Revolutionary Simulation Software for the 21st Century

Project Representative

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In this project, we chose six important sub-projects- turbulence simulation, internal flow computation for turbomachinery, analysis of heat transfer in a gas turbine, structural analysis, protein simulation, and nano-scale simulations- as representative topics from the fields of engineering, life science, and nanotechnology and achieved the following results.

In the turbulence simulation, we conducted one of world's largest unstructured large eddy simulation (LES) of air flow around a full-scale road vehicle. The main objective of our study was to look into the validity of LES for the assessment of vehicle aerodynamics, especially in the context of its possible application for unsteady or transient aerodynamic forces. First, the method was validated by comparing the reproduced organized flow structures around a vehicle with those obtained by wind tunnel measurement. Then, unsteady aerodynamic forces acting on the vehicle during transient yawing-angle changes were estimated and the relationship between the flow structures and the transient aerodynamic forces is examined. We found that LES can provide precious aerodynamic data, which conventional wind tunnel tests or RANS simulations are difficult to provide.

In the internal flow computation for turbomachinery, LES of internal flows of a mixed-flow pump was performed. The test pump had open impeller blades and diffuser vanes. The objective of this research was to verify the accuracy of the pump performance prediction by LES with a particular emphasis placed on the instability characteristics. The LES successfully predicted the instability characteristics. By analyzing computed flow fields, we can investigate the detailed mechanism leading to the instability characteristics.

In the analysis of heat transfer in a gas turbine, LES was used to predict heat transfer coefficients on a gas-turbine blade (PW6000). We computed the transitional boundary layer around the blade and predicted distribution of the static pressure and heat transfer coefficients on its surfaces.

In the field of structure analysis, FrontSTR enables analyses models with a billion degree of freedom. Test calculation on such large models showed FrontSTR's efficiency. The parallel ratio is more than 99.98%, and the performance in each process is about 4GFlops which is 50% of the peak.

In the protein simulation, we performed a series of benchmark FMO-MP2/6-31G calculations with the ABINIT-MP program on the Earth Simulator. A new route to integral transformation through DGEMM was created for the MP2 processing. The aricept-acetylcholinesterase complex (8,409 atoms and 46,831 AOs) was processed in 19.6 minutes with 4,096 VPUs, implying promising applicability of FMO-MP2 calculations to structure-based drug design.

In the nanoscale simulation, we have calculated the energy levels of the As As-donor state in Si, using the PHASE, which is

a first principles calculation code. We succeeded in calculating a 10,648-atom system using 4,096 CPUs on the Earth Simulator. In the system, the energy levels have been well converged.

Keywords: large eddy simulation, aerodynamic force, formula car, mixed-flow pump, gas-turbine blade, FMO, MP2, first principles calculation, As donor state

1. Assessment of unsteady aerodynamic forces on a passenger vehicle using LES [1][2][3]

The objective of this sub-project was to emphasize the validity LES by applying the high performance computing (HPC) technique to an aerodynamic assessment of automobiles.

In vehicle aerodynamics, greater attention is being paid to unsteady aerodynamic forces generated from sudden steering action, overtaking, or cross-wind conditions. It is difficult to measure such unsteady aerodynamics by conventional wind tunnel tests or RANS models. The advantage of LES, in addition to its high accuracy, is its possibility of capturing such unsteady forces, which will contribute to aerodynamic design innovations in automotive industry.

1.1 Reproduction of eddy structures around a vehicle

It is considered that unsteady aerodynamic forces are generated by unsteady eddy structures around vehicles. Thus, first, unsteady flow structures around a production sedan were visualized from numerical results obtained by ES, which was validated by a wind-tunnel measurement, as illustrated in Fig. 1. Our LES generally shows good agreement with experimental results.

