

MateriApps LIVE!の使い方・実演

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Contents

1. What is MateriApps ?

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/
Tutorial202004](https://github.com/cmsi/MateriAppsLive/wiki/Tutorial202004)**



名前	変更日	サイズ	種類
MateriAppsLive-3.0-amd64.ova	2020年4月14日 18:13	2.55 GB	Open V...Archive
MD5SUM	2020年4月14日 22:24	578 バイト	テキス…ディット
README-en.html	2020年4月14日 22:22	12 KB	HTML書類
README.html	2020年4月14日 22:22	13 KB	HTML書類
setup-en.pdf	2020年4月14日 22:22	1.4 MB	PDF書類
setup.pdf	2020年4月14日 22:22	1.6 MB	PDF書類
vbconfig.bat	2020年4月12日 19:30	111 バイト	書類
vbconfig.command	2020年4月12日 19:30	176 バイト	ターミ…クリプト
VirtualBox-6.1....6177-OSX.dmg	2020年4月12日 19:05	129 MB	ディスクイメージ
VirtualBox-6.1....136177-Win.exe	2020年4月12日 19:05	113 MB	Micros...lication

Motivations for developing MA

Users



How to find software ?
How to use software ?
Information about hands-on?
(Which software is better?)

Developers



Ads on software require much costs ...
(making web page and holding hands-on)

MA for users: a portal sites for software and related useful info.

MA for developers: a site for advertise their software

MA aims to be tabelog (食べログ) in the community of CMS.

Tabelog - the site you can search *restaurant* through ranking and reviews by users (口コミ)

MateriApps — A Portal Site of Materials Science Simulation

now 265 Apps
Inquiry / Application Request

JP / EN

MateriApps
A Portal Site of Materials Science Simulation

What's MateriApps? Call for reviews

Google Custom Search

Detailed search

News / Hands-on / Event List of Apps Search Apps Keywords Review Research Showcase Concierge

Try the app without installing 「MateriApps LIVE!」 MORE

Search by category

Electronic structure (solid state physics) Electronic structure (quantum chemistry) Molecular dynamics

Visualization/modeling Strong correlation/effective models Data analysis/supplementary tool

Continuum models Database Integrated Environment

Machine learning Quantum computing

News / Event

News Event

News / Hands-on / Event

News 2019 11/11

Monthly ranking has been updated.

- How to find & share information on software packages !

- Please add your software !

- Introducing 271 materials science applications and tools (as of 2020.4)
- Finding applications
 - search tags: features, targets, calculation methods/algorithms
- Information of applications
 - brief introduction, link to official pages, information installation, usage, etc
- Information of hands-on sessions, software update, etc
- New contents
Concierge, Review
- 16000+ pageviews / month, 5500+ unique visitors / month

Applications on MateriApps

- Introducing **271 materials science applications and tools** (as of 2020.5)

<p>DFT AkaiKKR★ OpenMX★ xTAPP★ ABINIT★ ... (78)</p>	<p>Quantum Chemistry FMO★ SMASH★ GAMESS★ DC★... (36)</p>	<p>Molecular Dynamics MODYLAS★ Gromacs★ ERmod★ MDACP... (31)</p>	<p>Lattice Models ALPS★ DSQSS BLOCK₍₅₂₎ DMRG++</p>
<p>Continuum Simulation ANSYS Multiphysics Octa ... (12)</p>	<p>Data Analysis CLUPAN★ phonopy★ (57)</p>	<p>Visualization fu★ TAPIOCA★(37)</p>	

Materials Database (11)

★ included in MateriApps LIVE!

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 6600+ 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: LAMMPS@MAL 6/18 (?) [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		

Files in “MateriAppsLive-3.0-dist”



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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: How to transfer files on VB to Host OS)

How to use H Φ in MA LIVE!

1. Start LXTerminal on MateriApps LIVE!

Setting for Japanese keyboard:
setxkbmap -layout jp

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

HPhi -s stan.in

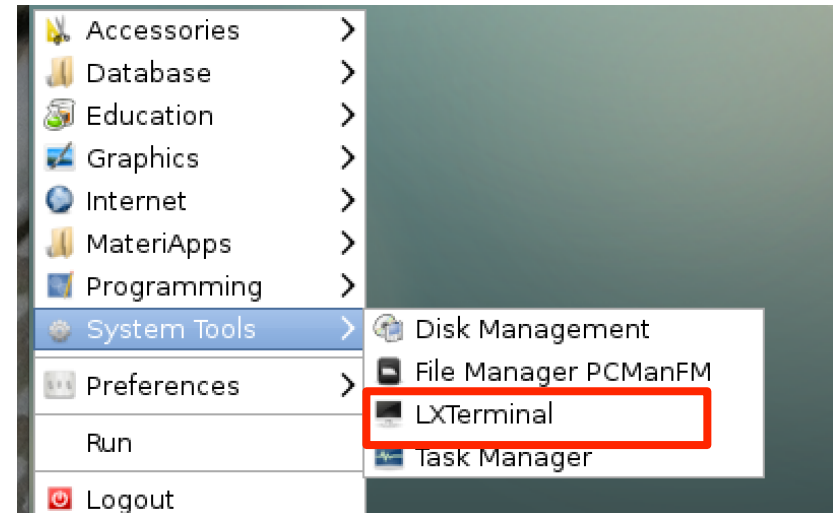
3. Please refer to the various input files in “/usr/share/hphi/samples”
[Some examples are shown on the next slides]

