Revolutionary Simulation Software for 21st Century

Project Representative

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In this project, we have chosen five important sub-projects- turbulence simulation, aeroacoustics noise simulation, structure 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 the world's largest engineering large eddy simulation (LES) of flow around a formula car (known as one of the most severe subjects in industry) to emphasize the validity of using high performance computing (HPC) technique to apply large-scale LES to industrial applications. The unstructured-grid LES code "FrontFlow/red" based on the Finite Volume (FV) scheme was intensively optimized for the execution on Earth Simulator, and we could successfully simulate the unsteady turbulent flow around the formula car using over 100 million. The software developed was also applied to a racing motorcycle and a commercial sedan with collaboration with industries, and validity of the method for the industrial use has been confirmed.

In the aeroacoustic simulation, we predicted aeroacoustic noise that is radiated from a low-speed axial flow fan, with a six-blade rotor installed in a casing duct. A one-way coupled simulation of LES and acoustical analysis was conducted. First, we performed LES by using FrontFlow/Blue. In the LES, we successfully captured a turbulent boundary layer on the rotor blade surfaces and predicted pressure fluctuation on the hub and rotor blade surfaces. Pressure fluctuations computed by the LES were fed to the acoustical analysis as a sound source. The predicted sound pressure level (SPL) agrees well with the measured SPL.

In the field of structure analysis, analysis of more than 100 million points is enabled by FrontSTR. We will try a more complicated analysis such as dynamic analysis or nonlinear analysis in the future. FrontSTR was designed for HEC environments and uses parallel and vector functions efficiently. It can be expected that the practical analysis range will be wider.

In the protein simulation, we recently developed a parallelized integral-direct algorithm for the configuration interaction singles with perturbative doubles correction (CIS(D)), and implemented it into the ABINIT-MP program of the multilayer fragment molecular orbital (MLFMO) scheme. We conducted FMO-MP2 and MLFMO-CIS(D) calculations on the Earth Simulator of realistic proteins consisting of tens of thousands of basis functions. The calculations were found to be highly accurate indicating that the ABINIT-MP program is easily applicable to realistic systems.

In the nanoscale simulation, we have calculated the energy levels of As donor state in Si, using the PHASE which is a first principles calculation code. Adopting the real number formalism for the wave functions, we succeeded in calculating 8,000-atom system. Thus, the uncertainty due to the overlap of donor wave functions in case of 5,800-atom system was completely eliminated. Next we undertook the analysis of conduction properties of DNA, which is considered as one of the building blocks for future nano-scale electronic devices. It is found that carriers hop along DNA with a velocity of about 1,000 cm/sec.

Keywords: large eddy simulation, aerodynamic force, formula car, aeroacoustics noise, FMO, MP2, CIS(D), First principles calculation, As donor state, DNA, Conjugate gradient methods, Finite Element method

1. Assessment of an aerodynamic force on a formula car using a large scale LES

The objective of this sub-project is to emphasize the validity of large eddy simulation (LES) by applying high performance computing (HPC) technique to an aerodynamic assessment of automobiles. For this purpose, the unstructured-grid LES code FrontFlow/red based on a finite volume (FV) scheme was intensively optimized for execution on the Earth Simulator.

Recently greater attention is going to be paid to unsteady aerodynamic force acting on automobiles, which is generated from sudden steering action, overtaking, or cross wind conditions and difficult to measure by the conventional wind tunnel tests or RANS models. The advantage of LES, in addition to its high accuracy, is its possibility of capturing such unsteady force, which will contribute to the aerodynamic design innovation in automotive industry.

1.1 Formula car (LOLA B03/51) [1]

LES of flow around a formula car, which is one of the most severe subjects in automotive industry from the viewpoint of both the demand of very high accuracy and pressed development time, was conducted on 100 nodes (800 CPUs) using 120 million elements. The simulation is, to the best of our knowledge, one of the world's largest engineering LES simulations. As shown in Table 1, the aerodynamic forces estimated show good agreement with the wind tunnel data (within several percent!). Various unsteady flow features around the car was investigated, and, as a typical example, effect of wheel rotation on the flow structure is visualized in Fig. 1. These results clearly indicate the effectiveness of large-scale LES in the very near future for the computation of flow around vehicles with complex configurations.

