

2020/08/01 [for version 2.7/3.1]

How to setup MaterApps LIVE!

MaterApps LIVE! Development Team

MateriApps — a Portal Site for Materials Science Simulation

- Aiming at the community formation through the promotion of application



since May 2013

- Introducing **273 materials science applications and tools** (as of 2020.8)
- Finding applications
 - search tags: features, targets, calculation methods/algorithms
- Information of applications
 - brief introduction, link to official pages, information installation, usage, etc
- Information of hands-on sessions, software update, etc
- Glossary of keywords, Concierge, Reviews
- 26000+ page views / month, 9000+ unique visitors / month

Applications on MateriApps

- Introducing **273 materials science applications and tools**

DFT

AkaiKKR★

OpenMX★

xTAPP★

ABINIT★

...

(79)

Quantum Chemistry

FMO★

SMASH★

GAMESS★

DC★ ... (37)

Molecular Dynamics

MODYLAS★

Gromacs★

ERmod★

MDACP... (31)

Lattice Models

ALPS★

DSQSS

BLOCK

DMRG++ (53)

Continuum Simulation

ANSYS Multiphysics

Octa ... (12)

Data Analysis

CLUPAN★

phonopy★ (58)

Visualization

fu★

TAPIOCA★ (37)

Database (11), Integrated Environment (4)
Machine Learning (17), Quantum Computing (6)

★ included in MateriApps LIVE!

Current status in computational materials science

- From developers' viewpoint
 - New algorithms should be implemented and used. Or, it will be forgotten ever existed.
 - It cost much to write and update documents
 - Development of software itself is hardly considered as scientific achievements
- From users' viewpoint
 - What kind of applications? Who develop them? Which application should I use for my problem?
 - Manual and documentation are not well prepared.
 - How to evaluate the accuracy of results?
- Goal of MateriApps project
 - **Forming of community in the field of computational materials science through the promotion of open source software**



