2022/09/19 [for version 4.0]

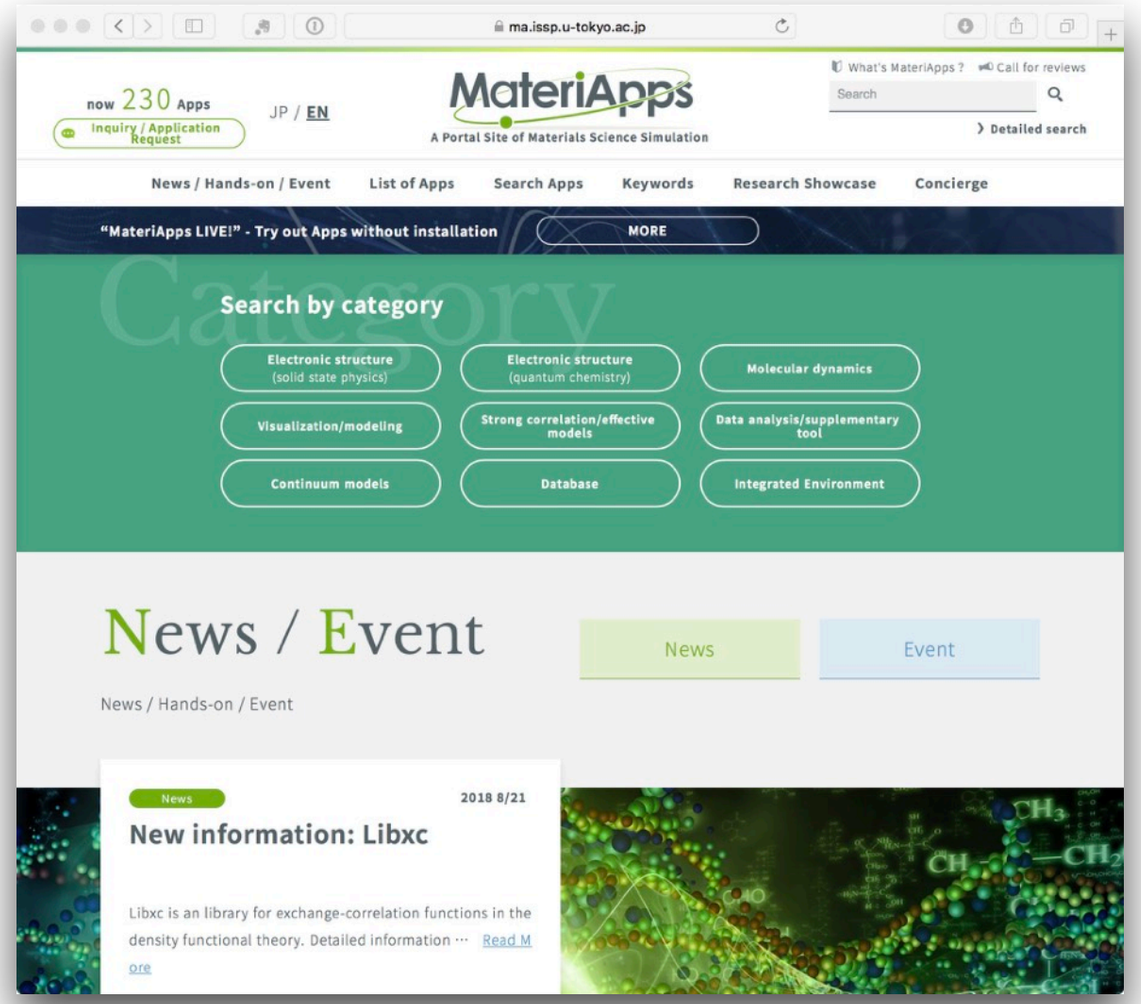
# How to setup MateriApps LIVE!

