materials modelling and discovery: the high-performance computing way

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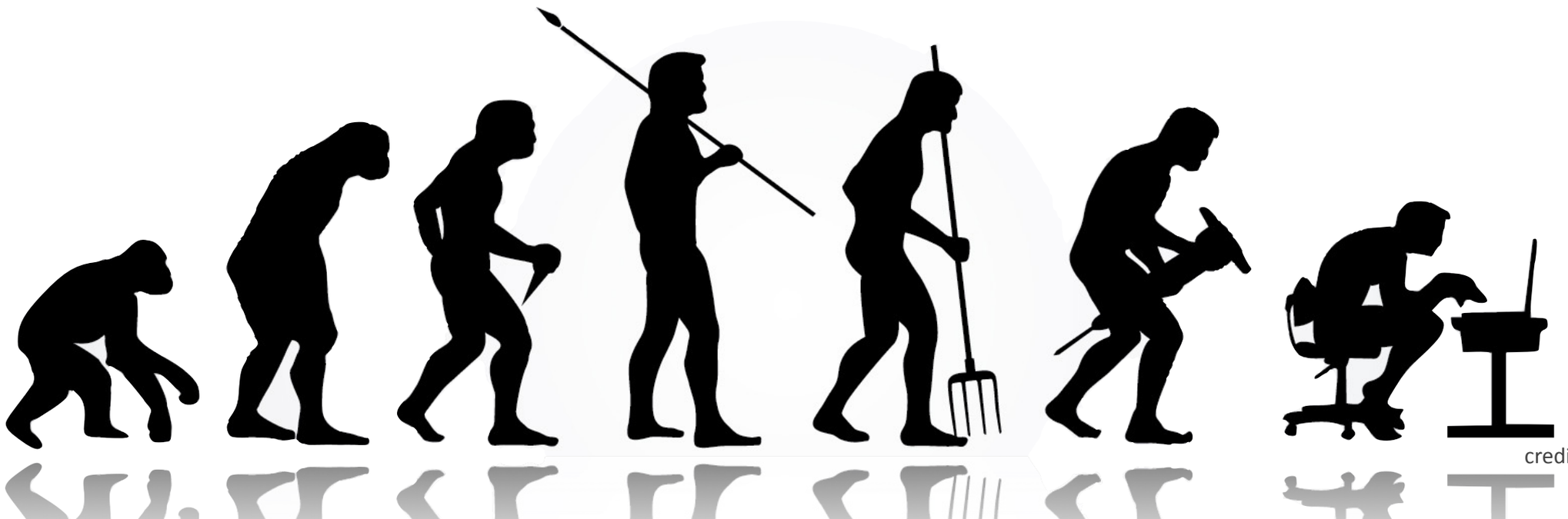
human ages are named after materials:

- 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

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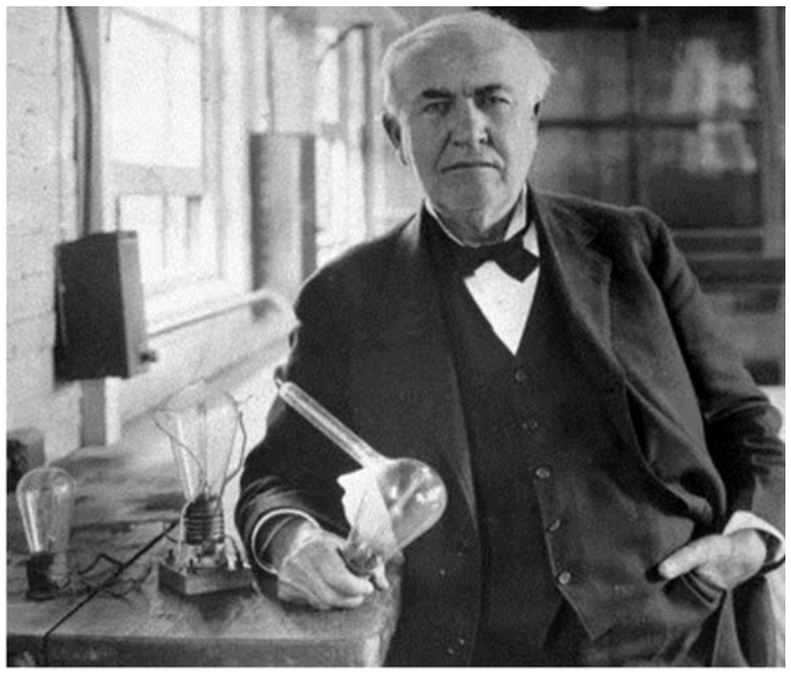

