13. Complex Phenomena Unified Simulation Research Team

13.1. Team members

Makoto Tsubokura (Team Leader)

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13.2. 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 cutting-edge 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.

13.3. Research Results and Achievements

13.3.1. Feasibility study of the building-cube method for complicated geometry

As a candidate of unified data structure for complicated and coupled phenomena, we focused on the building-cube method (BCM) proposed by Nakahashi[1]. The basic strategy of mesh generation by BCM is as follows: (1) Target flow field is decomposed into cubes of various sizes with their side length given as the exponent of 2 with respect to the minimum side length as one; (2) Each side of the cubes with the same size is subdivided at even intervals and uniform Cartesian mesh is generated in each cube. It should be noted that the number of grids is the same for all cubes with different sizes. The advantages of the BCM against the conventional unstructured grid used in the CFD of industrial applications are: Firstly, the data format is fully structured, making it easy to handle the hierarchical cash memories, and thus higher peak performance for single core is expected; Secondly, by allocating the same number of cubes for each core, exactly the same load balance including core to core communication is achieved, and thus higher parallel performance is expected. On the other hand, the disadvantage of the Cartesian mesh including the BCM is the treatment of the curved surface typically observed in industrial products. In this study, in addition to the conventional immersed boundary method to treat the curved surface by the voxel grid, additional methods are implemented to re-construct the solid surface information for flow simulation including the treatment of thin or thick-less geometry data. In fact these new methods turn the disadvantage of the solid body treatment in the Cartesian mesh into an advantage to the unstructured grid. By using the methods we could generate the numerical mesh by BCM without modifying the data defect in CAD data, such as little gaps or overlaps between two parts or unnecessary tapped hole on the surface.

The feasibility of the BCM including solid-surface treatment was tested in the real CAD data utilized in automotive industry, as shown in Fig. 1. Some data defections observed in the CAD data are indicated in Fig.2, in which the regions with red and cyan color show little gaps and overlaps between two parts, respectively. The number of the defections amounts to more than 1,000 places, and requires modification by hands if we generate conventional unstructured grids. Typically a couple of days are required for the modification in real industrial processes. On the other hand, we have confirmed that it took only less than 10 minutes including the automatic surface modification to generate BCM mesh of about 150 million cells, as shown in Fig. 3. In the mesh generation, the size of the analysis domain is given as 40m by 10m by 10m, which is divided by 87,558 cubes, and each cube is subdivided by 8x8x8 cells. In this case, the surface resolution is about 5mm on the vehicle surface.

Flow structures and the magnitude of flow velocity around the vehicle are visualized in Fig.4. The simulation was conducted on the K-computer using 512 CPUs. It took only about 4 wall-clock hours to obtain the result, including the mesh-generation time. The feasibility study has been successfully finished by validating the BCM for engineering CFD.

Fig. 1 CAD data of a full-scale road vehicle used in an industrial process.

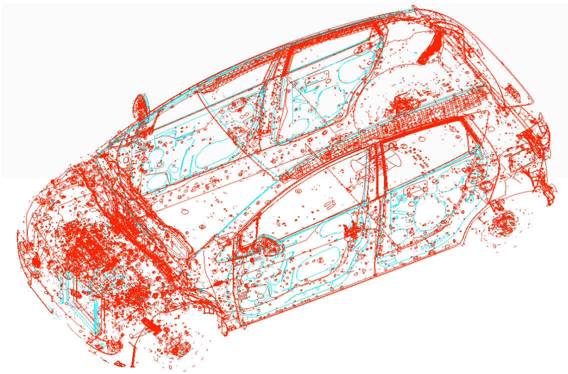


Fig. 2 Data defecting points in a CAD (red: gap, and cyan: overlap of two parts).

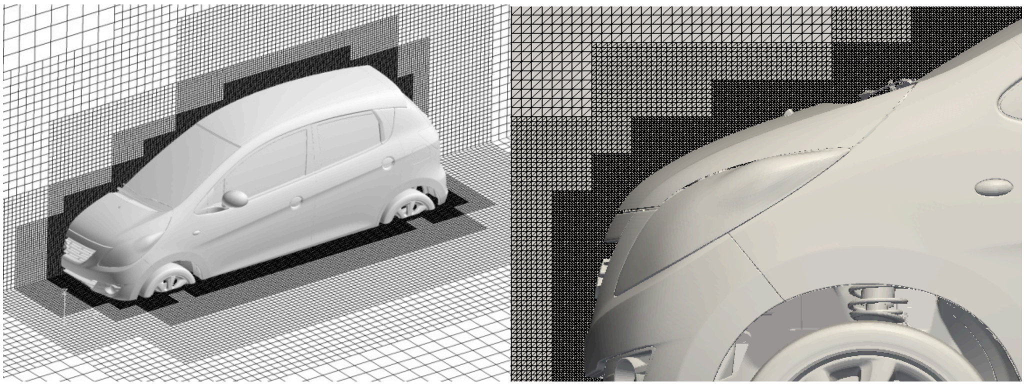


Fig. 3 BCM mesh generated around a full-scale vehicle using about 150 million cells.

