MateriApps Live!の導入とHΦの使用方法

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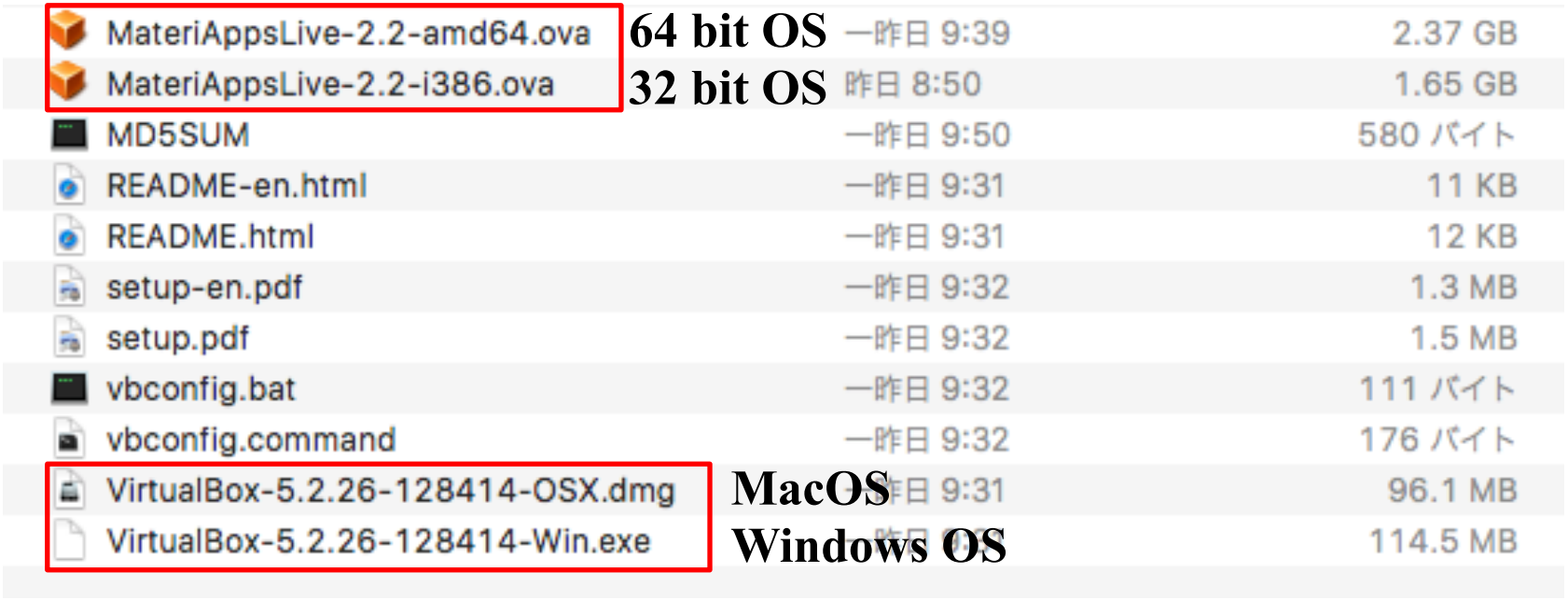
Note:

1. You can take the USB with you. Please install it on your PC and try it.

2. You can download VB in the following url:
https://www.virtualbox.org/wiki/Downloads

MaterialApps LIVE! can also be downloaded from the following site:
http://cmsi.github.io/MateriAppsLive/
(Please be careful that the file size of MateriApps LIVE! Distributed here is large, ~2GB)

Files in distributed USB



1. Copy VB and MateriAppsLive-*amd64.ova somewhere.
2. Starts VirtualBox Installer and install VirtualBox software.
3. Starts VirtualBox by double clicking “MateriAppsLive-*amd64.ova”. Click "Import" button in VirtualBox import window.

User: user
Password: live

Setting for Japanese keyboard:
setxkbmap -layout jp

MateriApps LIVE!

- Use in virtual machine (Debian Linux)
  - run on Windows, Macintosh, etc
  - just copy & click and get ready for materials science simulations without installation
- Pre-installed applications and tools
  - abinit, AkaiKKR, ALPS, CP2K, Feram ,ERmod, DSQSS, Gromacs, HΦ, LAMMPS, mVMC, OpenMX, Quantum Espresso, SMASH, xTAPP etc
  - ParaView, Tapioca, VESTA, VMD, XCrysDen…
  - GUI installer for GAMESS and VMD
- available from MateriApps LIVE! webpage
  - distributed 3000+ copies since 2013.7

Many apps have been already preinstalled in /usr/share /usr/bin

MateriApps LIVE! is useful in many situations!

- Hands on MateriApps LIVE!
  - MateriApps LIVE! Hands on
  - HΦ, mVMC, xTAPP, ALPS, DDMRG..
  - Coming Hands on: xTAPP 12/16 , DCore 12/26 [You can attend !]
- Lectures in university (tokyo-tech, tokyo science univ.)
  - Numerical Physics
  - Numerical Experiments (UNIX + C, LaTeX, version control system)
- Non-experts (experimentalists, researchers in industry or in computations science) can easily try to use applications [No compile !]
- Troubles in hands on are very rare ! (VirtualBox OVA ver.)
  Within 15 minutes you can finish setup
- Easy for trouble shooting and user supports
  because the environment is completely the same !

