materials modelling and discovery: the high-performance computing way

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human ages are named after materials:

- stone
- bronze
- steel and concrete
- coal and oil
- silicon ...
- ... what next?

credit: Nicola Marzari
we need novel **materials for**:

- energy harvesting, conversion, storage, efficiency
- environmental protection and reparation
- high-tech and high-value industries
- food safety and conservation
- experimental science (detectors, sensors, magnets)
- ...

... societal well being

credit: Nicola Marzari
materials’ discovery still based on intuition, blind search, and serendipity ...
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- Haber–Bosch ammonia synthesis used osmium as catalyst. Mittasch (BASF) tested more than 22,000 materials to identify the iron-based catalyst which is still used today.
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- Using state-of-the-art quantum-mechanical numerical modelling, Norskov showed in 2009 that CoMo is a more efficient and inexpensive catalyst.
what is QUANTUM ESPRESSO?

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ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation, and Optimization.
QUANTUM ESPRESSO is an initiative coordinated by the QUANTUM ESPRESSO Foundation, with the participation of SISSA, CNR, UniUD, CINECA, ICTP, EPFL, the University of Oxford, with many partners in Europe and worldwide.
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QUANTUM ESPRESSO is not a single application for quantum simulations; it is rather a distribution of packages performing different tasks and designed to be interoperable.

QUANTUM ESPRESSO is free software that can be freely downloaded. Everybody is free to use it and welcome to contribute to its development.
260,000+ lines of FORTRAN/C code
58 developers registered on GitLab/Hub
1000+ registered users
4000+ downloads for each new release
1000+ scientific papers per year
2 web sites (quantum-espresso.org, foundation@quantum-espresso.org) + 2 development portals on GitLab/Hub
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“NVIDIA Is So Far Ahead of the Curve”
— The Inquirer

GPU-accelerated Quantum ESPRESSO (QE-GPU) available @GitHub

This is an open-source custom version of Quantum ESPRESSO with embedded GPU support based on CUDA FORTRAN. This product has been made possible thanks to the effort of the NVIDIA HPC Software and Benchmarks Group. This
Schrödinger Inc. and the Quantum ESPRESSO Foundation announce an on-going development collaboration to integrate the Quantum ESPRESSO materials simulation program into the Schrödinger modelling suite.
MAX MAterials design at the eXascale
a distributed European Centre of Excellence for supercomputing applications in materials science

5 M€ / 2016-2018
That's all Folks!

these slides shortly at
http://talks.baroni.me