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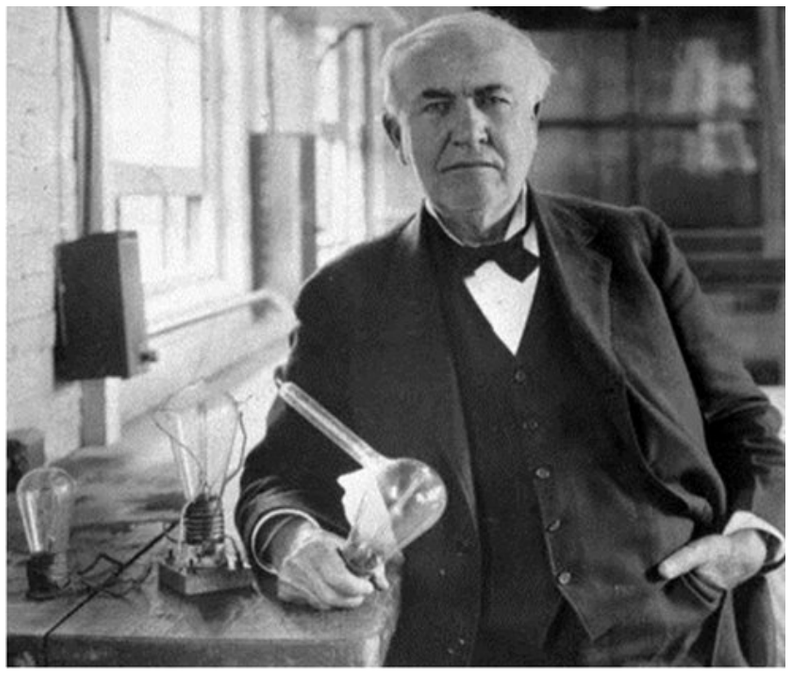
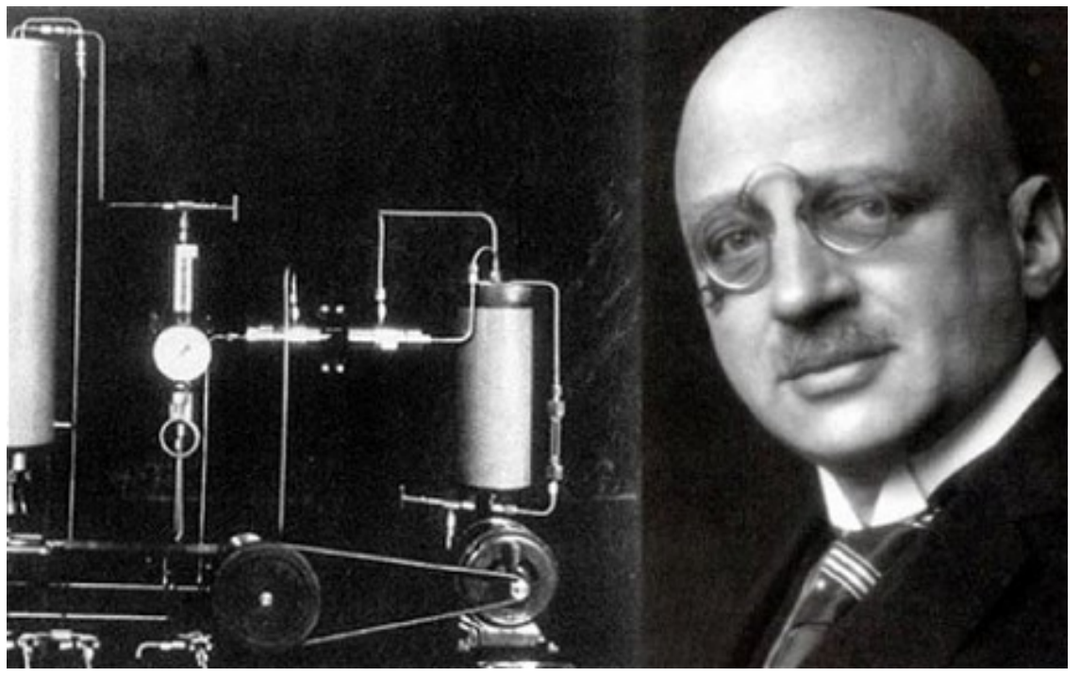
- Haber–Bosch ammonia synthesis used osmium as catalyst. Mittasch (BASF) tested more than 22,000 materials to identify the iron-based catalyst which is still used today.