Table 1 Aerodynamic coefficients.

	present LES		Wind tunnel
Cd	1.00 (incl. wheels)	0.56 (excl. wheels)	0.91 (incl. wheels)
Cl	-1.68 (incl. wheels)	-1.95 (excl. wheels)	-1.93 (excl. wheels)

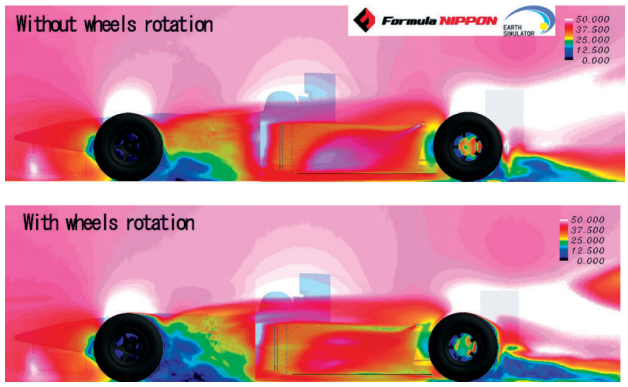

Fig. 1 Snapshots of the velocity distribution around a formula car with (below) or without (above) wheels rotation.

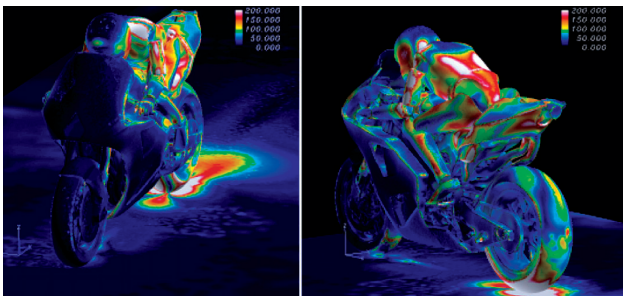

Fig. 2 Snapshots of the pressure fluctuation on the surface of the racing motorcycle (SUZUKI GSV-R) and rider.

1.2 Application to a racing motorcycle a commercial sedan and [2]

The software developed was successfully applied to the racing motorcycle (SUZUKI GSV-R in Fig. 2) and the commercial sedan (MAZDA Atenza in Fig. 3), and validity of the method for the industrial use has been confirmed through thorough comparison of reproduced eddy structures as well as the aerodynamic forces with the experimental data.

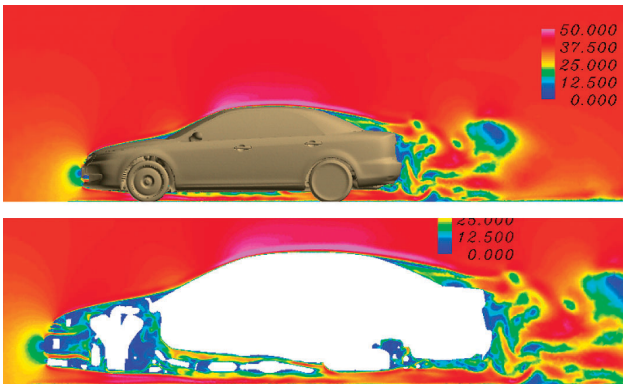

Fig. 3 Snapshots of the velocity distribution around the commercial sedan (MAZDA Atenza).

2. Prediction of aeroacoustic noise from an axial-flow fan

Aeroacoustic noise that is radiated from a low-speed axial flow fan with a six-blade rotor installed in a casing duct, is predicted by a one-way coupled simulation of the computa-

tion of the unsteady flow in the ducted fan and computation of the sound radiated to the ambient air. The former is performed by using our original LES (large eddy simulation) code, FrontFlow/blue[3–5], which is based on the Dynamic Smagorinsky Model (DSM) and multi-frame-of-reference dynamic overset finite element method (FEM). Computed pressure fluctuations on the hub, casing, and blade surfaces are fed to the following acoustical analysis as input data. The LES was performed on the Earth Simulator by using 40 nodes (320 CPUs). The latter (acoustical analysis) is performed by using a commercial code, SYSNOISE, which computes the sound field in the frequency domain on the basis of a boundary element method (BEM). In the acoustical analysis, the effects of the rotation of the blades and scattering of the incident sound at the blade surfaces on the sound field are neglected because they are presumably small for relatively low frequency sound radiated from a low-speed axial fan.

