MateriApps LIVE!の使い方・実演

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Contents

Have you already downloaded VirtualBox and MaterialApps LIVE! ?

https://github.com/cmsi/MateriAppsLive/wiki/OnlineTutorial

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 12000+ 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!
  - HΦ, mVMC, xTAPP, ALPS, DDMRG, QE, LAMMPS…
- 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!..

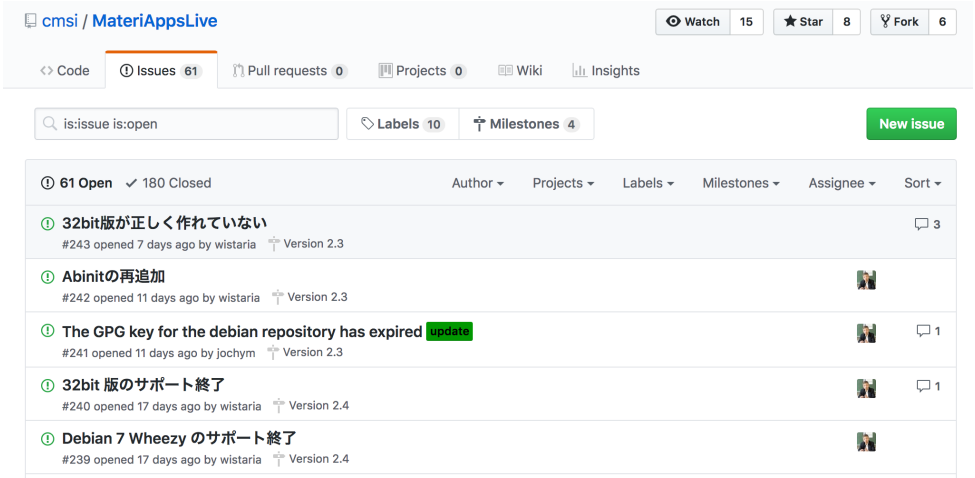
FAQ

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

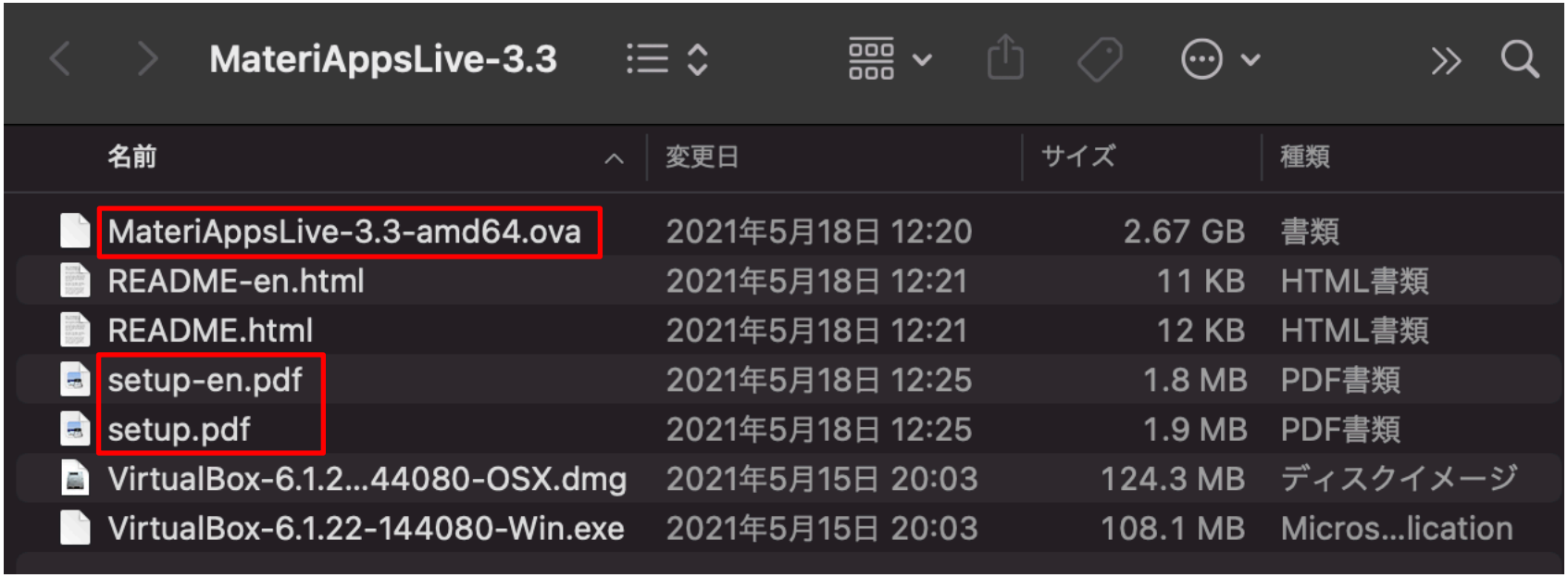
FAQ Frequently Asked Questions / よくある質問

- 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



Files in “MateriAppsLive-3.3-dist”



1. **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

2. **See setup.pdf to check Tips.**
   (ex: p15, How to transfer files on VB to Host OS)

How to use HΦ in MA LIVE!

