2016/03/08 [OVA]

How to setup MateriApps LIVE!

MateriApps LIVE! Development Team

MateriApps

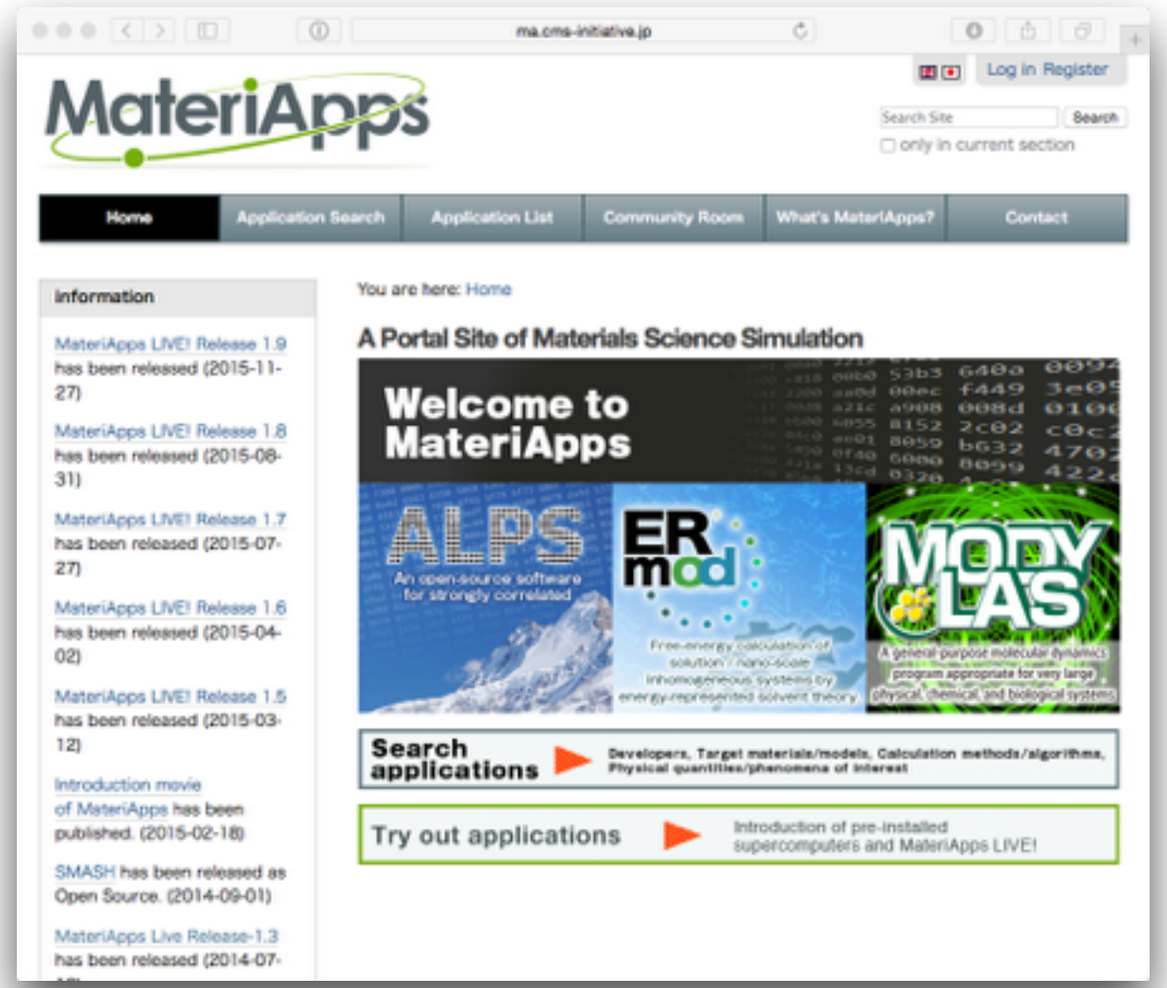
cmsi

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-*-i386.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 software**



- Introducing 170 materials science applications and tools (as of 2016.3)
- Finding applications
  - search tags: features, targets, calculation methods/algorithms
- Information of applications
  - brief introduction, link to official pages, information installation, usage, etc
- Forum for exchanging experiences
- Information of hands-on sessions, software update, etc
- 8000+ pageviews / month, 1500+ unique users / month

Applications on MateriApps

- Introducing 170 materials science applications and tools (as of 2016.3)

DFT
AkaiKKR☆
OpenMX☆
xTAPP☆
ABINIT☆
... (40)

Quantum Chemistry
FMO☆
SMASH☆
GAMESS☆
DC☆... (19)

Molecular Dynamics
MODYLAS☆
Gromacs☆
ERmod☆
MDACP...(19)

Lattice Models
ALPS☆
DSQSS
BLOCK
DMRG++ (25)

Continuum Simulation
ANSYS Multiphysics
Octa ... (12)

Data Analysis
CLUPAN☆
phonopy☆ (29)

Visualization
fu☆
TAPIOCA☆(28)

Materials Database (3)

☆ included in MateriApps LIVE!

