

# Electronic-structure codes

Iurii Timrov

*Theory and Simulation of Materials (THEOS), and  
National Centre for Computational Design and Discovery of Novel Materials (MARVEL),  
École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland*

13 June 2023, ASEMSA 2023 school

# Many codes for quantum chemistry, physics, and material science



Which one to choose?

**Electronic structure codes in quantum chemistry, physics, and materials science are computational tools used to simulate and study the electronic structure of atoms, molecules, and materials.**

**While there can be some overlap in their capabilities and features, there are also differences that arise due to varying theoretical approaches, algorithms, and target applications.**

**Examples of electronic-structure  
codes that are targeted mainly for  
physics and materials science**



**VASP (Vienna Ab initio Simulation Package)**: VASP is primarily used for solid-state physics and materials science calculations. It is based on DFT and employs plane-wave basis sets with pseudopotentials to describe electronic wave functions. VASP is known for its efficiency in handling large systems and is often used to study properties such as electronic structure, energetics, and much more.

**Commercial (\$\$\$-\$\$\$\$\$)**



**Abinit:** Abinit is another code widely used for studying solids within the framework of DFT. It utilizes a plane-wave basis set approach like VASP, and it offers a broad range of theoretical methods and approximations. Abinit is highly flexible and allows for a variety of calculations, including structural optimizations, electronic band structure calculations, and spectroscopic properties.

**Open-source (free)**



**Quantum ESPRESSO:** Quantum ESPRESSO is a suite of codes that encompasses various techniques for electronic structure calculations. It uses DFT, plane waves, and pseudopotentials as VASP and Abinit to study the properties of materials. It focuses on electronic structure, total energy calculations, phonons, magnons, spectroscopies, molecular dynamics simulations of solids, surfaces, and nanostructures.

**Open-source (free)**



**Siesta:** Siesta is designed specifically for simulating the electronic structure of nanostructured materials and molecular systems. It employs a localized basis set approach known as "linear combination of atomic orbitals" (LCAO). Siesta is efficient for large-scale calculations and is often used to study molecular adsorption, surfaces, and interfaces.

