	50	0.6	0.8	10000	10000
100%	c8ba..460	18 days ago	199	50	0.6	0.8	10000	10000
100%	c8ba..45f	18 days ago	149	50	0.6	0.8	10000	10000
100%	c8ba..45e	18 days ago	99	50	0.6	0.8	10000	10000

Figure 2. An example of snapshot of OACIS operation on a web browser is shown[1]. It browses status of specified jobs. A simulator named "ising2d" is prepared and registered on OACIS which execute a Monte Carlo simulation of the Ising model on square lattice with specified parameters: Lx, Ly, beta, h t_init and t_measure denoting lattice sizes in x and y directions, inverse temperature normalized by a spin-coupling constant, external field, number of Monte Carlo steps for initial relaxation and measurement, respectively. Each job is listed in a row.

3.2. Graph and network simulators

A benchmark program for the K computer aiming at car traffic simulation is made. Each car agent is driven at a given speed without interacting with any other cars, and it selects its way randomly at each corner. Geometrical parallelization is used: a given road network is divided into small areas geometrically, and each process on each computer node processes one of these small areas. Cars going out or coming into the area of each process are sent to or received from the process simulating corresponding areas.

Weak scaling of parallel performance was measured using a square-lattice road network(Figure 3). Lattice constant of this network corresponds to 100m, and each road segment has two lanes going to opposite direction with each other. Cars keep left lane. Initially, 16 cars are allocated par 100m of each lane. Velocity of each car is assigned uniformly randomly in a interval from 10Km/h to 60Km/h. Each node of the K computer processes area of 16×16, therefore totally 100m×16×16×2 lanes =51.2Km of lane per node, and 16×16×16×2=8192 cars in average per node. Time step Δt is 0.01sec and performance is measured for 1 million steps corresponding to 0.01sec$\times10^6$ steps = 10^4 sec is measured. The results from 9 nodes with 3×3 to 20,736 nodes(quarter nodes of the K computer) with 144×144 are plotted in Figure 4. The processes on the smallest 9 nodes simulate 73,728 cars on totally 460.8Km lanes, and the performance was 9.5MUPS(million update per second) per node. The largest 20,736 nodes treat 169,869,312 cars on 1,061,683.2Km, and the performance was 7.2MUPS per node, which is 24% slower than 9 nodes.

Strong scaling of parallel perfornace is measured using both the Japanese road network and the square-lattice network. The Japanese road network is based on the Open Street Map[6] and totally 1,310,000Km and 127,000,000 cars are simulated on the map(See Figure 5). The square-lattice network with the corresponding total length and number of cars is also used. This number of cars should be compared with 77,193,872, the number of car in Japan in the end of September 2014. Time step Δt is 0.01sec and performance is measured for 1 million steps corresponding to 0.01sec $\times10^6$ steps = 10^4 sec is measured. The performance with 324, 1,296, 5,184 and 20,736 nodes are plotted in Figure 6.

These results of strong scaling show peak around 5,184 nodes. Speed with 20,736 nodes is still faster than ones with 324 and 1,296 nodes. This will because the effect of cache memory. The speed of the Japanese traffic with 20,736 nodes was faster than 0.3MUPS per CPU core. And 0.3MUPS core will reasonably be expected when all nodes of the K computer is used which is 0.3MUPS$\times$8 cores = 2.4MUPS per node, and 2.4MUPS$\times$82.944 nodes = 0.20 TUPS(10^{12} UPS). This is a performance achieving a real-time simulation of two billion cars with Δt = 0.01 sec.

This is the performace with simplified car agents, each of which randomly moves around on the road network without interacting with other agents. In the more realistic model, car movement costs more calculations in each computer nodes. Therefore weight of communication between nodes becomes less. So parallelization of traffic simulation on the K computer will work efficiently if parallelized loads are well-balanced.

In summary, the benchmark results will imply that the K computer can achieve a real time or faster simulation of all the car traffic in Japan.

