MAX DRIVING THE EXASCALE TRANSITION

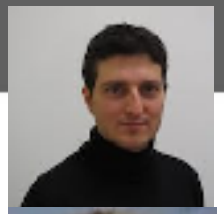
Industry and Materials design at the eXascale: bridging the gap

4 September 2019, 10:00 AM – 11:30 AM CET

#HPCForIndustry

MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

MaX Webinar: Industry and Materials design at the eXascale: bridging the gap






- 10:00 – 10:15: Welcome and Introduction – “Electronic structure and Materials modelling towards the exascale”, Andrea Ferretti, CNR Nano, Modena – Moderator
- 10:15 – 10:25: “High throughput screening and materials modelling in industry: success cases from MaX” Nicola Marzari, EPFL Lausanne
- 10:25 – 10:35: “Boosting the impact of the SIESTA code in the industry through HPC and HTC” Pablo Ordejon, ICN2 Barcelona
- 10:35 – 10:40: Q&A
- 10:40 – 10:50: “Quantum Mechanics on the Supermarket Shelf” Stefano Baroni, SISSA, Trieste
- 10:50 – 11:00: “HPC Services for Industry and SMEs. The European perspective on HPC” Carlo Cavazzoni, CINECA, Bologna
- 11:00 – 11:10: “Increasing the impact of Materials Modelling in Industry: the contribution of EMMC”, Gerhard Goldbeck, Executive Secretary EMMC
- 11:10 – 11:20: Q&A
- 11:20 – 11:25: Closing Remarks

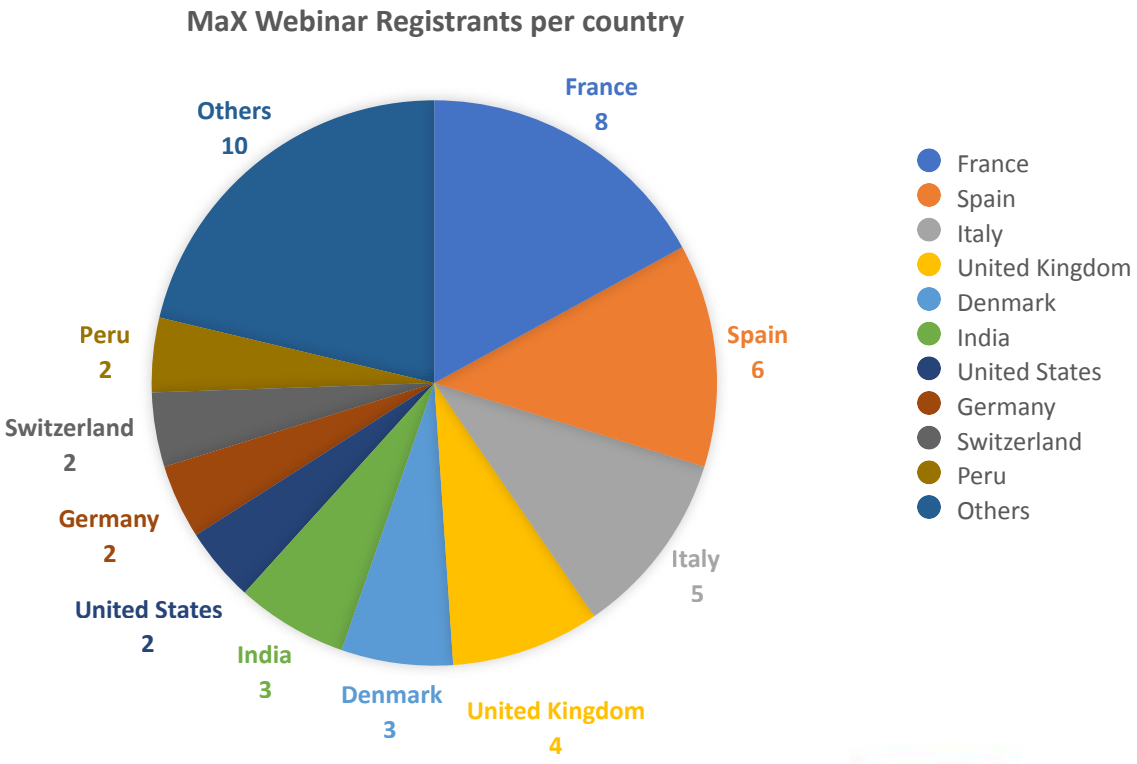
Webinar Participation

Industry and Materials design at the eXascale: bridging the gap

- Total of 47 registrants (4 September)
- 8 different countries across EU and 9 cross continental
- Breakdown Registrants per:

