# Introduction to application software developed in Japanese national projects and program for promoting research

Fugaku Topics

- Application Software on Fugaku
- Introduction to National Application Projects on Fugaku

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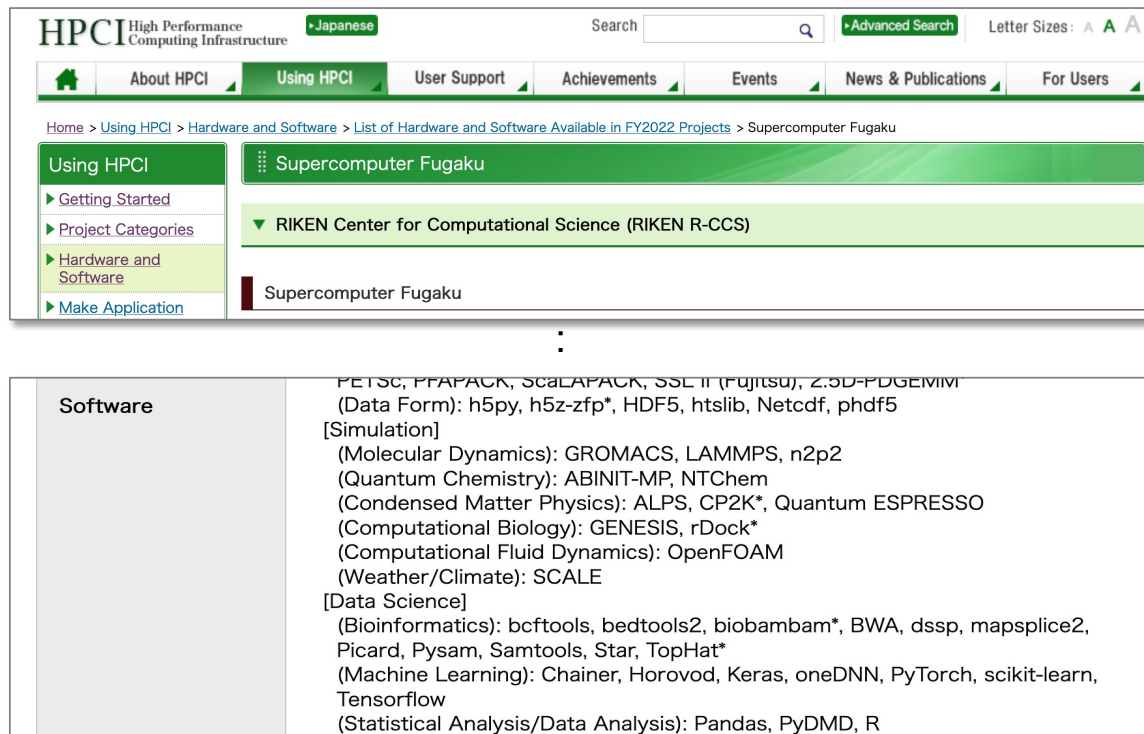
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# General software information

■ General software information, including libraries, on Fugaku

◆ https://www.hpci-office.jp/pages/e_r-ccs_riken_2022-2



◆ Further detailed software information will soon be available at the HPCI portal site.
● https://www.hpci-office.jp/pages/e_hardware_software?tab=software

# Major Community Software

■ Four pieces of Major Community Software*, LAMMPS, Quantum ESPRESSO, GROMACS, and OpenFOAM* have been pre-installed and are ***ready to use*** on Fugaku.

◆ https://www.hpci-office.jp/pages/e_appli_software?parent_folder=



> Useful information, such as example of running job-scripts, program information, and performance data on Fugaku, are provided.

# Japanese Application Software

■ Some pieces of Japanese national projects' software have been pre-installed or plan to be pre-installed on Fugaku.

■ These pieces of software are well optimized/tunned to Fugaku.

<u>List of the Japanese National Projects' Application Software, well optimized to Fugaku</u>

| Application Area | Software name | Features and contact point |
|---|---|---|
| Material Science and Biology | GENESIS[*1] | Molecular dynamics and modeling software for bimolecular systems such as proteins, lipids, nucleic acids, glycans, and their complexes<br>*https://www.r-ccs.riken.jp/labs/cbrt/* |
| | HΦ[*2] | An exact diagonalization package for a wide range of quantum lattice models (e.g. multi-orbital Hubbard model, Heisenberg model, Kondo lattice model)<br>*https://www.pasums.issp.u-tokyo.ac.jp/hphi/en/* |
| | MODYLAS[*2] | A general-purpose, molecular dynamics simulation program suited to the simulation of very large physical, chemical, and biological systems<br>*https://www.modylas.org/* |
| | NTChem[*1] | Comprehensive software for ab initio quantum chemistry calculations of large and complicated molecular systems<br>*https://www.r-ccs.riken.jp/software_center/software/ntchem/overview/* |

(Note) *1 : Pre- installed on Fugaku, *2 : Will be pre-installed on Fugaku by the end of March 2022

# Japanese Application Software

List of the Japanese National Projects' Application Software, well optimized to Fugaku (cont.)