[6] https://openstreetmap.jp/

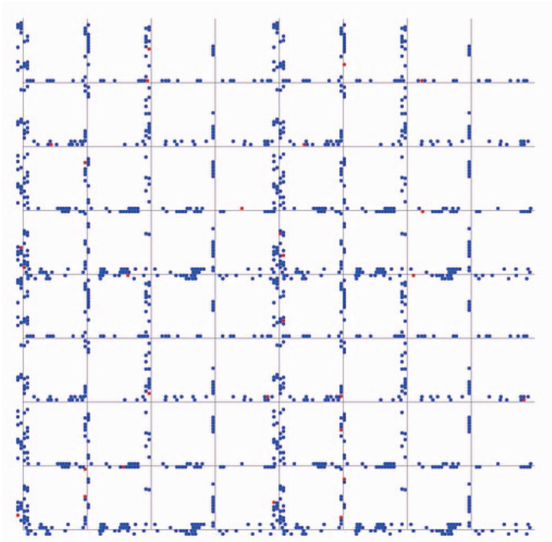


Figure 3: Traffic on the square-lattice road network is shown. Some segments have two traffic lanes for one direction on this figure, but the network for benchmark comprises one lane for each direction for all segments.

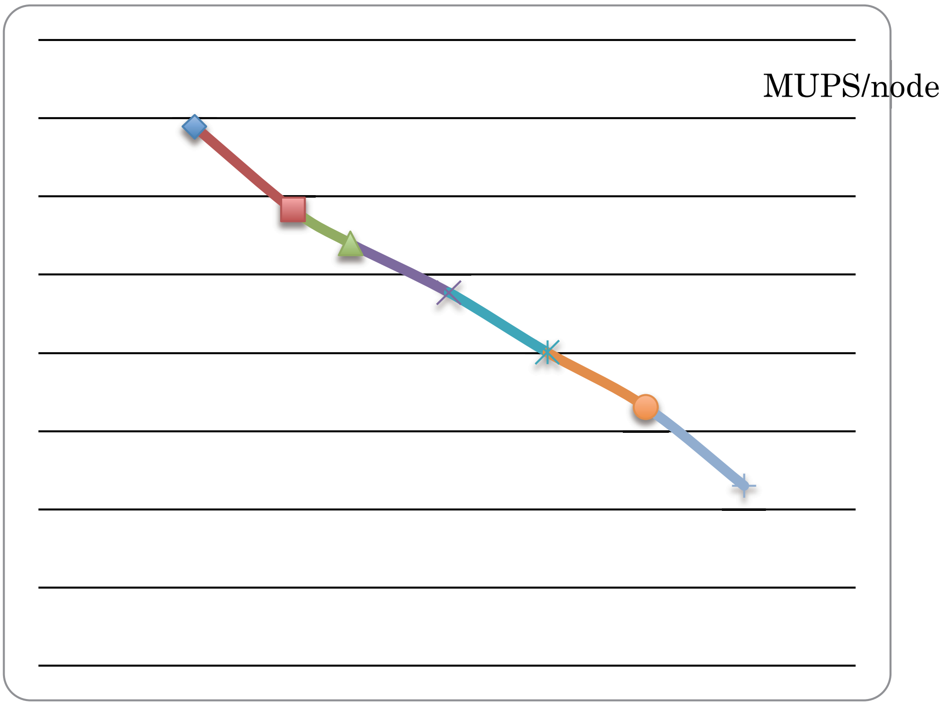
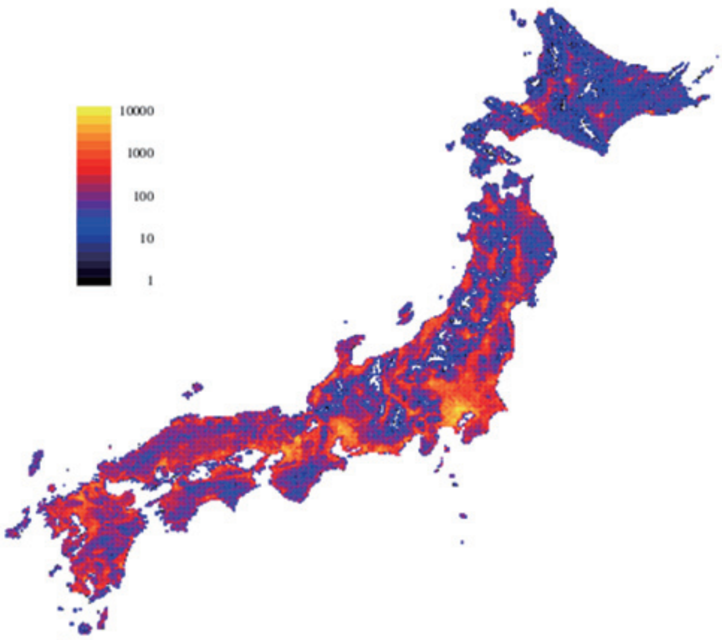


