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

Fugaku Topics

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

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  - General software information
  - Major Community Software
  - Japanese Application Software
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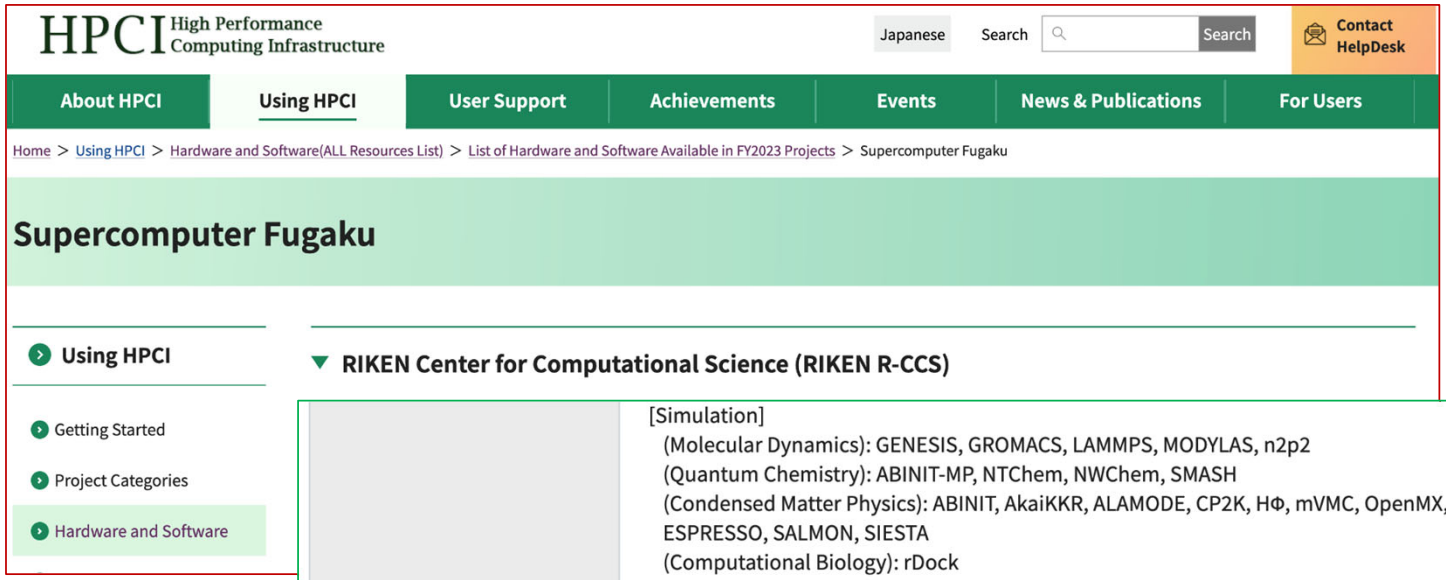
General software information

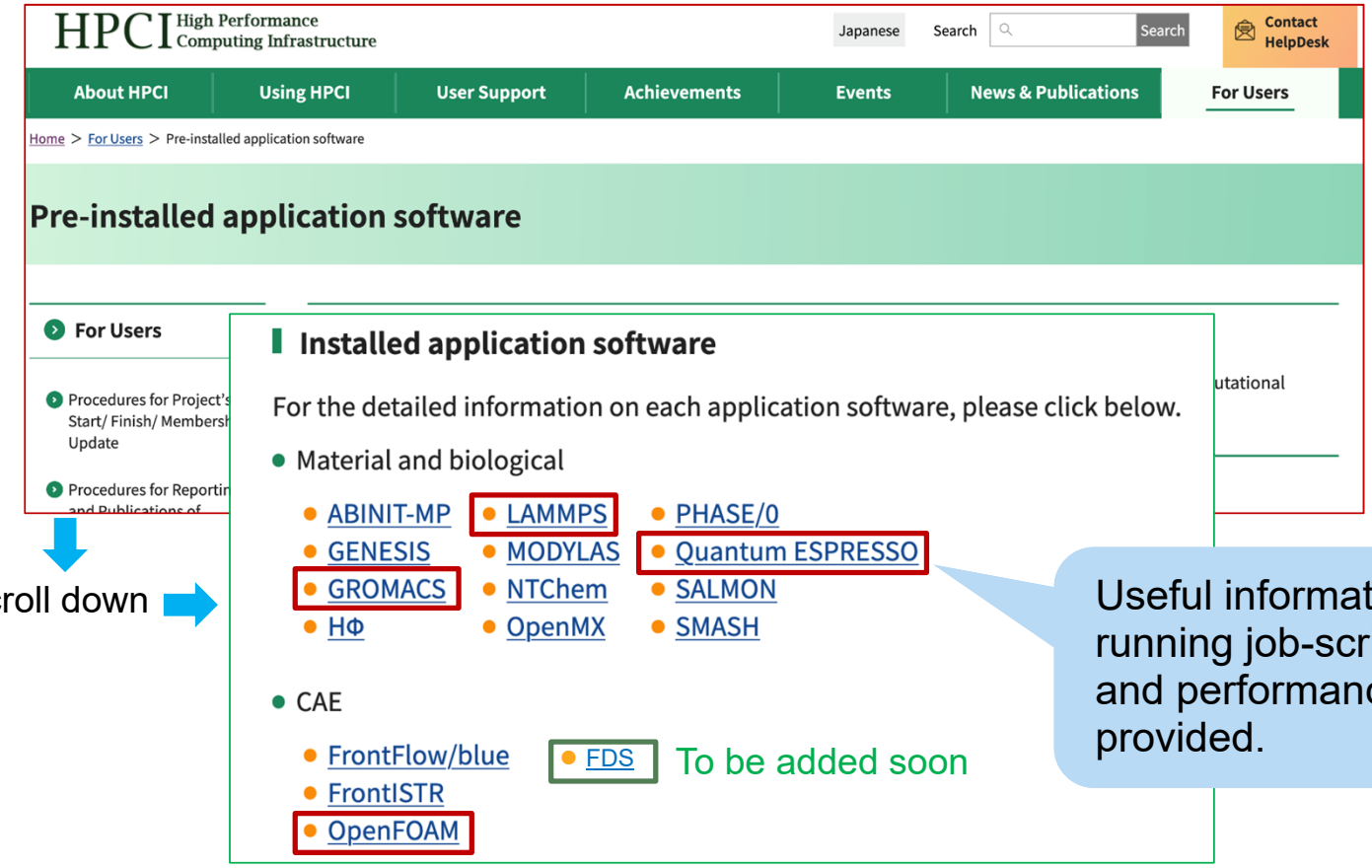
- General software information, including libraries, on Fugaku
  - https://www.hpci-office.jp/en/using_hpci/hardware_software_resource/2023/r-ccs_riken_2023-2