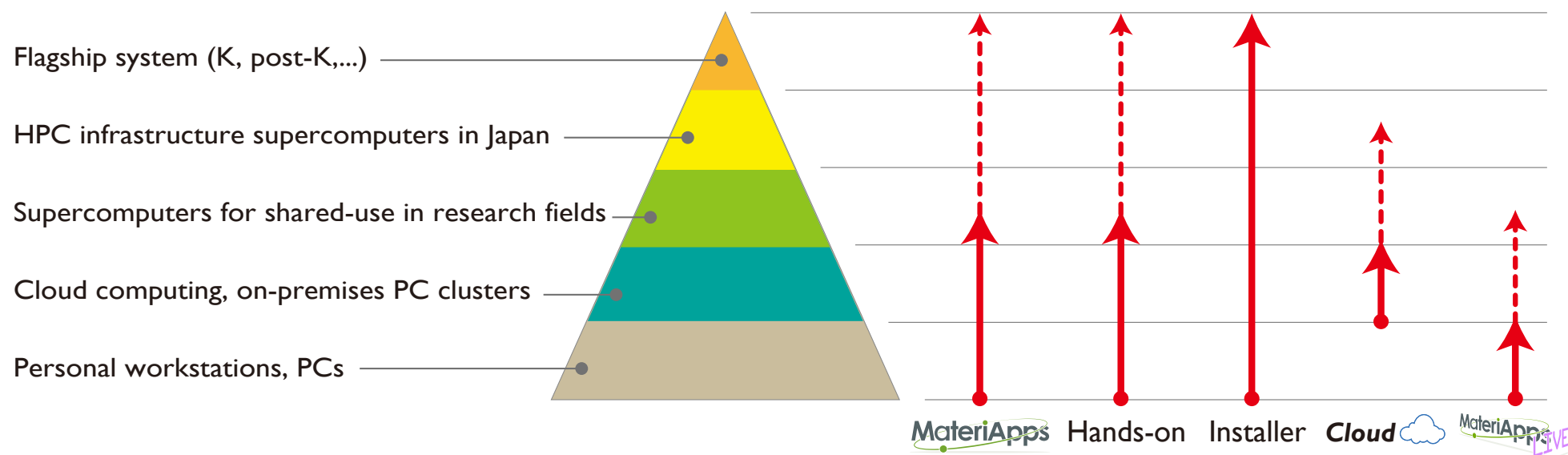
開発者



利用者

What MateriApps will provide

- To find and learn application software
 - catalog of application/tool on **MateriApps web**
- To start using application software
 - **MateriApps LIVE!**
- To active use application software
 - pre-installation to the K computer, supercomputers, etc: **MateriApps Installer**

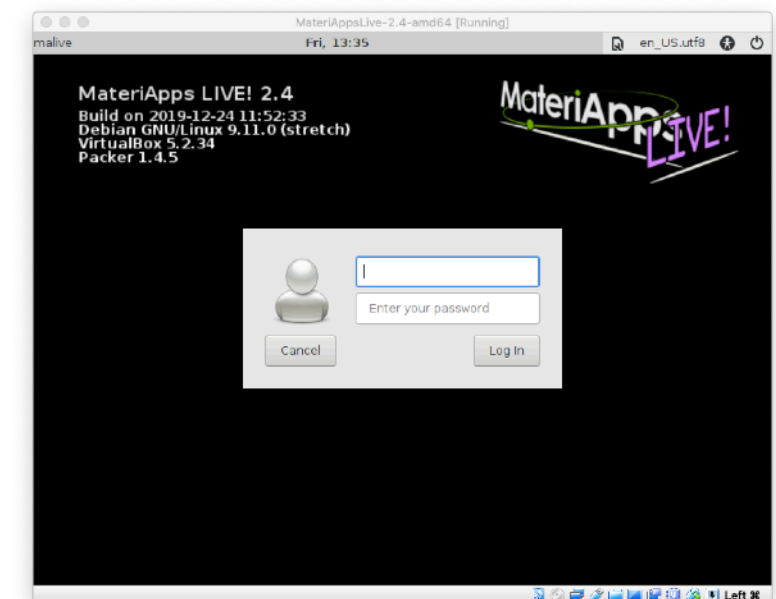


- Infrastructure for easily starting materials science simulations for theoreticians, experimentalists, researchers in companies, students, and more...

What is MateriApps LIVE! ?



- Live Linux bootable on virtual machine
 - run on Windows, Macintosh, etc
 - just boot and get ready for materials science simulations without installation
- Version 3.1 was published in Aug. 2020
- Pre-installed applications and tools
 - abinit, AkaiKKR, ALAMODE, ALPS, COQUEST, CP2K, DCore, DSQSS, H Φ , LAMMPS, mVMC, OpenMX, Quantum ESPRESSO, SMASH, xTAPP, etc
 - OVITO, ParaView, Tapioca, VESTA, VMD, XCrysDen...
 - GUI installer for CASINO, GAMESS, and VMD
- Available from MateriApps LIVE! webpage
 - c.a. 8700 copies distributed since July, 2013



MateriApps LIVE! is useful for ...

