Research on Innovative Simulation Software

Project Representative
Chisachi Kato — Center for Research on Innovative Simulation Software, Institute of Industrial Science (IIS), The University of Tokyo

Authors
Chisachi Kato — Institute of Industrial Science, The University of Tokyo
Makoto Tsubokura — Hokkaido University
Yoshinobu Yamade — Institute of Industrial Science, The University of Tokyo
Yuji Mochizuki — Rikkyo University
Katsumi Yamashita — NEC Soft, Ltd.
Tatsuya Nakano — National Institute of Health Sciences
Takenori Yamamoto — Toho University
Takahiro Yamasaki — Fujitsu Laboratories Ltd.
Takahisa Ohno — National Institute for Materials Science

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

In the vehicle aerodynamics simulation, we have developed a numerical method designed to predict unsteady aerodynamics of road vehicles based on the High-Performance Computing Large-Eddy Simulation (HPC-LES) technique. The method has been applied to a formula car subjected to sudden crosswinds, and unsteady aerodynamic forces were investigated in the context of the flow structures around the vehicle.

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 instability characteristics. The LES successfully predicted instability characteristics. We can investigate the detailed mechanism causing instability characteristics by analyzing computed flow fields.

In the protein simulation, we improved the ab initio fragment molecular orbital method program, ABINIT-MP, to treat the electronic state calculations of a protein in solution using the explicit water model on the Earth Simulator. The limit of the number of fragments has been increased by a factor of ten from 1,000 fragments to 10,000 fragments.

In the nanoscale simulation, we have investigated fundamental issues in developing next-generation silicon-based devises and researched chemical reactions closely related with construction of bio-nanodevice architectures.

Keywords: large eddy simulation, aerodynamic force, formula car, mixed-flow pump, FMO, solvation effects, First-principles calculation, First-principles molecular dynamics, Silicon devices, Bio-nanodevices, DNA, Cisplatin complex

1. Unsteady Aerodynamics of Formula Car in Wind Gust

In vehicle aerodynamics, greater attention is being paid to unsteady aerodynamic forces generated from sudden steering action, overtaking, or cross-wind conditions. Measuring such unsteady aerodynamics by conventional wind tunnel tests or RANS (Reynolds-Averaged Navier-Stokes) models is difficult. The advantage of LES, in addition to its high accuracy, is its capability of characterizing such unsteady forces, which will contribute to aerodynamic design innovations in the automotive industry. We have conducted one of the world's largest large eddy simulation (LES) studies of air flow around a formula car with 120 million numerical elements by optimizing the unstructured finite-volume LES code FrontFlow/red for execution on the Earth Simulator [1]. Thereby, the objective of this study is to develop a numerical

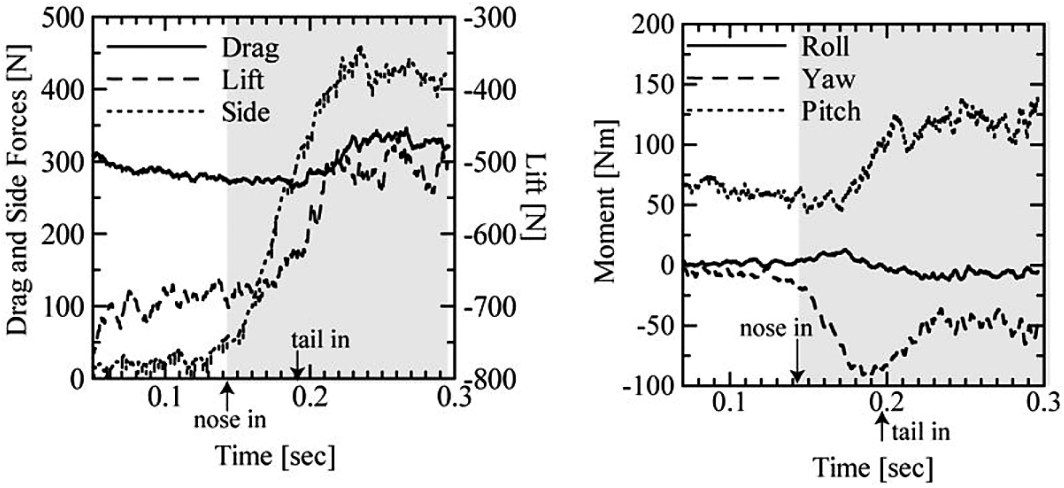

Fig. 1 Time history record of aerodynamic forces on the vehicle subjected to sudden crosswind (left: forces, right: moments). Shaded area indicates when the vehicle is in the crosswind region.

method, which predicts transient aerodynamic forces acting on a road vehicle.