Figure 4: Weak-scaling performance results using square-lattice road network are plotted. The horizontal axis shows number of nodes and the vertical axis shows performance measured by number of cars updated on each node per second with a unit of million. "MUPS" is an abbreviation for "million updates per second".



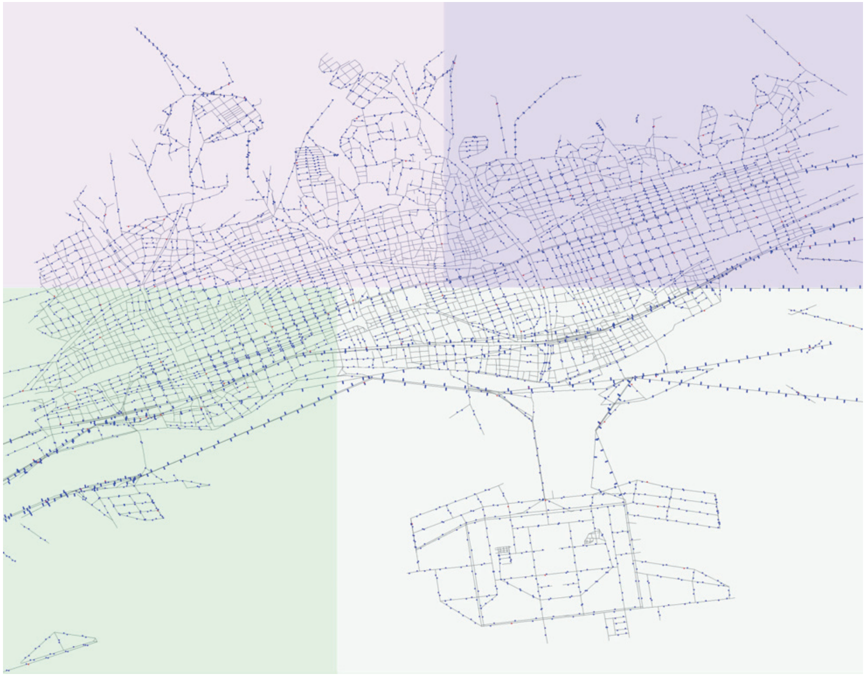


Figure 5: The Japanese road network used to evaluated the strong-scaling performance in Figure 6 is shown. Top: the network is visualized with density of crossing.
Bottom: magnified snap-shot focused at the Kobe city.