1. Start LXTerminal on MateriApps LIVE!

Setting for Japanese keyboard:

start menu⇒System Tools

⇒Switch to Japanese Keyboard Layout

2. Download the latest version of HΦ

```
sudo apt-get update
sudo apt-get install hphi
```

3. Make work direction and copy samples

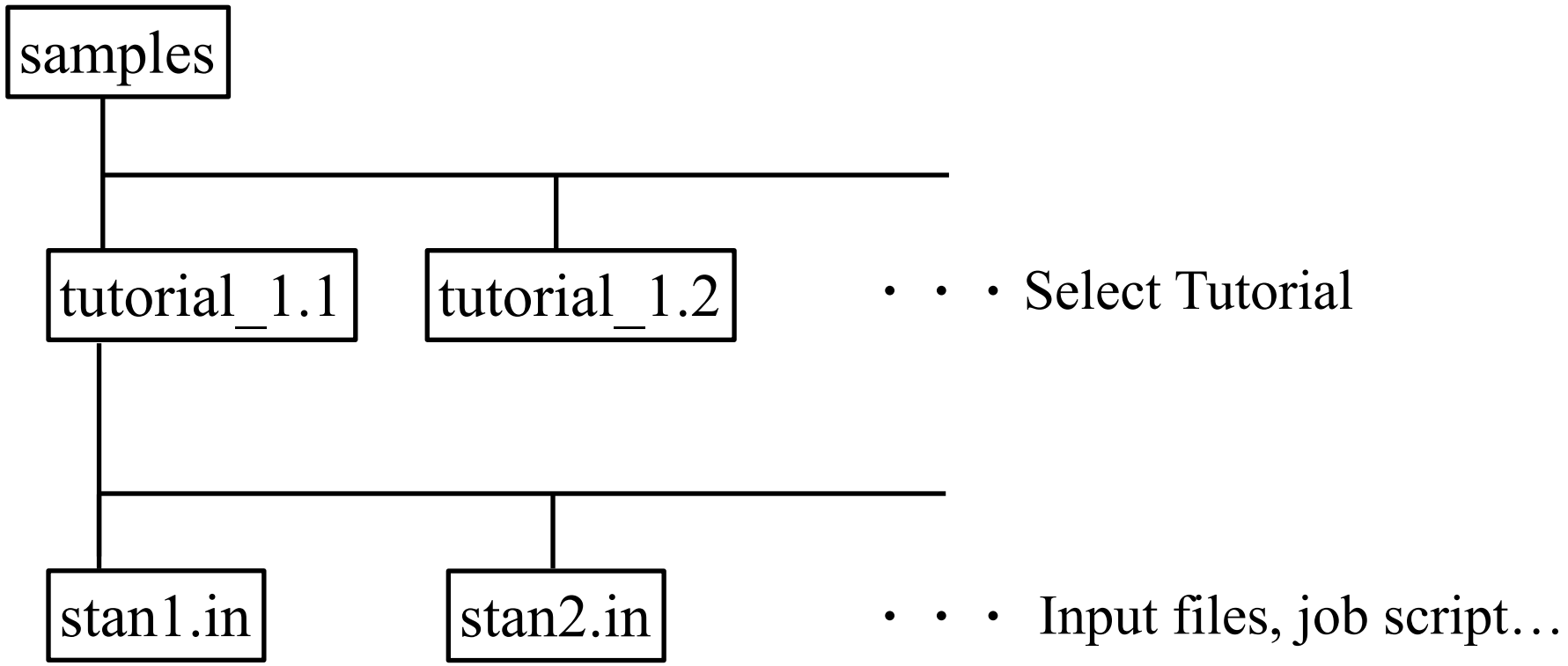
```
mkdir work
cd work
cp -r /usr/share/hphi/samples ./
```

※Commnad "HPhi" already exists in MAL. So, you can perform HΦ's simulations by executing the following command.

```
HPhi -s stan.in
```

Files/Directories in “samples”

https://issp-center-dev.github.io/HPhi/manual/develop/tutorial/en/html/index.html



How to use HΦ for standard models

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

```
L          = 2
model    = “SpinGC”
method   = “CG”
lattice    = “chain”
J            = 0.5
2S          = 1
H           = 2
```

ex. samples/tutorial_1.1/stan5a.in
(L=2 1d Heisenberg model,
GS by LOBCG method)

HPhi -s stan5a.in

./output : results are output

Method

Lanczos - ground state
CG - LOBCG
TPQ - finite-temperature
FullDiag - full-diagonalization
Time-Evolution - real-time dynamics

Important files

./output/zvo_energy.dat → energy
./output/zvo_Lanczos_Step.dat → convergence
./output/zvo_cisajs_eigen*.dat → one-body Green func.
./output/zvo_cisajscktalt_eigen*.dat → two-body Green func.

Demonstrations @ laptop

J1-J2 Heisenberg model (tutorial_1.5)

※online manual: https://www.pasums.issp.u-tokyo.ac.jp/hphi/doc/manual/

You can enjoy HΦ on your laptop !