We focused on gusty crosswinds as a typical case in which unsteady aerodynamics are expected to be crucial, and an innovative boundary condition for the side-wall of the computational domain was developed [2] to model a wind gust. The method was applied to a formula car and unsteady aerodynamics forces and flow structures were investigated. The time history record of the aerodynamic forces acting on the vehicle in a wind gust are illustrated in Fig. 1. Generally, the roll and yaw moments decrease, and the pitch moment increases under the crosswind condition, while serious undershoot is identified in the yaw moment during the transient process. The roll moment also shows a slight overshoot. These unsteady, nonlinear processes of aerodynamic forces that occur when the vehicle is subjected to sudden crosswinds are quite difficult to estimate by the conventional wind tunnel measurements, and our results clearly show the validity of CFD (Computational Fluid Dynamics) for studying such aerodynamic phenomena (Fig. 1).

Snapshots of the streamwise velocity and surface pressure distribution on the vehicle rushing into the crosswind region are shown in Figs. 2 and 3. At T = 0.14 sec right before the

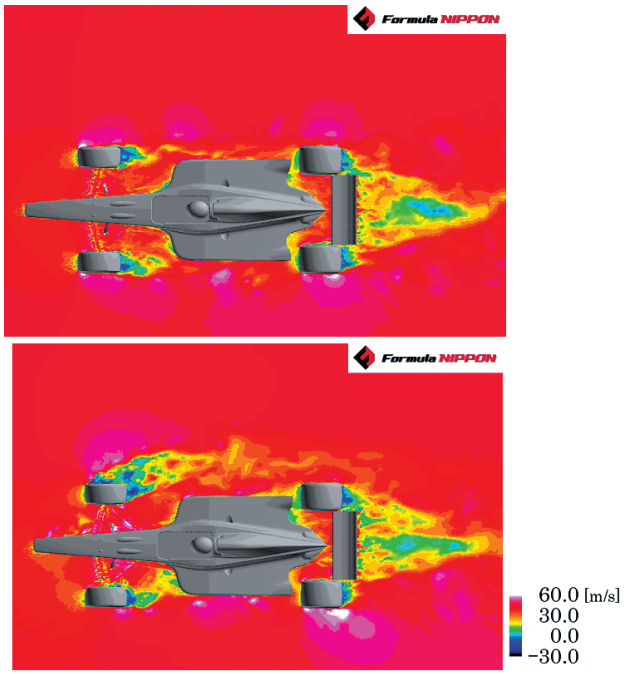

Fig. 2 Snapshots of streamwise velocity at T = 0.14 (above) and 0.20 (below) sec.

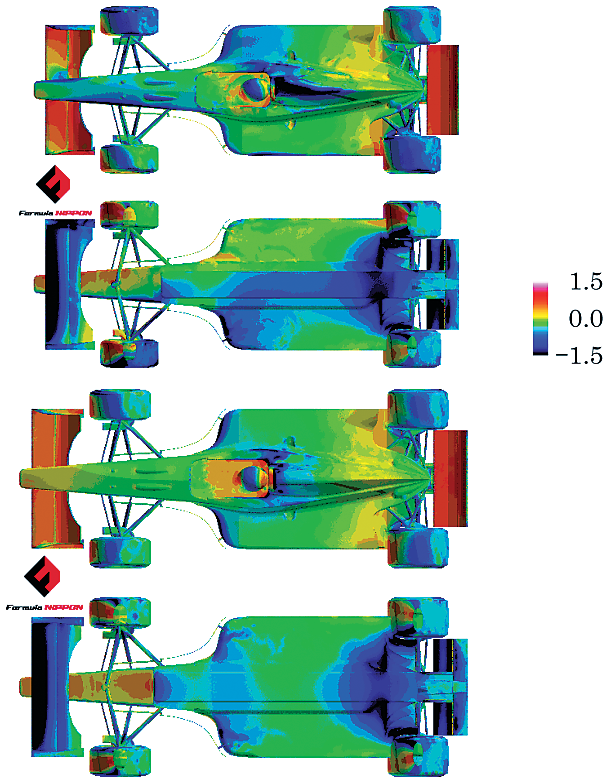

Fig. 3 Snapshots of surface pressure coefficient Cp on car body at T = 0.14 (above) and 0.20 (below) sec.