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 293 materials science applications and tools (as of 2022.9)
- 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
- 22,000+ page views / month, 6,000+ unique visitors / month (FY2021)

# Applications on MateriApps

- Introducing 273 materials science applications and tools

**DFT**
AkaiKKR☆
**OpenMX**☆
xTAPP☆
ABINIT☆
... (82)

**Quantum Chemistry**
**FMO**☆
**SMASH**☆
GAMESS☆
DC☆... (39)

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

**Lattice Models**
**ALPS**☆
DSQSS
BLOCK
DMRG++ (64)

**Continuum Simulation**
ANSYS Multiphysics
Octa ... (13)

**Data Analysis**
CLUPAN☆
phonopy☆ (59)

**Visualization**
fu☆
TAPIOCA☆(40)

Database (13), Integrated Environment (4)
Machine Learning (31), Quantum Computing (8)

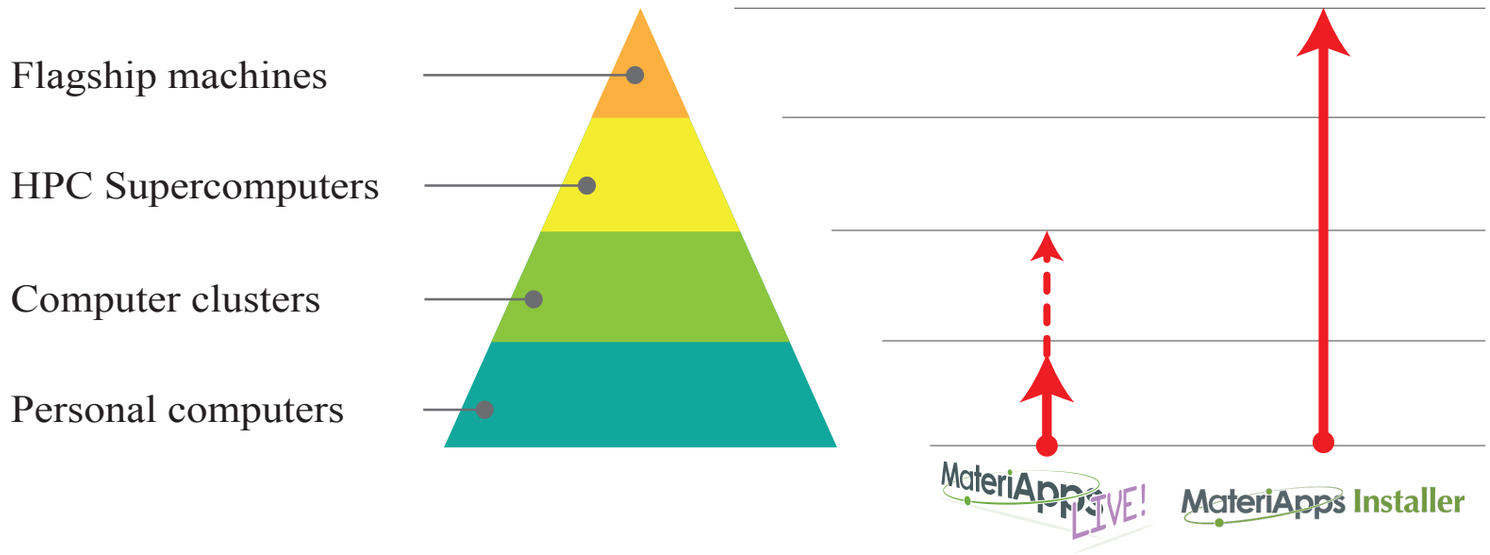
☆ included in MateriApps LIVE!

# 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


# What MateriApps will provide

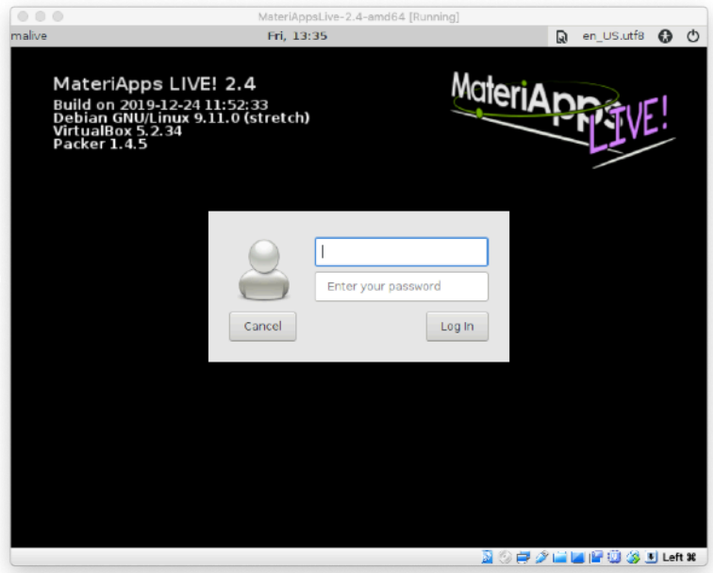
- To find and learn application software
  - catalog of application/tool on MateriApps web
- To start using application software
  - MateriApps LIVE!
- To active use application software
  - pre-installation to Fugaku, supercomputers, etc: MateriApps Installer




