

Installation guide for Quantum ESPRESSO on Windows

Feb. 6, 2017

1. Installing Quantum ESPRESSO

- ① Access to the website link below.

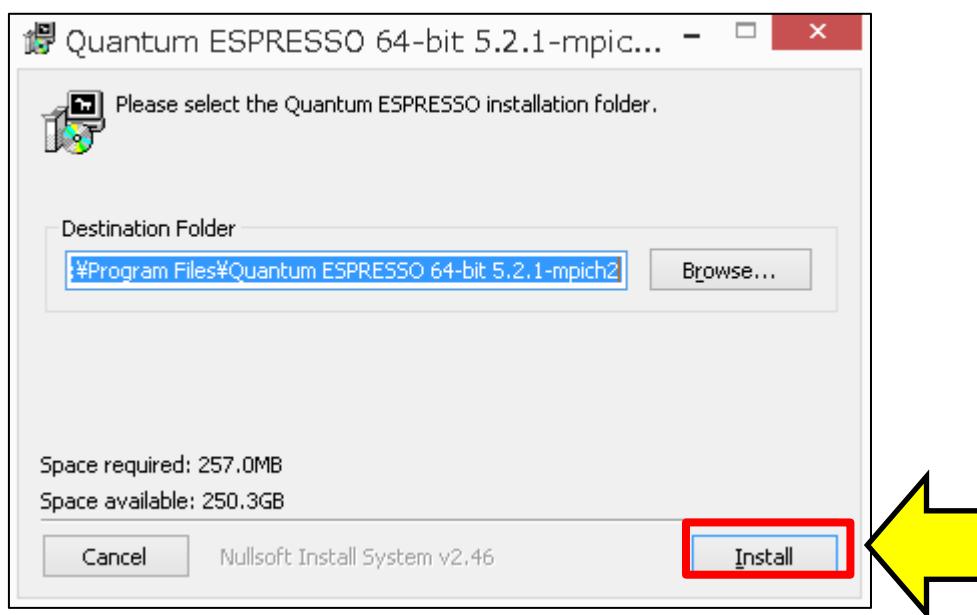
http://www.qe-forge.org/gf/project/q-e/frs/?action=FrsReleaseBrowse&frs_package_id=

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

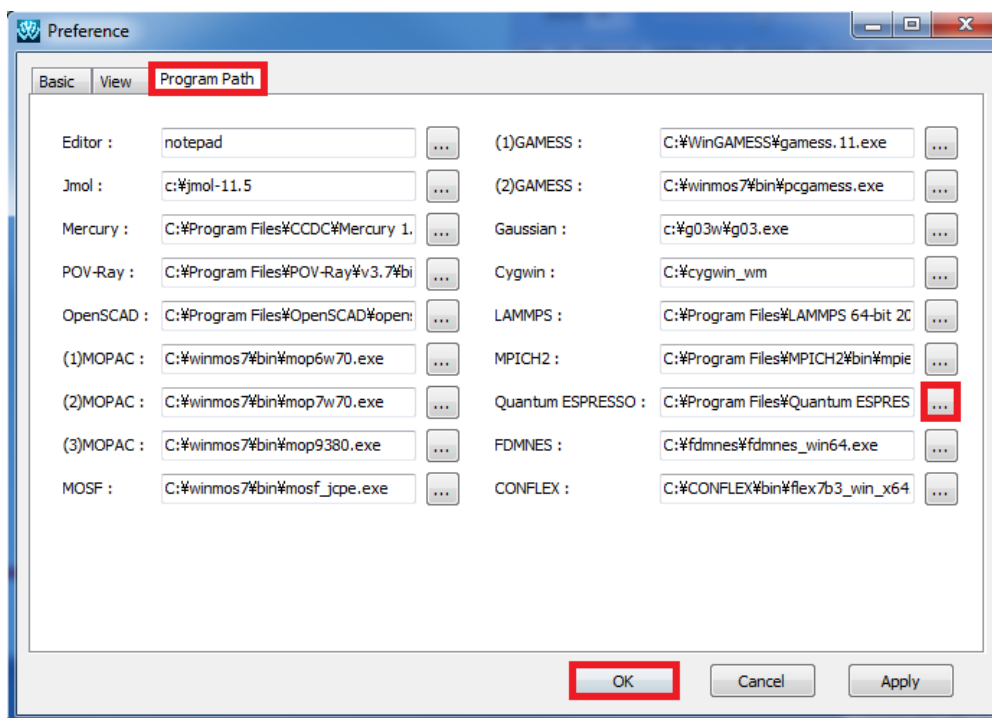
The screenshot shows the Forge website interface for Quantum ESPRESSO. The main content is a table of releases. The table has columns for Release Name, Release Date, Filename, File Size, and Download Count. The release 'QE-5.2.1' is highlighted with a red box. Within this release, the file 'qe-5.2.1-64bit-mpich2.exe' is also highlighted with a red box and a yellow arrow pointing to it.

Release Name	Release Date	Filename	File Size	Download Count		
QE-5.4.0	2016-04-24 00:00:00+02	GWW-5.4.0.tar.gz	482 KB	1487		
		PWQui-5.4.0.tar.gz	1 MB	1971		
		Phonon-5.4.0.tar.gz	2 MB	3823		
		neb-5.4.0.tar.gz	345 KB	2681		
		espresso-5.4.0.tar.gz	19 MB	21631		
		tddfpt-5.4.0.tar.gz	12 MB	4518		
		FPW-5.4.0.tar.gz	3 MB	2582		
		atomic-5.4.0.tar.gz	2 MB	4882		
		pwcond-5.4.0.tar.gz	202 KB	2297		
		QE-GPU-5.4.0.tar.gz	2 MB	922		
		test-suite-5.4.0.tar.gz	736 KB	1243		
		xspectra-5.4.0.tar.gz	4 MB	2627		
		QE-5.3.0	2016-01-09 00:00:00+01	qe-5.3.0-64bit-mpich2.exe	72 MB	7878
				neb-5.3.0.tar.gz	345 KB	5470
qe-5.3.0-64bit-serial.exe	72 MB			15635		
GWW-5.3.0.tar.gz	433 KB			1593		
tddfpt-5.3.0.tar.gz	9 MB			9223		
test-suite-5.3.0.tar.gz	733 KB			2221		
Phonon-5.3.0.tar.gz	2 MB			10292		
espresso-5.3.0.tar.gz	19 MB			37086		
QE-on-Windows.pdf	331 KB			3531		
atomic-5.3.0.tar.gz	2 MB			5958		
pwcond-5.3.0.tar.gz	202 KB			5301		
xspectra-5.3.0.tar.gz	4 MB			7670		
qe-5.3.0-32bit-mpich2.exe	60 MB			17421		
QE-GPU-5.3.0.tar.gz	2 MB			19187		
QE-5.2.1	2015-09-24 00:00:00+02	qe-5.2.0-32bit-serial.exe	60 MB	5970		
		PWQui-5.2.0.tar.gz	1 MB	2192		
		neb-5.2.1.tar.gz	345 KB	6613		
		PWQui-5.2.1.tar.gz	1 MB	10719		
		qe-5.2.1-64bit-serial.exe	70 MB	2901		
		xspectra-5.2.1.tar.gz	70 MB	8459		
qe-5.2.1-64bit-mpich2.exe		9616	2779	10842		

- 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].