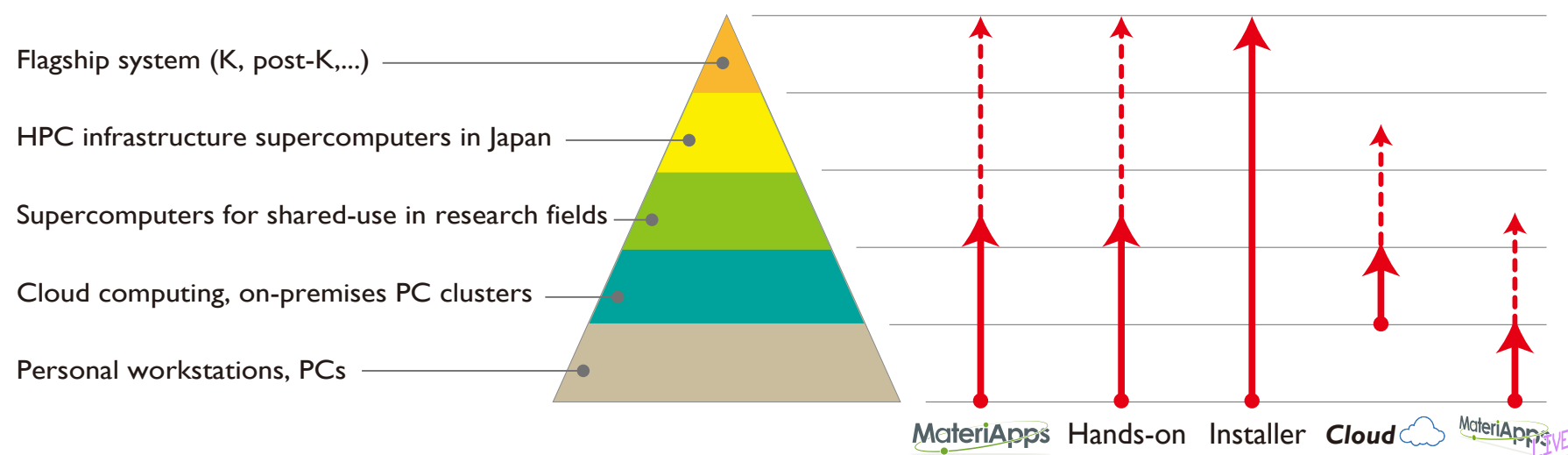
- Hands-on sessions using MateriApps LIVE!
 - MateriApps LIVE! Tutorials
 - $H\Phi$, xTAPP, ALPS, DCore, mVMC, ALAMODE, DDMRG, DSQSS, SALMON, CASINO, etc.
- Practices in lectures
 - Computational Physics
 - Computer Experiments (UNIX + C, LaTeX, VCS)
- Used by experimentalists, researchers in private companies
- Used by researchers in the field of computer science
- Easy setup (c.a. 15min) without no troubles
- Useful for operation check, trouble shooting, user support

Materials Science Simulation by MateriApps LIVE!



- Introduction / Setup
- First-principles band calculation (OpenMX / Quantum ESPRESSO / xTAPP)
- Simulation of solution by molecular dynamics (LAMMPS / Gromacs)
- Lattice model simulation (ALPS / H Φ / mVMC)
- Quantum chemistry calculation (in preparation)
- Hands-on materials are available at <https://github.com/cmsi/MateriAppsLive/wiki/MaLiveTutorial> (currently only in Japanese)

Wanna larger-scale simulations?

- For Debian/Ubuntu Linux workstations
 - Debian package for MateriApps LIVE! can be used
 - <https://github.com/cmsi/MateriAppsLive/wiki/UsingMateriAppsInDebian>
 - (Can also be installed on Google Colab)
- For PC clusters, clouds, supercomputers at ISSP and IT centers, Fugaku, etc
 - MateriApps Installer <https://ma.issp.u-tokyo.ac.jp/app/268>
 - Renewal underway as a software development and sophistication project at the University of Tokyo, 2020



What are included in USB Stick?