4. Execute the following commands:

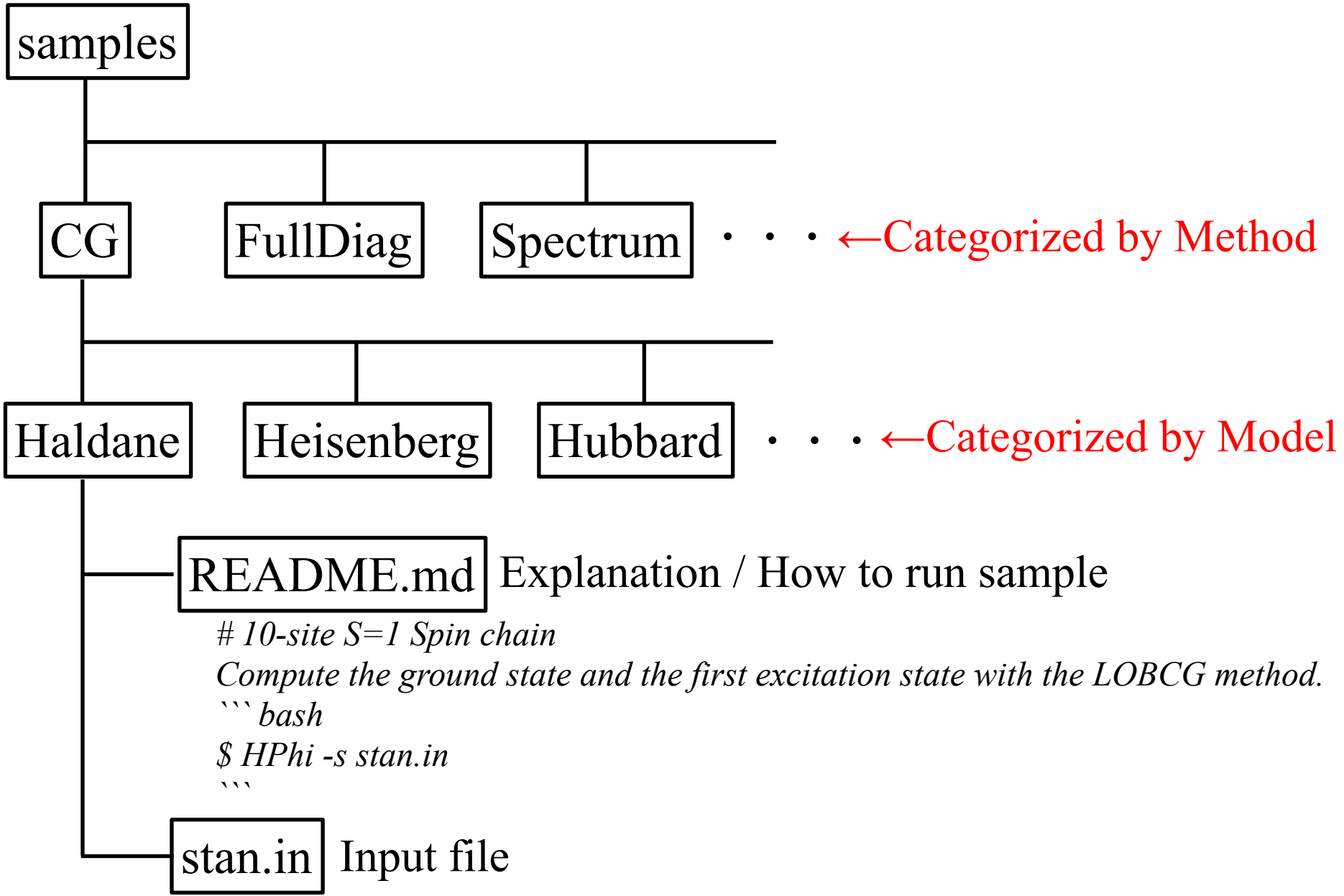
mkdir hphi

cd hphi

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



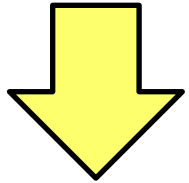
Files/Directories in “/usr/share/hphi/samples”



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

<code>./output/zvo_energy.dat</code>	→ energy
<code>./output/zvo_Lanczos_Step.dat</code>	→ convergence
<code>./output/zvo_cisajs.dat</code>	→ one-body Green func.
<code>./output/zvo_cisajscktalt.dat</code>	→ 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

Kitaev model ($S=1/2$): TPQ

※scripts for post process exists in “/usr/share/hphi/tool”

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

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.