**Open-source (free)**

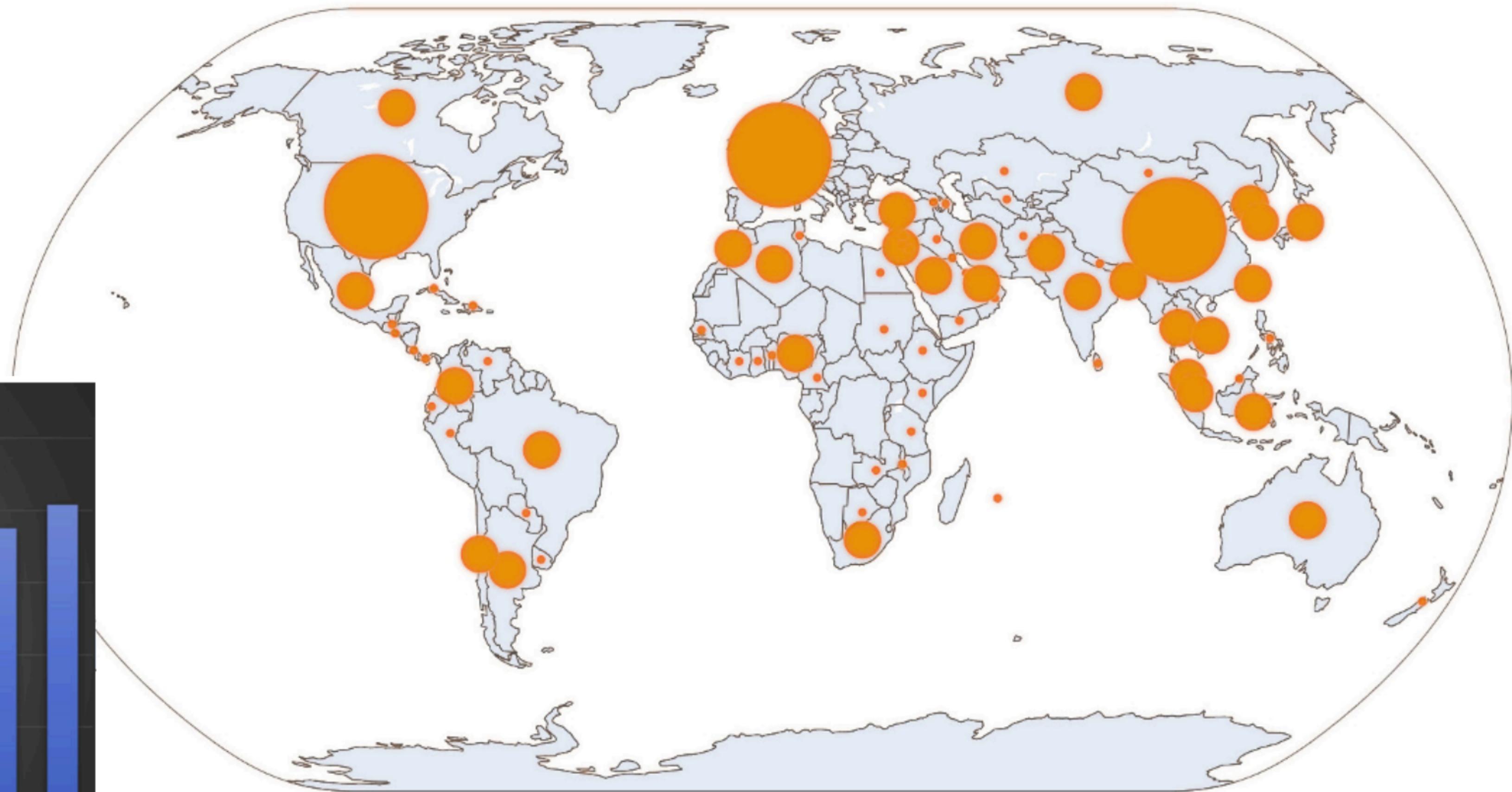
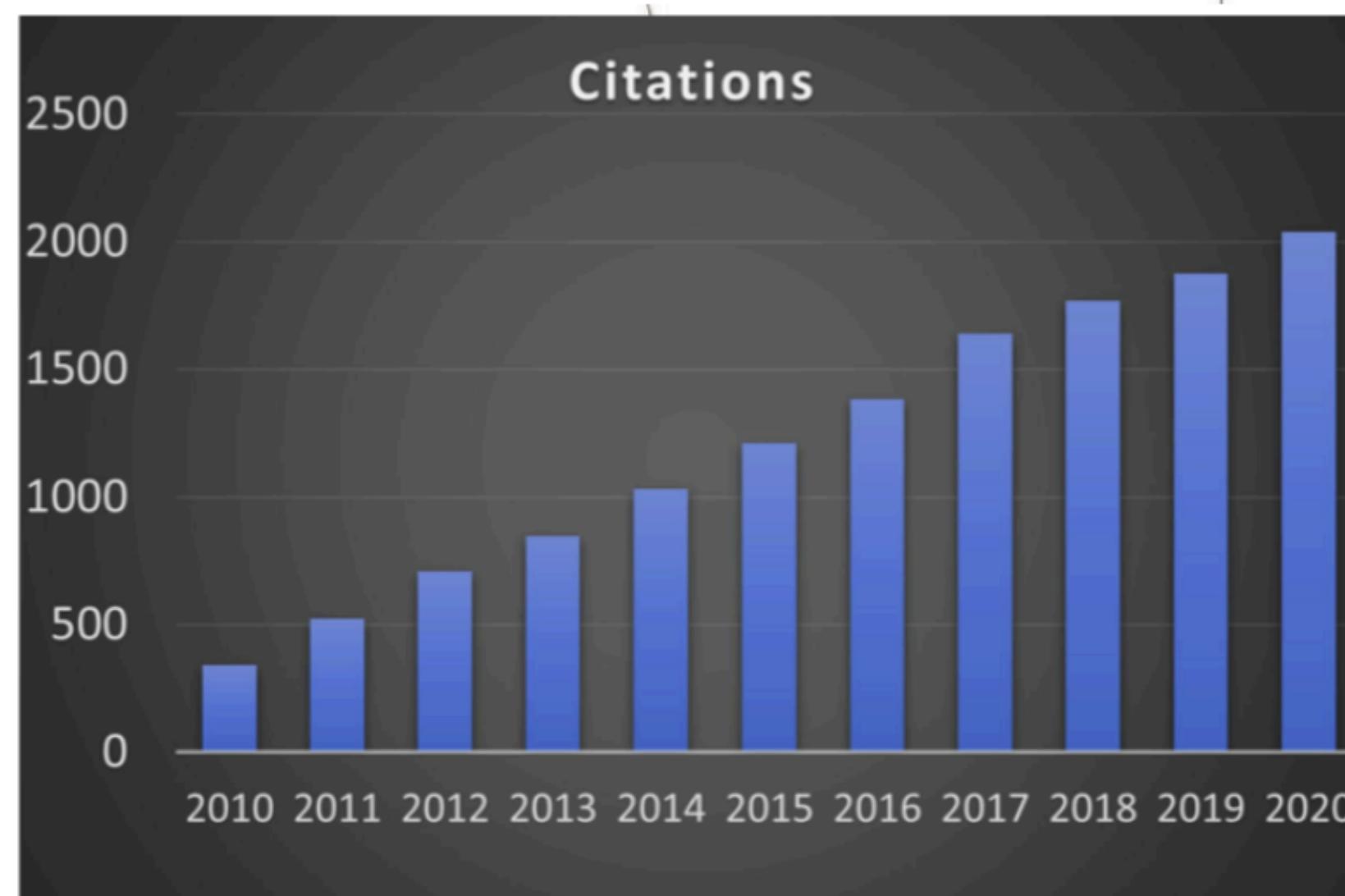
**During this ASE SMA school we will  
use Quantum ESPRESSO (week 1)**

