How to setup MateriApps LIVE!

MateriApps LIVE! Development Team

MateriApps

MateriApps — a Portal Site for Materials Science Simulation

- **Aiming at the community formation through the promotion of application**

since May 2013

- Introducing 277 materials science applications and tools (as of 2020.10)
- 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

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Applications on MateriApps

- Introducing 273 materials science applications and tools

DFT
AkaiKKR☆
OpenMX☆
xTAPP☆
ABINIT☆
...   (80)

Quantum Chemistry
FMO☆
SMASH☆
GAMESS☆
DC☆...   (38)

Molecular Dynamics
MODYLAS☆
Gromacs☆
ERmod☆
MDACP...(31)

Lattice Models
ALPS☆
DSQSS
BLOCK
DMRG++ (57)

Continuum Simulation
ANSYS Multiphysics
Octa ...   (12)

Data Analysis
CLUPAN☆
phonopy☆ (59)

Visualization
fu☆
TAPIOCA☆(37)

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

☆ included in MateriApps LIVE!

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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
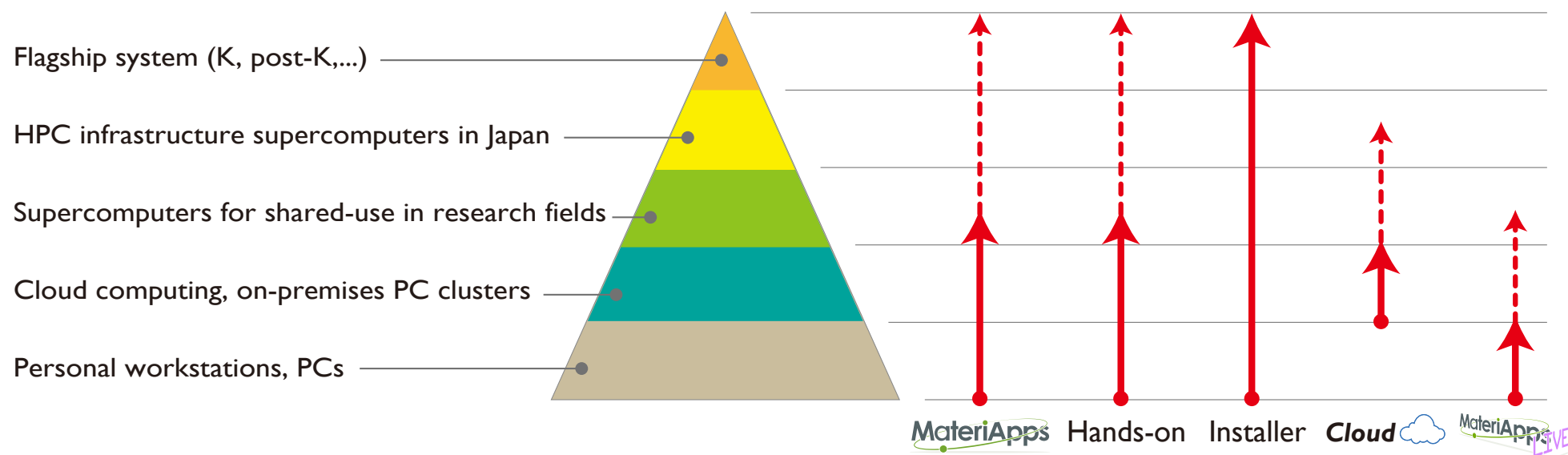
開発者