The LES that uses approximately 30 million hexahedral elements reproduced the transition to the turbulent boundary layer (TBL) on the suction surface of the rotor blades as well as the tip-leakage flow. The instantaneous vorticity magnitudes on the hub and rotor blade surfaces are shown in Fig. 4.

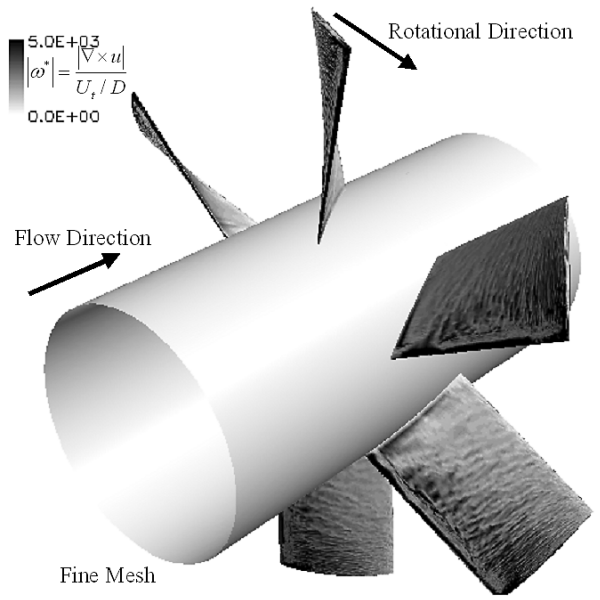

Fig. 4 Distribution of vorticity magnitude on hub and rotor blade surfaces.

We generate sound source data for an acoustical analysis by performing spectrum analysis and data mapping (from the LES mesh to the acoustical analysis mesh) for the pressure fluctuations predicted by the LES. A comparison of sound pressure level (SPL) is shown in Fig. 5. Reasonable agreement is obtained between the predicted and measured SPL evaluated 1.5 m upstream of the rotor blade center.

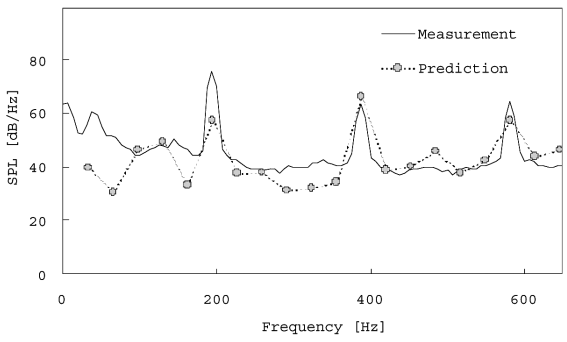

Fig. 5 Comparison of SPL.

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

The structural analysis code, FrontSTR, which has been developed in the FSIS project since 2003, is based on standard FEM techniques[6][7][8]. One of the most remarkable features of this code is high performance that is suitable for large-scale computational models with high end computing. The key issue is using HEC-MW, which is designed to utilize the high efficiency of various systems without changing the code.

3.1 Numerical experiments performed on Earth Simulator

We carried out two kinds of experiments.

1. We inspected the parallel efficiency by increasing the number of CPUs for the same size model.
2. We showed the possibility of large-scale computation by increasing the size of the model as the number of CPU increases.

The calculation time for a four-million-node model according to the number of CPUs is shown in Fig. 1.

According to Fig. 6, the increase in calculation speed between 8 and 256 CPUs is about a factor of 18. This means that the parallelizable fraction is 99.67%. Furthermore, we observe that the fraction increases as the model size becomes larger.

The model size that can be treated as the number of CPUs is increased is shown in Table 2. On the other hand, calculation time is almost constant. This shows that no matter how big calculation is possible if there are a sufficient number of CPUs. The calculation performance on each CPU is about 4 Mflops, which is 50% of peak performance.

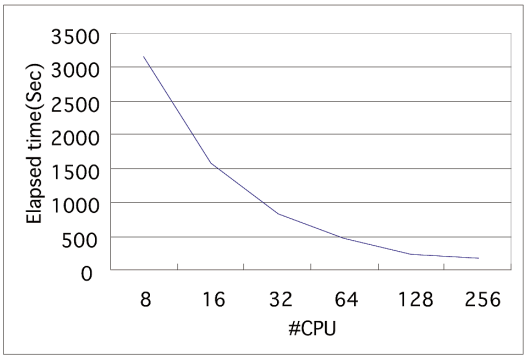

Fig. 6 Calculation time vs. number of CPUs.

