Development of MateriApps Installer

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Nowadays, computer numerical computation is indispensable for theoretical researches in materials science. For the advancement of computational materials science, efficient algorithms for solving equations of materials science are essential. Many excellent applications based on state-of-the-art algorithms have been created so far. In 2013, we launched a portal site for materials science simulations, MateriApps [1], to disseminate information about the developed software to experimentalists and corporate researchers. We have been disseminating information about the application.

One of the obstacles for users to start using published applications in materials science is installing software. MateriApps LIVE! [2] is an environment that allows users to quickly try out computational materials science applications on their laptops and other devices. MateriApps LIVE! is a Virtual Hard Disk Image (OVA) of VirtualBox that includes applications, OS (Debian GNU/Linux), editors, visualization tools, and other environments needed to get started with the tutorial. Using MateriApps LIVE!, it is possible to quickly set up a computing environment for participants in classes and software training sessions.

However, the environment provided by MateriApps LIVE! is not enough to proceed with full-scale simulations. Since MateriApps LIVE! runs as a virtual machine, its computational power is somewhat limited. To support users interested in larger-scale simulations, we had started the development of MateriApps Installer in 2013.

As FY2020 Project for Advancement of Software Usability in Materials Science (PASUMS), we have made several significant updates on MateriApps Installer: i) organized directory structure and scripts, ii) added full documentation and tutorials, iii) upgraded supported software, iv) supported new hardware [ISSP system B (ohtaka)], v) supported new compilers [GCC 10 and Intel oneAPI].

Version 1.0 of MateriApps Installer was released in March 2021, which includes install scripts for ALPS, ALPSCore, DSQSS, Quantum ESPRESSO, HΦ, Kω, LAMMPS, mVMC, OpenMX, RESPACK, and TeNeS. Also, it includes scripts for the following tools and libraries: Boost, CMake, Eigen3, FFTW, GCC, Git, GSL, HDF5, LAPACK, libffi, OpenBLAS, OpenMPI, OpenSSL, Python3, ScaLAPACK, Tcl/Tk, and zlib.

Using MateriApps Installer, the above material science applications have been preinstalled on the ISSP supercomputers (ohtaka and enaga). The source code of MateriApps Installer is freely available from GitHub [4]. MateriApps Installer is distributed under the GNU General Public License version 3 (GPLv3). However, the patch files for each software are distributed under the license of the software.

[1] `https://ma.issp.u-tokyo.ac.jp/`
[2] `https://cmsi.github.io/MateriAppsLive/`
[3] `https://www.pasums.issp.u-tokyo.ac.jp/mainstaller/`
[4] `https://github.com/wistaria/MateriAppsInstaller/`