Portal to Materials Science Simulation

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物質科学シミュレーションのポータル MateriApps

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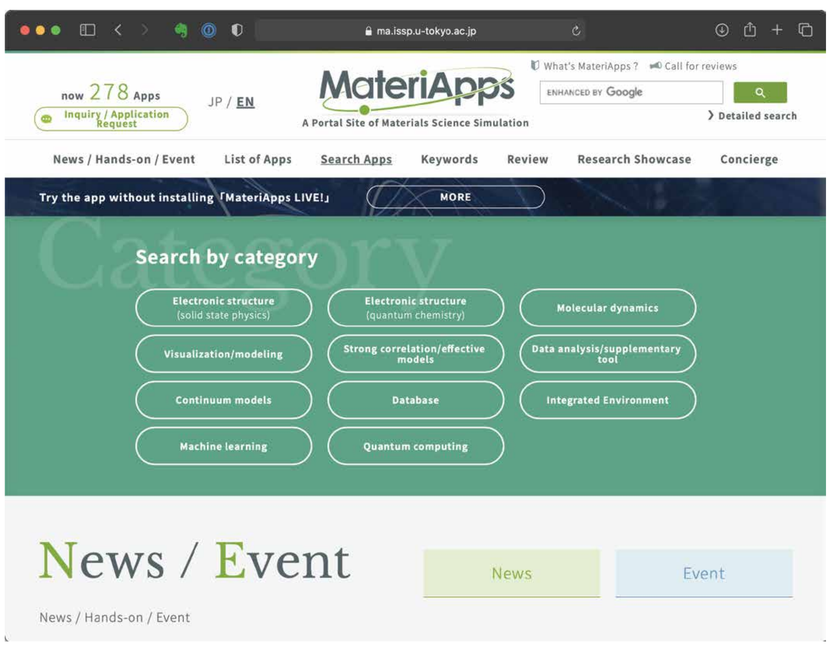
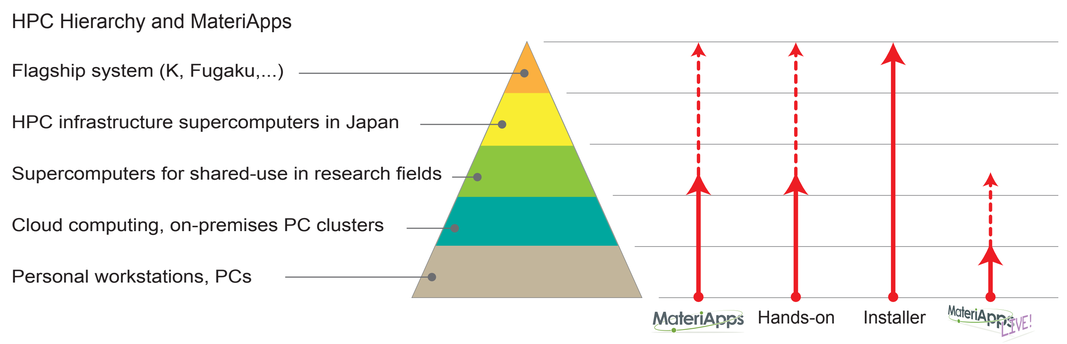
Goal of MateriApps Project

Formation of community in the field of computational materials science by promoting open-source software
Establlishment of infrastructure for easily starting simulations:
computational science experts, theoreticians, experimentalists, ...
researchers in academies, researchers in companies, students, ...
Sustainable development of materials science applications through growing community and infrastructure



What MateriApps will provide



For users:

To find application software - catalog of applications/tools on MateriApps web
To learn application software - CCMS hands-on sessions, web tutorials, reviews
To try application software - MateriApps LIVE!
To use application software - MateriApps Installer, pre-installation on supercomputers

For developers:

To make your application software more visible
MateriApps website has 23,000+ PVs and 8,000+ unique users per month
To make your application software more learnable
support for hands-on sessions, review pages
To make your application software easier to try and use
adding your applications to MateriApps LIVE! and MateriApps Installer

What's MateriApps LIVE!

Live Linux System that contains OS, editors, materials science applications, tools, etc. By booting up on VirtualBox, one can start simulations, e.g., first-principles calculation, molecular dynamics, quantum chemical calculation, lattice model calculation, etc, immediately. Suitable especially for trial use and education. Available from MateriApps LIVE! web page. 10,000+ downloads since May 2013.

What's MateriApps Installer

Collection of install scripts of open-source materials science applications and tools to macOS, Linux PC, cluster workstations, and supercomputers. Major applications has been pre-installed on supercomputer system at ISSP, UTokyo by using MateriApps Installer. MateriApps Installer version 1.0 will be published in Feb. 2021.