Table 2 Time invariance under varying #CPUs.

# of CPUs	8	16	32	64	128	256
# of Nodes (10^6)	4	8	16	32	64	128
Time (10^3 sec)	3.15	3.14	3.22	3.22	3.35	3.35

3.2 Practical calculations

In FrontSTR, static analysis and analyses of computationally higher complexity such as nonlinear or dynamic analyses are possible.

A pressure pump model is shown in Fig. 7. The Earth Simulator is 30 times faster than serial machines in calculations using this model. This high performance will lead to a wider variety of analyses.

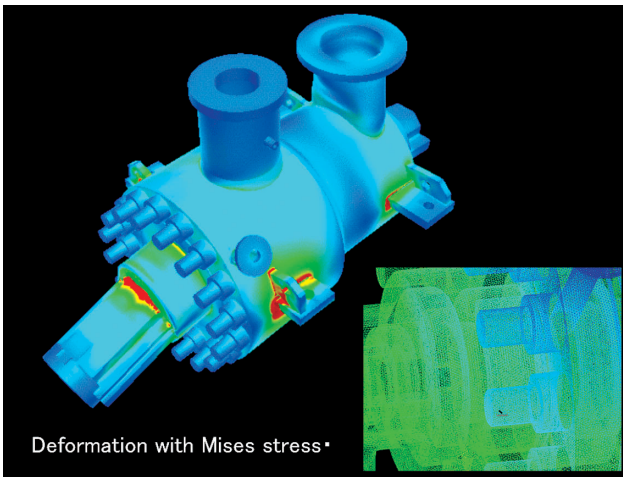

Fig. 7 Self-gravity analysis of 100 million D.O.F high-pressure pump model.

4. Protein Simulation

4.1 MLFMO-CIS(D) Method

Kitaura's fragment molecular orbital (FMO) method is a promising way of treating the issues of real-scale proteins in an ab initio fashion [9, 10]. In the ab initio FMO method, a molecule or a molecular cluster is divided into fragments, and the MO calculations on the fragments (monomers) and the fragment pairs (dimers) are performed to obtain the total energy that is expressed as a summation of the fragment energies and inter-fragment interaction energies (IFIEs).

The ABINIT-MP program that was originally developed by Nakano et al. for the parallelized Hartree-Fock (HF) calculations of proteins with FMO method has been extended in the "Revolutionary Simulation Software for 21st Century" and JST CREST projects. One of the most important extensions is the excited states calculation for large molecules such as protein and DNA with the configuration interaction singles with perturbative doubles correction (CIS(D)) method [11] proposed by Head-Gordon et al. [12].

The CIS(D) method provides the energy corrections both of the relaxation and differential correlation for the respective CIS excited states. The implementation of CIS(D) is based on our original algorithm for the second-order Møller-Plesset perturbation (MP2) calculations [13]. There is no need to communicate bulky intermediate data among worker processes of the parallelized execution. This CIS(D) code is then incorporated into a developer version of ABINIT-MP program, in order to improve the overestimation in excitation energies calculated by the CIS method in conjunction with the multilayer fragment molecular orbital scheme (MLFMO-CIS) [14]. Since the DAXPY and the DDOT operations are used in the most inner loop of each step of CIS(D) method [11], the vectorization of CIS(D) calculation is straightforward.

4.2 Benchmark Calculations

We conducted a series of benchmark calculations on the Earth Simulator. Here, we introduce three examples. The first is the FMO-HF calculation of $(Gly)_{512}$ alpha helix conformation at the HF/STO-3G level of theory. We used 512 nodes (4096 CPUs) of the Earth Simulator. The sustained performance was about 5.1 TFLOPS, and that is about 15% of the peak performance.