Current status in computational materials science

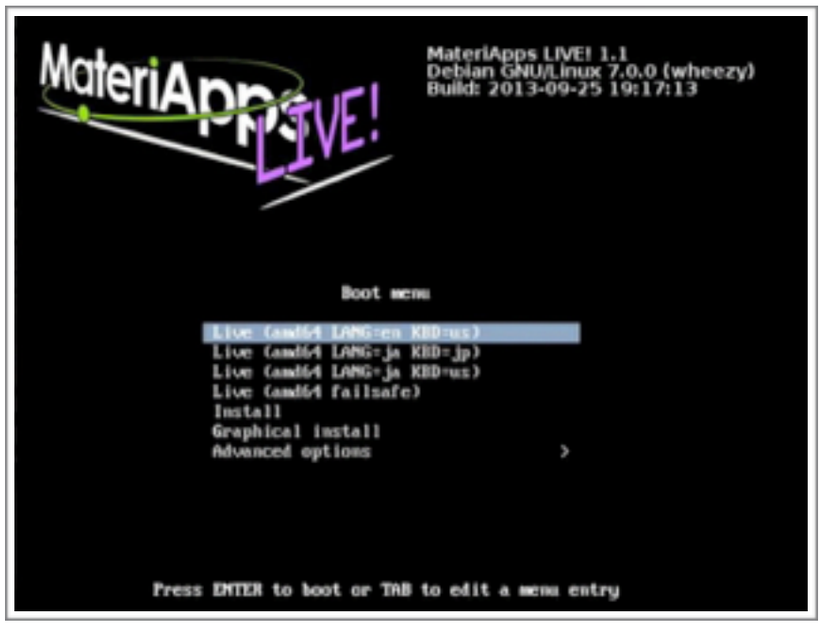
- From developers' viewpoint
  - New algorithms should be implemented and used. Or, it will be forgotten ever existed.
  - It cost much to write and update documents
  - Development of software itself is hardly considered as scientific achievements
- From users' viewpoint
  - What kind of applications? 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, major supercomputers, workstations, etc: MateriApps Installer
- Infrastructure for easily starting materials science simulations for theoreticians, experimentalists, researchers in companies, students, and more…

What is MateriApps LIVE! ?

- Bootable directly from USB stick, or in virtual machine (Debian Live Linux)
  - run on Windows, Macintosh, etc
  - just boot and get ready for materials science simulations without installation
- Version 1.10 was published on February 18, 2016
- Pre-installed applications and tools
  - ABINIT, AkaiKKR, ALPS, CP2K, Feram ,ERmod, DSQSS, Gromacs, LAMMPS, OpenMX, Quantum Espresso, SMASH, xTAPP, VESTA, etc
  - GUI installer for GAMESS and VMD
- available MateriApps LIVE! webpage



Let’s get started

✓Copy files in USB stick memory to hard disk

- copy all the files to your PC, e.g. to desktop

- Two ways to boot MateriApps LIVE!
  1. Start on virtualization software VirtualBox (explained in this document)
     - Simple, easy, reliable, but requires more memory
  2. Boot from USB stick memory
     - Run faster, but error-prone in some environment. Troublesome in setting up network

