Complex Phenomena Unified Simulation Research Team

1. Team members

Makoto Tsubokura (Team Leader)

Keiji Onishi (Postdoctoral Researcher)

Chung-gang Li (Postdoctoral Researcher)

Leif Niclas Jansson (Postdoctoral Researcher)

Rahul Bale (Postdoctoral Researcher)

Tetsuro Tamura (Visiting Researcher)

Ryoichi Kurose (Visiting Researcher)

Gakuji Nagai (Visiting Researcher)

Kei Akasaka (Visiting Researcher)

2. Research Activities

The objective of our research team is to propose a unified simulation method of solving multiple partial differential equations by developing common fundamental techniques such as the effective algorithms of multi-scale phenomena or the simulation modeling for effective utilization of the massively parallel computer architecture. The target of the unified simulation is supposed to be complex and combined phenomena observed in manufacturing processes in industrial circles and our final goal is to contribute to enhance Japanese technological capabilities and industrial process innovation through the high-performance computing simulation.

Most of the complex flow phenomena observed in manufacturing processes are relating to or coupled with other physical or chemical phenomenon such as turbulence diffusion, structure deformation, heat transfer, electromagnetic field or chemical reaction. While computer simulations are rapidly spreading in industry as useful engineering tools, their limitations to such coupled phenomena have come to realize recently. This is because of the fact that each simulation method has been optimized to a specific phenomenon and once two or more solvers of different phenomena are coupled for such a complicated target, its computational performance is seriously degraded. This is especially true when we utilize a high-performance computer such as "K-computer". In such a situation, in addition to the fundamental difficulty of treating different time or spatial scales, interpolation of physical quantities like pressure or velocity at the interface of two different phenomena requires additional computer costs and communications among processor cores. Different mesh topology and hence data structures among each simulation and treatment of different time or spatial scales also deteriorate single processor performance. We understand that one of the keys to solve these problems is to adopt unified structured mesh and data structure among multiple simulations for coupled phenomena. As a candidate of unified data structure for complicated and coupled phenomena, we focused on the building-cube method (BCM) proposed by Nakahashi[1].

[1]K. Nakahashi, High-Density Mesh Flow Computations with Pre-/Post-Data Compressions, Proc. AIAA 17th CFD Conference (2005) AIAA 2005-4876.

[2] P. L. Roe, Approximation Riemann solver, Parameter Vectors, and Difference Schemes, J. Comput. Phys. 43 (1981) 357-372.

[3] J. M. Weiss and W. A. Smith, Preconditioning Applied to Variable and Constants Density Flows, AIAA. 33 (1995) 2050-2056.

3. Research Results and Achievements

3.1. Development of a very large scale incompressible flow solver with a hierarchical grid system

This year, we have modified the main flow solver for incompressible flow developed last year in the context of its validation in a real development process on the massively parallel environment, including pre- and post-processing. For that purpose, we have utilized real production data (called as dirty CAD) provided by Suzuki Motor Company and Nissan Motor Company and conducted a full-scale vehicle aerodynamics simulation. Finally we have realized the world largest class vehicle aerodynamics simulation based on a real vehicle shape data by using 20 billion numerical cells. At the same time, we have started the accuracy inspection work using the wind tunnel experimental results. This numerical simulation enhanced the companies to utilize the K-computer for their own development purpose and two applications were submitted and accepted for the industrial use projects in FY 2014.

In addition, we have conducted a feasibility study of transient flow simulation around Tokyo station for the possible usage of assessing wind load on high-rise buildings. We will expand this project with the tight collaboration with Tokyo Institute of Technology and some construction companies under the K-computer's general use projects in FY2014.

We are planning to keep developing the software based on this framework in 2014, tackling for improvement of an accuracy of prediction adding numerical functions, physical model, and the tools for the usability improvement.