The second involves acetylcholinesterase (AChE), which is an important target protein for the design of new anti-

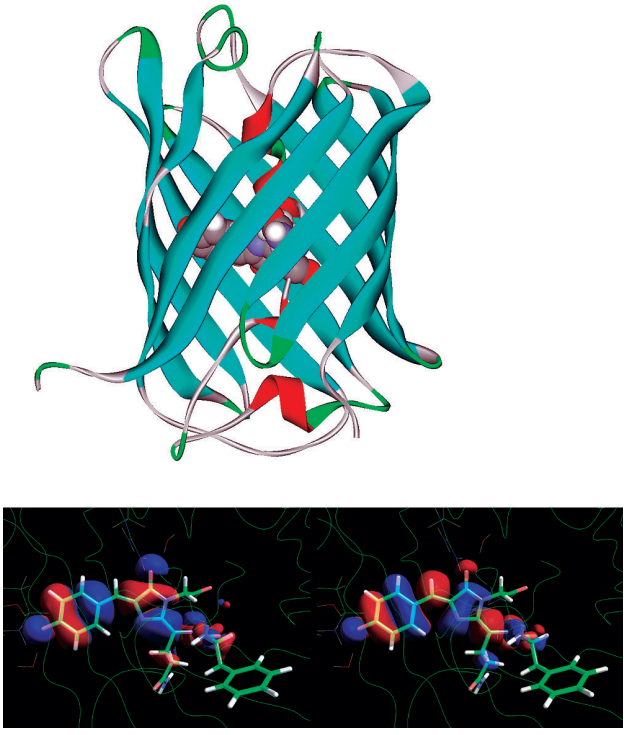

Fig. 8 Graphic representation of DsRed (PDB ID: 1ZGO) in solid-ribbon fashion. The pigment moiety located at the center of barrel is drawn with spheres. Hole (lower left graphic) and particle (lower right graphic) natural orbitals of the excited state of interest.

Alzheimer drugs. A full electron calculation for the AChE - aricept complex (PDB ID: 1EVE) was performed by the fragment molecular orbital (FMO) method on the Earth Simulator. The target system contains 532 amino acid residues and 8,409 atoms. The calculation at MP2/6-31G level of theory took only 3.0 hours with 128 nodes (1024 CPUs). This is the largest size to which the MP2 calculation has been applied.

The third is the MLFMO-CIS(D) calculation for a red fluorescent protein isolated from *Discosoma* coral (known as DsRed, Fig. 8) [15]. The calculated excitation energy of 2.30 eV is in good agreement with the experimental energy of 2.22 eV. The corresponding MLFMO-CIS(D)/6-31G job including the preceding FMO-HF stage required 20.2 hours on 20 cores of Xeon clusters. The same job took only 34.5 min on 128 nodes of the Earth Simulator. This was a promising timing for the target protein containing more than two hundreds residues (with 20 thousands basis functions) though the tuning of our program has still been in progress.

5. Nanoscale Simulation

5.1 As Donor state in Silicon

Last fiscal year we reported the energy structure of the As donor state in 5,832 Si atoms using the first-principles calculation code PHASE on the Earth Simulator. We demonstrated that the six folded As-donor levels in the effective-mass approximation split into three levels. The relative energy levels reproduced observed values precisely, while uncertainty about the absolute values remained due to the overlap of the donor wave function between adjacent cells. To escape the ambiguity, we tried to use a larger super-cell. We reduced the memory size by using the real-space formalism for the wave functions, and achieved a first-principles calculation of an 8,000-atom system (Fig. 9). The sustained peak performance of 10.7 TFlops was measured on 3,072 CPUs, which is 45% of the peak performance.

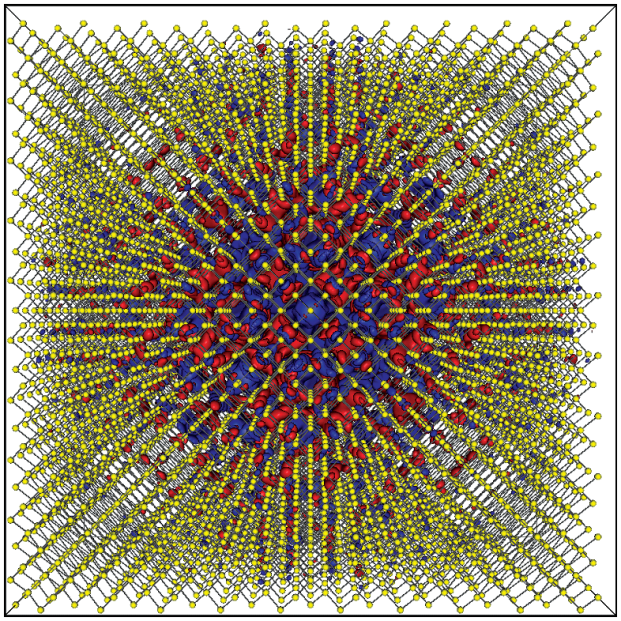

Fig. 9 Wave function of As-donor state in silicon. The yellow balls indicate 8,000 Si atoms in the super-cell, and an As atom is substituted for the center Si atom. The blue and red regions indicate the sign of the donor wave function.