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quantum mechanics and supercomputers can do more and faster …

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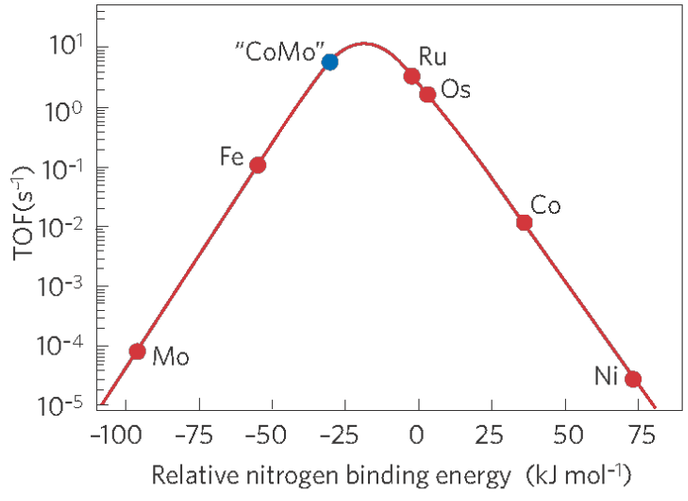
- Using state-of-the-art quantum-mechanical numerical modelling, Norskov showed in 2009 that CoMo is a more efficient and inexpensive catalyst

nature chemistry
REVIEW ARTICLE
PUBLISHED ONLINE: 19 MARCH 2009 | DOI: 10.1038/NCHEM.121

Towards the computational design of solid catalysts

J. K. Nørskov[1]*, T. Bligaard[1], J. Rossmeisl[1] and C. H. Christensen[2]



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QUANTUMESPRESSO

what is QUANTUM ESPRESSO?

QUANTUM ESPRESSO is an integrated suite of computer codes for atomistic simulations based on DFT, pseudo-potentials, and plane waves

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

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simulati[illegible] pseudo-potentials