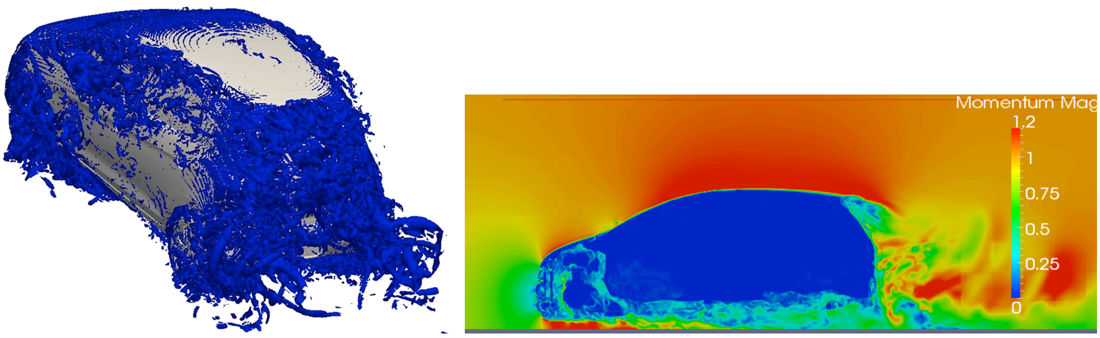


Fig. 4 Flow structures (left) and the magnitude of flow-velocity around the vehicle.

13.3.2 Feasibility study of a pre-conditioning compressible simulation for unified low to moderate Mach number turbulent flow

For the purpose of unifying the simulation, the fluid compressibility, turbulent effects and heat transfer should be taken into consideration simultaneously. In such kind of sever situation, the program which could only cope with the incompressible flow would be restricted for the practical applications. In order to solve the problem mentioned above, the preconditioning method which can be used on turbulent compressible flow in the full speed regions have been investigated and developed in the presently study.

The Roe scheme [2], Weiss and Smith preconditioning method and dual time stepping [3] have been implemented because of their sophisticated applicability on the transient state problems. For the sake of investigating the validation of this method on the low speed compressible turbulent flow ($M = 0.005$), the channel flow at $\mathrm{Re}_\tau = 180$ has been performed and all the simulation conditions are based on the direct numerical simulation based on the spectral method for incompressible flow conducted by Kim et al [4].

Figure 8 are the instant contour of the velocity magnitude and shows several noticeable turbulent characteristics. In the x_1x_2 plane, the flow field is unstable and contains different scales of the velocity magnitude near the wall. These phenomena are due to the turbulence injection from the wall. From the x_2x_3 plane, the injection can be observed more clearly near the wall. Besides, the streakline is also an important characteristic for the turbulence. In the x_1x_3 close the wall, there are several clear streaklines which can be easily distinguished.

Based on the present results mentioned above, there are several conclusions listed below. Firstly, this method can be used on very low Mach region and the result is in good agreement with the incompressible flow method. Secondly, it should be recognized that most of industry applications belongs the turbulence. This method also shows it has good capability on solving turbulence flow. Thirdly, preconditioning would change the temporal term and the governing equation is not suitable for transient state problems. Dual time stepping overcomes this disadvantage. From the turbulence statistical results, it can be known that the Roe scheme, Weiss and Smith preconditioning method and dual time stepping can be used on transient state problems. Therefore, this program will be a powerful tool on unifying the simulation method.

Besides, this method will be also a promising candidate for our next target-computational aeroacoustic (CAA). Basically, the study of aeroacoustic noise involves two academic fields. One is the compressible turbulent flow and the other is aeroacoustics. Usage of the results of the disturbance of density, pressure and velocity obtained from the compressible turbulent flow as an aeroacoustic source substitutes into the appropriate governing equations for example, Lighthill or Ffowcs Williams and Hawkings equations to calculate the noise propagation.

Due to the instinct of the compressible flow program, this method has the potential to accurately capture the density variation and turbulent fluctuations which are the main aeroacoustic source in the flow field. Therefore, the present program can be used to calculate the aeroacoustic source in the practical applications of controlling noise.