1.2 Unsteady aerodynamic forces during dynamic yawing angle change

The transient flow during a dynamic yaw-angle change was then visualized to investigate the relationship between the flow and the unsteady aerodynamic force. To mimic a sudden cross wind, the yaw angle of the vehicle was changed from 0 to -10 degrees in 0.05 second after the flow reached a fully developed state from the initial condition, then the angle was fixed at -10 degrees for 0.05 second and recovered to 0 degrees again in 0.05 second, as illustrated in the top panel of Fig. 2. The bottom panel plots the time series of the yawing moment acting on the vehicle. The profiles overshoot during the dynamic yaw-angle change and the absolute value is about three or four times larger than the ones when the motion is static (T = 0.15 ~ 0.20 sec). Such excess unsteady forces are successfully explained through the snapshots of the pressure distribution obtained by our LES (Fig. 3).

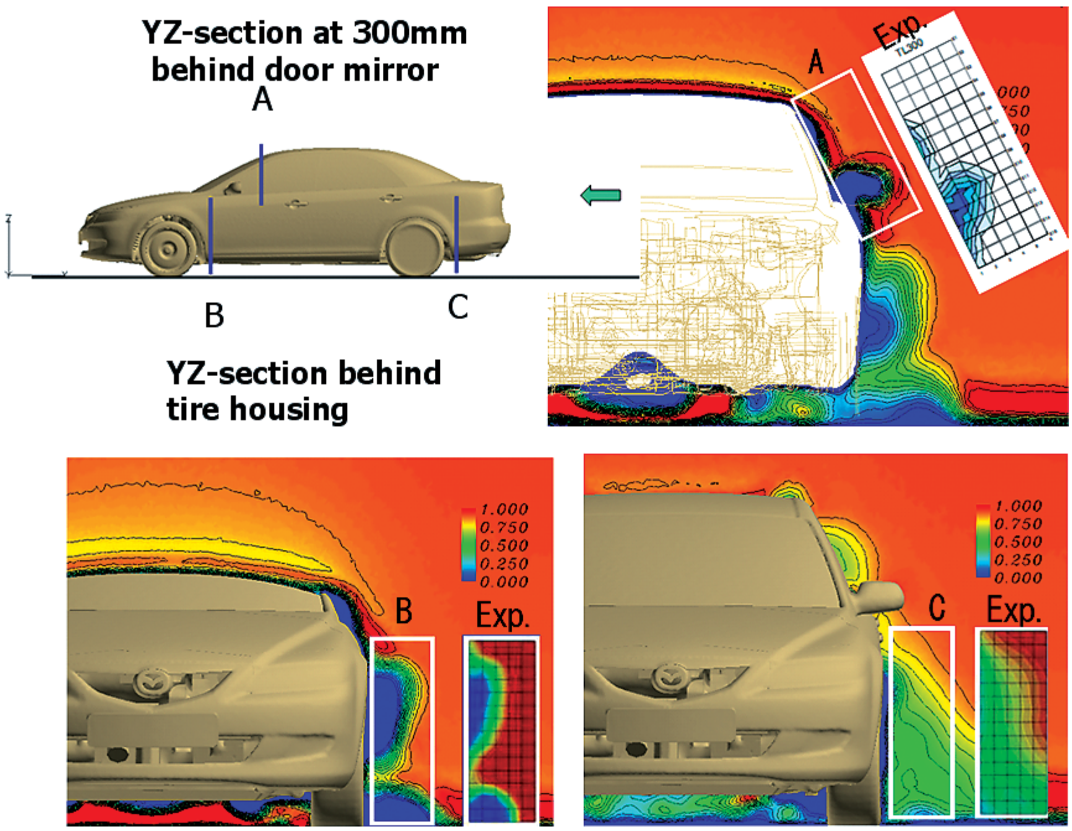

Fig. 1 Flow structures on the side of a vehicle (total pressure distributions) and its comparison with the wind-tunnel experiments.