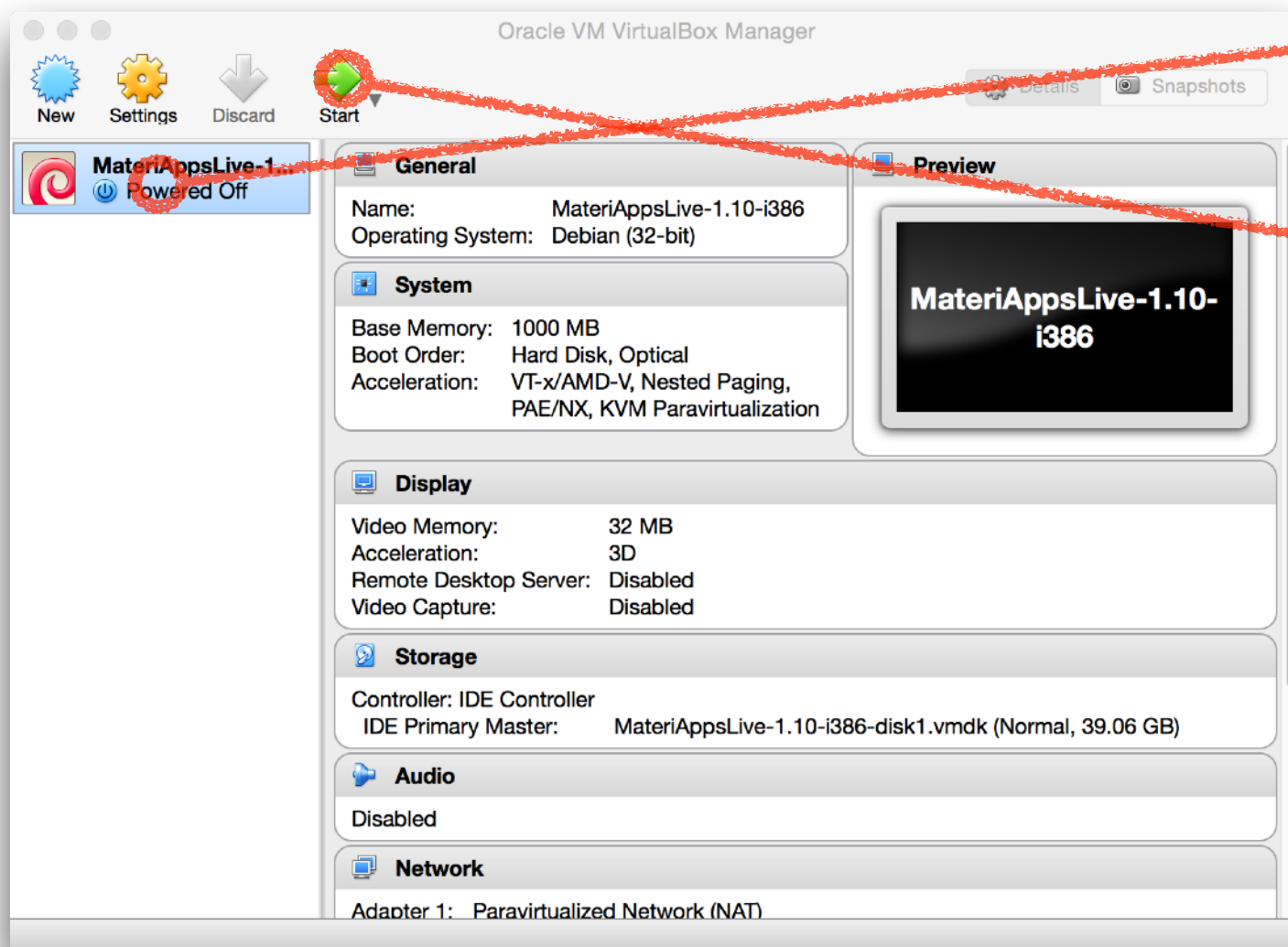
- MateriApps LIVE! USB  
 - setup.pdf, setup-en.pdf
this document
 - README.html, README-en.html
(copy from <https://github.com/cmsi/MateriAppsLive/wiki/MateriAppsLive-ova>)
 - VirtualBox Installer: VirtualBox-*-OSX.dmg, VirtualBox-*-Win.exe
(available at <https://www.virtualbox.org/wiki/Downloads>)
 - MateriApps LIVE! VirtualBox Disk Image: MateriAppsLive-*-amd64.ova
(available at <http://sourceforge.net/projects/materiappslive/files/>)