crosswind, the wake structure of the vehicle is almost symmetric with respect to the vehicle centerline. At T = 0.2 just after the entire body is subjected to the crosswind, the wake of the front wheel declines to about 30˚ with respect to the vehicle centerline, while the vehicle wake is not strongly affected by the crosswind. The coexistence of the declined wake created by the front wheels and the wake along the *x* direction created by the rear wheels are especially remarkable at T = 0.2 sec, which will contribute to nonlinear transient aerodynamic forces during this process.

As a result, we have demonstrated that HPC-LES can be a dominant aerodynamic assessment tool especially for unsteady aerodynamics, which would contribute to innovative aerodynamic design in the near future. As an ongoing study, we are now installing vehicle motion equations to estimate the vehicle behavior when the vehicle is subjected to unsteady aerodynamic forces.

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 mixed-flow pump with an open impeller and diffuser vanes was used as a test pump in this research. 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 [3] [4] [5]. 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. Surface-limited streamlines of time-averaged flow on blade surfaces at 55% are shown in Fig. 4. Performance curves of the pump predicted by coarse and fine LES are shown in Fig. 5. They agree with the measured one. In particular, the performance curve predicted by the fine LES agrees well measured one. We will analyze flow computed by the fine LES to understand the mechanism of instability characteristics.

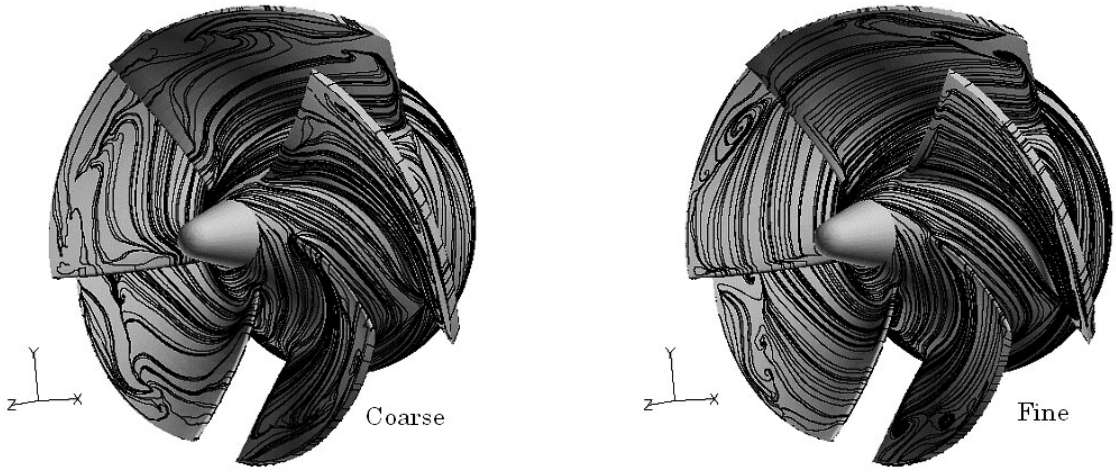

Fig. 4 Surface-limited streamlines of time-averaged flow on impeller blade surfaces at 55% flow rate [6].