want

利用者

MateriApps

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 3.2 was released in Oct. 2020
- Pre-installed applications and tools
  - abinit, AkaiKKR, ALAMODE, ALPS, CONQUEST, Feram, DCore, DSQSS, HΦ, LAMMPS, mVMC, OCTA, OpenMX, Quantum ESPRESSO, SMASH, TeNeS, xTAPP, etc
  - OVITO, ParaView, Tapioca, VESTA, VMD, XCrysDen…
  - GUI installer for CASINO, GAMESS, and VMD
- Available from MateriApps LIVE! webpage
  - c.a. 9500 copies distributed since July, 2013
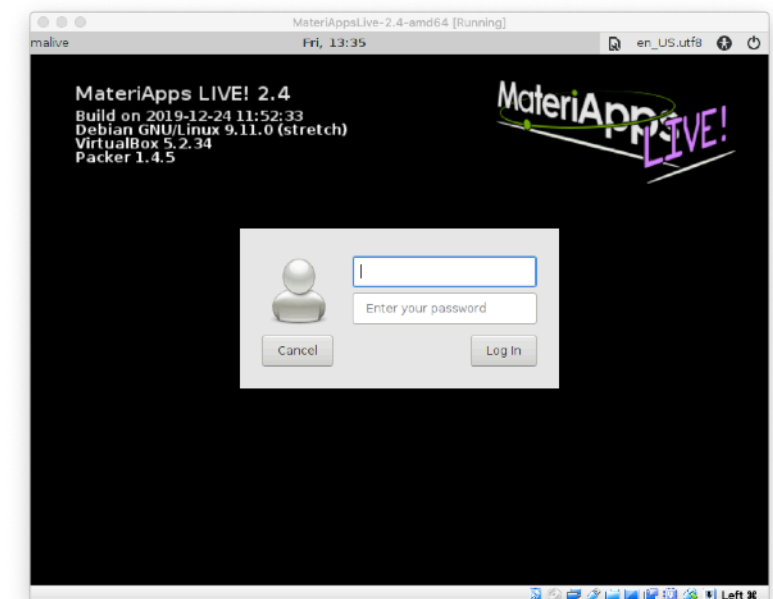
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MateriApps LIVE! is useful for ...

- Hands-on sessions using MateriApps LIVE!
    - MateriApps LIVE! Tutorials
    - HΦ, xTAPP, ALPS, DCore, mVMC, ALAMODE, DDMRG, DSQSS, SALMON, CASINO, TeNeS, 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 / HΦ / 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
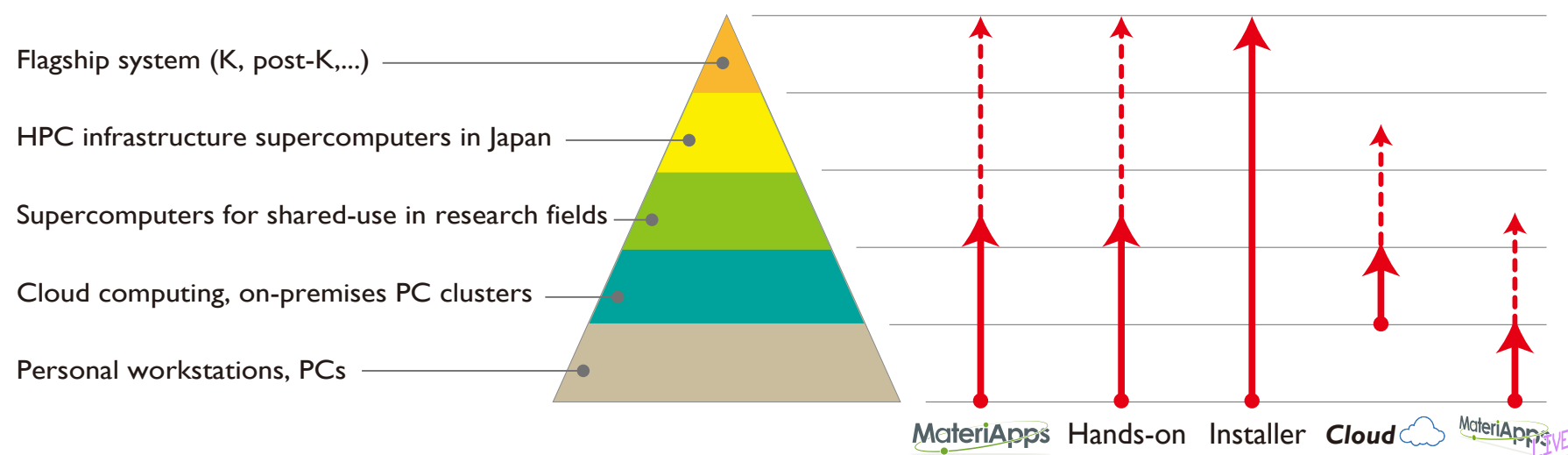
What are included in USB Stick?