ESPRESSO stands for opEn Source Pa[illegible]ectr[illegible]St[illegible]are,
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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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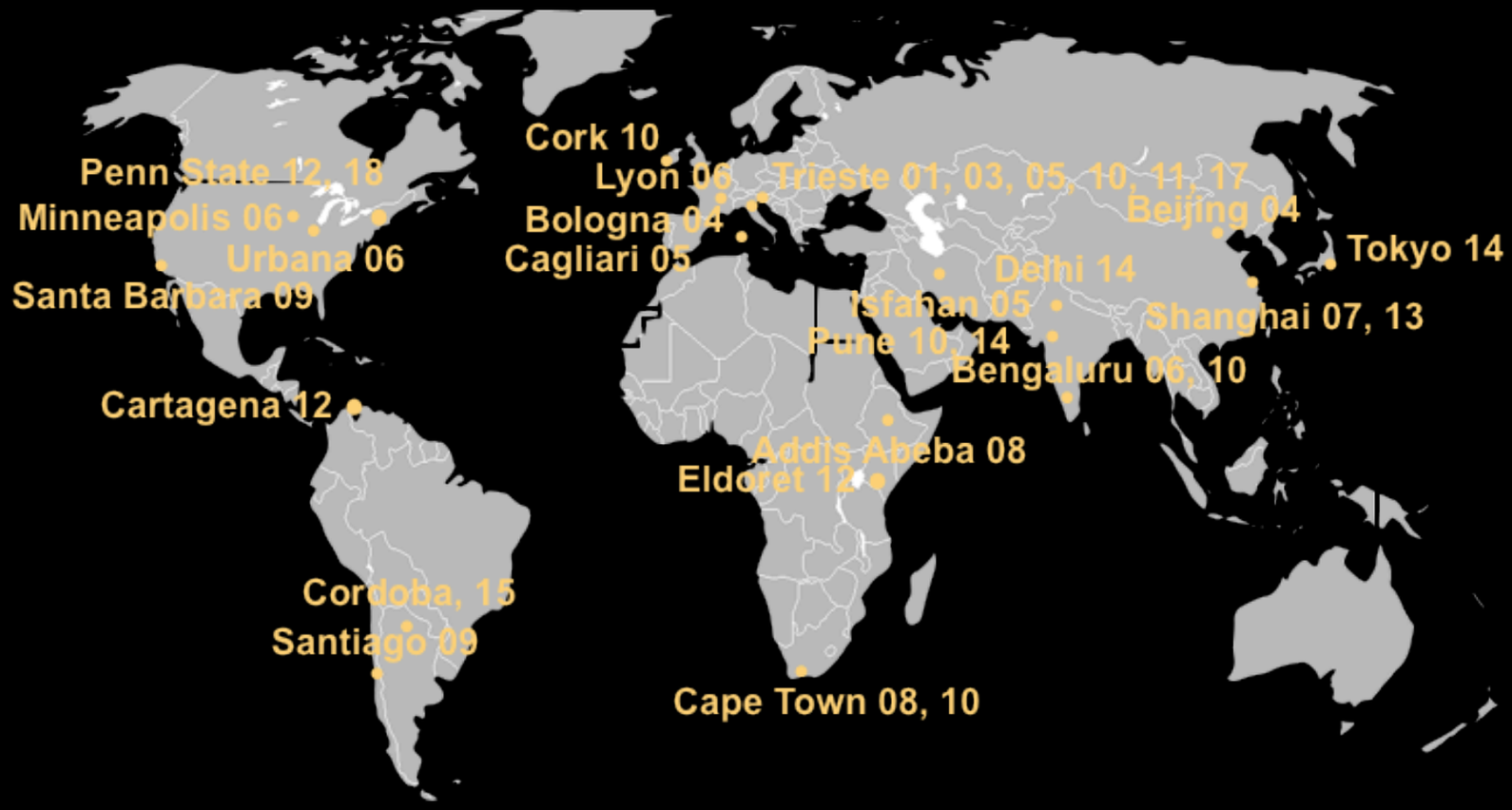
QUANTUM ESPRESSO is not a single application for quantum simulations; it is rather a distribution of packages performing different tasks and designed to be interoperable

QUANTUM ESPRESSO is *free* software that can be *freely* downloaded. Everybody is *free* to use it and welcome to contribute to its development

QUANTUM ESPRESSO in numbers

- 260,000+ lines of FORTRAN/C code
- 58 developers registered oh 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
- 1 popular international web discussion forum
- 36 international schools and training courses since 2001 (1500+ participants worldwide)