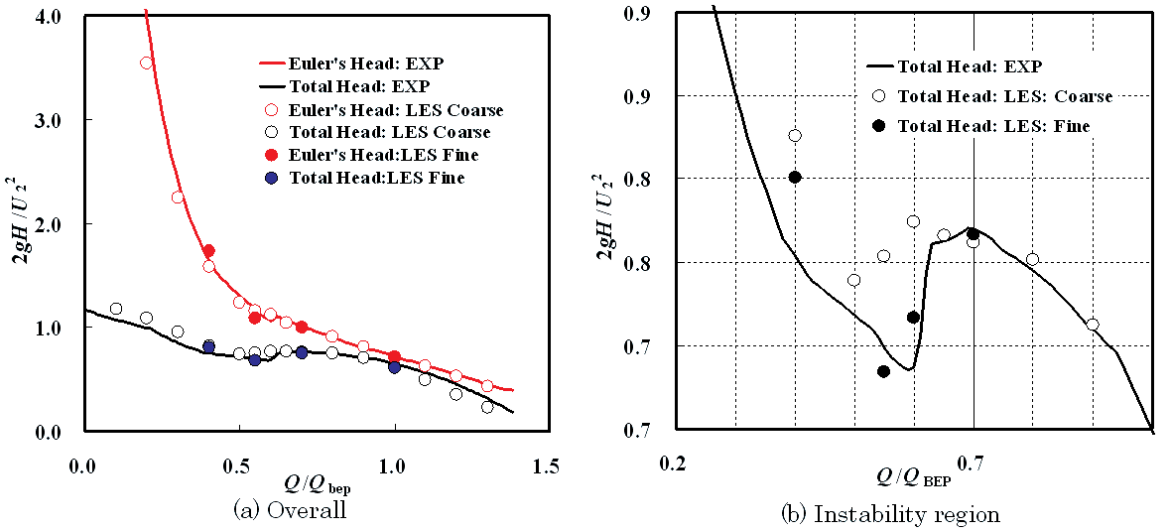

Fig. 5 Performance curve of pump predicted by LES [6].

3. Protein simulation

In the protein simulation, we improved the ab initio fragment molecular orbital method program, ABINIT-MP, to treat the electronic state calculations of a protein in solution using the explicit water model on the Earth Simulator. The limit of number of fragments has been improved by a factor of ten from 1,000 fragments to 10,000 fragments. Demonstrative calculations were performed using water droplet models (Fig. 6).

4. Nanoscale Simulation

4.1 Nanostructures of silicon (110) surface

We investigated the five-member ring structure on the Si(110) surface by first-principles calculations based on the density functional theory (DFT). The scanning tunneling microscope (STM) image of the proposed model [7] is shown in Fig. 7. We found that the proposed structure is metastable, and hence, consider that more stable structures would exist.

4.2 Silicon monovacancy

An ultrasonic determination suggested that there are high-symmetry (T_d) monovacancies in silicon wafers with very low impurity concentrations [8]. We studied the silicon monovacancy formation using large-scale first-principles calculations to examine this hypothesis. Simulations were carried out on three cubic cells at the sides of 10.86, 16.29, and 27.15Å including 63, 215, and 999 atoms, respectively. In the high vacancy concentration case (63-atom cell), the vacancy formation energy at the T_d symmetry is smaller than at the other symmetries D_{2d} and C_{2v}. However, we found that the formation energy at the D_{2d} symmetry decreases with increasing vacancy concentration and is the lowest in the largest simulation cell. This result confirms that the monovacancy structure is distorted due to the Jahn-Teller effect and suggests that other vacancy structures would exist.

4.3 Reactions between DNA and metal complexes

We consider that the reactions between DNA and metal complexes are useful for construction of bio-nanodevices and studied related chemical reactions using first-principles methods. We checked the hydration reaction of the cisplatin complex and the optimized structure of the cisplatin-guanine com-

