

MateriApps LIVE!の使い方・実演

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Contents

1. What is MateriApps LIVE! ?

2. Run MateriApps LIVE!

3. How to use HΦ on MateriApps LIVE!

**Have you already
downloaded VirtualBox
and MaterialApps
LIVE! ?**

**[https://github.com/cmsi/
MateriAppsLive/wiki/
OnlineTutorial](https://github.com/cmsi/MateriAppsLive/wiki/OnlineTutorial)**



名前	変更日	サイズ	種類
MateriAp...amd64.ova	2021年5月18日 12:20	2.67 GB	書類
README-en.html	2021年5月18日 12:21	11 KB	HTML書類
README.html	2021年5月18日 12:21	12 KB	HTML書類
setup-en.pdf	2021年5月18日 12:25	1.8 MB	PDF書類
setup.pdf	2021年5月18日 12:25	1.9 MB	PDF書類
VirtualBox...OSX.dmg	2021年5月15日 20:03	124.3 MB	ディスクイメージ
VirtualBox...0-Win.exe	2021年5月15日 20:03	108.1 MB	Micros...lication

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, $H\Phi$, 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>

cmsi / MateriAppsLive

Watch 15 Star 8 Fork 6

Code Issues 61 Pull requests 0 Projects 0 Wiki Insights

is:issue is:open Labels 10 Milestones 4 New issue

61 Open	180 Closed	Author	Projects	Labels	Milestones	Assignee	Sort
32bit版が正しく作れていない		#243 opened 7 days ago by wistaria			Version 2.3		3
Abinitの再追加		#242 opened 11 days ago by wistaria			Version 2.3		
The GPG key for the debian repository has expired	update	#241 opened 11 days ago by jochym			Version 2.3		1
32bit 版のサポート終了		#240 opened 17 days ago by wistaria			Version 2.4		1
Debian 7 Wheezy のサポート終了		#239 opened 17 days ago by wistaria			Version 2.4		

Files in “MateriAppsLive-3.3-dist”



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VirtualBox-6.1.22-144080-Win.exe	2021年5月15日 20:03	108.1 MB	Micros...lication

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

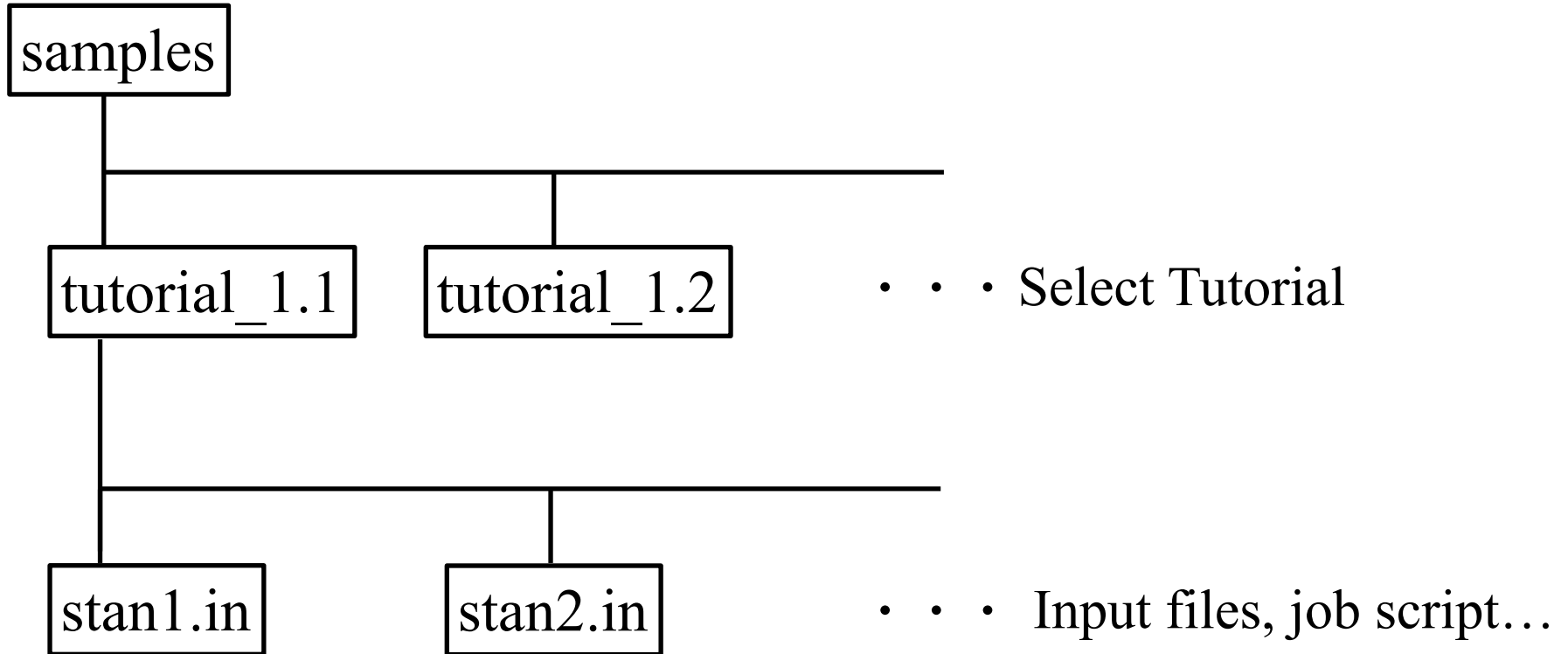
cp -r /usr/share/hphi/samples ./

※Command “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”

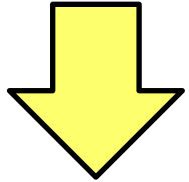
<https://issp-center-dev.github.io/HPhi/manual/develop/tutorial/en/html/index.html>



How to use H Φ 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
```



`HPhi -s stan5a.in`

`./output` : results are output

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.

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

Method

Lanczos - ground state

CG - LOBCG

TPQ - finite-temperature

FullDiag - full-diagonalization

Time-Evolution - real-time dynamics

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 $H\Phi$ on your laptop !