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 unified framework for large-scale multiphysics problems

Based on the Building Cube Method (BCM), we have developed a unified solver framework CUBE (Complex Unified Building cubE) for solving large-scale multphysics problems. The framework has a modular design where CUBE provides a core library containing kernel functionalities e.g. a mesh, flow fields and I/O routines. Solvers are then developed on top of the kernel by connecting necessary kernel modules together, forming a "solver" pipeline, describing the necessary steps to solve a particular problem.

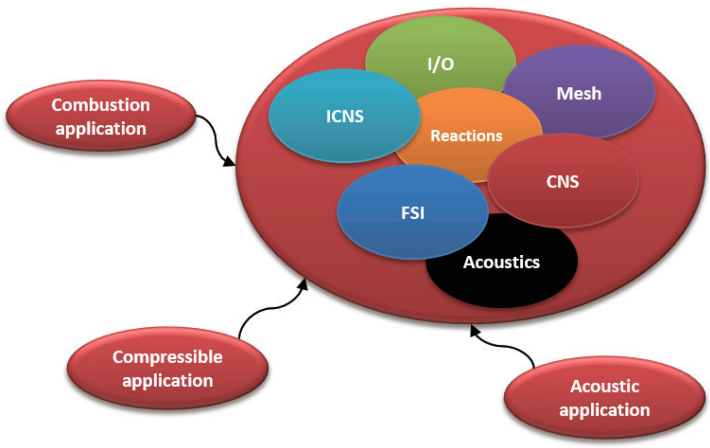
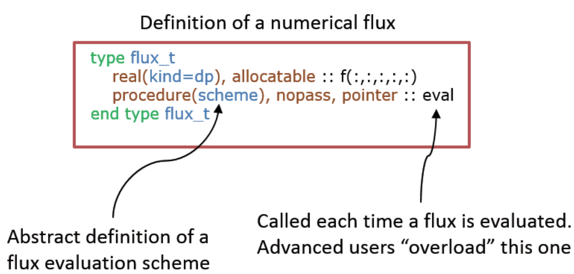


Figure 1. Framework of the unified solver CUBE.

Written in modern Fortran 2003, we have moved towards a fully Object-Oriented abstraction. Where a set of abstract classes defines canonical components of a solver, which is later overloaded by a real solver. Since the framework is targeted to different kinds of users, CUBE's framework already comes with a set of predefined solvers, intended for a general user.



By only providing simulation parameters and geometries, CUBE can be used as a regular flow solver. Advanced users can instead see CUBE as a library. And use it to develop own solvers, tailor-made for a particular application. Similar to other C++ based multiphysics frameworks, CUBE let advanced users overload certain kernel components in their application code. For example, if a user wish to write his own application specific flux evaluation routine, he would only need to overload the base definition of a numerical flux. Once done, the framework will execute the user's code instead of the one in the kernel every time fluxes are evaluated. This way we can keep CUBE's kernel small and general, without application specific code.

One of the recent addition to CUBE is its ability to handle chemical reactions. The current implementation aims towards a DNS/LES formulation, and supports both finite-rate and reduced reaction models as well as several species. In the case of reactive flow, we use a density based formulation and append an additional set of conservation laws to the flow problem.

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho\, u) = 0$$

$$\frac{\partial}{\partial t}\rho u + \nabla \cdot (\rho\, uu) = -\nabla p + \nabla \cdot \tau$$

$$\frac{\partial}{\partial t}\rho e_t + \nabla \cdot \left[\rho\, u\left(e_t + \frac{p}{\rho}\right)\right] = \nabla \cdot (u \cdot \tau) - \nabla \cdot q$$

$$\frac{\partial}{\partial t}\rho\, Y_k + \nabla \cdot (\rho\, Y_k u) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k$$

Figure 2. Navier-Stokes equations for a multi-species reactive mixture.

Here we have also strived for a general implementation, and have implemented most routines related to flow problems to handle both reactive and non-reactive flow. The kernel does not contain any reaction itself. Instead a user has to describe each reaction by himself in his application code and overload corresponding dummy reactions inside the framework.

Reactive flow is still under heavy development but an early example of this new feature is demonstrated below for a freely propagating premixed flame. Here the unit cube is filled with a fuel+air mixture, and one of the sides is heated in order to ignite the mixture.

