Kota Ido¹, Takeo Kato¹, Shusuke Kasamatsu², Naoki Kawashima¹, Takahiro Misawa¹, Yuichi Motoyama¹, Synge Todo¹,³,⁴, and Kanako Yoshizawa⁵

¹ISSP, UTokyo, ²Faculty of Science, Yamagata Univ., ³Dept. Phys., UTokyo, ⁴NIMS, ⁵RIST

A Portal Site of Materials Science Simulation

https://ma.issp.u-tokyo.ac.jp/en/

A Portal Site of Materials Science Simulation

Goal of MateriApps project
Formation of community in the field of computational materials science by promoting open-source software
Establishment 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

New Features
- Website renewal! (2018/04〜)
  - People in MateriApps become “Application Concierge”.
  - If you would like to ask “Application Concierge” about softwares (recommended apps, basic of numerical methods ...), please request !
  - Review of application has been added.
    24 (12) review pages are now available in Japanese (in English)

What MateriApps will provide for users
To find application softwares
   catalog of applications/tools/databases on MateriApps web
To learn application softwares
   CCMs hands-on session, web tutorials,
   Reviews on application pages
To try application softwares
   MateriAppsLIVE!
To use application softwares
   MateriApps Installer,
   pre-installed softwares on supercomputers
review page of “COMBO”

What MateriApps will provide for developers
To make your application softwares more findable
   MateriApps website has 15000+ PVs and 4000+ users per month
To make your application softwares more learnable
   we will help you to hold hands-on session,
   make review pages and query form for your application on MA web
To make your application softwares easier to try
   by adding your application in MateriAppsLIVE!
To make your application softwares easier to use on user’s (cluster) machine
   by adding your application in MateriApps Installer

MateriApps catalog
Contains 267 application softwares in the field of materials science
Electronic structure (solid state physics)
   OpenMX, RDFT, rTASSP, PHASE, AkaiKKR, ... (~80 applications)
   Gaussian, SMD/O, GAMESS, PIMD, PAICS, ... (~40 applications)
Strongly correlated systems/Effective models
   ALPS, HPhi, form, DISCUS, ... (~ 50 applications)
Continuum simulations
   OCTA, OpenFOAM, ANSYS Multiphysics, MMSP, ... (~10 applications)
Data analysis tools, Utilities
   C-Tools, OACIS, Phonopy, DC, REM, RSA, ... (~40 applications)
Machine learning
   COMBO, CySPY, iqsip, Xenonpy, ... (~17 applications)
Enables to search applications from several view-points
   Target (phenomena, observable)
     Molecular structures, Band calculation, Magnetization, ...
   Algorithm/methods
     Density functional theory, Exact diagonalization, Monte Carlo, ...

MA Installer
Install script of application softwares
Development tools:
   GCC, CMake, Git, Python, ...
Materials science softwares:
   ALPS, rTASSP, OpenMX, HPhi, Gromacs, ...
It covers several OS, machines
   GNU/Linux, Fujitsu FX,
   Mac OSX, Cygwin,
We have installed softwares on supercomputers by MA Installer
   K-computer, ISSP supercomputer system B, C, ...

Feel free to contact us (ma@cms-initiative.jp) for any comment or new software candidate to MateriApps!