| Application Area | Software name | Features and contact point |
|---|---|---|
| Material Science and Biology(cont.) | OpenMX*2 | An open source software for nano-scale material simulations based on Density Functional Theory, norm-conserving pseudopotentials, and pseudo-atomic localized basis functions<br>*http://www.openmx-square.org/* |
| | SALMON*2 | An open source software for ab-initio quantum-mechanical calculations of electron dynamics at the nanoscale that takes place in various situations of light-matter interactions<br>*http://salmon-tddft.jp/* |
| | SMASH*2 | Massively parallel open source software for quantum chemistry calculations with Hartree-Fock and Density Functional Theory<br>*https://smash-qc.sourceforge.io/* |
| | mVMC*2 | A low-energy solver for a wide ranger of quantum lattice models (multi-orbital Hubbard model, Heisenberg model, Kondo-lattice model) by using variational Monte Carlo method<br>*https://www.pasums.issp.u-tokyo.ac.jp/mvmc/en/* |
| | Phonopy*2 | An open source software for phonon calculations at harmonic and quasi-harmonic levels<br>*https://phonopy.github.io/phonopy/* |

(Note) *1 : Pre- installed in Fugaku, *2 : Will be pre-installed in Fugaku by the end of March 2022

# Japanese Application Software

List of the Japanese National Projects' Application Software, well optimized to Fugaku (cont.)

| Application Area | Software name | Features and contact point |
|---|---|---|
| Material Science and Biology(cont.) | ALAMODE*2 | An open source software designed for analyzing lattice anharmonicity and lattice thermal conductivity of solids <br> https://alamode.readthedocs.io/en/latest/ |
| | AkaiKKR*2 | A program package used for first-principles calculation of electronic structures of metals, semiconductors and compounds, in the framework of Density Functional Theory. <br> http://kkr.issp.u-tokyo.ac.jp/ |
| Computational Aided Engineering | FrontFlow/blue (FFB) *2 | A general-purpose flow solver, which is based on Large eddy simulation (LES) and capable of accurately predicting incompressible unsteady fluid-flows by using the Finite Element Method (FEM) for the spatial discretization method. <br> http://www.ciss.iis.u-tokyo.ac.jp/english/ |

(Note) *1 : Pre- installed in Fugaku, *2 : Will be pre-installed in Fugaku by the end of March 2022

◆ Please refer to the following HPCI portal page for further information.

https://www.hpci-office.jp/pages/e_appli_software?parent_folder=513

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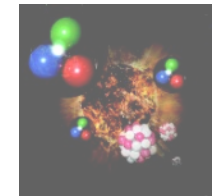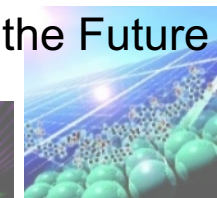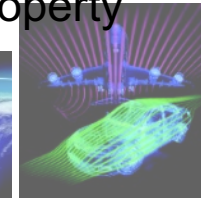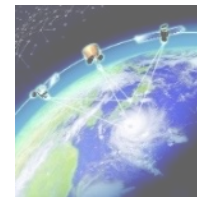
■ Summary

# Program for Promoting Researches on Supercomputer Fugaku

- Ongoing national application project called *"Program for Promoting Researches on Supercomputer Fugaku"*

  ◆ The program is funded by MEXT, Ministry of Education, Culture, Sports, Science and Technology of Japan, and around 40% of Fugaku resources are allocated to the program through the MEXT's open call.

  ◆ Projects with wide range of application, from basic science to engineering applications, are targeting at early creation of results using Fugaku.

  ◆ In following four focus areas , twenty-two (22) projects have been selected and are ongoing.

  - Area 1: Challenges for Solving Universal Problems of Mankind or Pioneering the Future
  - Area 2: Reinforcement of Efforts on Protecting People's Life and Property
  - Area 3: Enhancement of Industrial Competitiveness
  - Area 4: Research Infrastructure
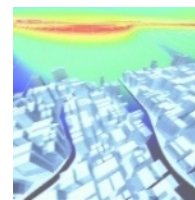
# Program for Promoting Researches on Supercomputer Fugaku

■ Area 1: Challenges for Solving Universal Problems of Mankind or Pioneering the Future

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 1 | Biomolecular dynamics and function in a living cell using atomistic and coarse-grained Simulations | Yuji Sugita, Riken *https://cbp.riken.jp/en/* |
| 2 | Unravelling origin of cancer and diversity by large-scale data analysis and artificial intelligence technology | Satoru Miyano, Tokyo Medical and Dental University *https://www.tmd.ac.jp/english/labs/dsc/* |
| 3 | Exploration of burning plasma confinement physics | Tomohiko Watanabe, Nagoya University *https://www.tmd.ac.jp/english/labs/dsc/* |
| 4 | Basic Science for Emergence and Functionality in Quantum Matter -- Innovative Strongly-Correlated Electron Science by Integration of "Fugaku" and Frontier Science | Masatoshi Imada, Waseda University *http://www.aoni.waseda.jp/imada/fugaku_en/fugaku_e_top.html* |
| 5 | Simulation for basic science: from fundamental laws of particles to creation of nuclei | Shoji Hashimoto, High Energy Accelerator Research Organization (KEK) *https://jicfus.jp/fugaku_pn/en/* |
| 6 | Toward a unified view of the universe: from large scale structures to planets | Junichiro Makino, Kobe University *https://jicfus.jp/fugaku_ap/en/* |
| 7 | Human-scale whole brain simulation with connectome analysis and structure-function estimation | Tadashi Yamazaki, The University of Electro-Communications *https://brain-hpc.jp/en/* |