If you have questions about MA LIVE!..

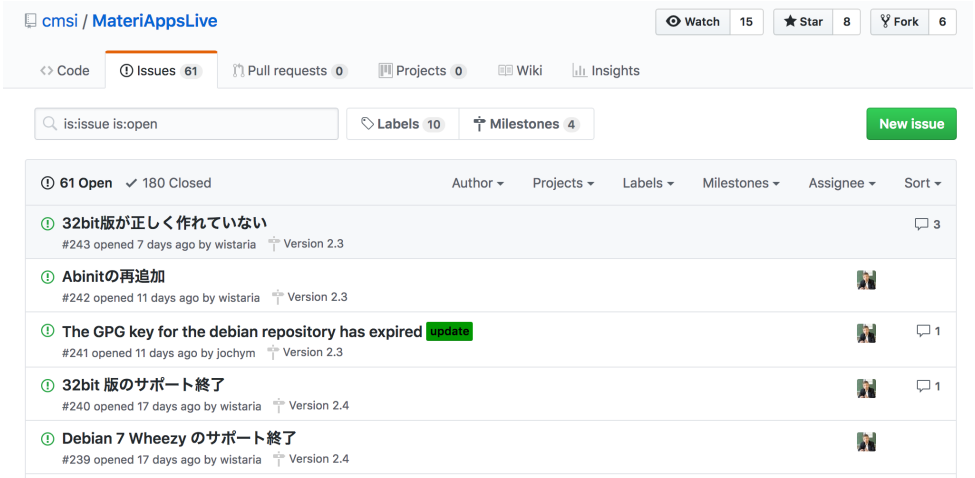
FAQ

https://github.com/cmsi/MateriAppsLive/wiki/FAQ#virtualbox

FAQ Frequently Asked Questions / よくある質問

- VirtualBox関連
- Software update / ソフトウェアアップデート
- Login and Logout / ログイン・ログアウト
- Keyboard / キーボード
- Japanese Input / 日本語入力
- Teminal / ターミナル

Forum https://github.com/cmsi/MateriAppsLive/issues



How to use HΦ in MA LIVE!

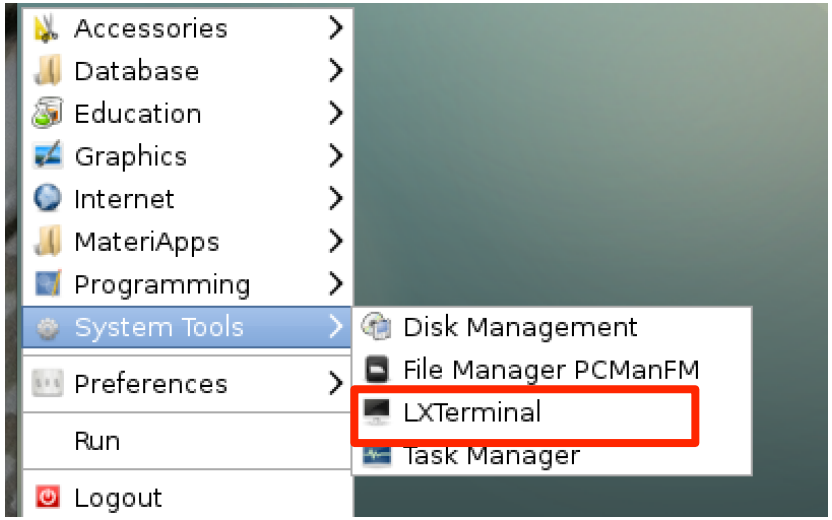
1. Start LXTerminal on Materi Apps LIVE!

2. Commnad “HPhi” already exists in MAL. So, you can perform HΦ’s simulations by executing the following command.

HPhi -s stan.in

3. Please refer to the various input files in “/usr/share/hphi/samples” [Some examples are shown on the next slides]

Setting for Japanese keyboard:
setxkbmap -layout jp

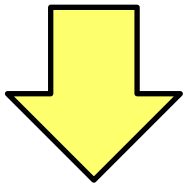


How to use HΦ for standard models

Only stan.in is necessary (< 10 lines) !

```
L         = 12
model     = “Spin”
method    = “CG”
lattice   = “chain”
J         = 1.0
2Sz       = 0
```

ex. L=12 1d Heisenberg model,
GS by LOBCG method



HPhi -s stan.in

./output : results are output

Method

Lanczos - ground state

CG - LOBCG

TPQ - finite-temperature

FullDiag - full-diagonalization

Important files

./output/zvo_energy.dat → energy

./output/zvo_Lanczos_Step.dat → convergence

./output/zvo_cisajs.dat → one-body Green func.

./output/zvo_cisajscktalt.dat → two-body Green func.

Demonstrations @ laptop

1D Heisenberg model (S=1/2): LOBCG

kagome Heisenberg model (S=1/2): TPQ

You can enjoy HΦ on your laptop !

How to build HΦ in MA Live!

If you want to use the latest version of HΦ, you may need to rebuild it.

1. git clone https://github.com/issp-center-dev/HPhi.git
2. cd ./HPhi
3. mkdir build
4. cd ./build
5. cmake ../
6. make
7. Binary “HPhi” is generated below HPhi/build/src.

You can install HΦ as described above,
if git, cmake c/fortran compilers and lapack are available in your environment.