Industry	Count
Education	7
Software - Other	6
Energy, Chemical, Utilities	4
High-Tech (hardware/other)	4
Aerospace & Defense	3
Consulting	2
Manufacturing	2
Others	19

Gender Preference	Count
Male	34
Female	13



DRIVING THE EXASCALE TRANSITION

Electronic structure and materials modelling towards the exascale

Andrea Ferretti
CNR-NANO, Modena, IT

Outline

MaX DRIVING THE EXASCALE TRANSITION

- intro - materials - exascale
- what is MaX
- context and activities
- what can we do for you ?


computational
materials **design** for …
ICT, digital economy
high-tech and high-value
manufacturing
energy harvesting, conversion,
storage, efficiency …
food safety and
conservation
biomedical research
and industries,
health
environmental protection
and reparation
technology advances
detectors, sensors, magnets, …
… qbit implementations
[…]
… well being

computational materials **design** for …

ICT, digital economy

high-tech and high-value manufacturing

energy harvesting, conversion, storage, efficiency …

food safety and conservation

biomedical research and industries, health

environmental protection and reparation

technology advances

detectors, sensors, magnets, …

… qbit implementations

[…]

… well being

accelerating discovery:
modelling, codes
data platforms, AI

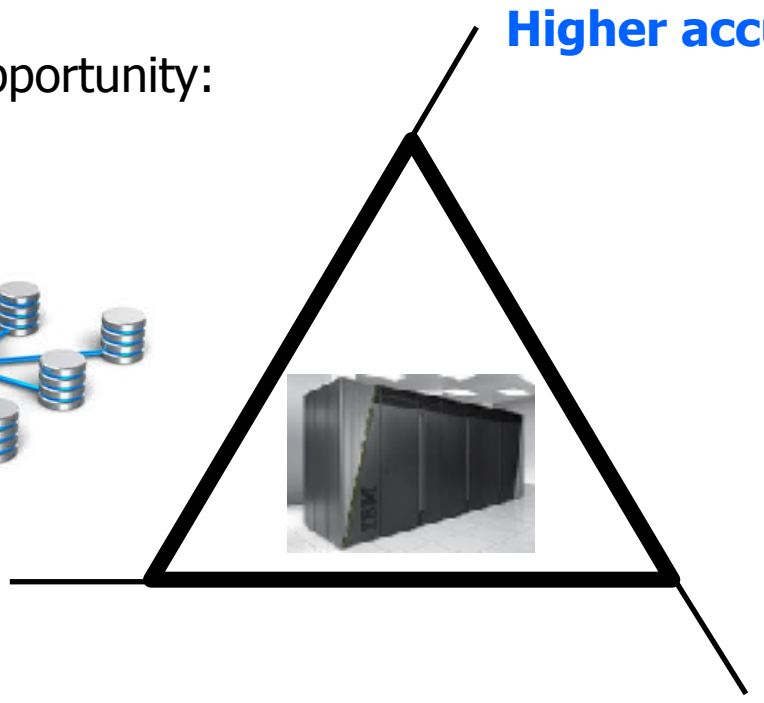
materials science @ exascale

MAX DRIVING THE EXASCALE TRANSITION

quantum mechanics based
atomistic modelling of materials
+
interfacing with **multiscale** approaches

- highly accurate (predictive)
- computationally demanding

the **exascale** opportunity:



HPC & exascale

MAX DRIVING THE EXASCALE TRANSITION

the exascale challenge
in high performance computing

- 10^18 flops/s
- 10^18 Bytes
- abrupt technology changes
- **action is needed** for full exploitation

HPC & exascale

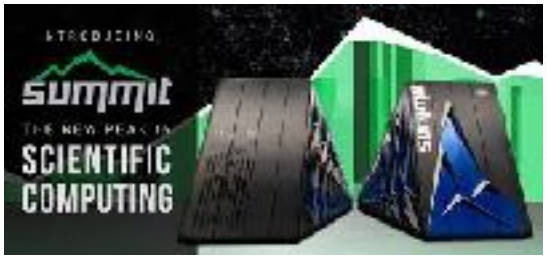
MAX DRIVING THE EXASCALE TRANSITION

the exascale challenge
in high performance computing

- 10^18 flops/s
- 10^18 Bytes
- abrupt technology changes
- **action is needed** for full exploitation
- **multiple** HW and SW stacks
- memory hierarchies