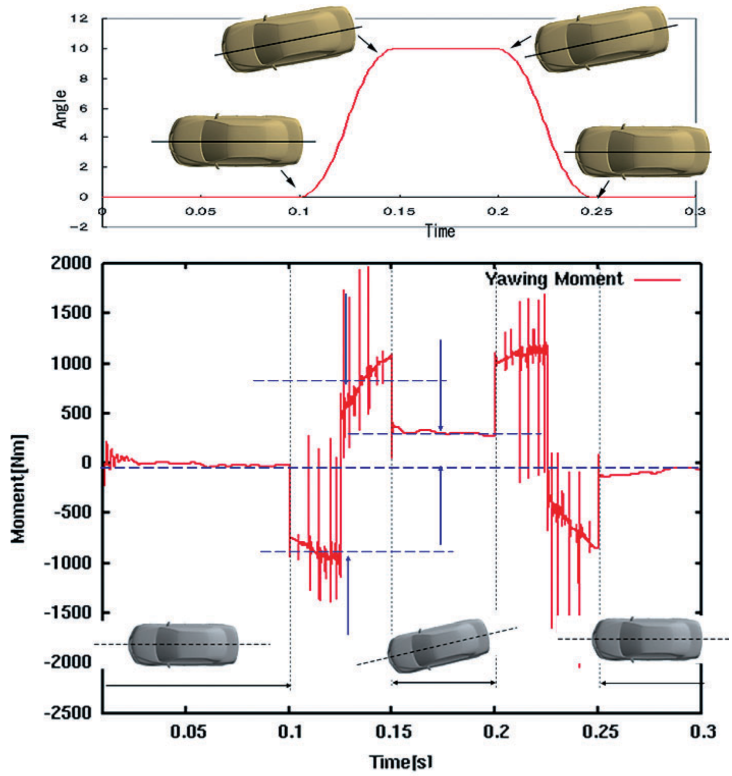

Fig. 2 Time history of the vehicle yawing angle (above) and the yawing moment obtained (below).

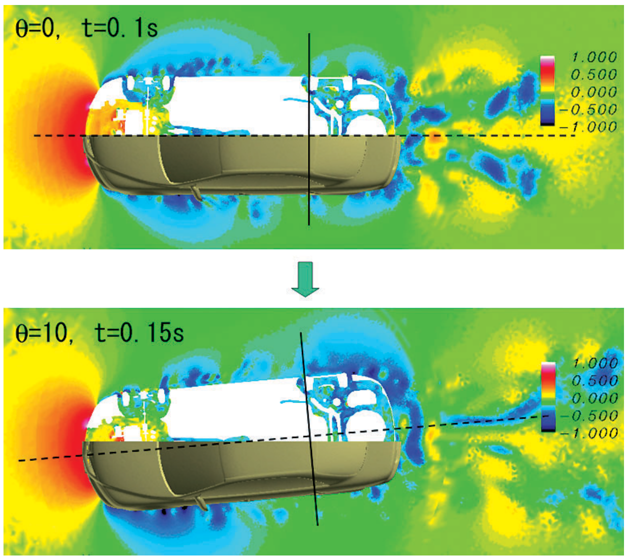

Fig. 3 Snapshots of the pressure distributions around the vehicle during the dynamic yawing-angle change.

2. Internal flow computation for turbomachinery

We performed LES of internal flows of a mixed-flow pump to achieve accurate predictions of pump performance for full flow-rate range. We especially focused on the flow rate where instability characteristics appear, which is about 50%~60% of the designed flow rate. A test pump in this research was a mixed-flow pump with an open impeller and diffuser vanes.

We used our original parallel LES code, FrontFlow/blue, to predict unsteady flows in the test pump. This code is based on the finite element method (FEM) with hexahedral elements and has second-order accuracy in both time and space [4][5][6]. For the LES, we prepared a coarse mesh composed of about 8 million elements and a fine one composed of 80 million elements. We intend to resolve the turbulent boundary layer on the blades of a pump by the fine mesh. Here, we show the results for the coarse mesh as preliminary results.

Figure 4 shows the Euler's head and total head computed by LES using the coarse mesh. We confirmed that the computed results agree with measured data (not shown). We successfully captured the pressure drop at the flow rate (50%~60% of designed flow rate) as in the measured data. We also confirmed that predictions of pump performance are improved by using the fine mesh, especially at the flow rate where instability characteristics appear. We will investigate the relationships between the internal flows and instability characteristics by analyzing the internal flow (e.g. stream lines on the impeller surface, see Fig. 5) in order to understand the mechanism of the instability characteristics.