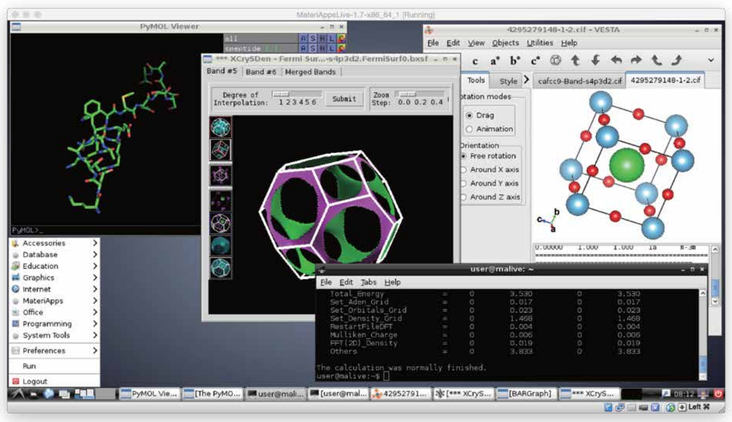
Details of MateriApps LIVE!

Features of this package

One can boot the Linux OS with a minimum procedure and obtain the environment for running materials science application programs immediately.

Available physical quantities/systems

[First-principles calculation] crystal structures, band structures, phonon dispersion, magnetization, electric polarization, surface/interface
[Quantum chemical calculation] molecular orbitals, spectrum analysis, chemical reaction
[Strongly correlated systems] specific heat, magnetic/dielectric susceptibility, phase transition
[Visualization tool] GUI for input/output, visualization of crystal structures, biomolecules, solutions



OS included in the package

Debian GNU/Linux basic system (withLXDE desktop)

Application programs included in the package

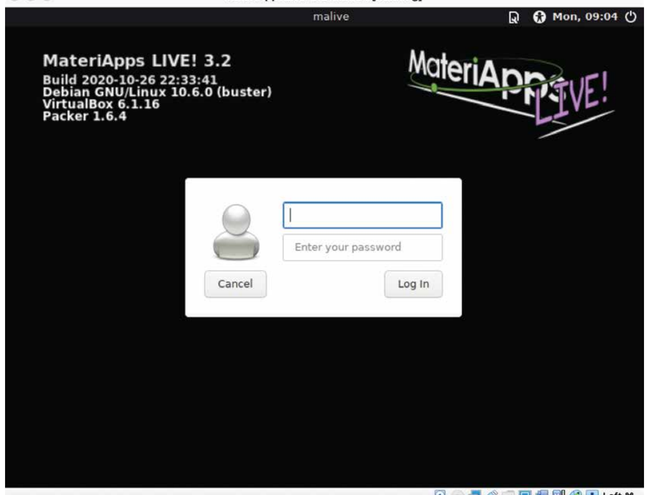
[First-principles calculation] ABINIT, AkaiKKR, Alamode, CONQUEST, OpenMX, Quantum ESPRESSO, RESPACK, SALMON, xTAPP
[Quantum chemical calculation] GAMESS, SMASH
[Molecular dynamics] Gromacs, LAMMPS, ERmod
[Strongly correlated systems] ALPS, DCore, DDMRG, DSQSS, HΦ, mVMC, TeNeS
[Tools] Avogadro, BSA, C-Tools, OpenDX, VMD, Paraview, Pymol, Rasmol, Tapioca, VESTA, XCrysDen
[Editors] emacs, nano, vim
[Development tools] gcc, g++, gfortran, python, ruby, python2/3, cmake, git

Operation environment

MateriApps LIVE! can be used on Windows, macOS, and Linux through the free virtualization software, VirtualBox.

History of versions and roadmap

2013/05/14 Launch of MateriApps LIVE! project
2013/07/24 Version 1.0 (based on Debian/Wheezy)
2018/08/26 Version 2.0 (based on Debian/Stretch)
2019/07/01 support for Debian/Buster, Ubuntu/Xenial, Ubuntu/Bionic
2020/04/14 Version 3.0 (based on Debian/Buster)
2020/08/01 Version 3.1 (support for Ubuntu/Focal)
2020/10/26 Version 3.1 (OCTA, TeNeS)
2021/03/xx Version 3.2 (support for ARM64 architecture)



MateriApps
Portal Site for Materials Science Simulation
https://ma.issp.u-tokyo.ac.jp/

MateriApps LIVE! on **GitHub**
https://cmsi.github.io/MateriAppsLive/

MateriApps LIVE! Tutorials
https://github.com/cmsi/MateriAppsLive/wiki/MaLiveTutorial

MateriApps Installer on **GitHub**
https://github.com/wistaria/MateriAppsInstaller