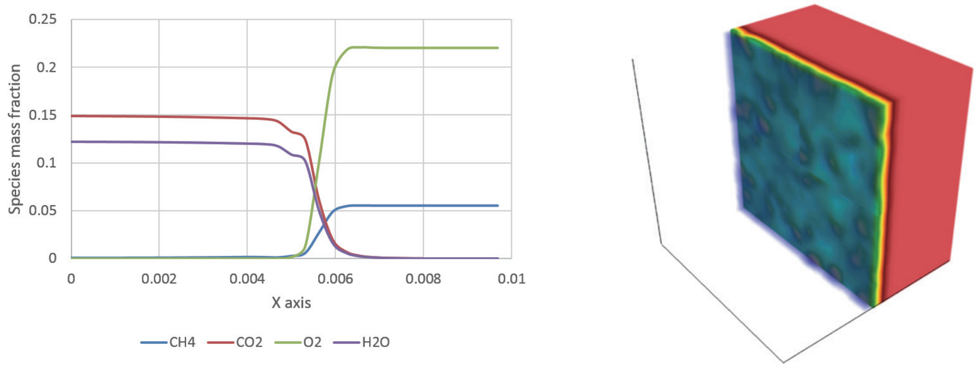


Figure 3. Species mass fraction (left) and Methane consumption at flame front (right).

As can be seen in Fig. 3, once the ignition process starts fuel is completely consumed and replaced with burnt products. Next year our aim is to continue this work and extend it to support reactive flow around as well as inside complex geometries.

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

The new software framework CUBE has been developed through this year, by conjunction with incompressible code which developed last year to realize the analysis in a real development process on the massively parallel environment, including pre- and post-processing.

We received a production vehicle CAD data from Mazda Motor Corporation and it's wind tunnel measurement data. The vehicle type is SUV which is relatively difficult to evaluate because it has large space in engine bay and narrow flow path within small parts affects the entire flow change acting on outside, especially under floor flow and grill opening drag.

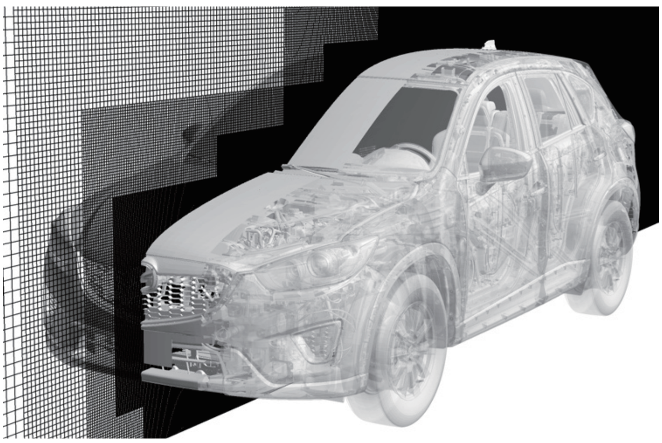


Figure 4. Overview of computational grid and geometry (provided by MAZDA Motor Company).

Figure 5. Flow visualization results of vortex structure

We have conducted basic validation of aerodynamic performance comparing with total pressure flow field which obtained by measurement. The typical flow characteristics especially longitudinal vortex structure around under floor, A-pillar vortex in wake region, side wake structure passed through front wheel arch has successfully reproduced. But, it was difficult to get high accurate results on the total drag force prediction because of the difficulty of integration on ‘dirty’ geometry data which is required to improve. To show the applicability on large scale analysis, we have conducted demonstration case using 27 billion numerical cells. Unfortunately we couldn’t run it enough longer to obtain the converged result due to the shortage of calculation resource, but MAZDA could decide to promote the results inside their organization, and continue the current research activity using our software in FY2015 by submitting the application and accepted the industrial use project on K-computer.

In addition, we have joined a research activity on Wind-HPC consortium which is organized by Tokyo Institute of Technology and several Japanese major construction companies. And provided our software. They are accepted the general use project on K-computer. The purpose of this project is to obtain accurate prediction on the wind pressure acting on building with a complicated shape, and very fine Cartesian grid. The actual urban area geometry has provided that is including housings, buildings, vegetation, and street, and so on. Then we provided a quick results using LES using very fine grids with large scale simulation for several are in Tokyo, then evaluated the turbulence characteristics on canopy and developed utilities to utilize the input boundary conditions on scale cascading condition. Finally, we have summarized the results to publish, it is still on going, and could get an upcoming post-K computer project regarding wind environment evaluation for building construction on severe climate condition.