Let's get started

- ✓ Copy files in USB stick memory to hard disk
 - copy all the files to your PC, e.g. to desktop
- ✓ Install VirtualBox by double-clicking the installer
 - For Windows: VirtualBox-*-Win.exe
 - For Macintosh: VirtualBox-*-OSX.dmg
- ✓ Import MateriApps LIVE!
 - double-click MateriAppsLive-*.ova
 - VirtualBox will start automatically and import window will open. Then press “import” button
 - VirtualBox Manager window will appear in two or three minutes
- Host (host OS): operating system (Windows, Mac OS X, etc) on which VirtualBox is running
- Virtual machine (guest OS): operating system (= MateriApps LIVE!) running on VirtualBox

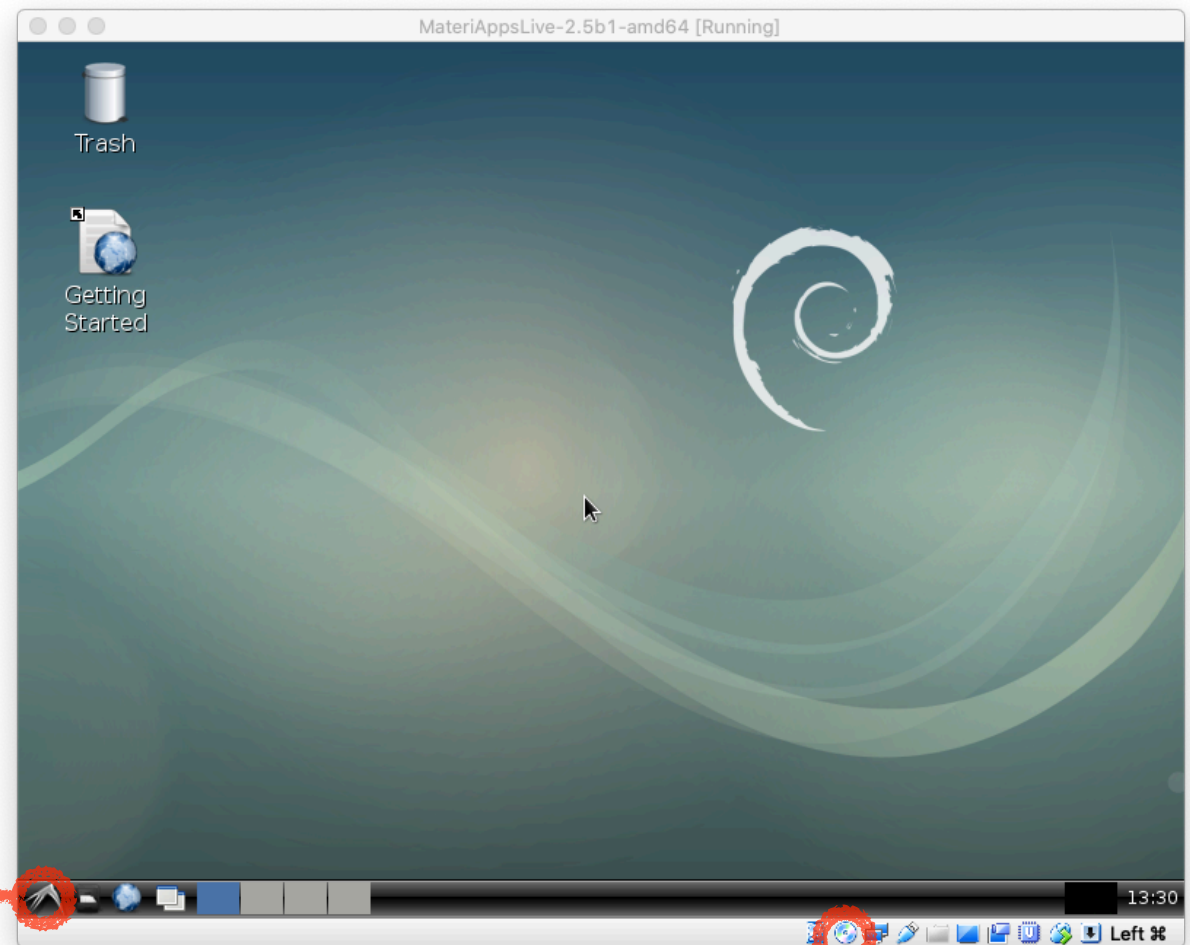
Boot in VirtualBox



1. Choose “MateriAppsLive...”
2. Press “Start” button.
3. Wait until login window will appear.

Login to MateriApps LIVE!

- Login by using
 - User name (login): *user*
 - Password: *live*
- Desktop (right) will appear
- *start menu*
- How to open a terminal window
start menu ⇒ “System Tools” ⇒ “LXTerminal”
- How to shutdown the virtual machine
start menu ⇒ “Logout” ⇒ “Shutdown”



CD-ROM button

Additional settings (1/2)

✓ Using Japanese keyboard

- start menu ⇒ “System Tools” ⇒ “Switch to Japanese Keyboard Layout”
- check if “@” key works correctly

✓ Changing resolution and scale of the virtual machine window

- Resolution (number of pixels): “800 x 600” by default
- Scale (pixel density): “200%” by default
- The resolution and scale can be changed from the “View” menu ⇒ “Virtual screen 1” of the host OS
- When using visualization software such as VESTA, OVITO, ParaView, set the resolution to “1024 x 768” or higher
- If characters are small and difficult to see, increase the scale

Additional settings (2/2)

- ✓ File sharing between host OS and virtual machine
 - shutdown the virtual machine, if it is running
 - choose MateriAppsLive-* in VirtualBox Manager window, then “Settings”
 - open “Shared Folders” tab and click “+” on the right
