

MateriApps Live!の導入とHΦの使用法

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Contents

- 1.From distributed USB, copy Virtual Box(VB), MateriAppsLIVE! to your own PC**
- 2.Install Virtual Box**
- 3.Run MateriAppsLIVE!: import from VB**
- 4.How to use HΦ on MateriAppsLIVE!**












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

 MateriAppsLive-2.2-amd64.ova	64 bit OS	一昨日 9:39	2.37 GB
 MateriAppsLive-2.2-i386.ova	32 bit OS	昨日 8:50	1.65 GB
 MD5SUM		一昨日 9:50	580 バイト
 README-en.html		一昨日 9:31	11 KB
 README.html		一昨日 9:31	12 KB
 setup-en.pdf		一昨日 9:32	1.3 MB
 setup.pdf		一昨日 9:32	1.5 MB
 vbconfig.bat		一昨日 9:32	111 バイト
 vbconfig.command		一昨日 9:32	176 バイト
 VirtualBox-5.2.26-128414-OSX.dmg	MacOS	昨日 9:31	96.1 MB
 VirtualBox-5.2.26-128414-Win.exe	Windows OS	昨日 9:31	114.5 MB

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, $H\Phi$, 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 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>

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		

How to use H Φ in MA LIVE!

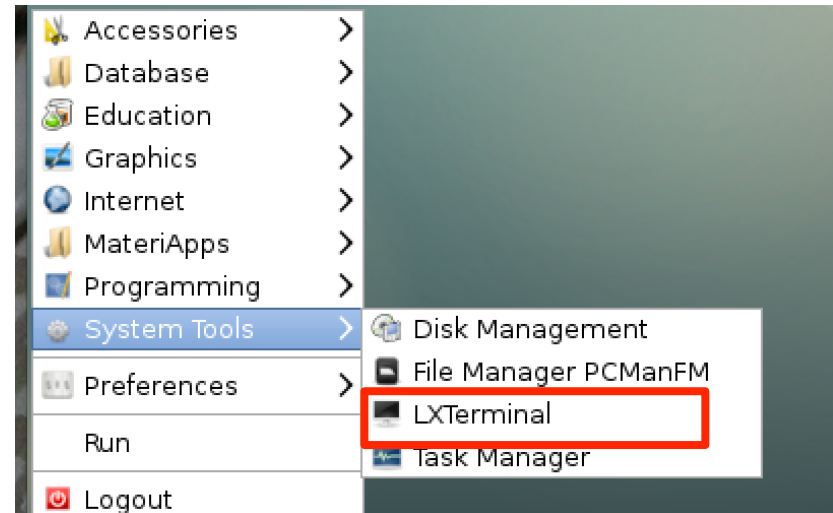
1. Start LXTerminal on Materi Apps LIVE!

2. Command “HPhi” already exists in MAL. So, you can perform H Φ '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]

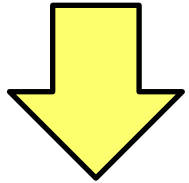
**Setting for Japanese keyboard:
`setxkbmap -layout jp`**



How to use H Φ for standard models

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

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



HPhi -s stan.in

`./output` : results are output

Important files

```
./output/zvo_energy.dat      → energy
./output/zvo_Lanczos_Step.dat → convergence
./output/zvo_cisajs.dat      → one-body Green func.
./output/zvo_cisajsccktalt.dat → two-body Green func.
```

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

Method

Lanczos - ground state

CG - LOBCG

TPQ - finite-temperature

FullDiag - full-diagonalization

Demonstrations @ laptop

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

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

You can enjoy $H\Phi$ 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.