5.2 DNA in water

DNA is expected to be one of the building blocks in future nanoscale electronic devices. We have calculated the structure and energetic properties of DNA, which is composed of GC-10 base pairs in water at room temperature. To trace the motion of DNA for sufficiently long times, we used the NAMD code, which is a classical molecular dynamics simulator, well tuned to bio-molecular systems. Selecting the geometries every ten psec, we have calculated the electronic structure of the DNA in detail using the PHASE code. As is shown in Fig.10, the HOMO and the LUMO are localized on a guanine and a cytosine, respectively, at each snapshot. They transfer to the neighboring guanine and cytosine in the course of 10 psec, indicating that the carriers hop along DNA with a velocity of about 1,000 cm/sec.

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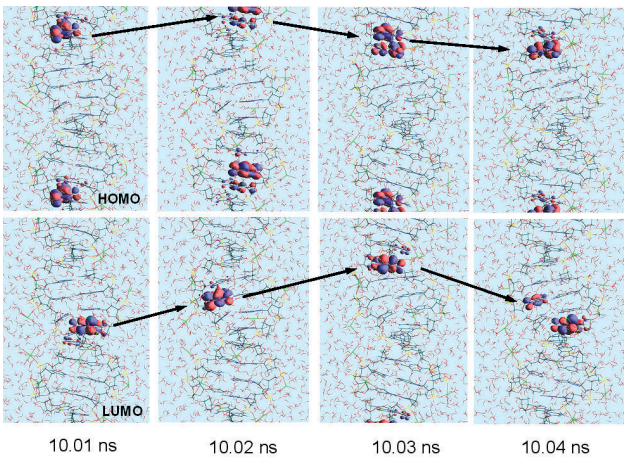

Fig.10 HOMO (upper figures) and the LUMO (lower figures) of the GC-ten base paired DNA in water at room temperature. The four geometries are taken from the classical MD simulation every 10 psec. The DNA and the water molecules are indicated by the blue and red lines, while the green lines indicate the position of Mg couter-ions.

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戦略的革新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、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、産業界で最も過酷な設計開発要件の一つといえるフォーミュラカーを対象とした1億2千万要素世界最大規模LES解析を実現し、風洞実験データとの比較から定常空力の高精度予測を実証した(誤差数%)。また、開発したソフトウェアを産業界との連携の下、レース用二輪車(スズキ)と市販セダン(マツダ)に適用し、その実用性を示した。

また、騒音予測では、軸流ファンから発生する空力騒音に着目し、LES解析により動翼表面の圧力変動(音源)を解析した後に、音響解析を実施し周囲の音場を予測した結果は、実験データと良好に一致した。

構造シミュレーションでは、1億点を超える大規模な構造解析に取り組み、256CPUの並列計算にて1億3000万点の計算が可能になった。並列化率99.8%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)法に基づいたプログラムに、望月らによるMLFMO-CIS(D)法を用いた高精度励起状態計算エンジンの組込みを行い、地球シミュレータ512ノード(4096プロセッサ)で、実効性能5.1TFLOPSを達成した。また128ノードを用い、アセチルコリンエステラーゼ－アリセプト複合体のFMO-MP2計算を3.0時間で、赤色蛍光タンパク質(DsRed)のMLFMO-CIS(D)計算を34.5分で実行できた。

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。波動関数の実数表現を採用することにより、8,000原子系の計算に成功し、昨年行った5,800原子の計算で問題となっていたドナー準位間の重なりを除去することができた。ついで、次世代ナノデバイスの構成部品の一つとして着目されているDNAのエネルギー構造の解析を行い、電子や正孔は1,000 cm/秒の速度で運動していることを明らかにした。

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, CIS (D),
ドナー準位, 第一原理計算, DNA