2019/12/24 [version 2.4]

How to setup MateriApps LIVE!

MateriApps LIVE! Development Team

MateriApps

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)
  - VirtualBox configuration scripts: vbconfig.*
    (available at https://github.com/cmsi/MateriAppsLive/tree/master/ova)
  - MateriApps LIVE! VitualBox Disk Image: MateriAppsLive-*-amd64.ova
    (available at http://sourceforge.net/projects/materiappslive/files/)

MateriApps — a Portal Site for Materials Science Simulation

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

since May 2013

- Introducing 268 materials science applications and tools (as of 2019.12)
- 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
- New! - Glossary of keywords, Concierge, Reviews
- 16000+ page views / month, 5500+ unique visitors / month

Applications on MateriApps

- Introducing 268 materials science applications and tools

DFT
AkaiKKR☆
OpenMX☆
xTAPP☆
ABINIT☆
... (77)

Quantum Chemistry
FMO☆
SMASH☆
GAMESS☆
DC☆... (36)

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

Lattice Models
ALPS☆
DSQSS
BLOCK
DMRG++ (50)

Continuum Simulation
ANSYS Multiphysics
Octa ... (12)

Data Analysis
CLUPAN☆
phonopy☆ (57)

Visualization
fu☆
TAPIOCA☆(38)

Database (11), Integrated Environment (3)
Machine Learning (17), Quantum Computing (4)

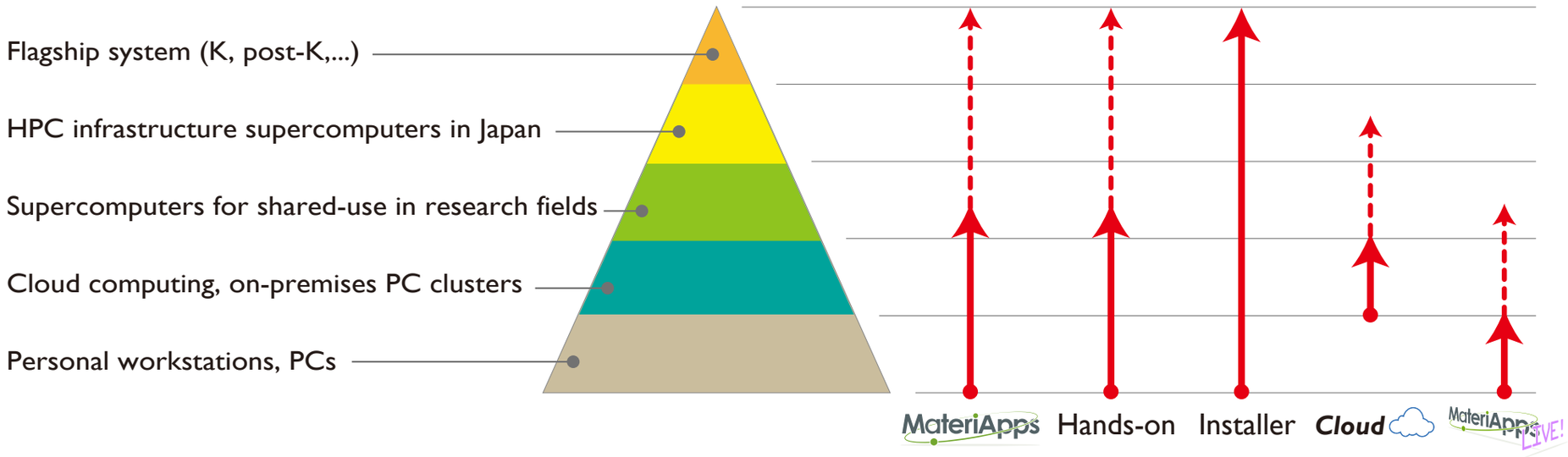
☆ included in MateriApps LIVE!