- 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! VitualBox 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: VirutalBox-*-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
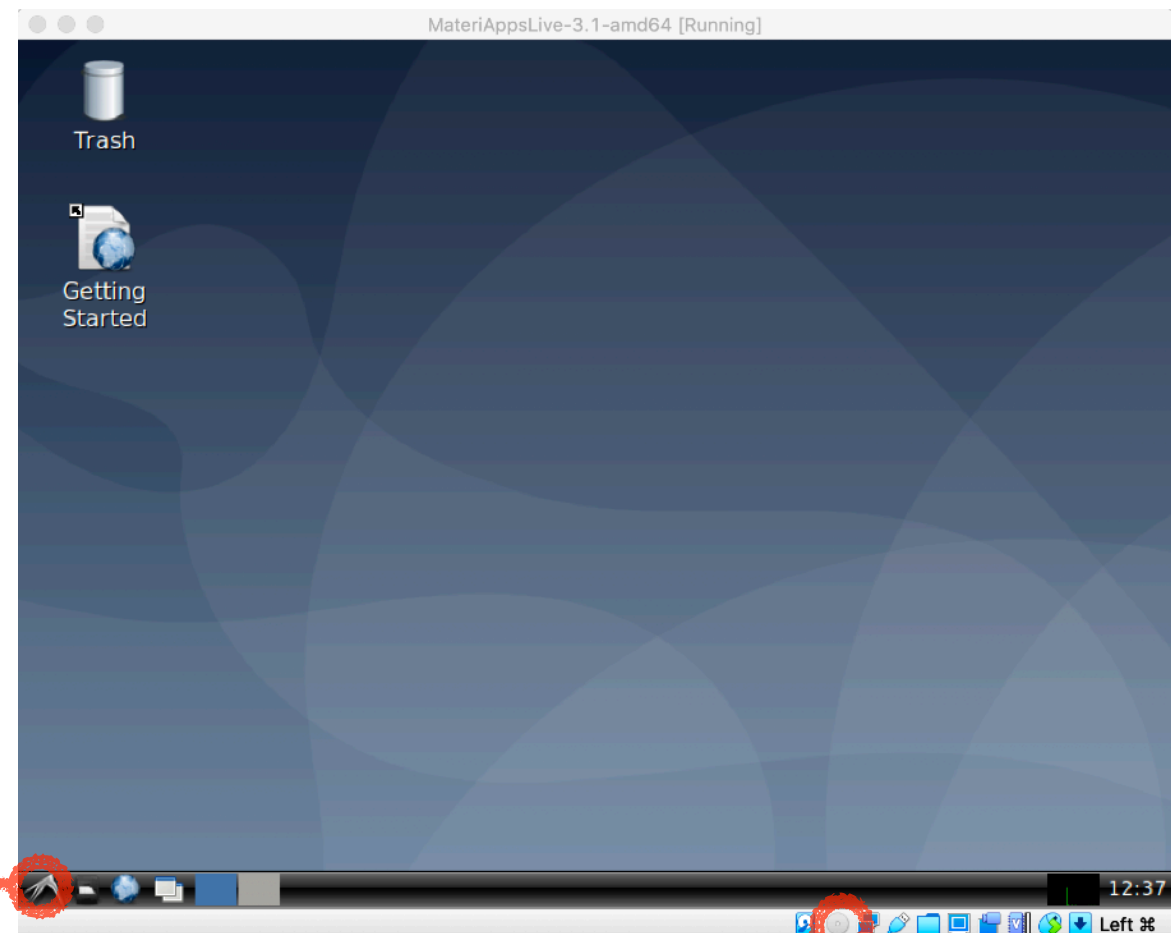- Virtual machine (guest OS): operating system (= MateriApps LIVE!) running on VirtualBox