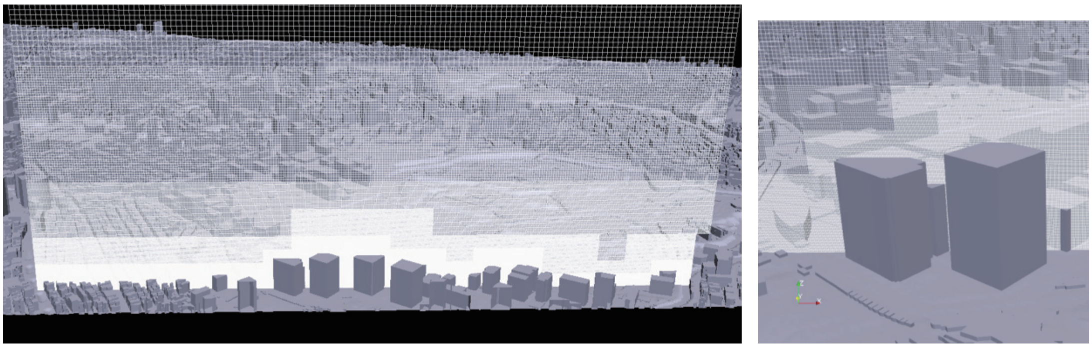


Figure 6. Overview of computational grid for wind environment analysis around Tokyo station area.

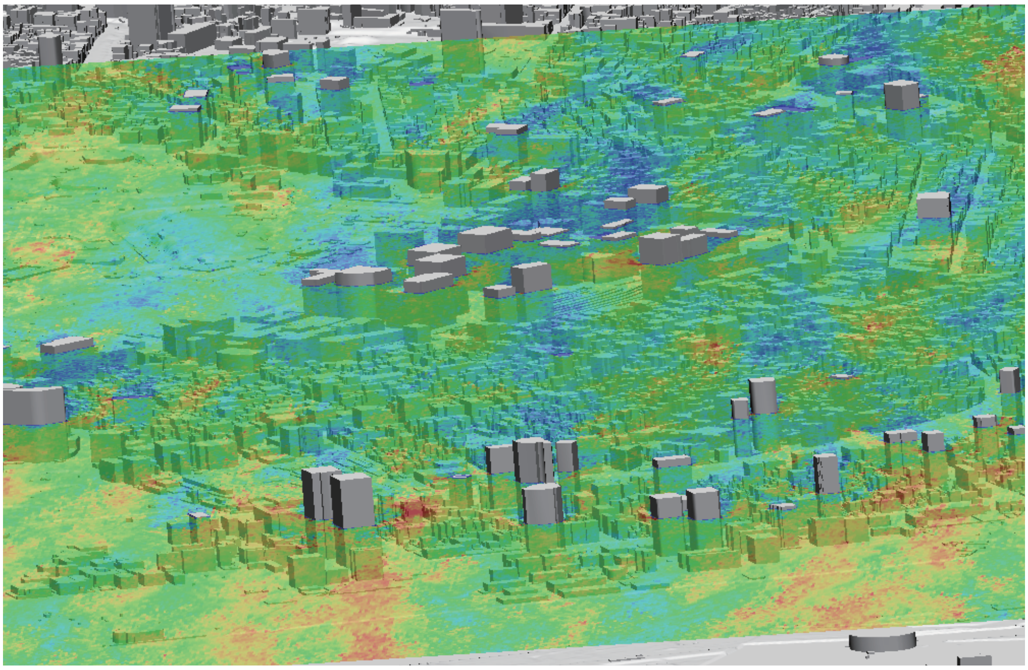


Figure 7. Example of the flow field results around Tokyo bay area.