Booting in VirtualBox

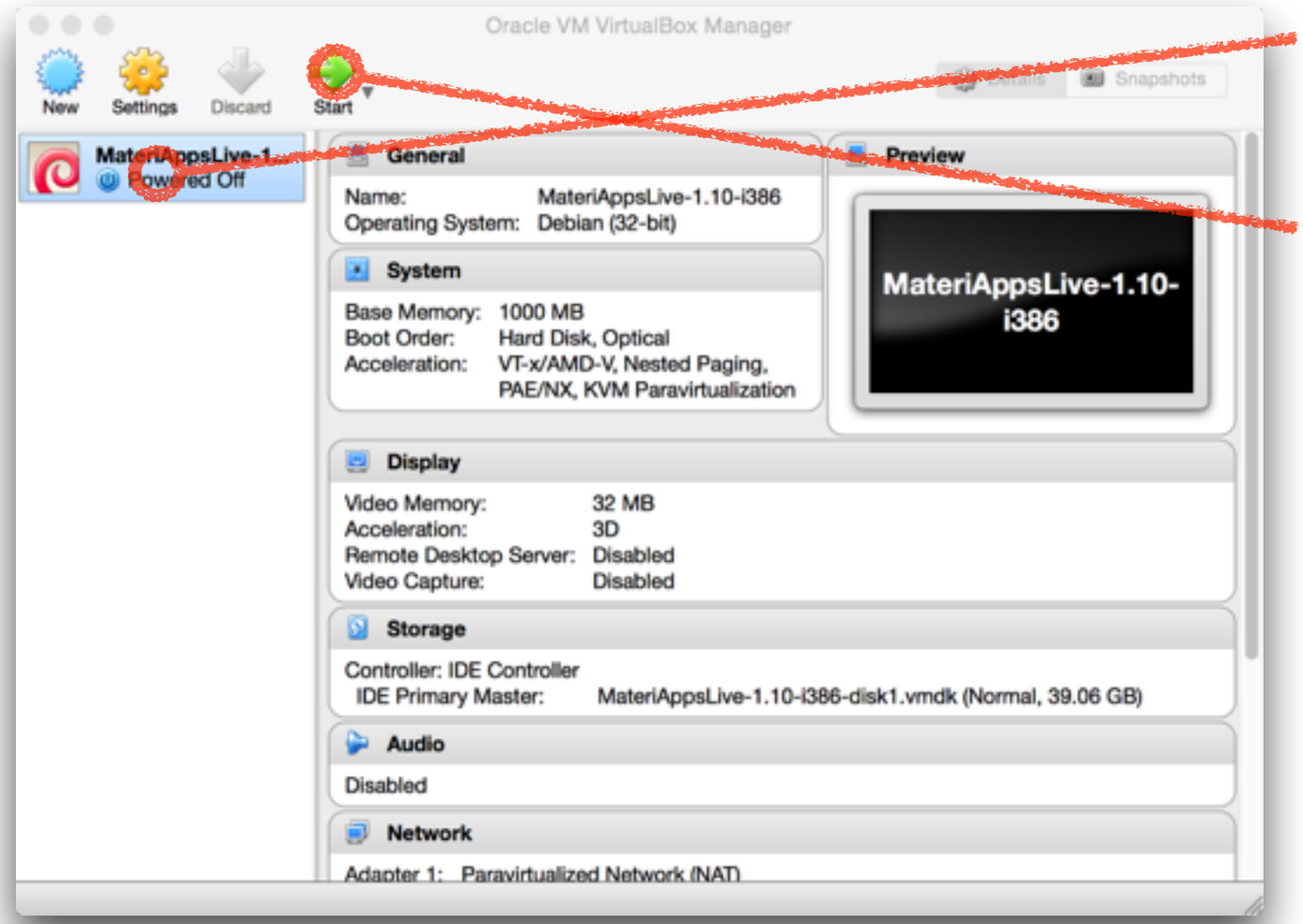
- ✓ Install VirtualBox by double-clicking the installer
  - For Windows: VirutalBox-5.*-Win.exe
  - For Macintosh: VirtualBox-5.*-OSX.dmg
- Import MateriApps LIVE!
  - double-click MateriAppsLive-*-i386.ova
  - VirtualBox will start automatically and import window will open. Then press “import” button
  - 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.sh”* 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).