**You will also hear about other codes  
such as Yambo (spectroscopies),  
deMon2k (quantum chemistry), and  
TBPW (basic DFT) (week 2)**

# Quantum ESPRESSO

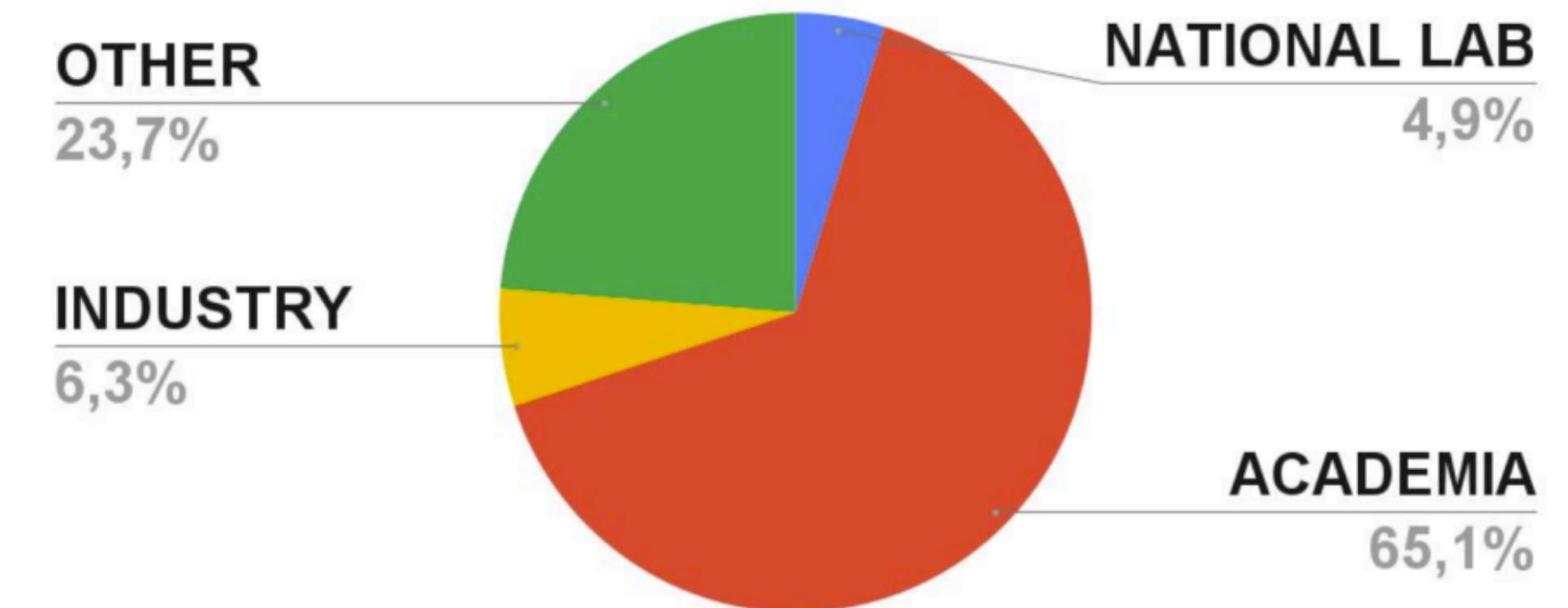
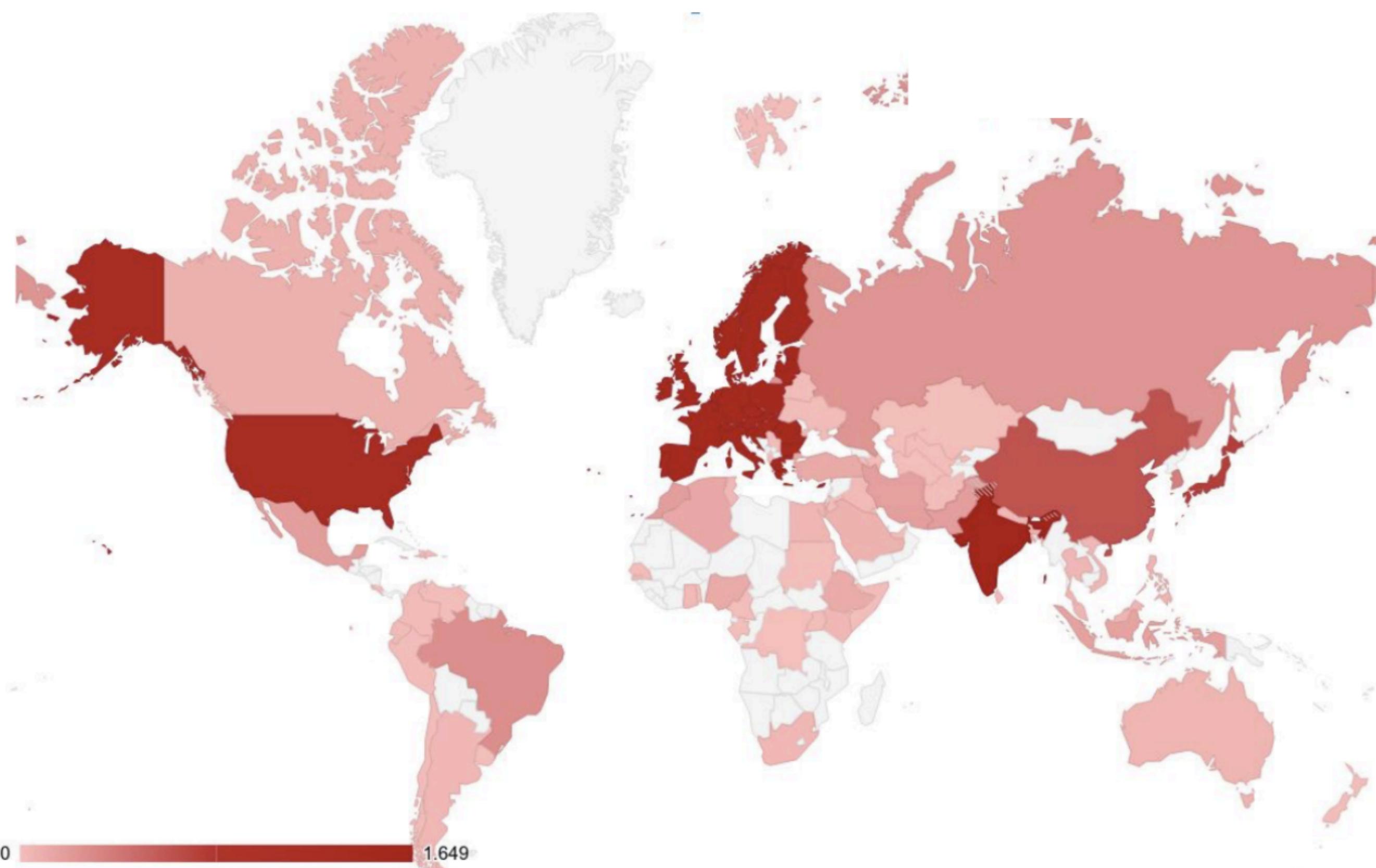
"ESPRESSO" stands for  
"opEn-Source Package for Research in  
Electronic Structure, Simulation, and  
Optimization"