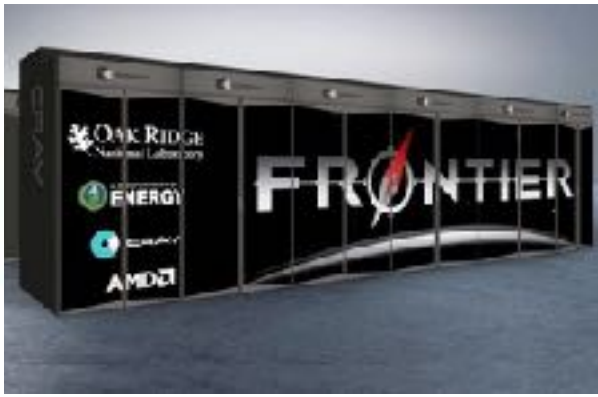
eg in the US:

Frontier: AMD EPYC + AMD GPU



Summit: IBM power + NVIDIA GPUs

Aurora: CRAY + Intel Acc



The EuroHPC Joint Undertaking

EuroHPC
Joint Uncertaking

A legal funding entity

- **28 Participating States + EC**
- **Budget 2019-2020: ~1.4 B€**
  Proposed 2021-27: 2.7 B€

to develop **the whole HPC ecosystem**:
machines, applications, data, training…

https://eurohpc-ju.europa.eu/

The EuroHPC Joint Undertaking

EuroHPC
Joint Uncertaking

A legal funding entity

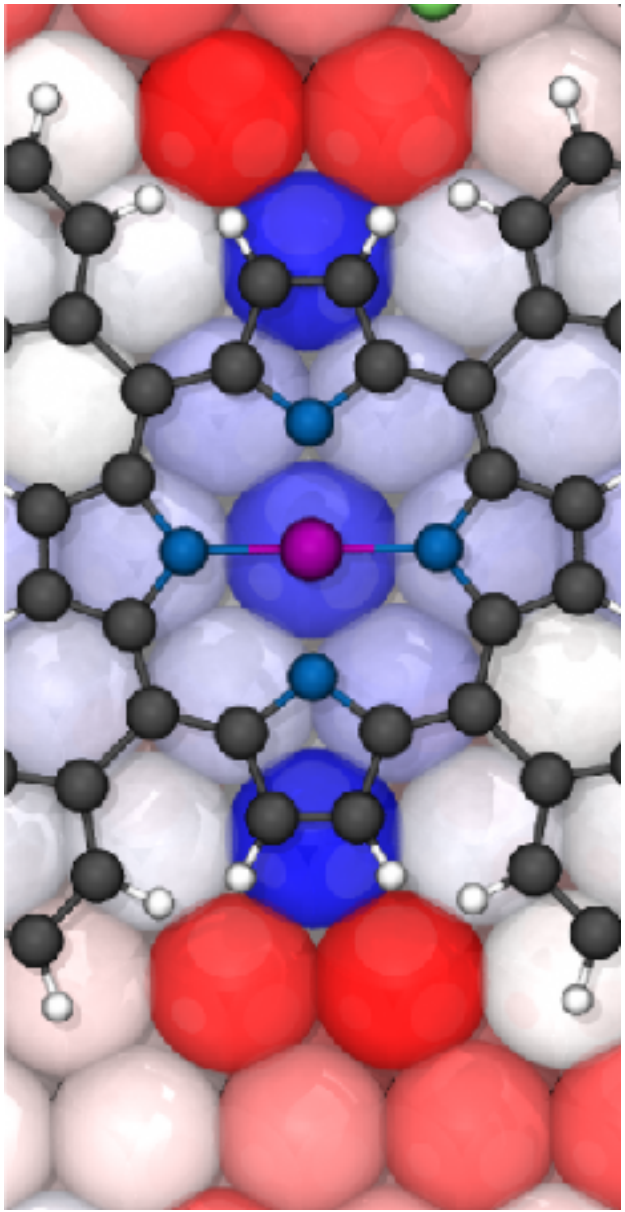
- **28 Participating States + EC**
- **Budget 2019-2020: ~1.4 B€**
  Proposed 2021-27: 2.7 B€