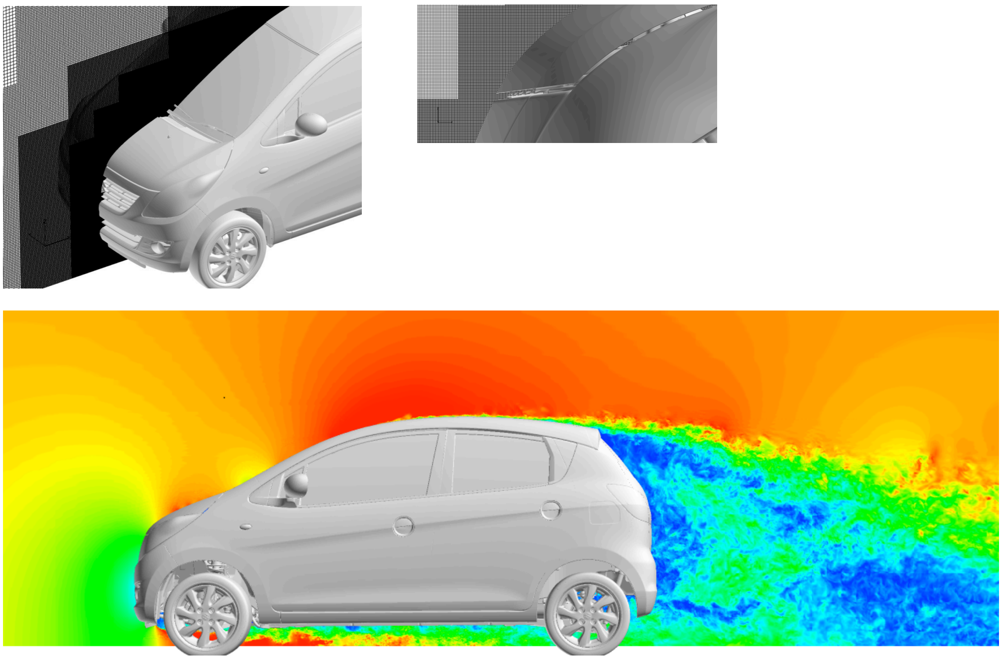
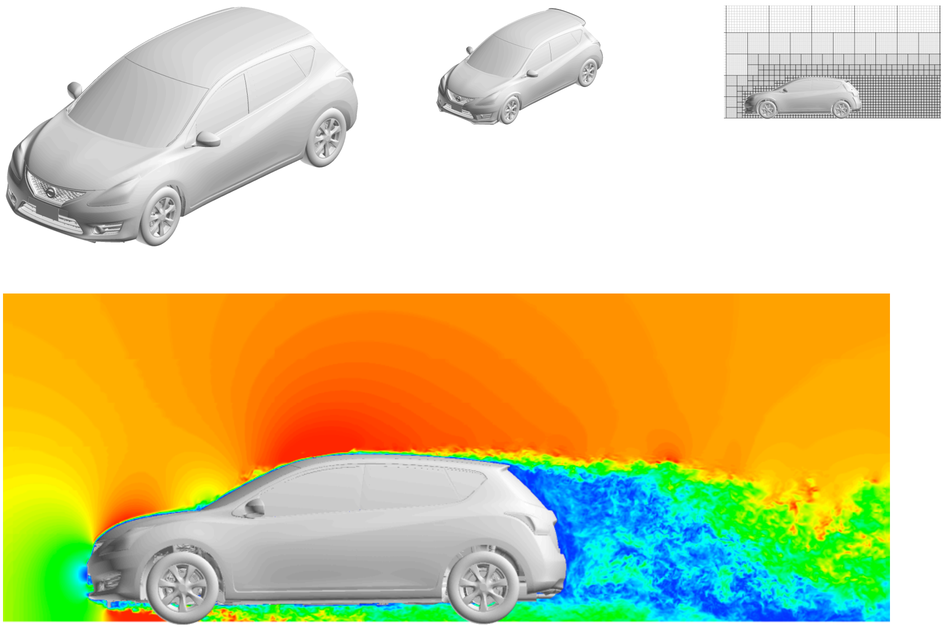


Fig. 1. Practical application of large scale full vehicle aerodynamics simulation using 20 billion cells (Suzuki Motor Company).