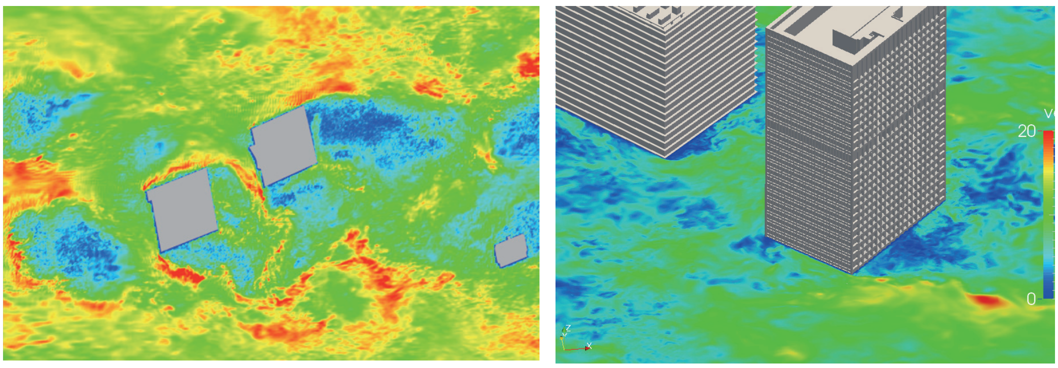


Figure 8. Detailed flow result showing specific building, showing the interaction of vortex and structure.

[1] Onishi, K., Tsubokura, M., Obayashi, S., and Nakahashi, K., "Vehicle Aerodynamics Simulation

for the Next Generation on the K Computer: Part 2 Use of Dirty CAD Data with Modified Cartesian Grid Approach," SAE Int. J. Passeng. Cars - Mech. Syst. 7(2):528-537, 2014, doi:10.4271/2014-01-0580.

[2] Onishi, K., Tsubokura, "Large-scale Simulation of Full Vehicle Aerodynamics using Cartesian Grid Approach optimized on K-computer", JSAE Paper Number: 20145232, No.24-14, 2014.

[3] Onishi, K., Tsubokura, M., Obayashi, S., and Nakahashi, K., "Practical applications for the computational vehicle aerodynamics on the massively parallel supercomputer: Part 2, hierarchical cartesian grid approach utilizing dirty CAD data", proceedings of 11th World Congress on Computational. Mechanics (WCCM XI). July 21, 2014, Barcelona, Spain.

[4] Onishi, K., Tsubokura, M., "Optimized preprocessing of tens of billions of grids in a full-vehicle aerodynamic simulation on the K-computer", INTERNATIONAL VEHICLE AERODYNAMICS CONFERENCE, Oct. 15th, 2014, Loughborough, UK.

[5] Tamura, T., Tsubokura, M., Nozu, T., Onishi, K., "HPC-based LES for wind forces on building in Tokyo", proceedings of 11th World Congress on Computational. Mechanics (WCCM XI). July 21, 2014, Barcelona, Spain.

[6] Tamura,T., Nozu, T., Tsubokura, M., and Onishi, K.,"LES of turbulent boundary layer flow over urban-like roughness elements", 67th Annual Meeting of the APS Division of Fluid Dynamics, Volume 59, Number 20, 2014, BAPS.2014.DFD.L25.5.

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

Aeroacoustics is one of the most important subjects in industrial applications such as vehicle aeroacoustics, fan noise in electronic devices and jet noise reduction … etc. In order to use the unified program developed by our team on this kind of topics to help industries to control the noise, the adaptability for turbulent flows, absorbing boundary condition to obtain accurate results, and immersed boundary condition for complex geometry have been developed and validated.

Fig. 9 shows the comparison of normalised turbulence intensities with the results of Kim [1] done by direct numerical simulation (DNS). It is indicated that under the condition of $\Delta t^{+} < 0.32$, our numerical scheme can accurately capture the turbulence phenomena. Through this study, the adaptability for turbulent flows of our numerical scheme is validated and the guide line of the parameters is also builded. The present results have been published in International Journal of Computational Fluid Dynamics [2].