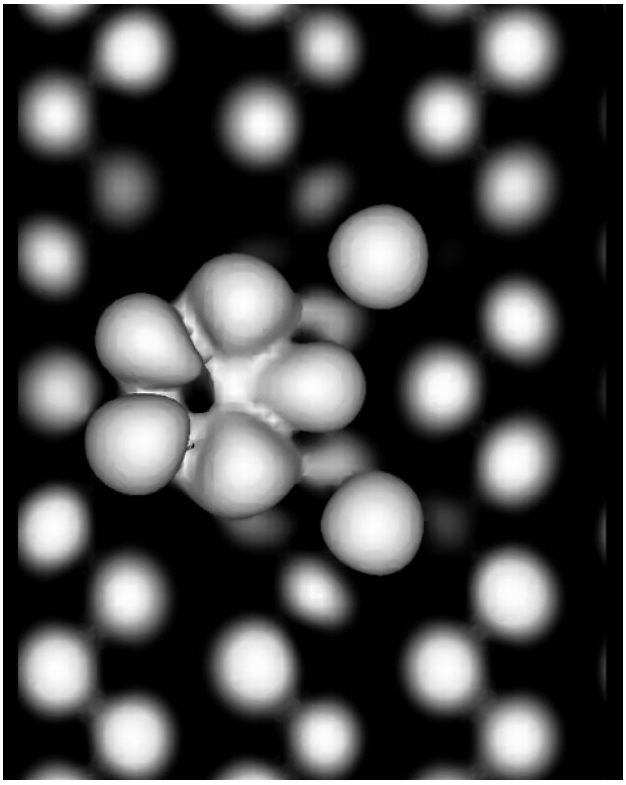

Fig. 7 Scanning tunneling microscope image of proposed model of five-member ring structure on Si(110) surface [7].

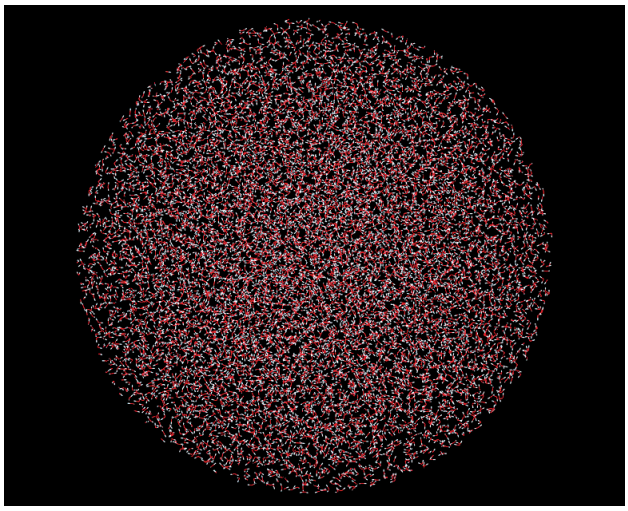

Fig. 6 Graphic representation of water droplet model (R = 42.0Å, 10,189 water molecules).

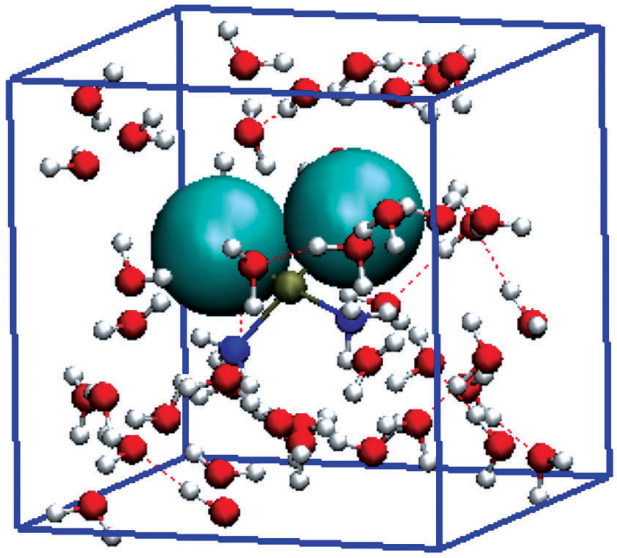

Fig. 8 First-principles molecular dynamics of cisplatin complex in aqueous solution.

plex. We found the results are in good agreement with ones obtained by DFT-level chemical methods. We also implemented the metadynamics method [9] into the PHASE code to efficiently simulate rare events in a chemical reaction. This method was applied to the analysis of the substitution reaction between a water molecule and a chlorine atom of the cisplatin complex in aqueous solutions, as shown in Fig. 8.

4.4 Reactions of DNA on solid surfaces

The self-assembly of DNA on solid surfaces is a key phenomenon of bio-nanostructure fabrications. We simulated the adsorption and self-assembled structures of adenine on Cu(110) surfaces. The simulated STM image of self-assembled structures agrees with the experimental one [10]. We also implemented the van der Waals interaction correction in the PHASE code to simulate the reaction of DNA strands on solid surfaces accurately. The correction makes the distance between the stacked DNA base pair (A-T) agree with ones obtained by a high-accuracy chemical method.