# Program for Promoting Researches on Supercomputer Fugaku

■ Area 2: Reinforcement of Efforts on Protecting People's Life and Property

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 1 | Promotion of innovative drug discovery infrastructure for acceleration of precision medicine | Yasushi Okuno, RIKEN<br>*https://www.r-ccs.riken.jp/en/research/ddpd/* |
| 2 | Overcoming heart failure pandemic with innovative integration of multi-scale heart simulator and large-scale clinical data | Toshiaki Hisada, UT-Hesrt Inc.<br>*http://ut-heart.com/index.html* |
| 3 | Large-scale numerical simulation of earthquake generation, wave propagation and soil amplification | Takane Hori, Japan Agency for Marine-Earth Science and Technology<br>*http://www.jamstec.go.jp/fugaku-earthq/en/* |
| 4 | Large Ensemble Atmospheric and Environmental Prediction for Disaster Prevention and Mitigation | Masaki Satoh, The University of Tokyo<br>*https://cesd.aori.u-tokyo.ac.jp/fugaku/index_en.html* |

■ Area 3: Enhancement of Industrial Competitiveness

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 1 | Computational and Data Science Study for ET Revolution by Development of Next-Generation Battery and Fuel Cell | Yoshitaka Tateyama, National Institute for Materials Science<br>*https://www.nims.go.jp/fugaku-denchi/en/index.html* |
| 2 | Digital Twins of Real World's Clean Energy Systems with Integrated Utilization of Super-simulation and AI | Shinobu Yoshimura, The University of Tokyo<br>*https://postk6.t.u-tokyo.ac.jp/en/* |

# Program for Promoting Researches on Supercomputer Fugaku

■ Area 3: Enhancement of Industrial Competitiveness (cont.)

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 3 | Multiscale simulations based on quantum theory toward the developments of energy-saving next-generation semiconductor devices | Atsushi Oshiyama, Nagoya University<br>*https://fugaku-semicon.jp/en/index.html* |
| 4 | Development of high-performance permanent magnets by large-scale simulations and data-driven approaches | Takashi Miyake, National Institute of Advanced Industrial Science and Technology<br>*https://unit.aist.go.jp/cd-fmat/index_en.html* |
| 5 | Environment-Compatible Chemical Substances | Nobuyuki Matubayasi, Osaka University<br>*http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html* |
| 6 | Research and development of innovative fluid-dynamics simulations for aerodynamical/hydrodynamical performance predictions by using Fugaku | Chisachi Kato, The University of Tokyo<br>*http://www.ciss.iis.u-tokyo.ac.jp/english/project/* |
| 7 | Leading research on innovative aircraft design technologies to replace flight test | Soshi Kawai, Tohoku University<br>*http://www.klab.mech.tohoku.ac.jp/index.html* |
| 8 | Creation of data infrastructure for data-driven polymer materials research | Ryo Yoshida, The Institute of Statistical Mathematics<br>*http://daweb.ism.ac.jp/yoshidalab/index_e.html* |

# Program for Promoting Researches on Supercomputer Fugaku

■ Area 3: Enhancement of Industrial Competitiveness (cont.)

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 9 | Smart design in the Society 5.0 era on the supercomputer "Fugaku" | Makoto Tsubokura, Kobe University<br>*https://www.lab.kobe-u.ac.jp/csi-cfd/index_e.html* |
| 10 | Realization of innovative light-energy conversion materials using Fugaku | Takahito Nakajima, RIKEN<br>*https://www.riken.jp/en/research/labs/r-ccs/comput_mol_sci/index.html* |

■ Area 4: Research Infrastructure

| No. | Project Name | Project Representative and Contact Information |
|---|---|---|
| 1 | Development of personalized medical support technology based on simulation data science of whole brain blood circulation | Shigeo Wada, Osaka University<br>*https://sites.google.com/site/biomechwadalaben/home?authuser=1* |

▢ : Bio and Life Science    ▢ : Material Science    ▢ : Engineering    ▢ : Basic Science    ▢ : Weather, Climate and Earth Science

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# Summary

- Various compilers, libraries and AI tools are provided in the program development environment of Fugaku.

- Major community software is ready to use for your research on Fugaku.

- Japanese useful application software, well optimized to Fugaku, also is pre-installed or will be pre-installed on Fugaku.

- Several national projects are ongoing on Fugaku for advanced research and expected to achieve early outcome through Fugaku power.

We are open to Collaborative Research.

Please contact each Software Developer or Research Projects.

**HPCI Portal site**

https://www.hpci-office.jp/folders/english

**For inquiries about applications, contact the Help Desk.**

https://www.hpci-office.jp/pages/e_helpdesk/



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