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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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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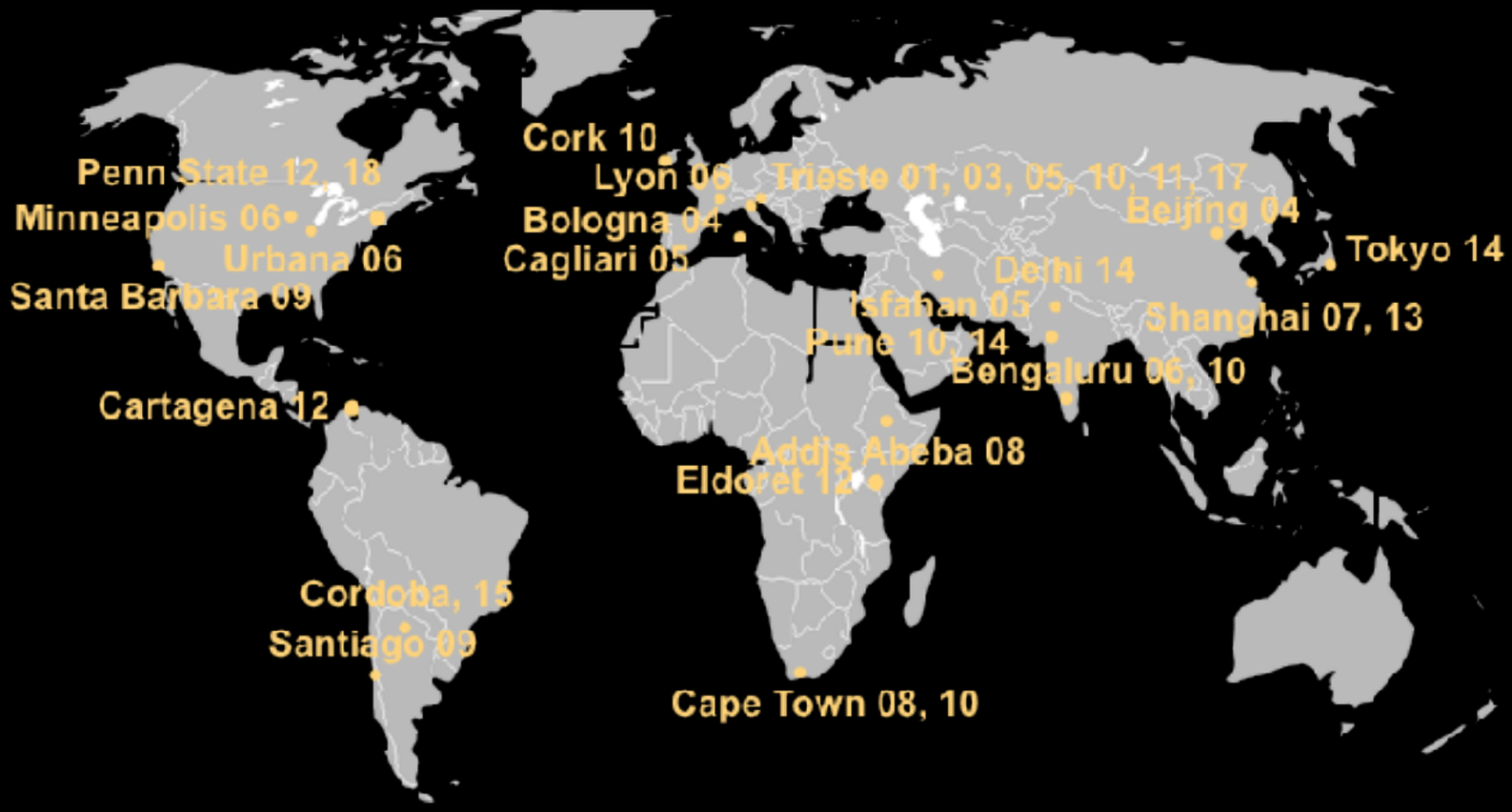
QUANTUM ESPRESSO is not a single application for quantum simulations; it is rather a distribution of packages performing different tasks and designed to be interoperable