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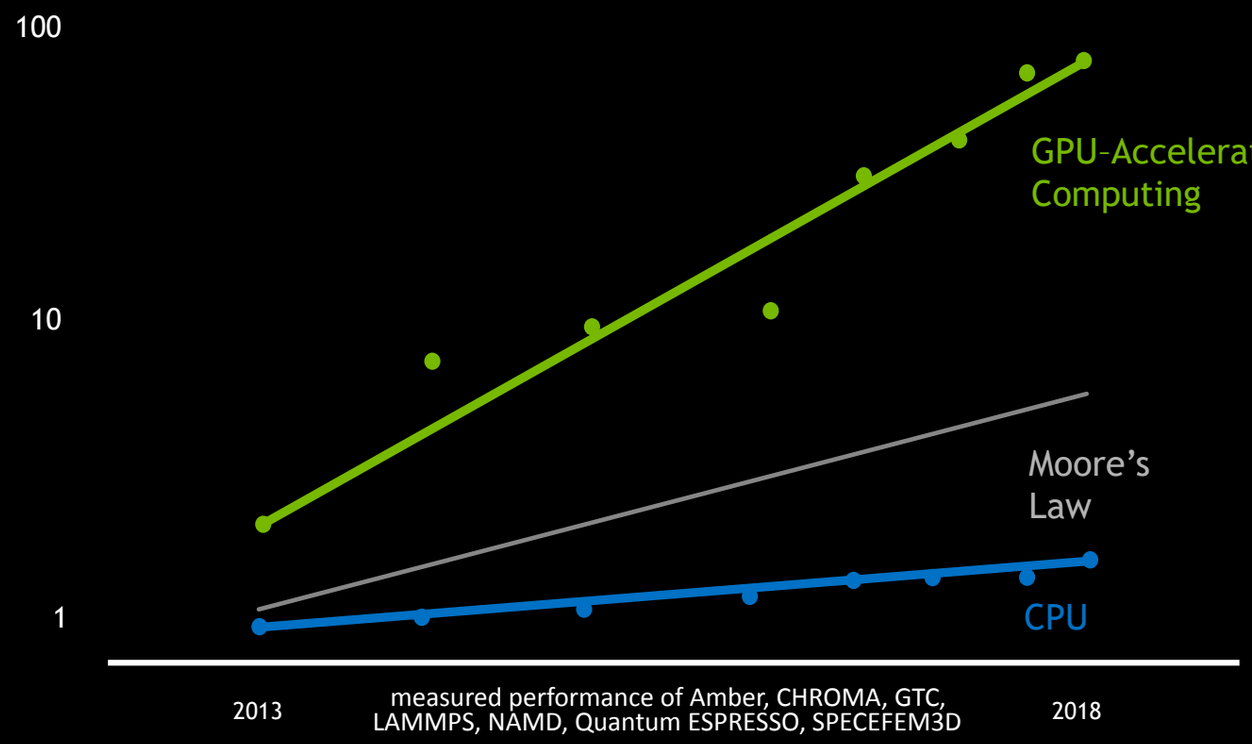
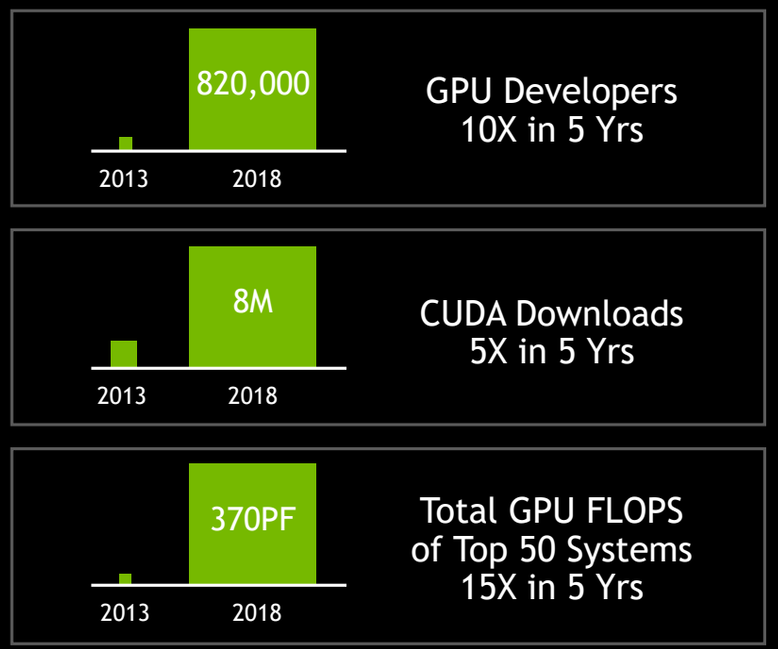
towards the exascale