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

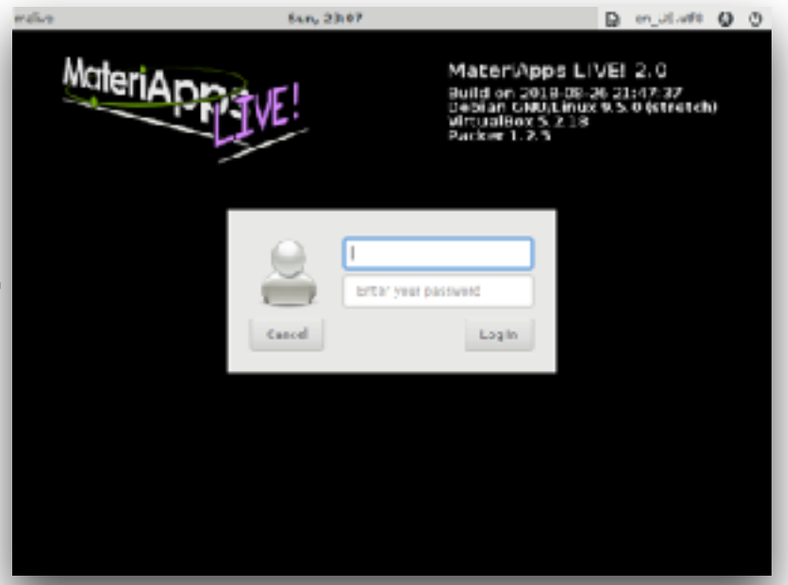
- To find and learn application software
  - catalog of application/tool on MateriApps web
- To start using application software
  - MateriApps LIVE!
- To active use application software
  - pre-installation to the K computer, supercomputers, etc: MateriApps Installer



- 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 2.4 was published in December 2019
- Pre-installed applications and tools
  - abinit, AkaiKKR, ALAMODE, ALPS, CP2K, Feram, ERmod, DCore, DSQSS, HΦ, LAMMPS, mVMC, OpenMX, Quantum ESPRESSO, SMASH, xTAPP, etc
  - OVITO, ParaView, Tapioca, VESTA, VMD, XCrysDen…
  - GUI installer for GAMESS and VMD
- Available from MateriApps LIVE! webpage
  - c.a. 6400 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, 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