 - click “v” on the right of “Folder Path”, choose “Other...”, and select the folder to be shared
 - check “Auto-mount” box and press “OK”. Then press “OK” again
 - the folder specified above can be accessed as /media/sf_... after restarting the virtual machine
- ✓ Browsing contents of ISO image file (*.iso) from the virtual machine
 - click CD-ROM icon at the bottom of the virtual machine window frame, select “Choose disk image ...”, and select the ISO image file
 - contents of ISO image file are accessible via /media/cdrom0

Tips

- ✓ Copy & Paste: How to paste strings copied from a PDF file on host OS?
 - right click on terminal window ⇒ “Paste”
 - or press “V” with “shift” and “control” keys
 - right click ⇒ “Copy”, or “shift + control + C” to copy a string
- ✓ Completion/history/sequential search of command lines and filenames
 - Hit the tab key in the terminal to complete the command name or the filename
 - Hit the “↑” key in the terminal to trace back the history of commands
 - Execute the “history” command in the terminal to display the list of commands executed
 - Hit “Ctrl + r” in the terminal to search the commands executed so far (reverse incremental search)

MateriApps planning & production

- Administration:
 - Center for Computational Materials Science, Institute for Solid State Physics, University of Tokyo (ISSP-CCMS)
- MateriApps Development Team
 - Kota Ido (ISSP), Shusuke Kasamatsu (Dept. of Phys., Yamagata Univ.), Takeo Kato (ISSP), Naoki Kawashima (ISSP), Hikaru Kouta (ISSP), Synge Todo (Dept. of Phys., Univ. of Tokyo/ISSP), Masahito Fukuda (ISSP), Kanako Yoshizawa (RIST)
 - (contract) Yusuke Konishi and Gotai Yamada
- Cooperation:
 - Research Organization for Information Science and Technology (RIST)
- Sponsor
 - Elements Strategy Initiative
 - Program for Promoting Researches on the Supercomputer Fugaku: DPMSD (Development of high-performance Permanent Magnets by large-scale Simulations and Data-driven approaches)