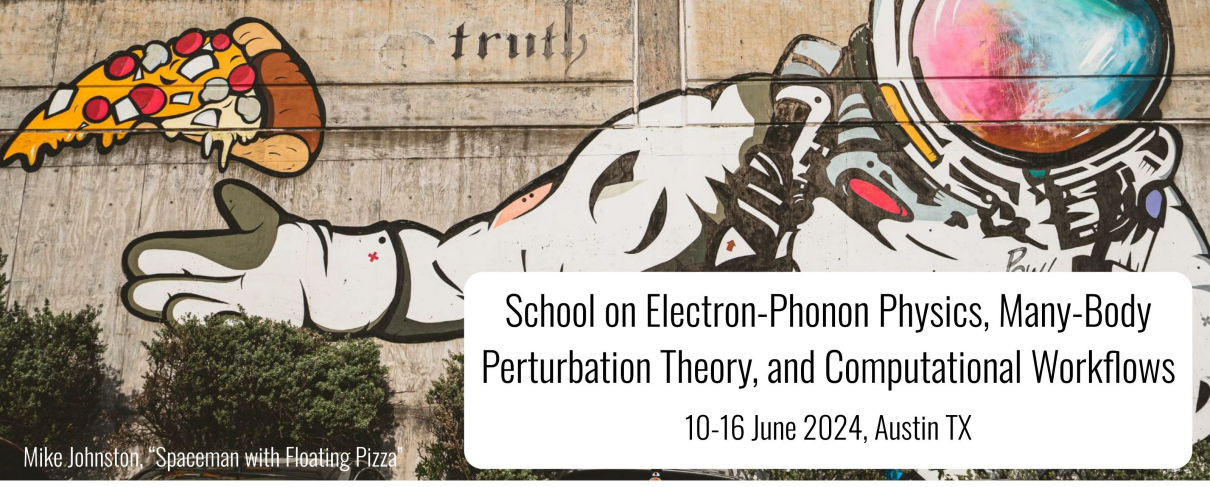


Mike Johnston, "Spaceman with Floating Pizza"

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

NSF

TACC
TEXAS ADVANCED COMPUTING CENTER

ODEN

Hands-on Mon.4

Phonon calculations with QUANTUM ESPRESSO

Paolo Giannozzi

Dept. Mathematics, Computer Science, Physics, University of Udine, Italy
and CNR-IOM, Trieste, Italy

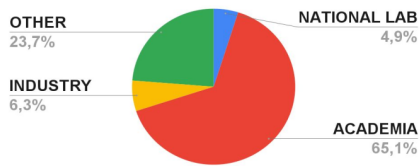
About QUANTUM ESPRESSO

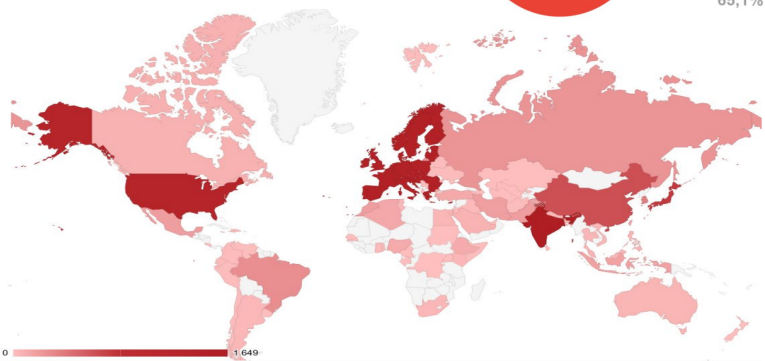
- An open-source *distribution* (an integrated suite) of codes for electronic-structure calculations; organized into several packages
- Web site `http://www.quantum-espresso.org`, contains links to all relevant resources
- Documentation online at `https://www.quantum-espresso.org/documentation/` and in `Doc/`, `PW/Doc/`, `PHonon/Doc/` subdirectories
- Development takes place on `http://gitlab.com/QEF/q-e`
- Development funded by the QUANTUM ESPRESSO Foundation and by the European Union H2020 Project MaX - Materials at the Exascale

The Quantum ESPRESSO project

Geographic distribution of downloads of QE from the website since the beginning of 2022