Booting in VirtualBox

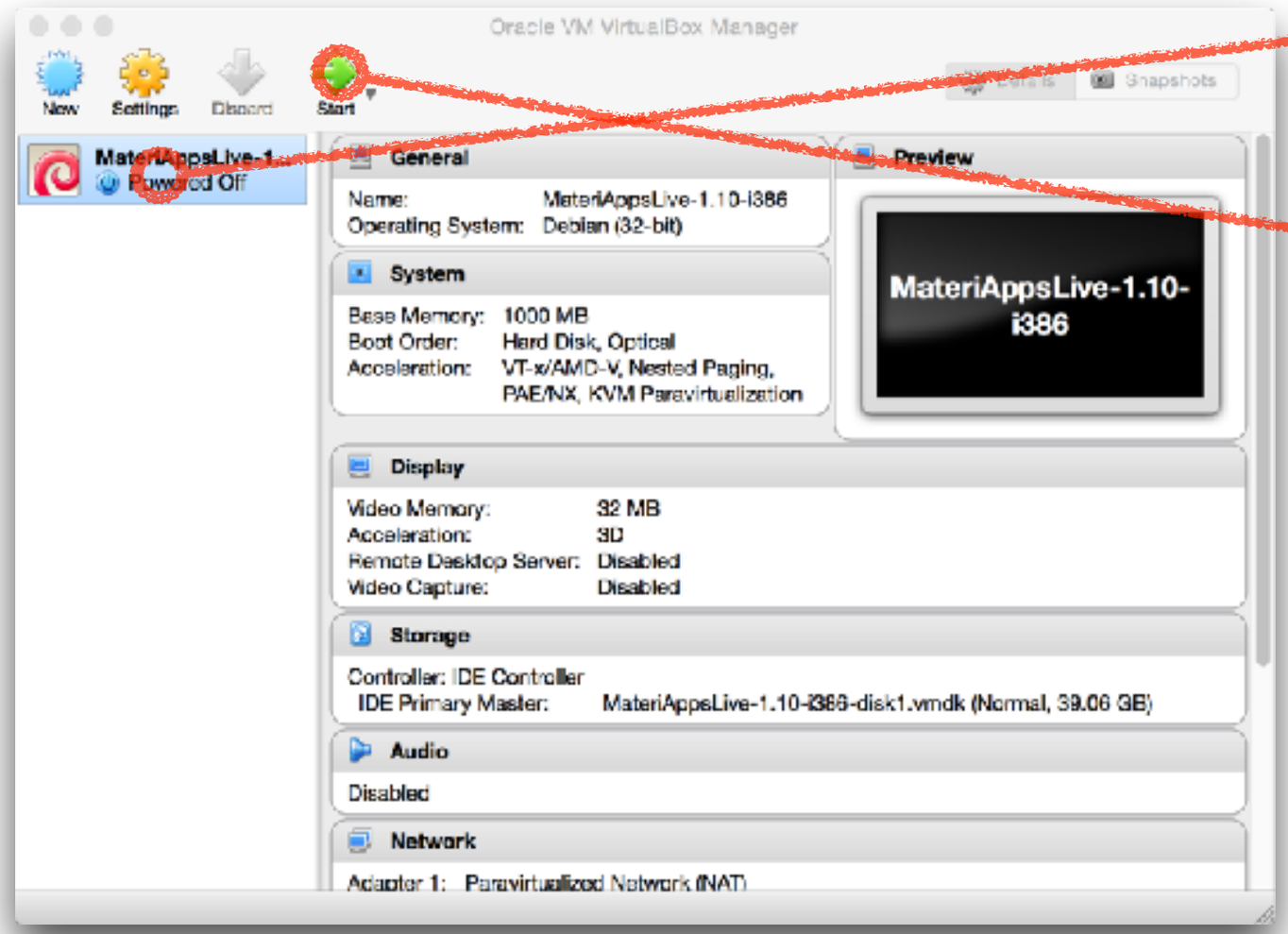
- ✓ Copy files in USB stick memory to hard disk
  - copy all the files to your PC, e.g. to desktop
- ✓ Install VirtualBox by double-clicking the installer
  - For Windows: VirutalBox-5.*-Win.exe
  - For Macintosh: VirtualBox-5.*-OSX.dmg
- ✓ Import MateriApps LIVE!
  - double-click MateriAppsLive-*-amd64.ova
  - 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

Setting up VirtualBox

- ✓ Setup: disabling unnecessary popup messages
  - on Windows: double click “vbconfig.bat”.
  - on Mac OS X: double click “vbconfig.command”, or run “*sh vbconfig.command*” in terminal software.
- ✓ Setup: enabling access from virtual machine to hard disc on host OS
  1. Choose MateriAppsLive-* in VirtualBox Manager window, and press “Settings”.
  2. Open “Shared Folders” tab and click “+” on the right.
  3. Click “v” on the right of “Folder Path”, choose “Other…”, and select the folder to which the files have been copied from the USB stick memory.
  4. Check “Auto-mount” box and press “OK”. Then press “OK” again.
  5. The folder specified in step 3 can be accessed as /media/sf_… after booting the virtual machine (explained in the following pages).