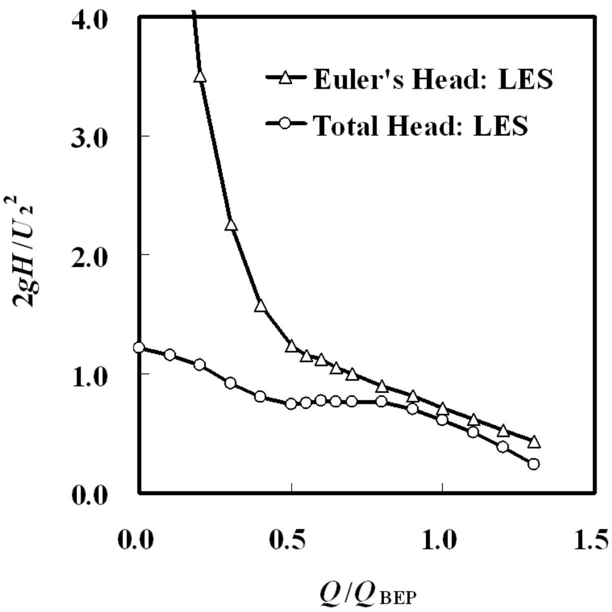

Fig. 4 The Euler head and total head computed by LES.

3. Analysis of heat transfer in a gas turbine

Accurate predictions of the transition and heat transfer distributions are crucial to the design of various kinds of turbomachinery. This paper presents the results of numerical predictions of heat transfer coefficient on a gas-turbine blade using LES. We used an in-house CFD code, Front Flow/blue [4][5][6] in the LES. We computed the transitional boundary layer around a gas-turbine blade and predicted heat transfer coefficients on the blade's surfaces.

The test blade in this research was a turbine blade of a PW6000 jet engine, developed by Pratt & Whitney. This blade is regarded as the benchmark for studies of the prediction of heat transfer coefficients and it has been used in many studies and experiments [7][8].

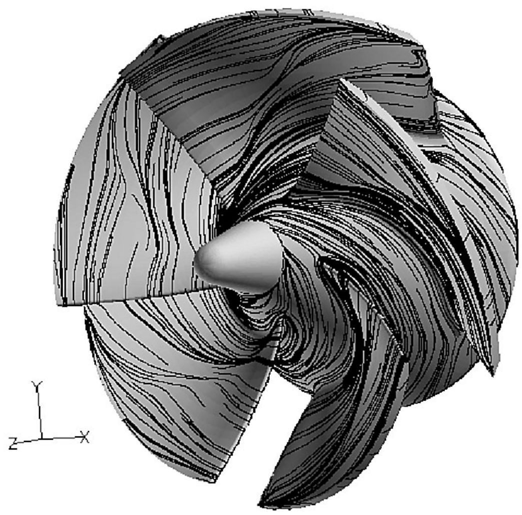

Fig. 5 Stream lines on rotor blades (designed point).

The instantaneous distribution of the magnitude of vorticity computed by the LES is represented in Fig. 6. It can be seen that on the suction side, strong vorticity is captured from the transition point. Near the transition point, the vorticity is higher, and in the fully developed turbulence region, the streak structure is captured.

In Fig. 7, Stanton numbers measured by Radomsky

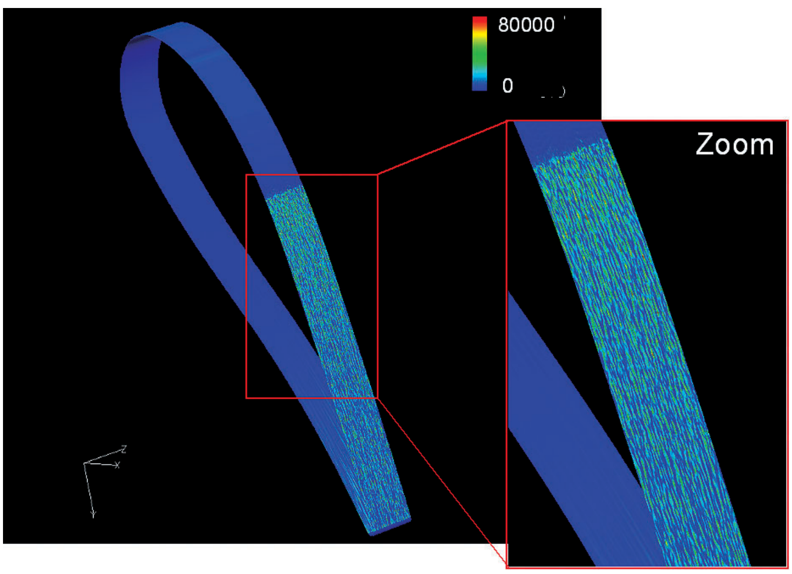

Fig. 6 Magnitude of vorticity distribution on the blade's surface.