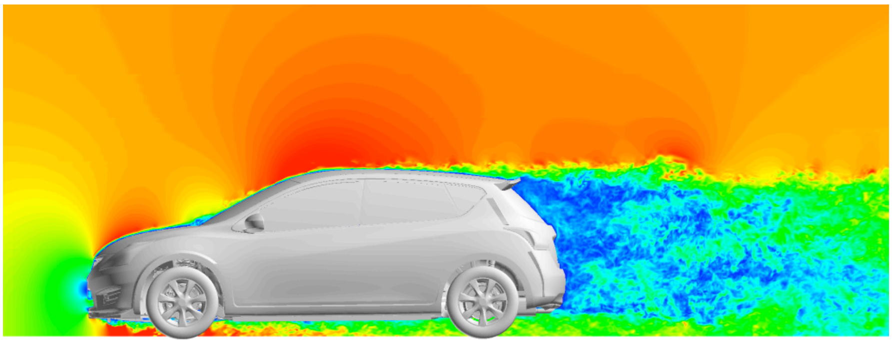


Fig. 2. Analysis of aerodynamic parts effect on full scale vehicle model (Nissan Motor Company).

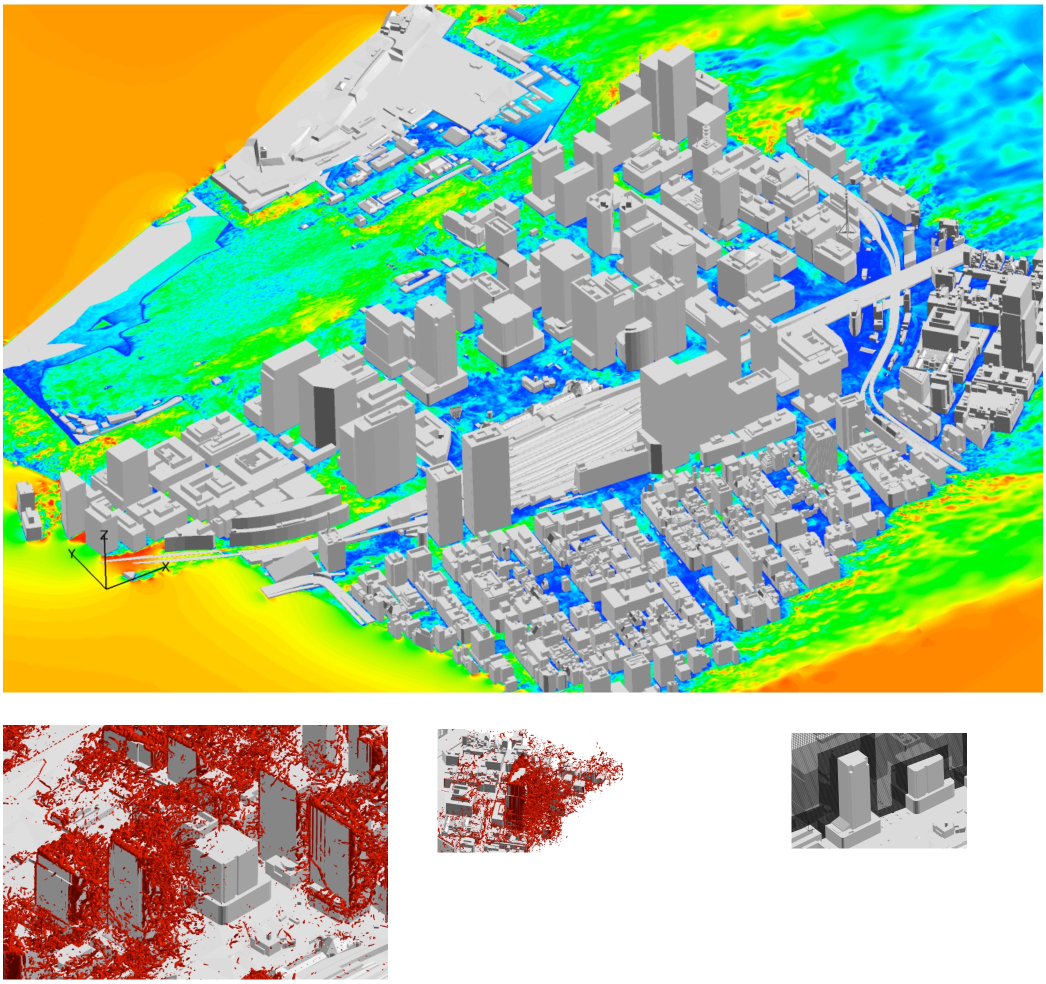


Fig. 3. Wind environment analysis around Tokyo station area.

3.2 Development of unified compressible flow solver for unified low to moderate Mach number turbulence with hierarchical grid system

For the purpose of applying CFD on practical applications, the program with the characteristics of high performance computing, massive parallelization, the ability to handle the complex geometry, suitable from low to high Mach numbers, and adaptability for turbulence is necessary.

Therefore the Roe scheme [2], Weiss and Smith preconditioning method and dual time stepping [3] based on hierarchical data structure have been implemented to unify the solver. Table I shows the weak scaling test of the solver. For 8 CPUs, the peak performance is almost 15% which is much higher than incompressible solver. Additionally, with the increment of the CPUs from 8 to 4096 CPUs, the peak performance just slightly decreases around 1.5% which shows excellent scalability of massive parallelization.

Table I. Weak scaling test.