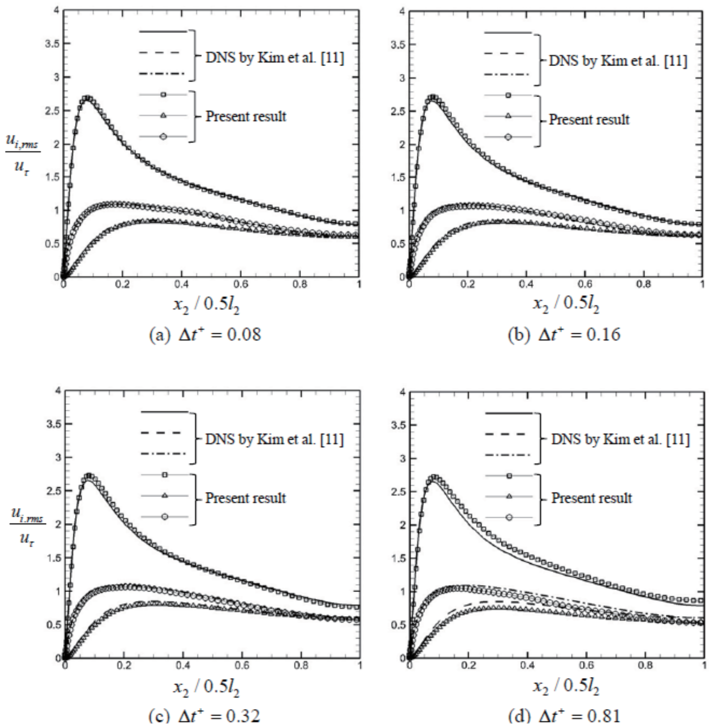
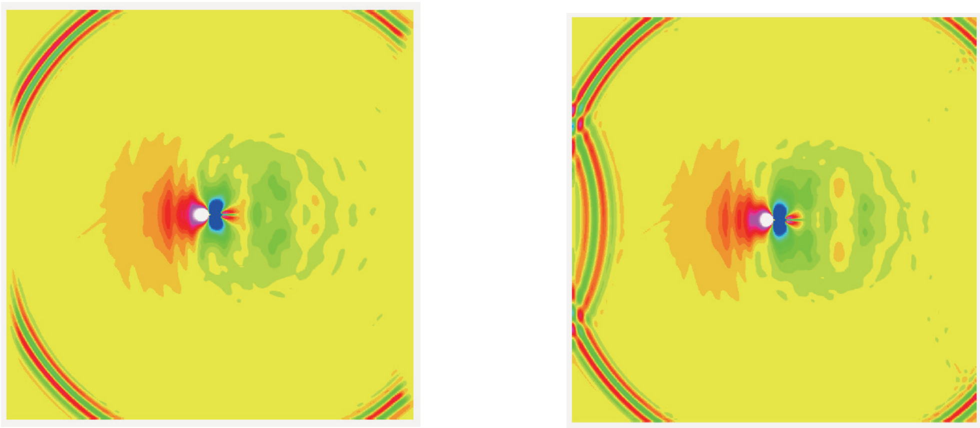


Figure 9. The comparison of normalised turbulence intensities with the results of Kim [1].

[1] Kim J, Moin P and Moser R, Turbulence statistics in fully developed channel flow at low Reynolds number, J. Fluid Mech. (1987) 133-166.

[2] C. G. Li, M. Tsubokura and K. Onishi, Feasibility investigation of compressible direct numerical simulation with a preconditioning method at extremely low Mach numbers, Int. J. Comput. Fluid Dyn. (2014) 411-419.

Because the order of the difference for the pressure between the aeroacoustic field and flow field is very large, the special treatment for the boundary is necessary to prevent the pollution on the aeroacoustic field. The absorbing boundary has been developed to handle the above issue. Fig. 10 shows the pressure fluctuation propagation across the boundary. In Fig 10(a), because the absorbing boundary is added in the left side, the pressure fluctuation can leave the computational domain without any reflection. On the other hand, in Fig 10(b), due to the lack of the absorbing boundary, the reflection of the pressure fluctuation affects the field.



(a) With absorbing boundary (b) Without absorbing boundary

Figure 10. The pressure fluctuation propagation.

With adaptability for turbulent flows and absorbing boundary condition, acoustic on a cascade of flat plate has been conducted. Owing to the complex phenomena and mechanism of the acoustic, the numerical scheme with high accuracy and immersed boundary condition for compressible flow are needed to capture the interaction of the pressure fluctuation between acoustic field and flow field. Fig. 11 shows the Instantaneous pressure fluctuation magnitude. The acoustic pressure is radiated from the plate can be clearly observed and the pressure fluctuation propagation can be well captured.