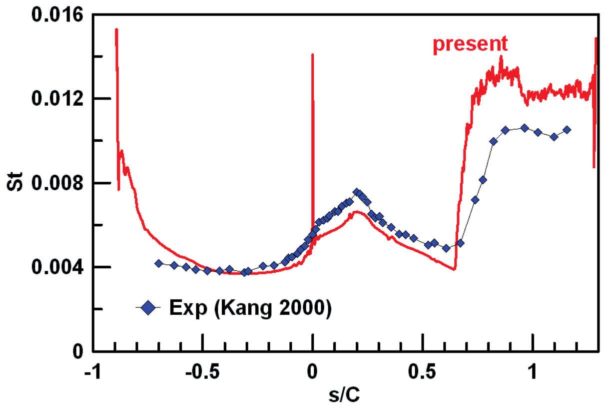

Fig. 7 Stanton number distribution on the blade's surface.

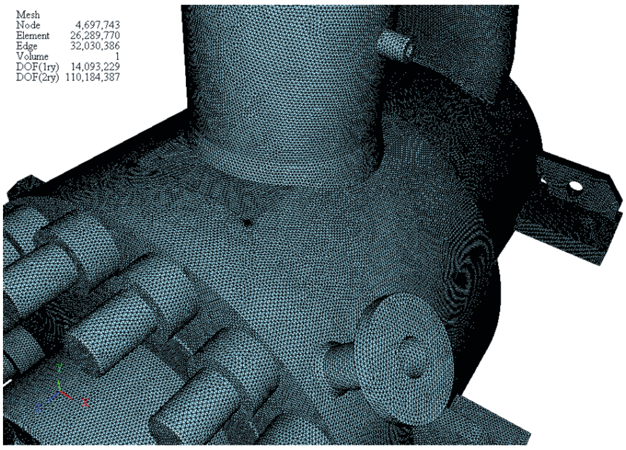

Fig. 8 Mesh of the model.

(2000) [7] and those computed by LES are compared. This calculation could not predict the heat transfer quantitatively. In the turbulent region and the pressure side, the Stanton number is overestimated, and in the other region, it is underestimated. The shapes of both results are similar, however, so the prediction is achieved qualitatively.

4. Structural analysis with high precision for large-scale industrial machines

The structural analysis code, FrontSTR, which has been evolving in the FSIS project since 2003, is based on standard FEM techniques[[9][10][11]. One of the most remarkable features of this code is high performance that is suitable for large-scale computational models with high end computing. FronsSTR's advantage is the use of HEC-MW, which is designed to utilize the high efficiency of various systems without changing the code.

4.1 Numerical experiments performed on Earth Simulator

We carried out two experiments.

In the first experiment, we used we measured parallel efficiency using a test model (a cubic model).

The results are summarized in Table 1. The test model comprised 32,768,000 node points (98,304,000D.O.F) and an eight-point hexahedral element.

Table 1 Static analysis time on the Earth Simulator.

Number of CPUs	Calculation time (sec)
64	3224.827
128	1669.418

The estimated parallel ratio by Amdahl's law is 99.9428%.

The expected number of CPUs on which the parallel efficiency is 50% will be 1748 CPUs.