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Boot in VirtualBox
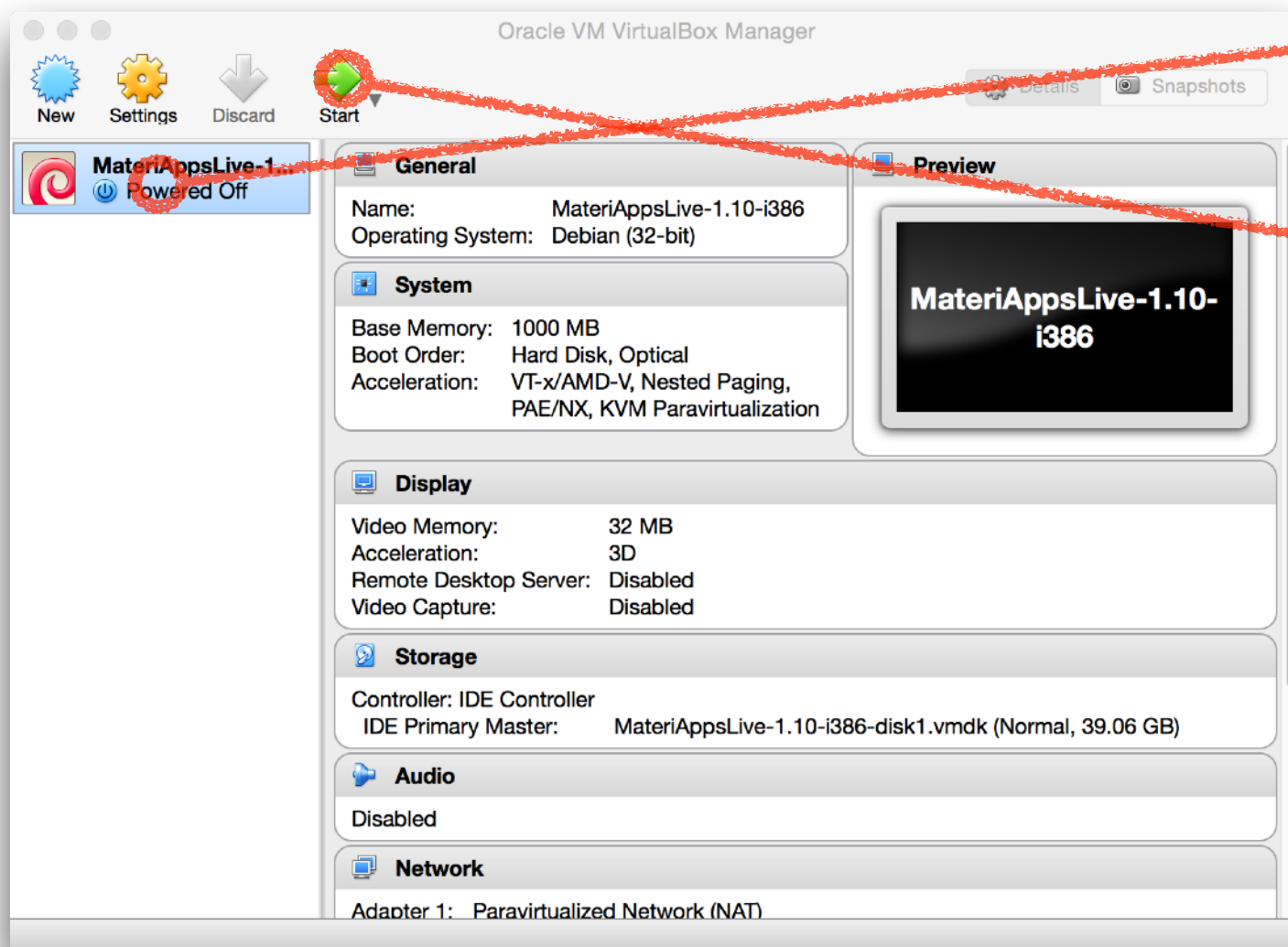
1. Choose "MateriAppsLive…"

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

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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:
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    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)