References

[1] Tsubokura, M., Kitoh, K., Oshima, N., Nakashima, T., Zhang, H., Onishi, K., and Kobayashi, T., "Large Eddy Simulation of Unsteady Flow around a Formula Car on Earth Simulator", SAE 2007 Trans. J. of Passenger Cars -Mechanical Systems, 2007-01-0106, 2007.

[2] Tsubokura, M., Nakashima, T., Ikenaga, T., Onishi, K., Kitoh, K., Oshima, N., and Kobayashi, T., "HPC-LES for the Prediction of Unsteady Aerodynamic Forces on a Vehicle in a Gusty Cross-flow Condition, SAE Technical Paper Series 2008-01-300, 2008.

[3] Kato, C. and Ikegawa, M., "Large Eddy Simulation of Unsteady Turbulent Wake of a Circular Cylinder Using the Finite Element Method", ASME-FED (1991), 117, pp.49–56.

[4] Kato, C., Kaiho, M. and Manabe, A., "An Overset Finite-Element Large-Eddy Simulation Method With Application to Turbomachinery and Aeroacoustics", Trans. ASME, Journal of Applied Mechanics, 70 (2003), pp.32–43.

[5] Kato, C. *et al*., "Numerical prediction of sound generated from flows with a low Mach number", Computers & Fluids, 36, 53–68 (2007).

[6] Shimizu, H., *et al*., "Large Eddy Simulation of a Mixed-Flow Pump", Proceeding of Turbomachinery Society of Japan, Osaka, Sep, 2008.

[7] Stekolnikov, A.A. *et al*., "Long-Range Surface Reconstruction: Si(110)–(16×2)", Phys. Rev. Lett. 93, 136104 (2004).

[8] Goto T. *et al*., Phys. Soc. Jpn. 75, 44602 (2006).

[9] Iannuzzi, M. et al., "Efficient Exploration of Reactive Potential Energy Surfaces Using Car-Parrinello Molecular Dynamics", Phys. Rev. Lett. 90, 238302 (2003).

[10] Chen, Q. *et al*., "Self-Assembly of Adenine on Cu(110) Surfaces", Langmuir 18, 3219 (2002).

革新的シミュレーションソフトウェアの研究開発

プロジェクト責任者
加藤　千幸　　東京大学生産技術研究所　革新的シミュレーション研究センター
著者
加藤　千幸　　東京大学生産技術研究所　革新的シミュレーション研究センター
坪倉　　誠　　北海道大学
山出　吉伸　　東京大学生産技術研究所　革新的シミュレーション研究センター
望月　祐志　　立教大学
山下　勝美　　NECソフト(株)
中野　達也　　国立医薬品食品衛生研究所
山本　武範　　東邦大学
山崎　隆浩　　(株)富士通研究所
大野　隆央　　(独)物質・材料研究機構

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、突風時にフォーミュラカーに作用する非定常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。解析には、約800万要素の小規模メッシュおよび約8,000万要素の大規模メッシュを用いた。本解析により予測した水力性能は全流量域にわたり、実験値とよく一致することが確認された。特に、大規模メッシュを用いた解析では、性能曲線に現れる右上がり特性(不安定特性)を定量的に予測できることを確認した。本解析により、ポンプの不安定特性が発生する際の特徴的な流れ構造を抽出することができた。

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について、溶媒分子の電子状態を露に扱った水溶液中のタンパク質の電子状態計算を可能するために、これまでの限界であった1,000フラグメントから、10倍の10,000フラグメントのFMO計算を行うための改良を行った。

ナノシミュレーションでは、次世代シリコンデバイスの開発で重要となる基礎事項について研究するとともに、バイオナノデバイスの基本設計の構築と関連深い化学反応の研究を行った。

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, ポンプ, FMO, 溶媒効果, 第一原理計算,
第一原理分子動力学, シリコンデバイス, バイオナノデバイス, DNA, シスプラチン錯体