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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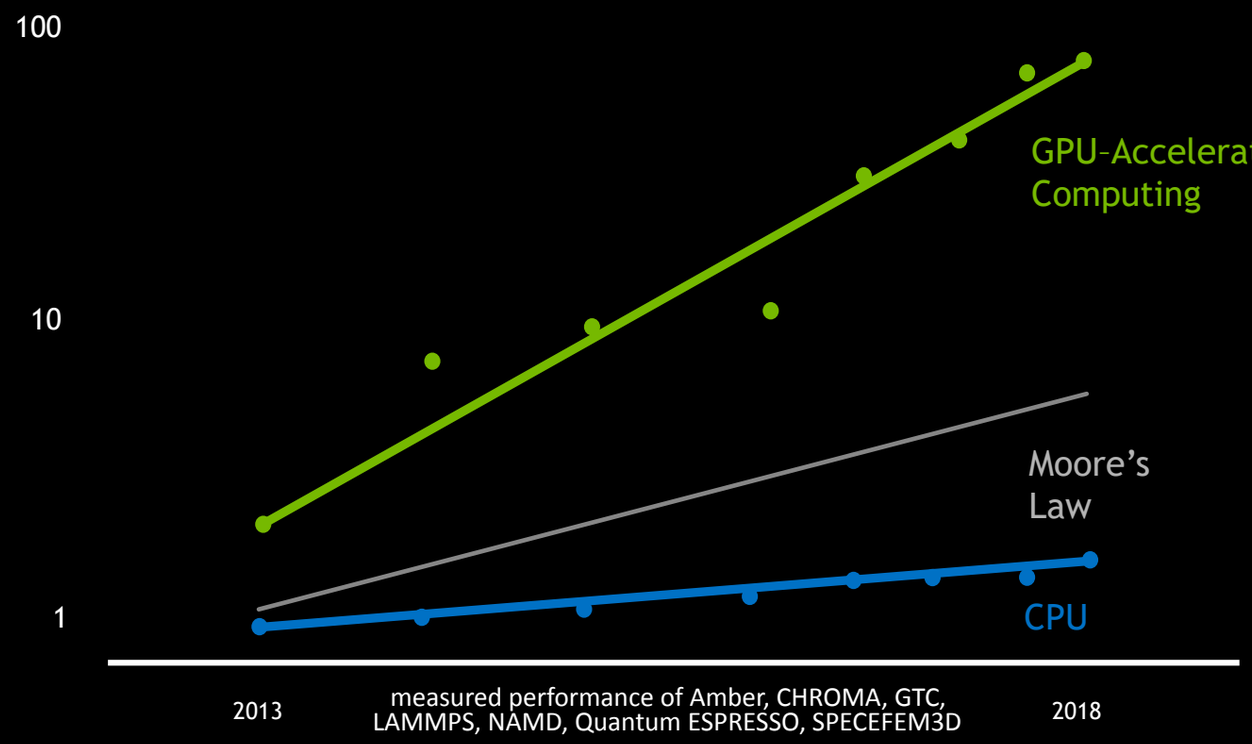
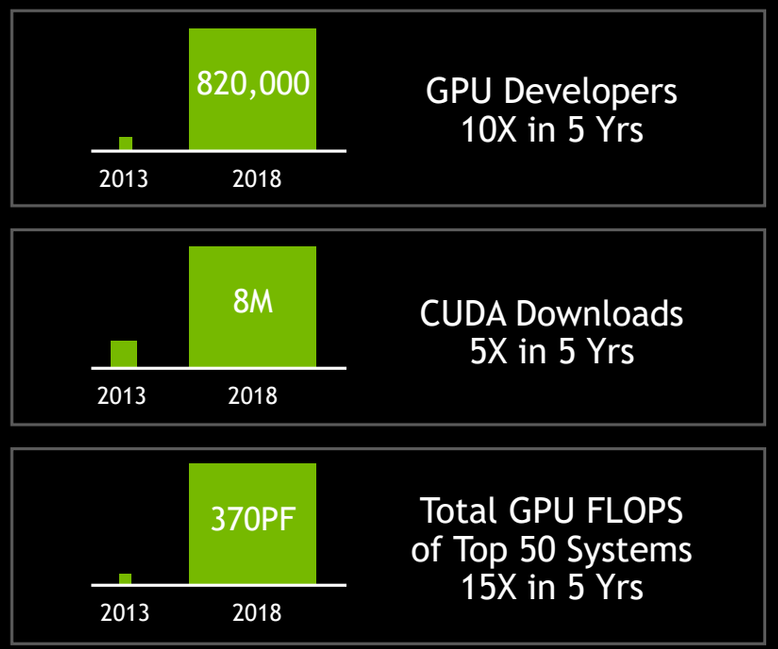
towards the exascale