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

Major Community Software

- Five pieces of Major Community Software, ***LAMMPS, Quantum ESPRESSO, GROMACS, OpenFOAM, and FDS*** have been pre-installed and are ***ready to use*** on Fugaku.
  - https://www.hpci-office.jp/pages/e_appli_software?parent_folder=



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

Japanese Application Software (1)

- 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.

List of the Japanese National Projects' Application Software

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 *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) *https://www.pasums.issp.u-tokyo.ac.jp/hphi/en/*
	MODYLAS*1	A general-purpose, molecular dynamics simulation program suited to the simulation of very large physical, chemical, and biological systems *https://www.modylas.org/*
	NTChem*1	Comprehensive software for ab initio quantum chemistry calculations of large and complicated molecular systems *https://www.r-ccs.riken.jp/software_center/software/ntchem/overview/*

(Note) *1 : Pre- installed on Fugaku, *2 : New version will be pre-installed on Fugaku by the end of March 2023

Japanese Application Software (2)

List of the Japanese National Projects' Application Software (cont.)

Application Area	Software name	Features and contact point
Material Science and Biology(cont.)	OpenMX*1	An open source software for nano-scale material simulations based on Density Functional Theory, norm-conserving pseudopotentials, and pseudo-atomic localized basis functions *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 *http://salmon-tddft.jp/*
	SMASH*2	Massively parallel open source software for quantum chemistry calculations with Hartree-Fock and Density Functional Theory *https://smash-qc.sourceforge.io/*
	ABINIT-MP*1	An application software for efficient quantum chemical calculations of large molecules such as proteins based on the fragment molecular orbital (FMO) method *https://www.cenav.org/abinit-mp-open_ver-1-rev-10/* (in Japanese)

(Note) *1 : Pre- installed on Fugaku, *2 : New version will be pre-installed on Fugaku by the end of March 2023

Japanese Application Software (3)

List of the Japanese National Projects' Application Software (cont.)

Application Area	Software name	Features and contact point
Material Science and Biology(cont.)	mVMC*1	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 *https://www.pasums.issp.u-tokyo.ac.jp/mvmc/en/*
	Phonopy*1	An open source software for phonon calculations at harmonic and quasi-harmonic levels *https://phonopy.github.io/phonopy/*
	ALAMODE*2	An open source software designed for analyzing lattice anharmonicity and lattice thermal conductivity of solids *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. *http://kkr.issp.u-tokyo.ac.jp/*

(Note) *1 : Pre- installed on Fugaku, *2 : New version will be pre-installed on Fugaku by the end of March 2023

Japanese Application Software (4)

List of the Japanese National Projects' Application Software (cont.)

Application Area	Software name	Features and contact point
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. *http://www.ciss.iis.u-tokyo.ac.jp/english/*
	FFX*3	An application software for high-precision fluid flow simulations based on the Lattice Boltzmann Method *https://www.jstage.jst.go.jp/article/seisankenkyu/70/1/70_43/_pdf* (in Japanese)
	FFVHC-ACE*3	An application software for predictive evaluation of aircraft aerodynamic phenomenon based on the high-fidelity compressible flow Large-eddy simulation (LES) analysis *https://fugaku100kei.jp/assets/data/e_hpcimag_08.pdf*

(Note) *1 : Pre- installed on Fugaku, *3 : Application software will be pre-installed for the first time as common use on Fugaku by the end of March 2023

- 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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Program for Promoting Researches on Supercomputer Fugaku

- Ongoing national application projects 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.
  - Twenty-two (22) projects are ongoing. Nineteen (19) projects among them will finish at the end of March 2023, and several new projects will start in April, 2023.
    - 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/*

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

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 *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. *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 *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 *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 *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 *https://postk6.t.u-tokyo.ac.jp/en/*

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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 *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 *https://unit.aist.go.jp/cd-fmat/index_en.html*
5	Environment-Compatible Chemical Substances	Nobuyuki Matubayasi, Osaka University *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 *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 *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 *http://daweb.ism.ac.jp/yoshidalab/index_e.html*

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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 *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 *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 *https://sites.google.com/site/biomechwadalaben/home?authuser=1*

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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 of the Software Developers or Research Projects.

How to access HPCI Portal site pages in English

Access
https://www.hpci-office.jp
and press the “English” button on the top

You can change Japanese to English by pressing the “English” button on each page.

For inquiries about applications, contact the Help Desk.

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

General Information on Fugaku and HPCI

https://fugaku100kei.jp/e/exhibit/