Using a practical model (High pressure pump model of

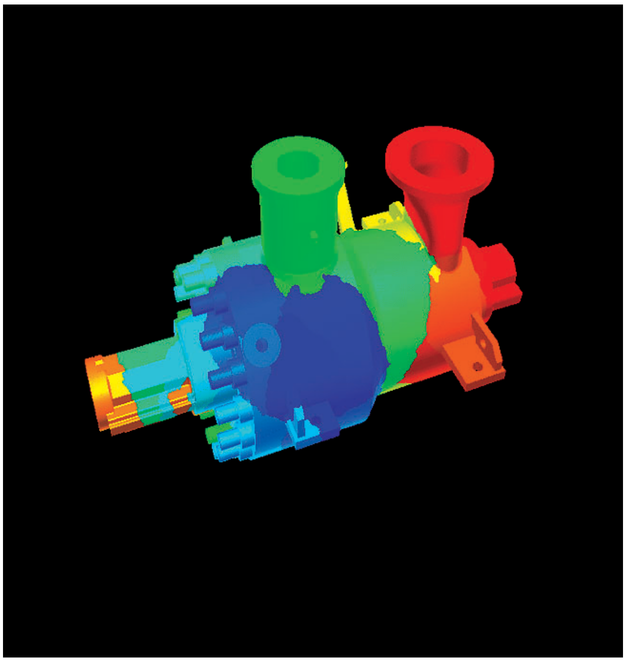

Fig. 9 Domain decomposition of the model (32 domains).

36,728,129 node points, Fig. 8, Fig. 9) a static linear analysis was performed. The calculation time was about 1 hour. Comparing to the conventional serial machines, we found the Earth Simulator is about thirty times faster.

5. Protein simulation

In protein simulation, we have reported a series of benchmark FMO-MP2/6-31G calculations with the ABINIT-MP program on the Earth Simulator in collaboration with the JST-CREST project [12]. A new route to the integral transformation through DGEMM was created for the MP2 processing. The aricept-acetylcholinesterase complex (8,409 atoms and 46,831 AOs, Fig.10) was processed in 19.6 minutes with 4,096 VPUs, implying a promising applicability of FMO-MP2 calculations to structure-based drug design. The largest target computed was an influenza HA antigen-antibody system consisting of a total of 14,086 atoms (921

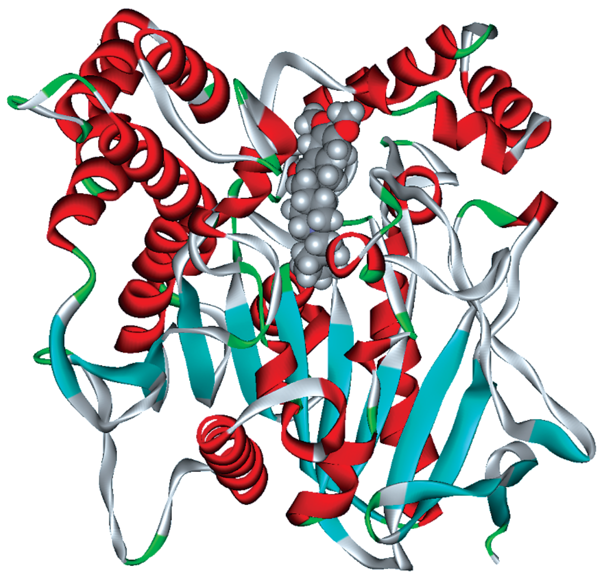

Fig. 10 Graphic representation of aricept-acetylcholinesterase complex (PDB ID: 1EVE). Aricept molecule is drawn with spheres.

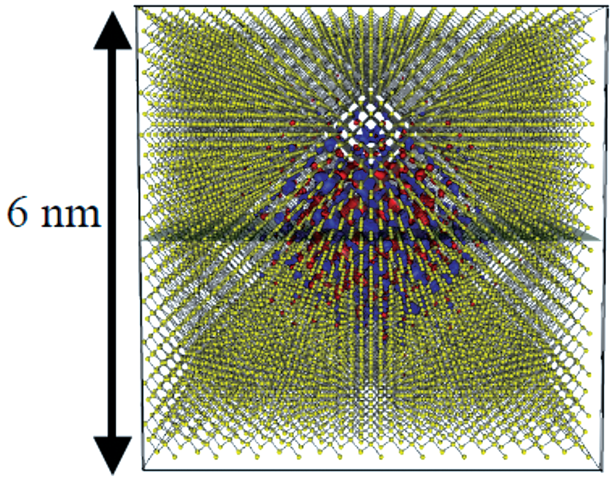

Fig. 11 The wavefunction of the As-donor state in silicon. The yellow balls indicate 10,648 Si atoms in the super-cell, and an As atom is substituted for the center Si atom. The blue and red regions indicate the sign of the donor wavefunction.

