

Installation guide for Quantum ESPRESSO on Windows

Jul. 17, 2018

1. Installing Quantum ESPRESSO

- ① Access to the website link below.

<http://rpm.lammps.org/qe4win/release/index.html>

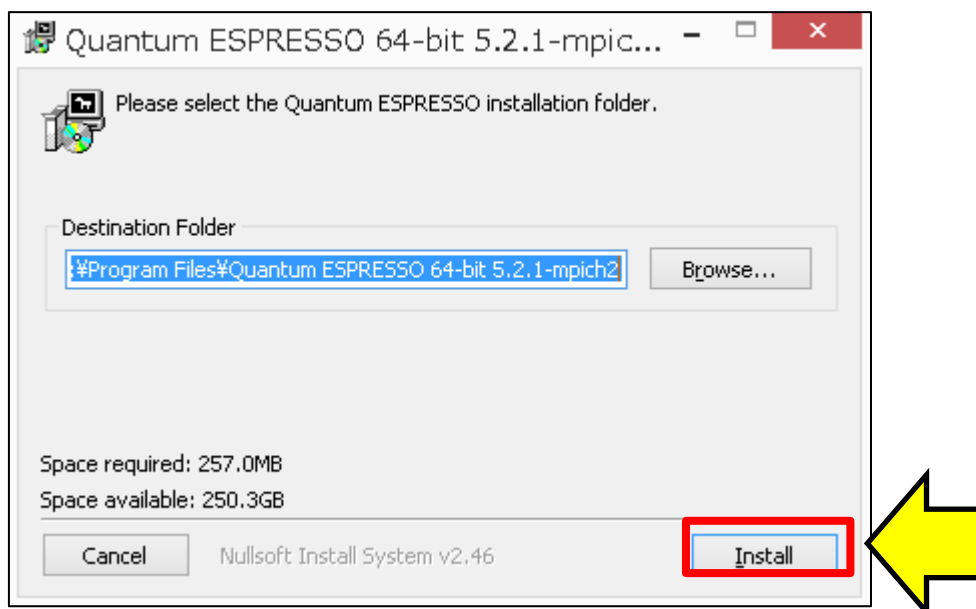
Download 'qe-5.2.1-64bit-mpich2.exe'. If using 32-bit Windows-OS, choose 'qe-5.2.1-32bit-mpich2.exe'.

LAMMPS-ICMS Binaries Repository: qe4win/release

Contents of release

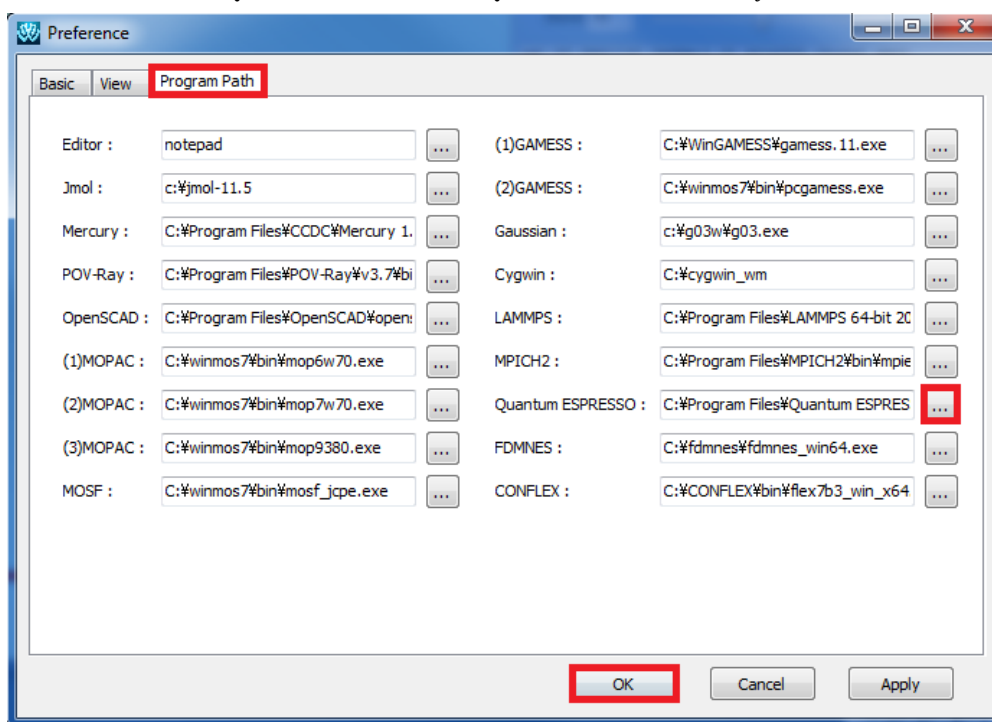
| [DIR] | (Up one level) |
|------------------|---|
| 2015-04-03 16:05 | QE-on-Windows.pdf |
| 2016-01-15 15:40 | qe-5.3.0-64bit-serial.exe |
| 2016-01-15 15:42 | qe-5.3.0-64bit-mpich2.exe |
| 2016-01-15 15:36 | qe-5.3.0-32bit-serial.exe |
| 2016-01-15 15:38 | qe-5.3.0-32bit-mpich2.exe |
| 2015-09-30 16:59 | qe-5.2.1-64bit-serial.exe |
| 2015-09-30 16:59 | qe-5.2.1-64bit-mpich2.exe |
| 2015-09-30 16:59 | qe-5.2.1-32bit-serial.exe |
| 2015-09-30 16:59 | qe-5.2.1-32bit-mpich2.exe |
| 2015-06-26 16:10 | qe-5.2.0-64bit-serial.exe |
| 2015-06-26 16:10 | qe-5.2.0-64bit-mpich2.exe |

- ② Double-click the installer file, and click [Install]



- ③ Launch Winmostar, and select [Tools]-> [Preference].

- ④ On [Program Path] tab window (see the fig. below), register the executable file (pw.exe) under bin folder in Quantum ESPRESSO (QE) installation directory.



The default setting is [C:\Program Files\Quantum ESPRESSO 64-bit 5.2.1-mpich2\bin\pw.exe]. If using 32-bit Windows-OS, set to [C:\Program Files\Quantum ESPRESSO 32-bit 5.2.1-mpich2\bin\pw.exe].

2. Installing cygwin_wm

Access to https://winmostar.com/en/gmx4wm_en.html, download the latest cygwin_wm_*.exe, and follow the instructions. Note that you can skip this step when cygwin_wm has been already installed.

3. Getting and setting MPICH

- ① Access to <http://rpm.lammps.org/windows.html>
- ② Download and save [[mpich2-1.4.1p1-win-x86-64.msi](#)] or [[mpich2-1.4.1p1-win-ia32.msi](#)]. If you use 32-bit version of QE, choose the latter.
- ③ Double-click the installer file (.msi) and follow the instructions.
- ④ Launch Command Prompt with the administrator authority.
- ⑤ Move to bin in MPICH installation folder.

```
c:\> cd "c:\Program Files\MPICH2\bin"
```
- ⑥ Execute the following command.

```
bin> smpd.exe -install
```

- ⑦ Launch Winmostar and select [Tools]-> [Preference]. In Preference window, click [...] button at MPICH2, and register the executable file mpiexec.exe. Click [OK].