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

# What's MateriApps LIVE!

- Debian Linux running on a virtual machine (VirtualBox)
  - works on Windows, Intel Mac, etc (Docker edition available for Apple Silicon)
  - just boot and get ready for materials science simulations without installation
- Version 4.0 was released in Sep 2022
- Pre-installed applications and tools
  - abinit, AkaiKKR, ALAMODE, ALPS, CONQUEST, Feram, DCore, DSQSS, HΦ, LAMMPS, mVMC, OCTA, OpenMX, Quantum ESPRESSO, PHYSBO, SMASH, TeNeS, xTAPP, etc
  - OVITO, ParaView, Tapioca, VESTA, VMD, XCrysDen.
  - GUI installer for CASINO, GAMESS, and VMD
- Available from MateriApps LIVE! webpage
  - c.a. 14,000+ copies distributed since July, 2013

# 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)

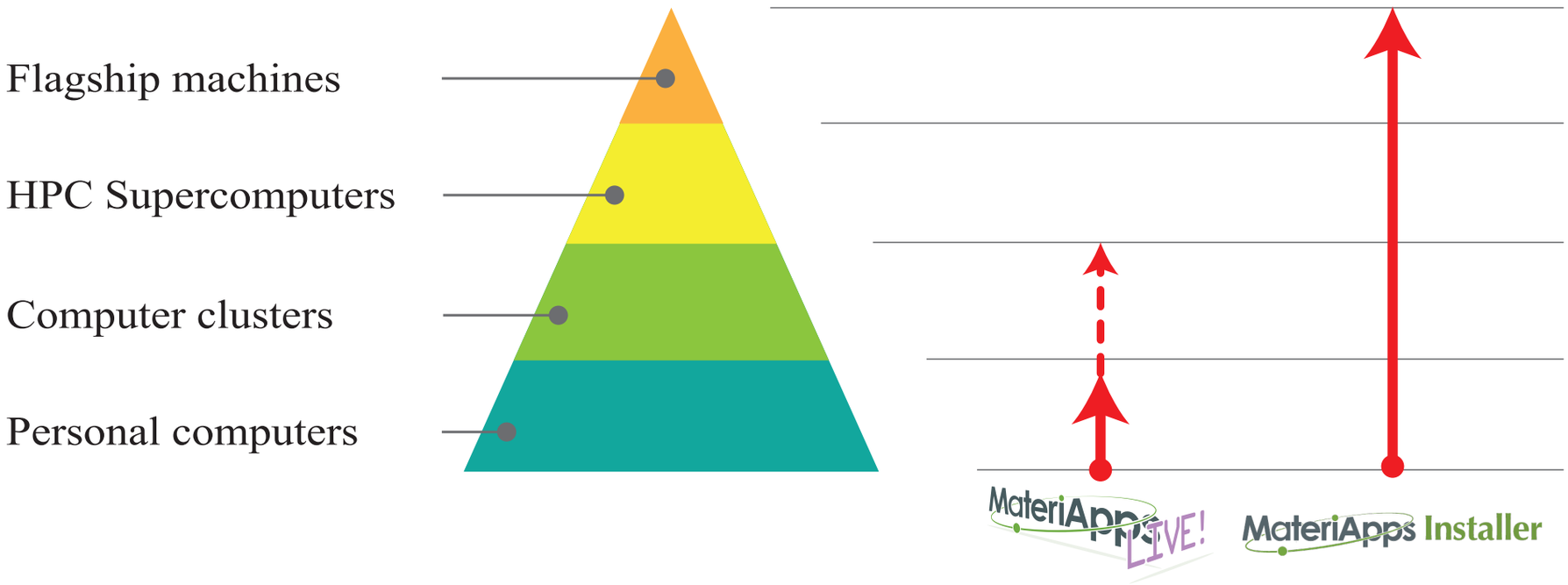
- Hands-on materials are available at https://github.com/cmsi/MateriAppsLive/wiki/MaLiveTutorial (currently only in Japanese)