residues) and thus having 78,390 AOs. This FMO-MP2 job could be completed in less than one hour (53.4 minutes) with 4,096 VPUs, where its cost factor relative to the FMO-HF job was only 2.7. Reasonable timing and efficiency were observed in benchmark tests, indicating the promising ability of FMO-MP2 for high-throughput executions on a few thousand VPUs.

6. Nanoscale simulation

6.1 As-donor state in silicon

Last fiscal year, we reported the energy structure of the As-donor state in 8,000 Si atoms using the first-principles calculation code PHASE on the Earth Simulator. We demonstrated that the six-fold As-donor levels in the effective-mass approximation split into three levels. We achieved a first-principles calculation of a 10,648-atom system. The ground-state wavefunction of the 1s donor state, which has A1 symmetry, is shown in Fig.11. The sustained peak performance of 16.2 TFlops was measured on 4,096 CPUs, which is about a half of the theoretical peak performance. This work was a finalist for the Gordon Bell Prize in 2007 [13], but unfortunately we did not win the award.

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革新的シミュレーションソフトウェアの研究開発

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本プロジェクトでは、工学（次世代デジタルエンジニアリング）、生命科学、ナノテクノロジーの分野で核となる流体シミュレーション、構造シミュレーション、タンパク質シミュレーション、ナノシミュレーションを取り上げそれぞれ次の成果を得た。

まず、デジタルエンジニアリング技術の一つとして流体シミュレーションでは、ハイパフォーマンスコンピューティング(HPC)を用いた大規模ラージエディシミュレーション(LES)による自動車空力解析に着目し、その有用性の検討、実証を目的とする。特に実験では予測の難しい非定常空力特性に着目し、スライディング機構を導入することで、車両ヨー角の動的変化時に作用する空気力の予測に成功した。

2つ目として、斜流ポンプ内部流れのLES解析を実施した。テストポンプはオープンインペラおよびディフューザを有する。本解析の目的は、全流量において水力性能を予測するとともに、低流量側で生じる不安定特性の発生メカニズムを解明することである。本解析により、不安定特性を含めた全流量域の水力性能の予測が可能であることが確認された。

3つ目としては、ガスタービン翼の熱輸送分布を予測した。従来の研究では、遷移モデルを含むRANSを用いた予測手法が主流であったが、本研究では、翼面の乱流遷移をLES解析により直接的に予測することにより、熱輸送分布の高精度予測を試みた。翼周りの圧力分布および熱輸送分布の予測値を実験値と比較した結果、良好に一致することが確認できた。

構造シミュレーションでは、10億自由度程度の大規模な構造解析に取り組んだ。ソルバー本体としてはその規模に十分耐えうることを検証し、並列化性能などを測定した。並列化率99.98％以上、対ピーク性能50％以上を維持している。

タンパク質シミュレーションでは、非経験的フラグメント分子軌道(FMO)法プログラムABINIT-MPのMP2計算エンジンへlevel 3 BLAS (DGEMM)の導入を行い、地球シミュレータ128ノード(1,024プロセッサ)を用い、アセチルコリンエステラーゼ－アリセプト複合体のFMO-MP2計算に従来は3.0時間かかっていたところが、1.5時間と2倍に高速化された。さらに512ノード(4,096プロセッサ)を用いることで、わずか19.6分で実行できた。

ナノシミュレーションでは、ナノシミュレーションでは、シリコン中のヒ素が作るドナー準位のエネルギー構造を解析した。地球シミュレータの512ノード(4,096プロセッサ)を用いることで、これまで行ってきた中で最大規模である10,648原子系の計算を成功させ、実行性能16.2TFLOPSを達成した。このサイズでドナー準位が十分に収束していることが確認できた。

キーワード：ラージエディ・シミュレーション，空力，空力騒音，自動車，構造解析，共役勾配法，FMO，MP2，ドナー準位，第一原理計算