“NVIDIA Is So Far Ahead of the Curve”

—The Inquirer





For 30 years, the dynamics of Moore’s law held true. But CPU performance scaling has slowed. GPU computing is defining a new, supercharged law. It starts with a highly specialized parallel processor called the GPU and continues through system design, system software, algorithms, and all the way through optimized applications. The world is jumping on board.

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

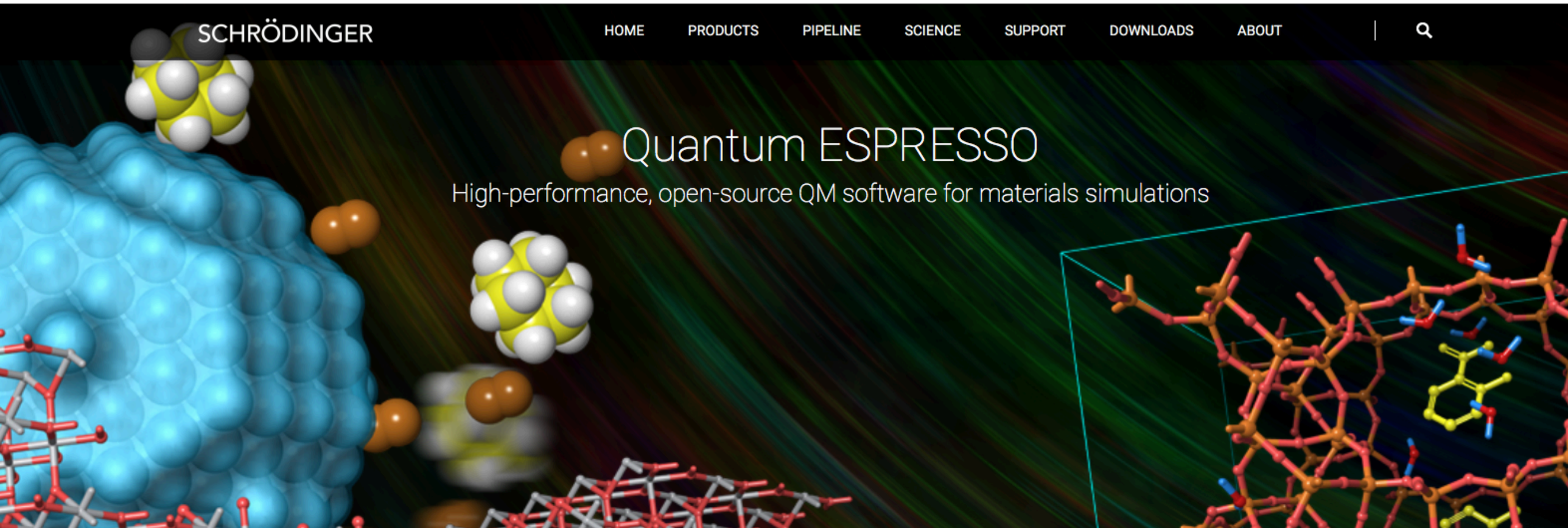
This is an open-source custom version of Quantum ESPRESSO with embedded GPU support based on CUDA FORTRAN. This product has been made possible thanks to the effort of the NVIDIA HPC Software and Benchmarks Group. This

QUANTUM ESPRESSO goes to the market

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

SCHRÖDINGER

QUANTUM ESPRESSO FOUNDATION



MAX MAterials design at the eXascale

a distributed European Centre of Excellence for supercomputing applications in materials science

Stockholm

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MAX

5 M€ / 2016-2018

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