

Installation guide for Quantum ESPRESSO on Windows

Jul. 17, 2018

1. Installing Quantum ESPRESSO

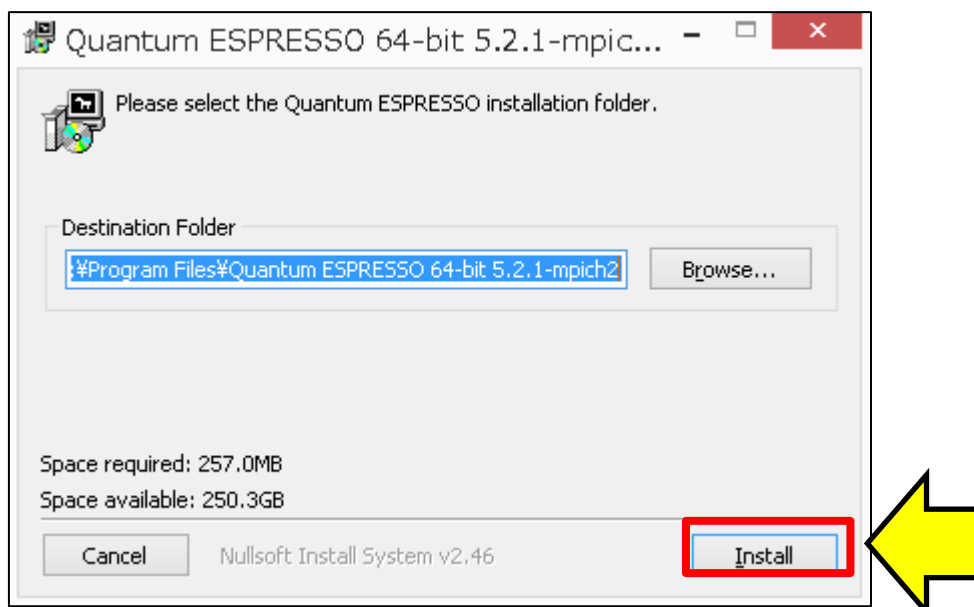
- ① Access to the website link below.

<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'.

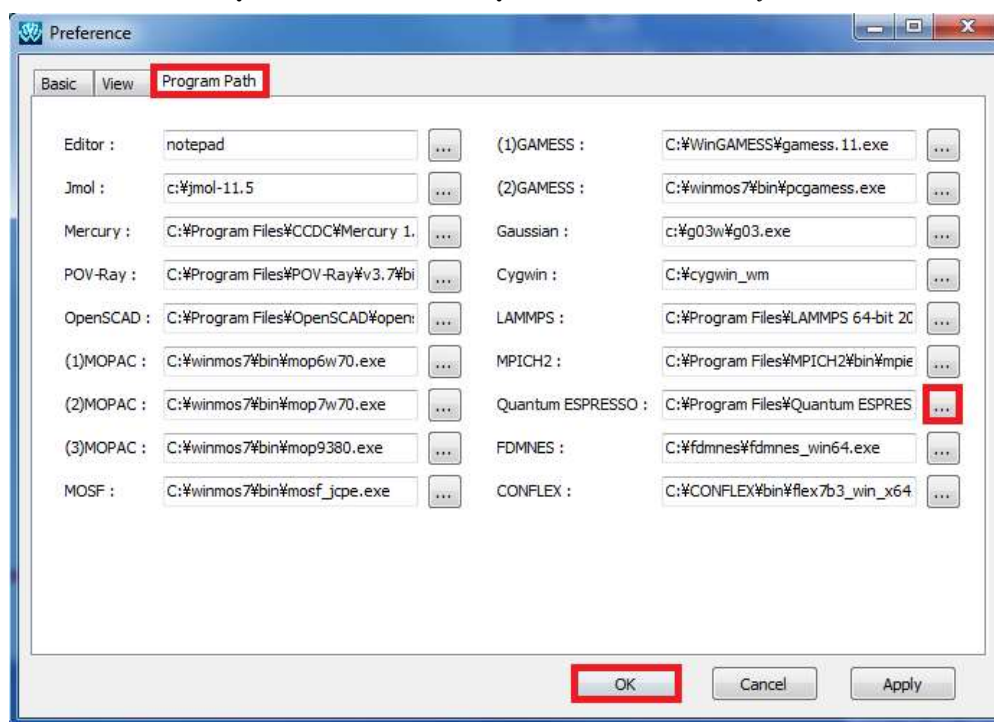


- ② Double-click the installer file, and click [Install]



- 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].