# MateriApps LIVE! (Docker edition)

- MateriApps LIVE! 4.0 (Docker Edition) (Sep 2022)
  - Docker edition released at the same time in addition to VirtualBox edition
  - Supports Apple Silicon (M1/M2) Macs on which VirtualBox does not work
    - Supports Intel Macs as well
    - Should also work on Intel Windows, but scripts are not yet available
  - Docker Image is available on Docker Hub
    - https://hub.docker.com/r/malive/malive
- How to start MateriApps LIVE! (Docker edition)
  - https://github.com/cmsi/MateriAppsLive/wiki/GettingStartedDocker

# 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



# MateriApps LIVE! (VirtualBox edition)

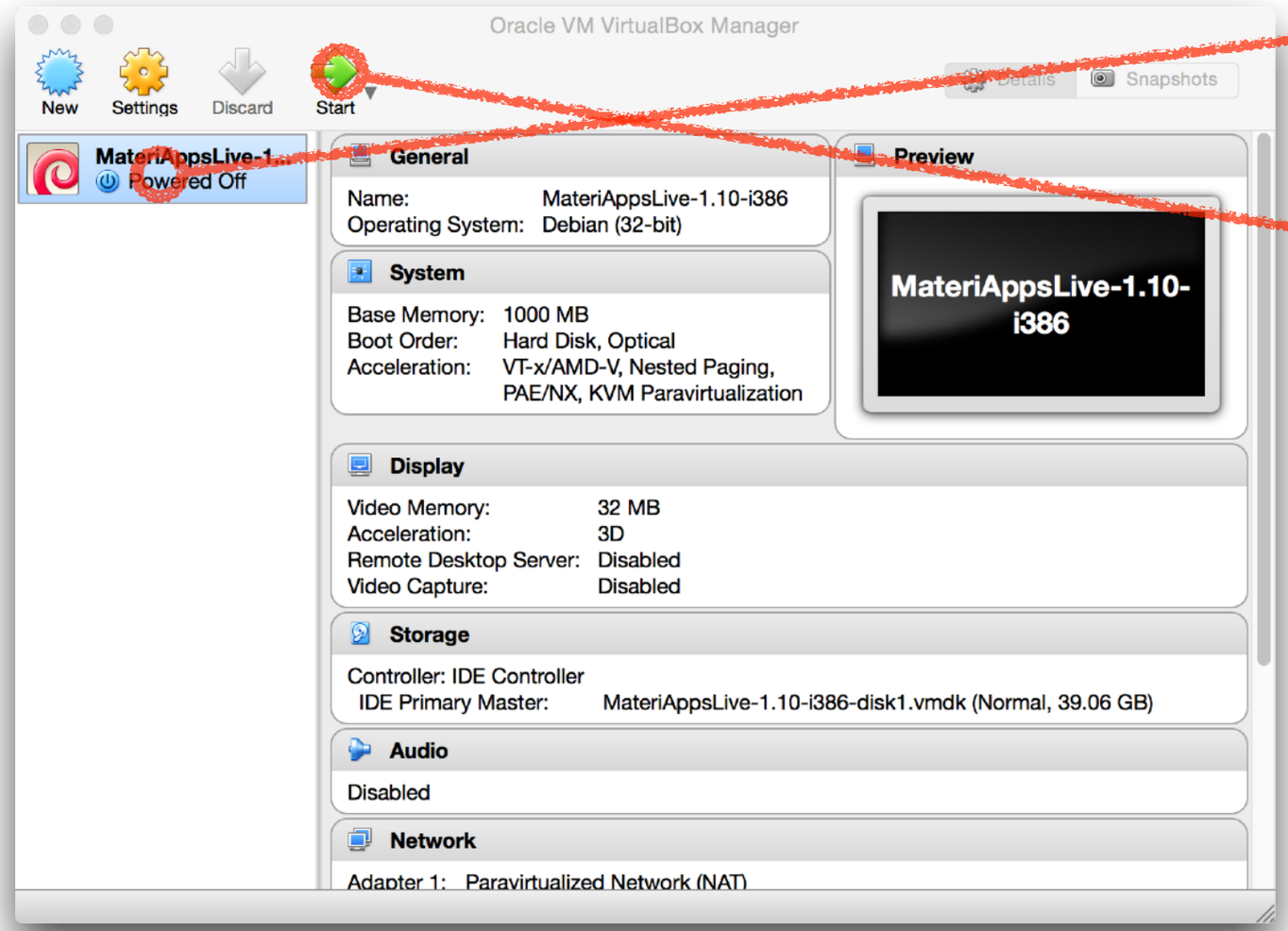

- Distribution files
  - setup.pdf, setup-en.pdf
    this document
  - README.html, README-en.html