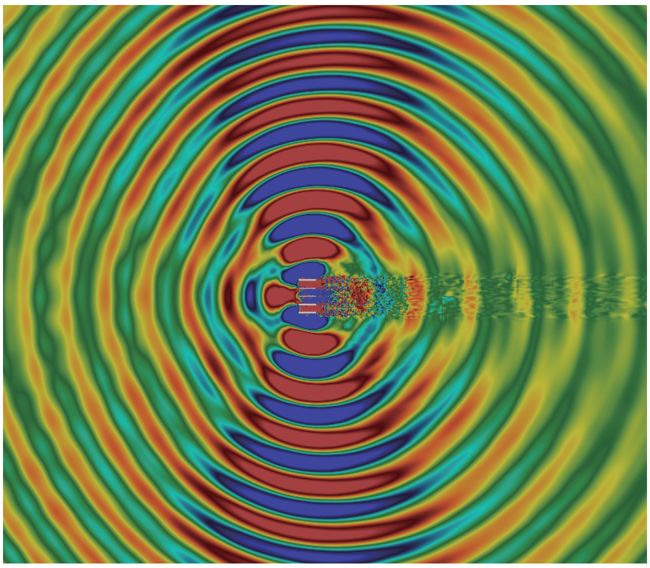


Figure 11. Pressure fluctuation

Based on the present results mentioned above, the computational aeroacoustic (CAA) on the vehicle will be conducted for the next year. Fig. 12 shows the preliminary results performed by the compressible program. The flow field around the whole car is simulated and the complex geometry of the car be well presented.

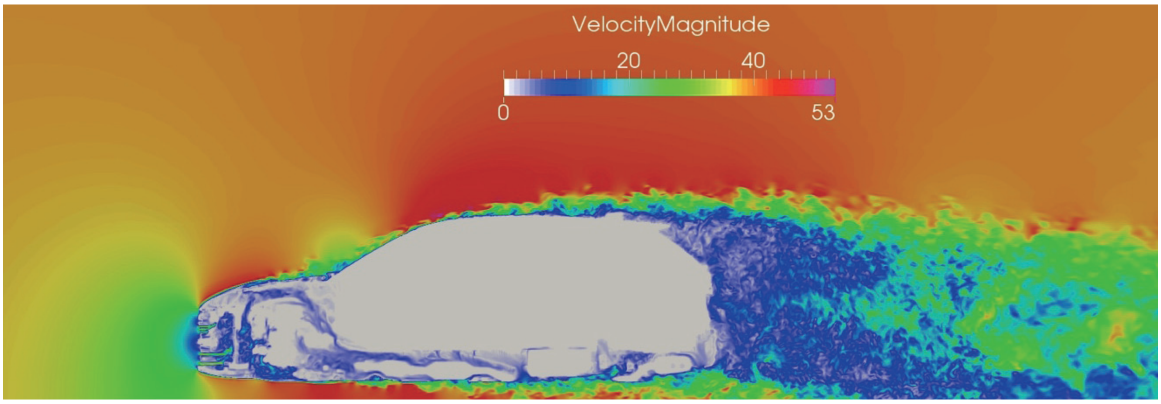


Figure 12. Velocity magnitude

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.

A fully Eulerian (FE) and Lagrangian-Eulerian based immersed boundary method (IBM) was implemented and tested. Through the FE-IBM we were able to obtain promising results with small-scale test cases in FY13. As was pointed out in the last report in FY13, the key limitation/drawback of the fully Eulerian based method is in the lack of its ability to accurately capture and maintain the original shape of the structure. This limitation of the fully Eulerian methods can partially be alleviated by using higher order advection schemes for the colour function that is used to represent the structure. In the case where the colour function is a level set, the limitation can be further alleviated through the reinitialization process. The higher order advection schemes, and the reinitialization process in the case of level set, are able to represent the shape of structures that have simple geometries with no sharp changes in curvature (eg. a sphere, torus, etc.). But, for more complex real-world geometries, which involve sharp changes and discontinuities in curvature, the ability of FE methods to retain original shape over time is lacking. The maintenance of the shape of the structure over time is limited by the grid scale and numerical diffusion. While the numerical diffusion can be reduced by higher order schemes, the grid resolution necessary for accurately representing and maintaining the shape of the structure is prohibitively small.

Owing to the limitation of FE methods for IBM discussed above, it was decided that the capabilities and limitations of Lagrangian-Eulerian (LE) based IBM need to be reassessed. The two main limitations of LE approach and possible resolution of these limitations are discussed below.

I. LE methods involve expensive interpolation operators between the Lagrangian mesh and the Eulerian mesh.

The interpolation between Lagrangian and Eulerian meshes, for a given point on the Lagrangian mesh, involves searching a set of nearest neighbouring Eulerian mesh points. It is this searching operation that makes the interpolation expensive. To overcome this limitation we have developed a *Lagrangian BCM data structure*. This new data structure eliminates the 'search' step of the interpolation. The nearest set of Eulerian neighbours are now located by simple inexpensive *arithmetic operations* rather than expensive search operations. The *Lagrangian BCM data structure* has been recently added to the code with the unified framework: Complex Unified Building cubE method (CUBE)

II. Moving structures involve moving Lagrangian meshes which increases the difficulty of load balancing.

A dynamic load balancing method has been implemented in the Unified BCM framework (CUBE). The dynamic load balancing technique in use can easily be modified to account for a mobile Lagrangian mesh. This is done by assigning a larger weight to BCM cubes with Lagrangian mesh during grid partitioning.