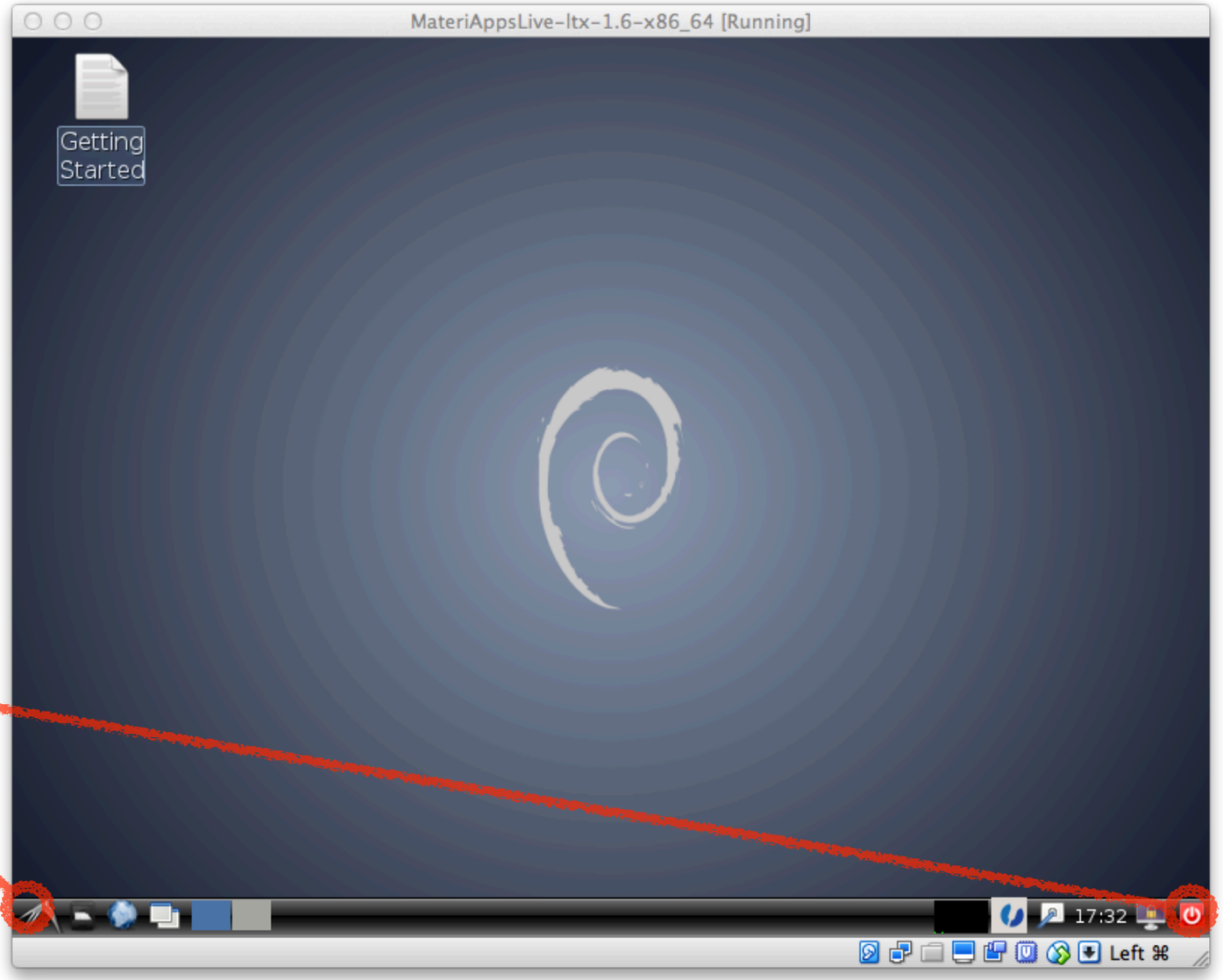
Booting in VirtualBox



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

Login to MateriApps LIVE!

- Login window will appear in a few minutes
- Login by using
  - User name (login): *user*
  - Password: *live*
- Desktop (right) will appear
- Important buttons
  - start menu
  - logout



Copy & paste, Japanese keyboard

- 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
- Setup for using Japanese keyboard
  - start menu ⇒ “System Tools” ⇒ “LXTerminal”
  - type “*setxkbmap -layout jp”* and “return” in terminal window
  - check if “@” key works correctly
  - (To revert to US keyboard: “*setxkbmap -layout us”*)

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 planning & production

- Administration:
  - Center for Computational Materials Science, Institute for Solid State Physics, University of Tokyo (ISSP-CCMS)
- MateriApps Administration Team
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- Cooperation:
  - Research Organization for Information Science and Technology (RIST)
  - Materials research by Information Integration Initiative, NIMS (MI2I)
- Sponsor
  - Post-K Priority Issue 7
  - Elements Strategy Initiative
  - Professional Development Consortium for Computational Materials Science (PCoMS)
  - TIA “Kakehashi”