Nodes	$N_{cube} \times N_x \times N_y \times N_z$	N_{ave}	Elapse time (s)	Data Transfer	Peak(%)
8	$512 \times 16 \times 16 \times 16$	64	54.23	5.03s (9.3%)	14.94
64	$4096 \times 16 \times 16 \times 16$	64	58.99	6.78s (11.5%)	13.74
512	$32768 \times 16 \times 16 \times 16$	64	60.11	6.77s (11.3%)	13.48
4096	$262144 \times 16 \times 16 \times 16$	64	60.12	6.71s (11.2%)	13.48

Immersed boundary is implemented to cope with the complex geometry. Fig. 4 shows the vortex contour around a vehicle at Reynolds number 1000.The flow field disordered by the complex shape and mirror is obvious.

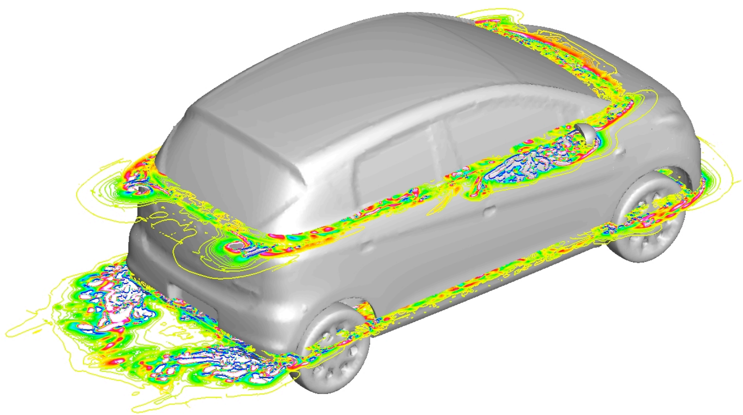


Fig. 4. Vortex contour.

Due to the instinct of the compressible flow, the problem can also be used for our next target: computational aeroacoustics (CAA). The pressure propagation with sine wave in the condition of 30 PPW is conducted and shown in Fig. 5. The comparison with the exact solution is shown in Fig.3. From the Fig. 5, it can be observed that the amplitude keeps decreasing from the pressure source to the outside. This kind of decay is direct proportion to $P = x^{-0.5}$ and the results in Fig. 6 is in good agreement with the exact solution $P = x^{-0.5}$ when CFL number is smaller than 0.5.