“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

MAX MAterials design at the eXascale

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

Cambridge

Jülich

Gent

Zürich

Lausanne

Lugano

Trieste & Udine

Grenoble

Modena, Bologna, Scandiano, Pisa

Barcelona

MAX

8.5 M€ / 2018-2021


QUANTUM ESPRESSO
FOUNDATION

qef/Objects

coordinate and support research, education, and outreach within the QUANTUM ESPRESSO community

own the trademarks and protect the open-source character of QUANTUM ESPRESSO

raise funds to foster the QUANTUM ESPRESSO project

/the Company

PRIVATE COMPANIES LIMITED BY GUARANTEE

ARTICLES OF QUANTUM ESPRESSO FOUNDATION

INDEX TO THE ARTICLES

PART 1
INTERPRETATION AND LIMITATION OF LIABILITY

1. Defined terms
2. Liability of members

PART 2
DIRECTORS
DIRECTORS' POWERS AND RESPONSIBILITIES

3. Directors' general authority
4. Members' reserve power
5. Directors may delegate
6. Committees

DECISION-MAKING BY DIRECTORS

7. Directors to take decisions collectively
8. Unanimous decisions
9. Calling a directors' meeting
10. Participation in directors' meetings
11. Quorum for directors' meetings
12. Chairing of directors' meetings
13. Casting vote
14. Conflicts of interest
15. Records of decisions to be kept
16. Directors' discretion to make further rules

APPOINTMENT OF DIRECTORS

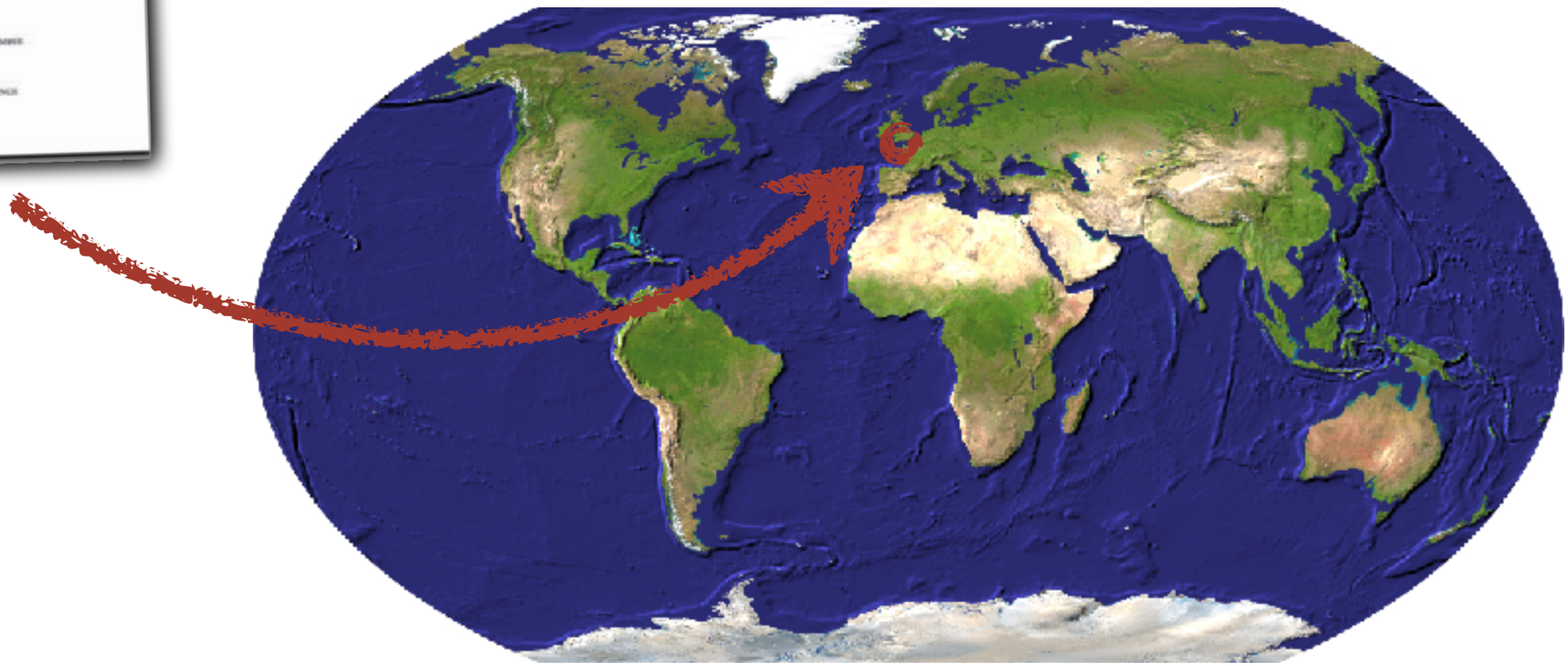
17. Methods of appointing directors
18. Termination of director's appointment
19. Directors' remuneration
20. Directors' expenses