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 of QE

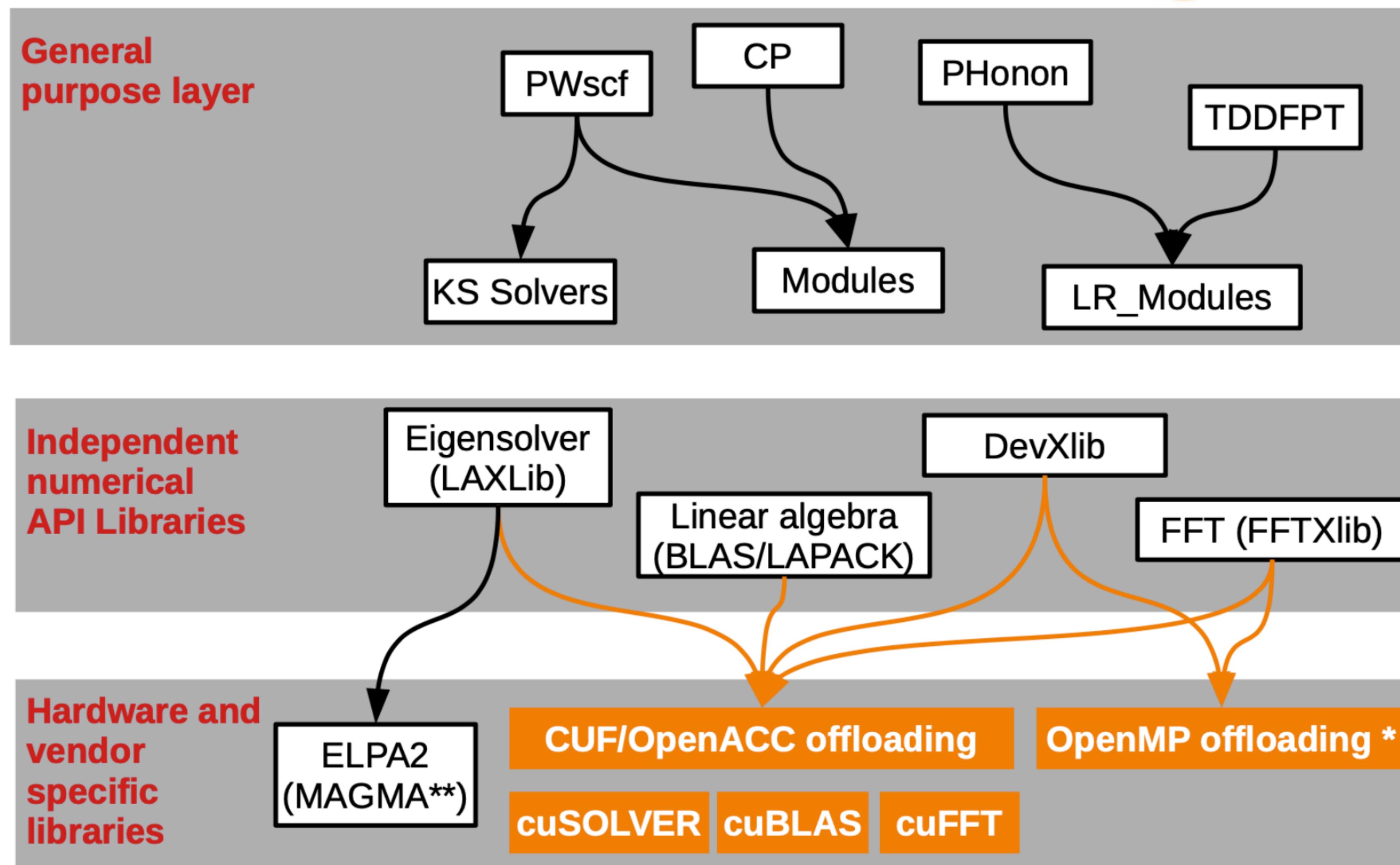
Nearly **10000 download** of the code from the website since the beginning of 2022, mostly from Europe, USA, India and China



Geographic distribution and main professional fields of people who have downloaded QE from the website since the beginning of 2022

Data by courtesy of the Quantum ESPRESSO foundation

# Quantum ESPRESSO structure



# Quantum Mobile

Activities Sun 18:32

Quantum Mobile is a Virtual Machine for computational materials science

It provides a uniform environment for quantum mechanical materials simulations

Simulation codes are set up and ready to be used either directly

The desktop environment includes a vertical dock on the left with icons for Home, Applications, and a Dash button. The desktop itself has several files and folders: README.md, RELEASE\_NOTES.txt, Trash, Homepage, and HK\_getcode.py.

Logos for MARVEL, QUANTUM MOBILE, and MAX are displayed at the bottom right.

MARVEL  
NATIONAL CENTRE OF EXCELLENCE IN RESEARCH

QUANTUM MOBILE

MAX DRIVING THE EXASCALE TRANSITION

# Happy computing!