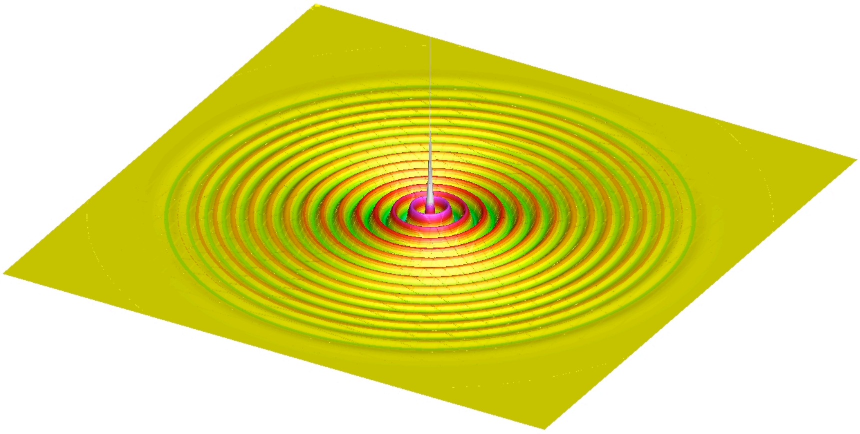


Fig. 5. Pressure propagation with sine wave.

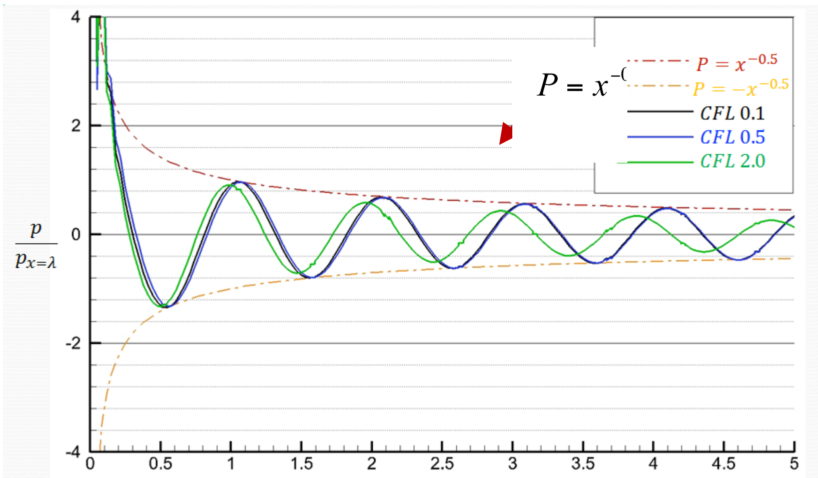


Fig. 6. The comparison with the exact solution.

Based on the present results mentioned above, this unified solver is a sophisticated and powerful tool for practical applications. In order to broaden the suitability on industrial field, the CAA on the vehicle will be conducted for next year.

3.3 Development of a unified framework for incompressible and compressible flow solver

Based on the Building Cube Method (BCM), our unified framework is a merge of the previous flow solvers in our group (incompressible and compressible). Written in modern Fortran 2003, the framework has a modular design, where each solver is an independent module, written by the user or provided by the core library itself. These modules can then be connected together to form a "solver" pipeline, describing the steps necessary to solve a particular multiphysics problem.

The framework utilize different hybrid parallelization strategies, mainly MPI across nodes together with OpenMP for intra-node parallelism, and MPI I/O for efficient parallel and scalable I/O operations. On a single node our framework achieve around 10-14% of peak flops, and a parallel efficiency of 80-90%, depending on the particular problem at hand (see Fig. 7).