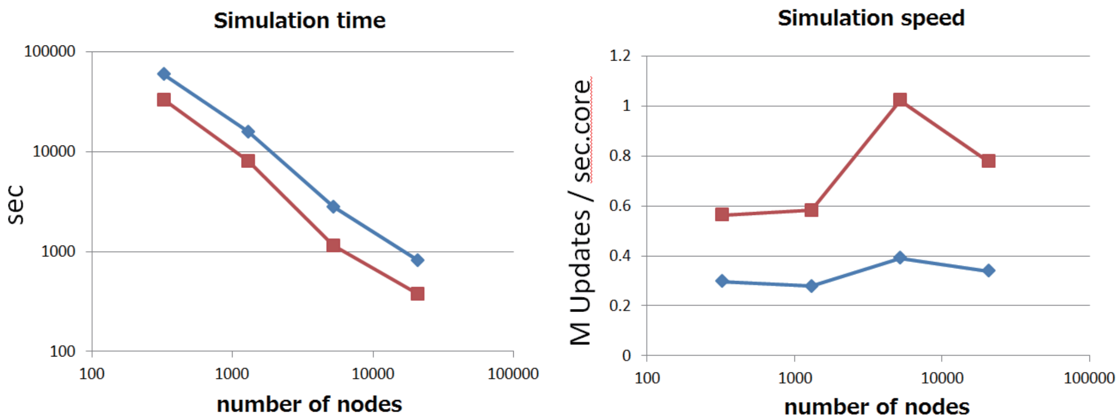


Figure 6: Results of strong-scaling parallel performance are plotted. Blue diamond denotes the results with the Japanese road network, and red square with the square-lattice network. Left:

4. Schedule and Future Plan

In the following years, a beta version of the OACIS is released to the public, and tools of visualization and simulation design will be developped. And a graph simulation and analysis tool working on K-computer up to its full node will be developped.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Yohsuke Murase, János Török, Hang-Hyun Jo, Kimmo Kaski, János Kertész, "Multilayer weighted social network model", Physical Review E, vol.90 (2014) 052810.
2. Hiroshi Watanabe, Masaru Suzuki, Hajime Inaoka, and Nobuyasu Ito, "Ostwald ripening in multiple-bubble nuclei", Journal of Chemical Physics, vol.141 (2014) 234703.

(2) Conference Papers

1. Yohsuke Murase, Takeshi Uchitane, and Nobuyasu Ito, "A tool for parameter-space exploration"、Physics Procedia 57 (2014) pp. 73-76.

(3) Invited Talks

1. Nobuyasu Ito, "Simulation study of liquid-gas transition", International Conference "Smart functional materials for shaping our future" (Debrecen, Hungary, 19-20 September 2014) .

(4) Posters and presentations

1. Hiroshi Watanabe, Masaru Suzuki, Hajime Inaoka, and Nobuyasu Ito, "Huge-Scale Molecular Dynamics Simulation of Multi-Bubble Nuclei", NCSA Blue Waters Symposium for Petascale Science and Beyond(Champaign, Illinois, USA, May 2014).
2. Hajime Inaoka and Nobuyasu Ito, "Implementation of a breadth-first search algorithm on a massive-parallel computer", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014),.
3. Yuta Asano, Nobuyasu Ito, Hajime Inaoka, Yohsuke Murase, Tetsuo Imai, and Takeshi Uchitane, "Traffic Simulation of Kobe-city", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014).
4. Takeshi Uchitane, "A software for managing a lot of jobs and their results", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014).
5. Yohsuke Murase, et al.“A Universal Lifetime Distribution for Multi-Species Systems”, Social Modeling and Simulation + Econophysics Colloquium 2014, (Kobe, Japan, Nov. 2014)
6. Yohsuke Murase, et al.“Multilayer weighted social network model”Social Modeling and Simulation + Econophysics Colloquium 2014, (Kobe, Japan, Nov. 2014), awarded as the Best Poster Prize
7. Hajime Inaoka and Nobuyasu Ito, "Molecular Dynamics Simulation of Pool Boiling of a Lennard-Jones Liquid", International Symposium on Extended Molecular Dynamics and Enhanced Sampling Nosé Dynamics 30 Years(Keio University, Tokyo, Japan, Nov. 2014).

8. Yohsuke Murase,et al. “Multilayer weighted social network model”, 5th AICS International Symposium.
9. Takeshi Uchitane, “OACIS - A tool for social simulation execution and its applications", The 5th AICS Symposium, 2014.

(5) Patents and Deliverables

OACIS, a job management application, released on April 1st, 2014.