    (copy from https://github.com/cmsi/MateriAppsLive/wiki/MateriAppsLive-ova)
  - VirtualBox Installer: VirtualBox-*-OSX.dmg, VirtualBox-*-Win.exe
    (available at https://www.virtualbox.org/wiki/Downloads)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

# Let's get started

- ✓ Download distribution files
- ✓ 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

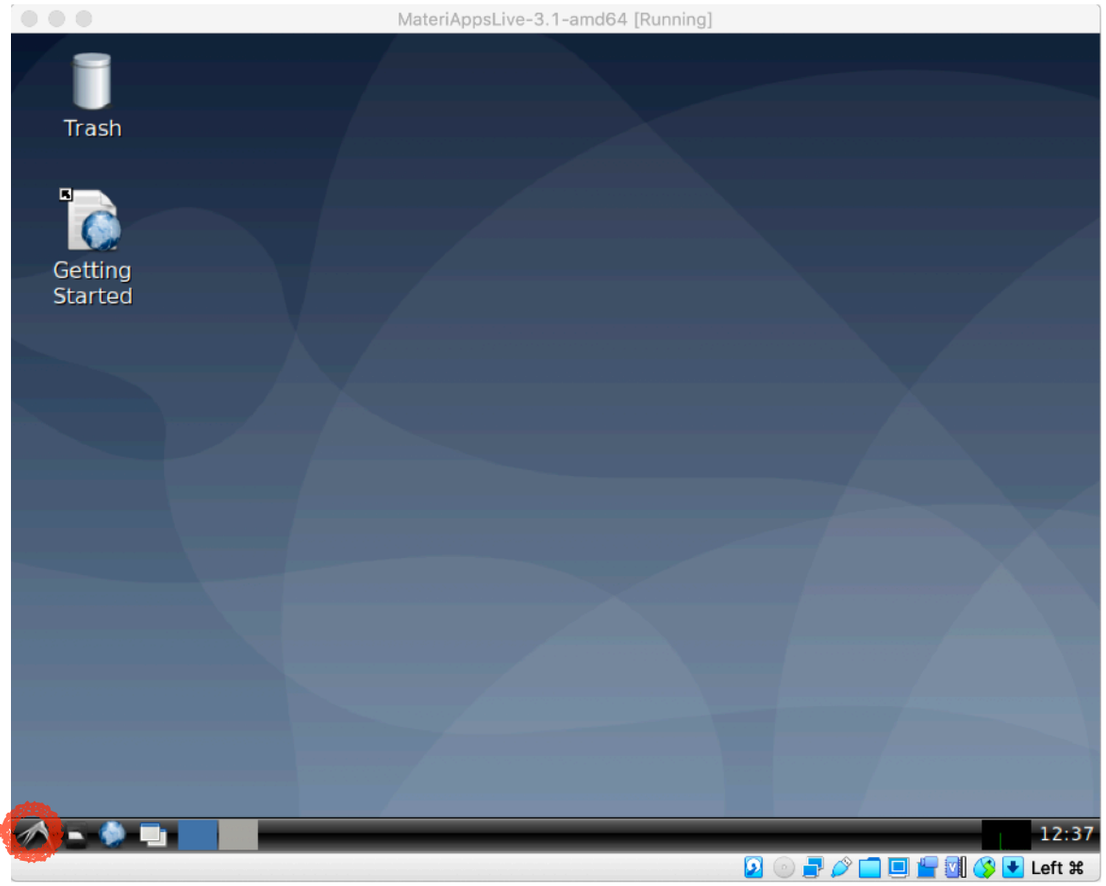
# Boot in VirtualBox




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”

# 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
- ✓ 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

# 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), Jun Yamazaki (ISSP)
  - (contract) Academeia (Yusuke Konishi, Masashi Noda, 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)