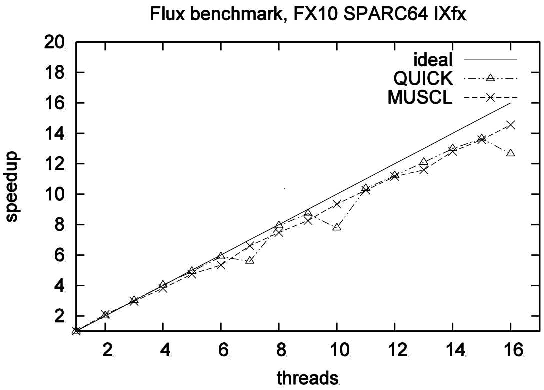


Fig. 7. Single node performance for a incompressible (QUICK) and compressible (MUSCL) scheme.

In order to scale to a large number of MPI tasks we have developed a new multithreaded halo-exchange algorithm. Traditionally, halo-exchange is performed using non-blocking communication, overlapping communication with computation. Our multithreaded approach adds an additional layer on top of this, overlapping packing and sending of communication buffers, performed by one OpenMP thread, with local computation performed in the remaining threads, reducing load imbalance between threads, and improving application performance with up to 20% at scale (see Fig 8.).

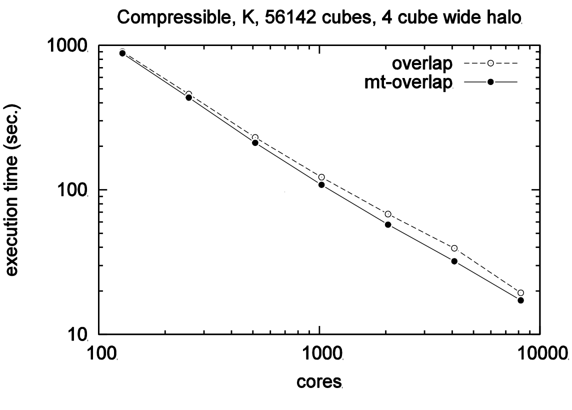


Fig. 8. Execution time for the compressible solver using two different halo-exchange algorithms, the traditional (overlap) and our new multithreaded implementation (mt-overlap).

Our feasibility study of new programming models has also led to the development of a low latency hybrid parallelization of the framework, based on Coarray Fortran together with OpenMP. Furthermore, the framework's modular design allow us to easily interface with routines written in other programming languages, and to target various kinds of current and future accelerators.

3.4 Unified flow and structure simulation based on the immersed boundary methods

Most fluid structure interaction (FSI) problems, encountered in industrial processes and biological systems, involve one or more the following scenarios: Complex motion of structures relative to fluid, motion of structures induced by fluid flow, and deformation of structures induced by fluid forces. Thus, to address FSI problems of practical significance it is necessary to model the afore mentioned scenarios of FSI.

Several approaches for FSI involving deformable and moving structures have been developed over the last four decades. Broadly, these methods fall under two categories Lagrangian-Eulerian (LE) methods and full Eulerian (FE) methods. In LE methods, the structure is represented on a Lagrangian mesh and the fluid on an Eulerian mesh, where as in FE method both structure and fluid are represented on an Eulerian mesh.

The fundamental difference between LE methods and full Eulerian method is the manner of information exchange between fluid and the structure. In LE methods, the information between Lagrangian and Eulerian meshes (i.e. structure and fluid, respectively) is exchanged through operators such as the, so-called, pseudo-delta function. These operators are computationally very expensive and are not suitable for large scale industrial FSI problems. In comparison with LE methods, full Eulerian method does not require any information exchange because both the fluid and the structure are represented on the same Eulerian mesh. Another drawback of LE methods is the issue of load balancing in parallel implementations for moving IB. Moving IB require dynamic load balancing, increasing the difficulty of implementation. Thus, due to lower computational cost and relative ease of implementation, we prefer FE methods over LE methods.