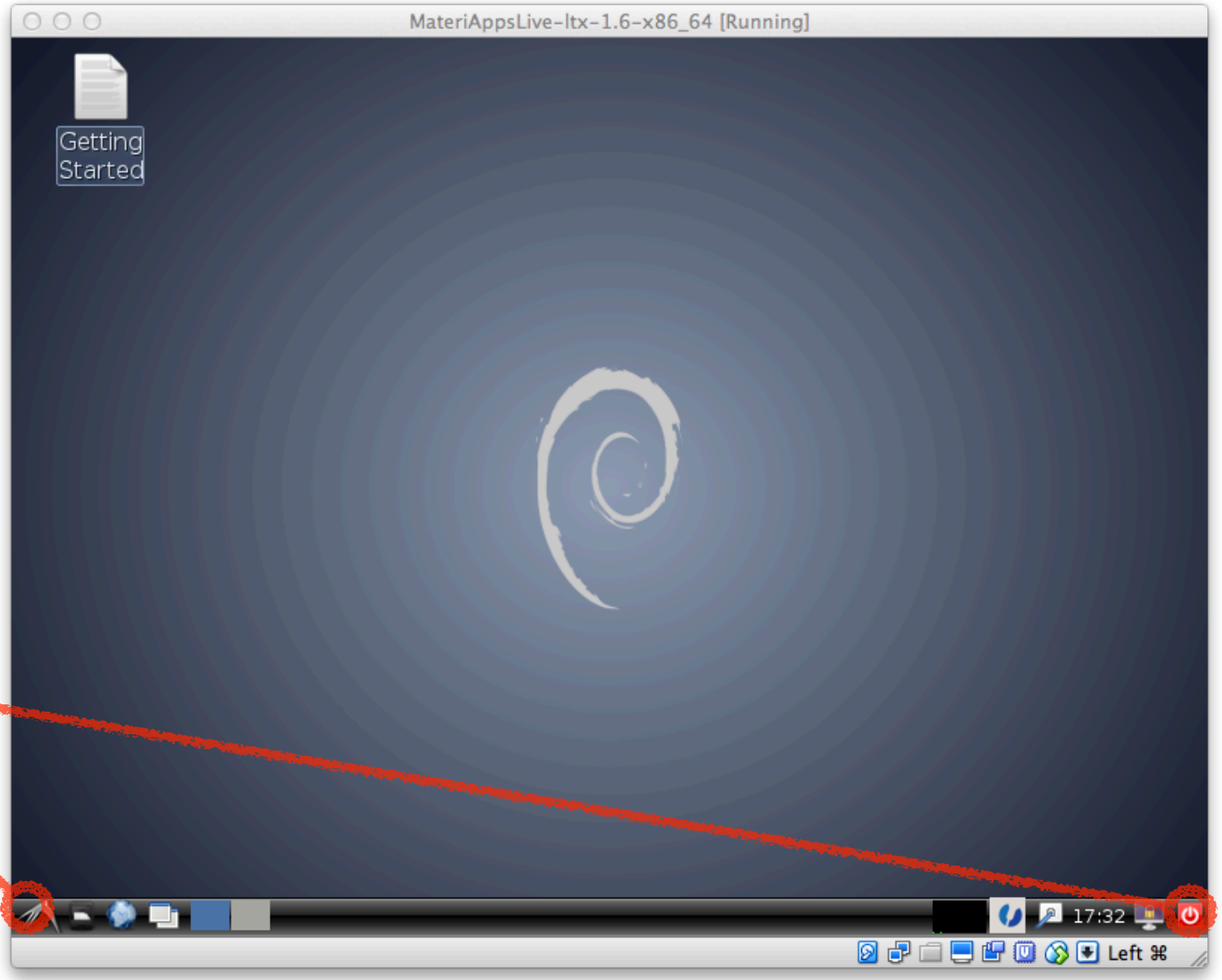
Booting in VirtualBox



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



Japanese keyboard, copy & paste

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

- Starting MateriApps LIVE!
- First-principles band calculation
  - first-principles software: OpenMX
  - input preparation: C-Tools, visualization: VESTA, fermi surface: XCrysDen
- Simulation of solution by molecular dynamics
  - general purpose MD software: Gromacs
  - visualization tool: VMD
- Monte Carlo simulation of phase transition in spin models
  - simulation package for strongly correlated lattice models: ALPS
  - visualization tool: ParaView
- Quantum chemistry calculation (in preparation)

- Hands-on materials are available at http://www.slideshare.net/cms_initiative/clipboards/materiappslive (currently only in Japanese)

MateriApps planning & production

- Hosting:
  - Computational Materials Science Initiative (CMSI); The Institute for Solid State Physics, The University of Tokyo (ISSP); Institute for Molecular Science, National Institutes of Natural Sciences (IMS); Institute for Materials Science, Tohoku University (IMR)
- Planning, Production, and User Support
  - CMSI Public Relations Subcommittee
  - MateriApps Administration Team
    - Synge Todo (Department of Physics, University of Tokyo/ISSP), Takeo Kato (ISSP), Ryo Igarashi (CMSI-ISSP), Syusuke Kasamatsu (ISSP), Naoki Kawashima (ISSP), Hikaru Kouta (CMSI-ISSP), Yusuke Konishi (CMSI-ISSP), Yayoi Terada (CMSI-IMR), Masashi Noda (CMSI-IMS), Haruhiko Matsuo (RIST), Kanako Yoshizawa (RIST), Kazuyoshi Yoshimi (ISSP)
    - (contract) Shoichi Sasaki (Ageha), Shigehiro Tsuchida (Ageha)
- Cooperation:
  - CMSI Elements Strategy Initiative Center; Center for Computational Materials Science, ISSP; Theoretical and Computational Chemistry Initiative, IMS; Computational Materials Research Initiative, IMR