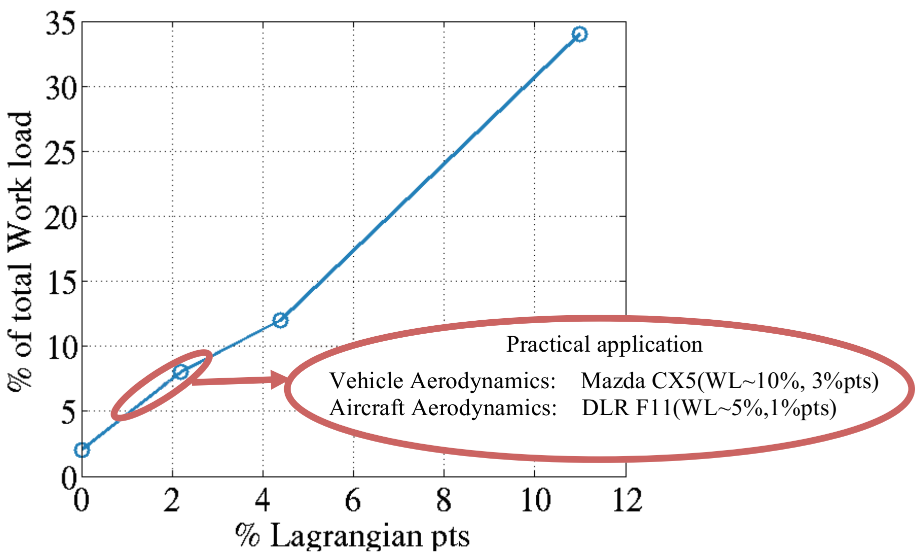


Figure 13. Profiling data for LE based IBM. Percentage of total time spent on Lagrangian operations plotted against proportion of Lagrangian points relative to BCM mesh size, i.e (No. Lagrangian pts)/ (BCM mesh size) * 100.

Reinit Iterations	20	50	100	200
% Work Load	9	19	32	48

Table 1. A comparison of percentage time spent on reinitialization of the level set for increasing reinitialization iterations (Note: These are crude extrapolated estimates.).

Performance comparison LE vs FE: Fig. 13 shows the results of performance evaluation of LE based IBM solver. In the figure percentage work load (WL) is plotted against proportion of Lagrangian points relative to the number of Eulerian mesh points (BCM mesh size). The work load ranges from 2% for 0.01% Lagrangian points to 34% for 10% Lagrangian points. The Lagrangian-Eulerian approach is practical only if the WL of Lagrangian operations is less than 20%. Real world applications of interest to our research are vehicle aerodynamics, aircraft aerodynamics, urban flow dynamics, etc. As is highlighted, in Fig. 13 for practical application of interest the percentage of Lagrangian points ranges from 1% to 4%.; for proportion of Lagrangian points in this range, the work load ranges from 5% to 12%. We believe that this amount for work load for the Lagrangian is reasonable for practical applications.

In Table 1 we present the performance analysis of Fully Eulerian based IBM solver, where the structure is represented by a level set function. As alluded to above, level set undergoes distortion due to motion of the structure and numerical diffusion. This distortion has to be corrected at every time step of the solver, which is done through the reinitialization process. Reinitialization is an iterative process that is carried out until the level reaches the desired state (in our case, accurate representation of the shape of the structure). The number of iterations necessary for the level set to reach the desired state depends on several factor, namely: complexity of the geometry, problem size, etc. For simple geometries like a sphere, the iteration necessary are of the order of O(10), more complex geometries like a vehicle the number is of the order of O(100). The work load of the reinitialization ranges from 9% to 48% for 20 to 200 iterations. For most practical applications, anywhere between 20 to 100 iterations would necessary, the load corresponding to these iterations ranges between 9% to 30%.

Despite our a priori expectation that a Fully Eulerian approach would be computationally less expensive, we find that the Lagrangian based approach has a slight edge over Fully Eulerian approach.