We have adapted the LE based IB method developed by Sharma and Patankar into an FE based IB for Rigid IB dynamics. Through this method we will have the capability to investigate flow induced motion of rigid bodies, flow due to specified motion of rigid bodies as well as flow around immobile rigid bodies. In Fig. 9, as an example of a preliminary test case, the gravity induced motion of a rigid sphere is shown. We use the FE method developed by Sugiyama et al. to model the dynamics of deformable IB. To test our implementation we carried out simulation of the motion and deformation of a compliant sphere placed in a cavity flow (see Fig. 10).

In FE based IB methods, the IB is represented on the Eulerian mesh through a colour function such as volume of fluid (VOF) or through a level set of a distance function. The position and velocity of the function representing the IB is updated through the hyperbolic advection equation $\frac{\partial f}{\partial t} + \boldsymbol{u} \cdot \nabla f = 0$, where f is either the VOF or the level set function, and $\boldsymbol{u}$ is the fluid velocity field. The accuracy with which sharpness of the IB-fluid interface, and volume and shape of the IB are maintained throughout IB's motion and deformation depends on the advection scheme used for solving the advection equation, and on the type of the function f chosen to represent IB. We are currently doing a literature survey (and testing) of the available advection schemes to find an accurate and inexpensive advection scheme for the equation of motion of the IB.

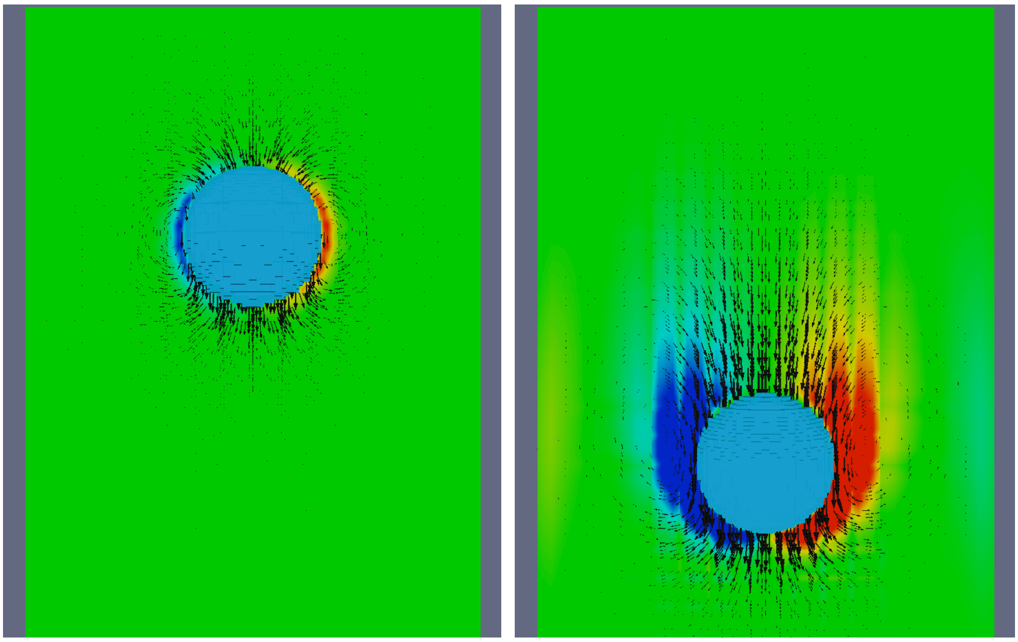


Fig. 9. Gravity induced motion of a rigid sphere at Re = 40. Left: Flow field at t = 0.1 sec. Right: Flow field at t = 1.9 sec. The colour contours represent vorticity and the arrows represent the velocity vector.