PART 3
MEMBERS
BECOMING AND CEASING TO BE A MEMBER

21. Applications for membership
22. Termination of membership

ORGANISATION OF GENERAL MEETINGS

- Cambridge-based non profit company limited by guarantee
- public company articles



/Members

- Scuola Internazionale Superiore di Studi Avanzati, Trieste
- Ecole Polytechnique Fédérale de Lausanne
- University of Oxford
- International Centre for Theoretical Physics, Trieste
- Consiglio Nazionale delle Ricerche, Italy
- CINECA supercomputing center, Bologna
- University of North Texas
- the Foundation is open to new groups / institutions wishing to join

/the Business Model

where the foundation's money goes to

- dissemination (web sites, web-based community-oriented users' assistance)
- training (mainly, international schools)
- funding (micro-) prizes and super-computing grants
- code development and community-oriented code gluing

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where the foundation's money come from

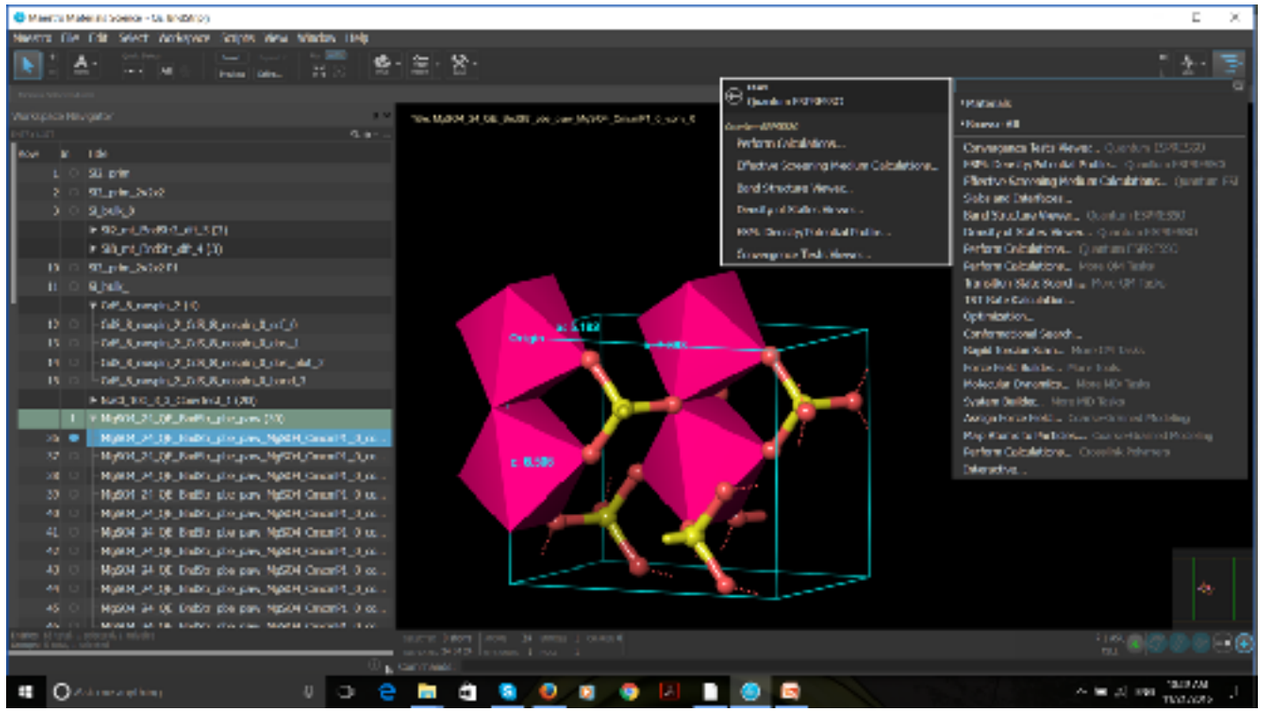
- membership fees
- (micro-) donations
- academic and corporate training
- brokering of custom-tailored code development / porting / optimization / benchmarking

/the Business Model

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®

QUANTUMESPRESSO

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