[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 Application development		Porting guideline		
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. Makoto Tsubokura, Andrew Hamilton Kerr, Keiji Onishi, Yoshimitsu Hashizume: Vehicle Aerodynamics Simulation for the Next Generation on the K-computer: Part 1 Development of the framework for fully unstructured grids up to 10 billion numerical elements, SAE International Journal of Passenger Cars – Mechanical Systems, 7(2): 2014-01-0621(2014)
2. Keiji Onishi, Makoto Tsubokura: Vehicle Aerodynamics Simulation for the Next Generation on the K computer: Part 2 Use of Dirty CAD Data with Modified Cartesian Grid Approach, SAE International Journal of Passenger Cars – Mechanical Systems, 7(2): 2014-01-0580(2014)

3. Chun-Gang Li, Makoto Tsbuokura, Keiji Onishi: Feasibility Investigation of Compressible Direct Numerical Simulation with Preconditioning Method at Extremely Low Mach Numbers, International Journal of Computational Fluid Dynamics, vol.28, Issue 6-10, pp.411-419 (2014)
4. 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.
5. 坪倉誠，大西慶治：HPC-LES を活用した自動車用数値風洞の開発，ターボ機械（ターボ機械協会誌），vol.42, No.5, pp.36（324）-43（325）（2014）
6. 坪倉誠，大西慶治：自動車の大規模空力シミュレーション　―非構造格子 vs. 構造格子―，情報処理（情報処理学会誌），vol.55, No.8, pp.823-828 (2014)

(2) Conference Papers

7. **Makoto Tsubokura**, Ryuya Kobayashi, Shoya Ota, Shinji Okamine, Kinzan Ryu, Toshio Onuma, Nobuhiro Sasuga: The Effect of Wheel Geometry on the Total Aerodynamic Drag of a Road Vehicle, 32nd AIAA Applied Aerodynamics Conference (16-20, June, 2014, Hyatt Regency Atlanta, Altanta, GE), AIAA-2014-3126 (2014)
8. Kohei Nara, **Makoto Tsubokura**, Jun Ikeda: A Numerical Analysis of Unsteady Aerodynamics of Formula Car during Dynamic Cornering Motion, 32nd AIAA Applied Aerodynamics Conference (16-20, June, 2014, Hyatt Regency Atlanta, Altanta, GE), AIAA-2014-3138 (2014)
9. Jing Li, **Makoto Tsubokura**, Masaya Tsunoda: Numerical Investigation of Drag Crisis of a Sphere and the Effect of Surface Roughness, 10th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements (17-19, September, 2014, Don Carlos Resort, Marbella, Spain)
10. Keiji Onishi, **Makoto Tsubokura**: Optimized preprocessing of tens of billions of grids in a full-vehicle aerodynamic simulation on the K-computer, Proceedings of the 2014 International Vehicle Aerodynamics Conference (14-15, October, 2014, Holywell Park, Loughborough, Great Britain), pp.149-158 (2014)

(3) Invited Talks

11. 坪倉誠：「京」が拓いた新たなものづくり　～自動車空力設計を例に～，未来をひらくスーパーコンピュータ　～「京」からその先へ限りなき挑戦～（理研計算科学研究機構、高度情報科学技術研究機構主催）（2014 年 8 月 23 日、24 日、科学技術館、東京）
12. 坪倉誠 : HPC-CFD が拓く自動車空力シミュレーション :（2014 年 12 月 19 日、JAXA

相模原キャンパス）

(4) Posters and presentations

13. Andrew H. Kerr, Keiji Onishi, **Makoto Tsubokura**: Practical Applications for the Computational Vehicle Aerodynamics on the Massively Parallel Supercomputer: Part 1, Framework for the Fully Unstructured Finite Volume Cells, 11th World Congress on Computational Mechanics (WCCM XI), July 20-25, 2014, Barcelona, Spain (2014)
14. Keiji Onishi, **Makoto Tsubokura**, Shigeru Obayashi and Kazuhiro Nakahashi: Practical Applications for the Computational Vehicle Aerodynamics on the Massively Parallel Supercomputer: Part 2, Hierarchical Cartesian Grid Approach Utilizing Dirty CAD Data, 11th World Congress on Computational Mechanics (WCCM XI), July 20-25, 2014, Barcelona, Spain (2014)

(5) Patents and Deliverables