A journey through electronic structure and materials modelling at the exascale

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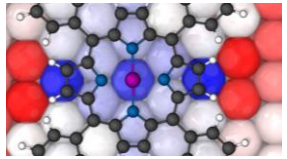
A European Centre of Excellence for materials design



U. G. E. Perera, Phys. Rev. Lett. 105, 106601 (2010)

Disruptive innovation in the simulation and discovery of materials and processes from:
predictive first principles methods + extreme computing

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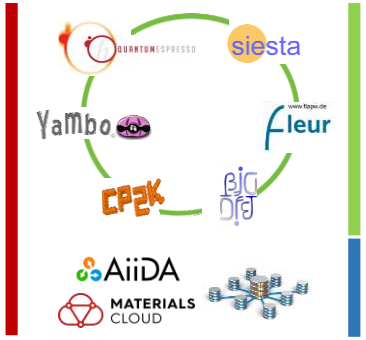
Codes and ecosystem developers

Tier0 HPC centres

Technology partners

Communications, training and disseminations

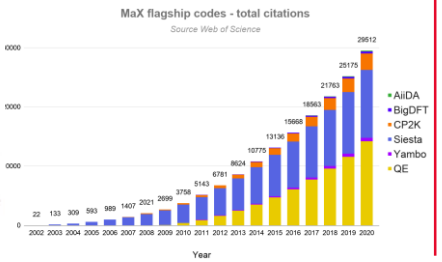
How: codes, data, co-design, users



- 6 flagship **open source codes** + impact on other codes and interoperability
- a dedicated platform to enable **automated high-throughput screening**: workflows, turn-key solutions, curated data, analytics
- **users**: dedicated tool for automated simulations, training

World-wide community: >4400 total citations of MaX flagship codes in 2020

Geographical distribution of author affiliations in the globe

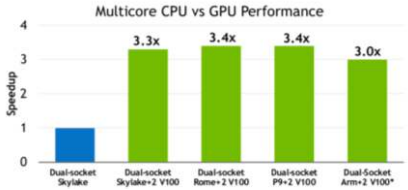


From laptops to supercomputers: performance on GPU

MaX flagship codes are all parallel oriented and ready for GPU-accelerated architectures

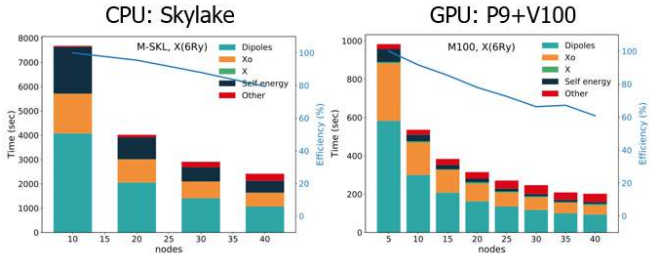
Porting of QUANTUM ESPRESSO *on GPUs*

AUSURF112



Performance of QE on different host machines equipped with Nvidia GPUs, in collaboration with NVIDIA

Porting of Yambo *on GPUs*



complete **GW workflow** for a defected TiO2 crystal; small system, **stress test;** data obtained on Marconi100, 4 MPI tasks/node; 4 V100 GPUs/node

MaX for users

- Codes — open source, powerful, green, matching industry standards; ready to go modules & libraries; come with automated workflows
- Consulting — high-level support for industry, ISVs ...; turn-key solutions
- Training — hands-on schools, tutorials, hackathons; training through research in MaX labs; dedicated training for industry; resources for online training
- Support — code and documentation download; basic and advanced support; containers

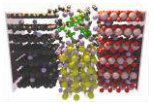
Materials modelling and electronic structure

Quantum mechanics based atomistic modelling of materials

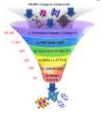
Electronic structure methods: highly accurate, predictive, compute-intensive

Materials modelling using HPC:

complexity

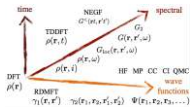


HTC screening



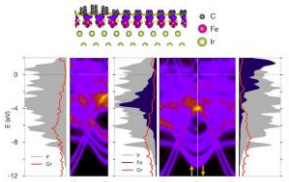
A. K. Singh, Nat. Commun. 10, 443 (2019).

accuracy



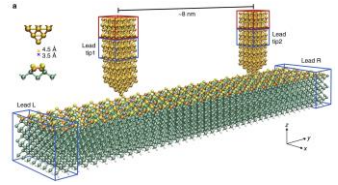
Scientific use cases

Structural, electronic and magnetic properties



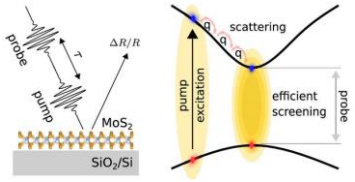
C. Cardoso *et al.*, Phys. Res. Materials 5, 014405 (2020)

Electronic transport



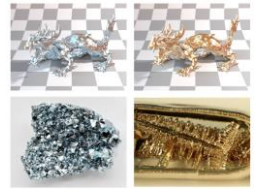
M. Kolmer *et al.*, Nat. Comm. 10, 1573 (2019)

2D semiconductors and excitons



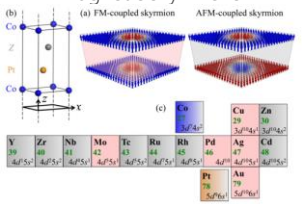
V. Smejkal *et al.*, ACSNano 15,1, 1179-1185 (2021)

Optics and colorimetry



G. Prandini *et al.*, Npj computational materials 5, 129 (2019)

Magnetic skyrmions



H. Jia *et al.* Phys. Rev. Mat. 4, 094407 (2020)

Thermal conductivity

F. Grasselli *et al.*, Nat. Comm. 11, 3605 (2019)

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