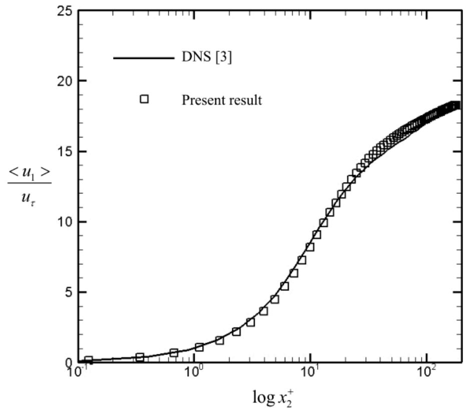


Figure 5. The distributions of mean velocities

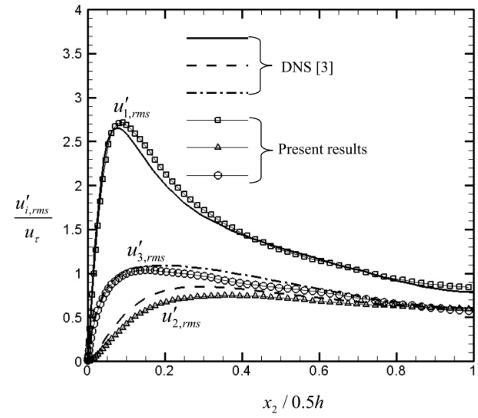


Figure 6. The distributions of turbulent intensities

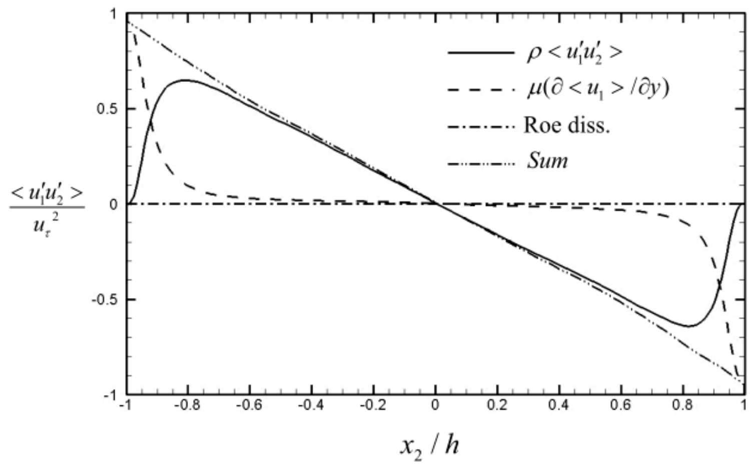
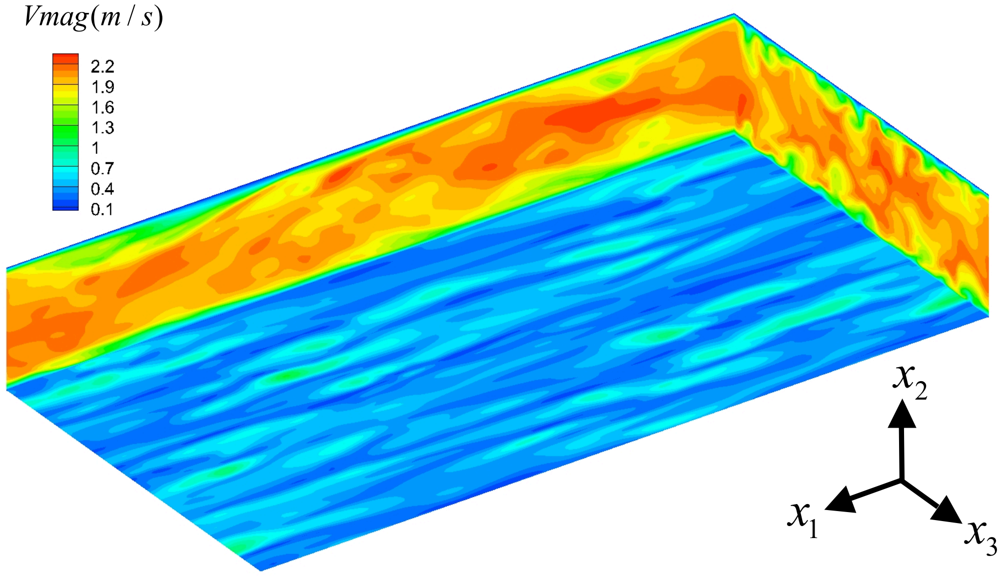


Figure 7. The distributions of Reynolds stress



Figures 8. The instant contour of the velocity magnitude

[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] J. Kim, P. Moin and R. Moser, Turbulence statistics in fully developed channel flow at low Reynolds number, J. Fluid Mech. 177 (1987) 133-166.

13.4. 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	

13.5. Publication, Presentation and Deliverables

(1) Journal Papers

-None

(2) Conference Papers

-None

(3) Invited Talks

1. Makoto Tsubokura: Next-generation design system for aerodynamics/thermal management for road vehicle development, K-computer symposium 2012 (15th, June, 2012 at Univ. Kobe, Shin-Kokusaikaigijou) in Japanese
2. Makoto Tsubokura: Vehicle-aerodynamics development using supercomputer and challenge for the new mystery of aerodynamics, Supercomputer K wo shiru tsudoi in Kanazawa(4th, August, 2012 at Kanagawa Bunkyoukaikan) in Japanese
3. Makoto Tsubokura: Vehicle-aerodynamics development using supercomputer and challenge for the new mystery of aerodynamics, Supercomputer K wo shiru tsudoi in Kanazawa(4th, August, 2012 at Kanagawa Bunkyoukaikan) in Japanese

(4) Posters and presentations

-None

(5) Patents and Deliverables

-None