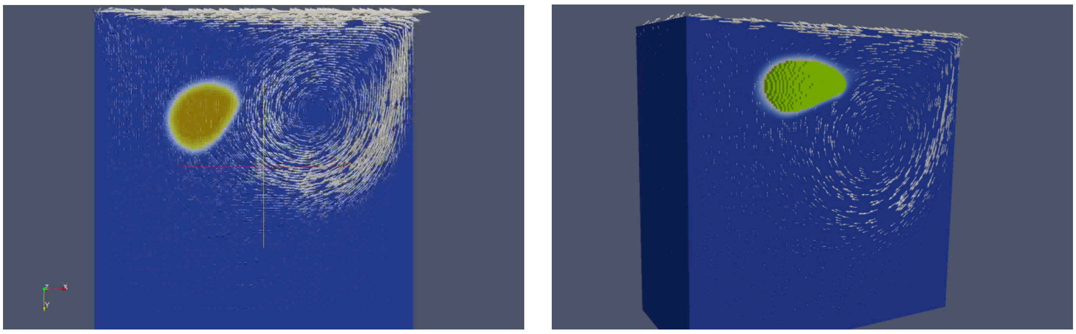


Fig. 10. A compliant deformable sphere place in a cavity flow at Re = 100. Left: Flow field and configuration of the sphere represented on a 2D place through the center of the deformed sphere. Right: Same as left pane but represented in 3D and at a different time instant.

[1] K. Nakahashi, High-Density Mesh Flow Computations with Pre-/Post-Data Compressions, Proc. AIAA 17th CFD Conference (2005) AIAA 2005-4876.
[2] P. L. Roe, Approximation Riemann solver, Parameter Vectors, and Difference Schemes, J. Comput. Phys. 43 (1981) 357-372.
[3] J. M. Weiss and W. A. Smith, Preconditioning Applied to Variable and Constants Density Flows, AIAA. 33 (1995) 2050-2056.

4. Schedule and Future Plan

(1) Five-year objectives and goals toward 2017

a. Construction and development of the simulation technology for bringing out the performance of K computer

b. Proposal of the technological trend of HPC simulation toward EXA-scale

(2) Long-term objectives

a. Establishment of the research and development center for industrial simulation technology

b. Contribution to computer science by expanding the developed simulation technology to different fields

(3) Time schedule

	2012	2013	2014	2015	2016	2017
Proposal of the project	Interview to the industry and feasibility study	Making specification list for the development				
Building light libraries		Library development		Porting guideline		

Application development

Development of the coupling algorithms for the PETA-scale computing		Development of the scaling algorithms	Development of the coupling algorithms			
Validation studies		PETA-scale applications			Performance test of the post PETA-scale applications	

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] W. S. Fu*, C. G. Li, M. Tsubokura, Y Huang and J. A. Domaradzki, An Investigation of Compressible Turbulent Forced Convection by an Implicit Turbulence Model for Large Eddy Simulation, Numerical Heat Transfer, Part A: Applications 64 (2013) 858-878.

(2) Conference Papers

[2] 大西　慶治，坪倉　誠, "階層型直交格子を用いた大規模自動車複雑形状空力解析", 日本機械学会 2013 年度年次大会, (2013).

[3] Onishi, K., Tsubokura, M., “Enhancement of Wall Boundary Condition for Dirty CAD on Building Cube Method based Immersed Boundary”, The 10th International Conference on Flow Dynamics (ICFD2013), (2013).

[4] Onishi, K., Obayashi, S., Nakahashi, K., Tsubokura, M., “Use of the Immersed Boundary Method within the Building Cube Method and its Application to Real Vehicle CAD Data”, AIAA-2013-2713, (2013)

[5] C. G. Li, M. Tsubokura, An implicit turbulence model for Preconditioned-Roe scheme by using Truncated Navier-Stokes Equations, 66th Annual Meeting of the APS Division of Fluid Dynamics.

(3) Invited Talks

[6] M. Tsubokura, “スパコン「京」の産業利用成果”, HPC 産業利用スクール「京」特別コース（スパコン技術産業応用協議会主催）, Jan. 15, 2014.

[7] M. Tsubokura, “「京」コンピュータが可能にする未来の自動車空力シミュレーション”, スーパーコンピュータ「京」を知る集い in 盛岡（理化学研究所主催）, Dec. 7, 2013.