35000+ downloads
20000+ citations
50000+ authors

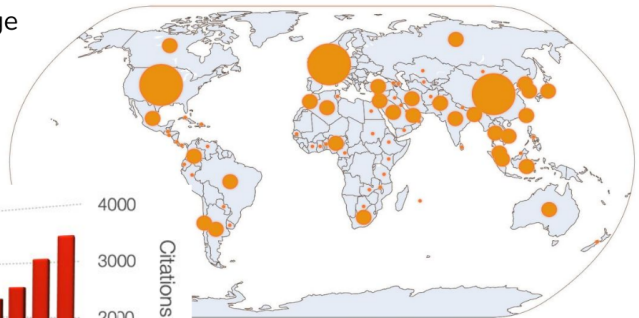




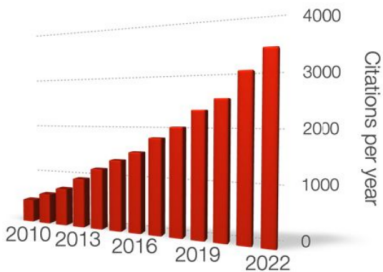
Data provided by the courtesy of the QUANTUM ESPRESSO foundation

The Quantum ESPRESSO project

QUANTUM ESPRESSO is an **open initiative** involving a large community of developers and contributors from different **regions of the world**



Geographic distribution of the authors of the articles citing the main reference articles as QUANTUM ESPRESSO



Data provided by the courtesy of the QUANTUM ESPRESSO foundation

Practical phonon calculation in QUANTUM ESPRESSO

First step: scf calculation *at equilibrium positions* (performed by `pw.x`). Compute $n(\mathbf{r})$ and $\psi_{\mathbf{k},v}$ over the Irreducible Brillouin Zone for the symmetry group of the material.

- Single phonon calculation at finite wave-vector **q**
  - Generate $\psi_{\mathbf{k},v}$ and $\psi_{\mathbf{k}+\mathbf{q},v}$ in the Irreducible Brillouin Zone relative to the small group of **q**; Calculate $C(\mathbf{q})$, diagonalize, produce $\omega(\mathbf{q})$ and $u(\mathbf{q})$ (code `ph.x`)
- Single phonon calculation at Γ wave-vector (**q**=0)
  - Calculate $C(\mathbf{q}=0)$, diagonalize, produce $\omega(\mathbf{q}=0)$ and $u(\mathbf{q}=0)$ (code `ph.x`)
    For polar materials: calculate non-analytical terms that are missing from $C(\mathbf{q}=0)$ (LO-TO splitting are absent from $\omega(\mathbf{q}=0)$): specify option `epsil=.true.` to `ph.x` (will calculate and store in output file Z^* and ϵ^∞).
  - Impose Acoustic Sum Rule (ASR), add the nonanalytic LO-TO splitting, calculate cross sections (code `dynmat.x`)

Practical phonon calculation (2)

- Complete phonon dispersion calculation
  - Perform many single-phonon calculations on a uniform grid of wave-vectors $\mathbf{q}_i$, including $\mathbf{q} = 0$ (if system is polar, calculate in the latter case Z^* and ϵ^∞); save all $C(\mathbf{q}_i)$ (and Z^*, ϵ^∞) (code `ph.x` with option `ldisp=.true.`)
  - Perform inverse FFT of the $C(\mathbf{q}_i)$, obtain interatomic force constants in real space $C(\mathbf{R})$. For polar materials: a term having the same behavior for $\mathbf{q} \to 0$ as the non-analytic term is subtracted from $C(\mathbf{q}_i)$ before the Fourier Transform and re-added to $C(\mathbf{R})$, so that no problem related to the non-analytic behavior and related long-range character arises in the Fourier Transform (code `q2r.x`)
- Calculate phonons at any wave-vector, diagonalizing the dynamical matrix:

$$D_{st}^{\alpha\beta}(\mathbf{q}) = \frac{1}{\sqrt{M_s M_t}} \sum_{\mathbf{R}} C_{st}^{\alpha\beta}(\mathbf{R}) \exp(i\mathbf{q}\cdot\mathbf{R})$$

using code `matdyn.x`

Examples of this tutorial

- **Silicon** (LDA) in the diamond structure: a nonpolar insulator
  - Understand the procedure
- **AlAs** (LDA) in the zincblende structure: a polar insulator
  - Understand the importance of macroscopic electric fields
- **Pb** in the fcc structure: a metal, with important spin-orbit interactions
  - Understand the importance of a proper Fermi-surface sampling
  - Observe the effects of spin-orbit interactions

About parallelization

You may take advantage of parallelization of the `pw.x` and `ph.x` codes by using

```
ibrun -np N code-to-be-run
```

where `N` is the number of processors, `ibrun` is a (machine-dependent) launcher software. Performs parallelization over plane waves (and real-space grids as well).

For small runs, it is not worth to set `N` larger than $\simeq 4-8$. You can use instead

```
ibrun -np N code-to-be-run -nk M
```

(alternatively: `-npool M`) that divides the `N` processors into `M` "pools", of `N/M` processors (must be an integer!). Parallelizing over plane waves takes place inside a pool, while parallelization over **k**-points takes place among pools.

NOTE: plane-wave parallelization is the only one that distributes (almost) all memory