9 Centres of Excellence

ChEESE

a European CoE for materials design

MAX DRIVING THE EXASCALE TRANSITION



disruptive innovation in the simulation and discovery of materials and processes from:

predictive first principles methods

+

extreme computing

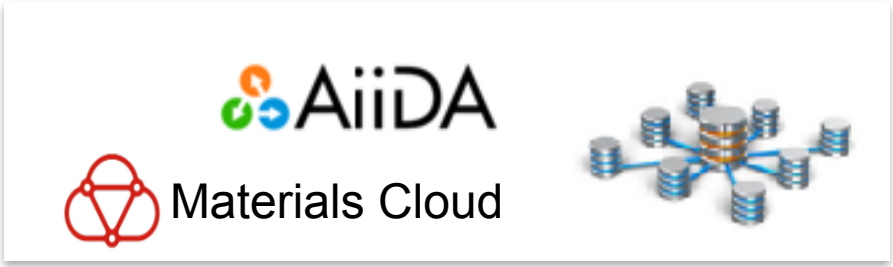
MAX

MaX: a European Centre of Excellence for materials design

MaX coordinator: CNR-NANO, Modena, IT

How: codes, data, codesign, users

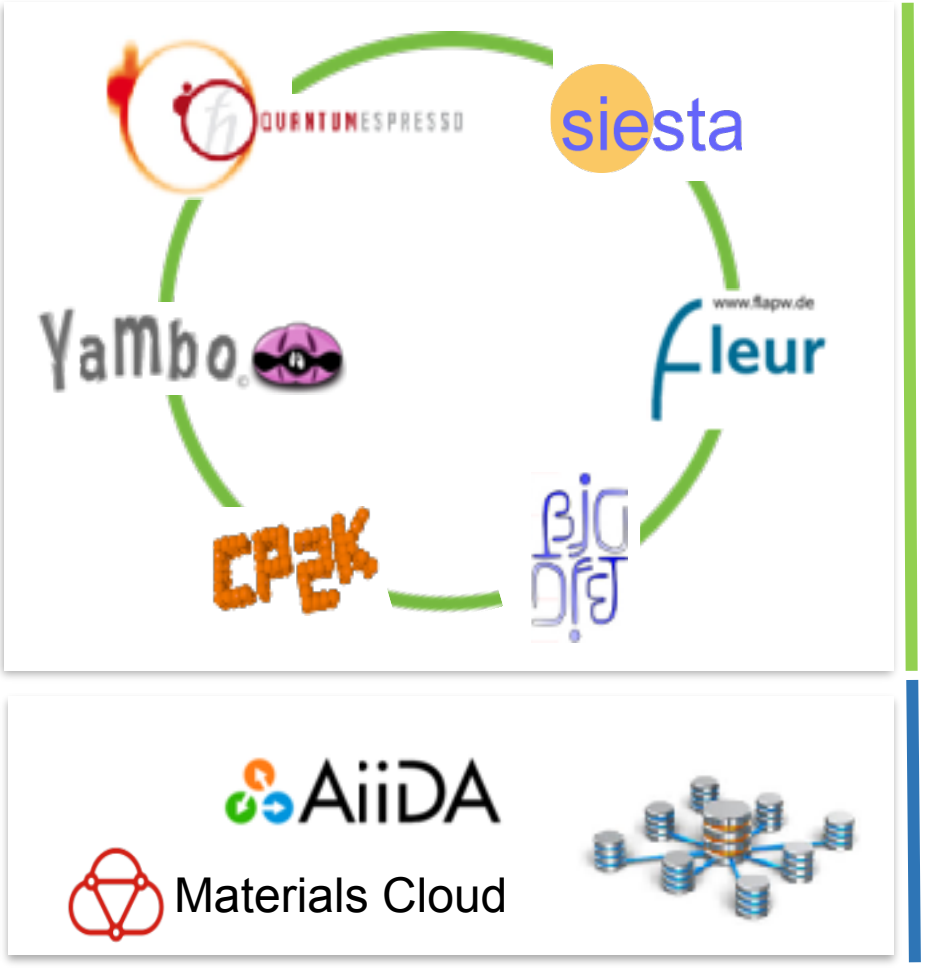
MAX DRIVING THE EXASCALE TRANSITION



- start from successful and widely used open-source, **community codes** in quantum materials simulations
- make them **scalable and optimized** for current and **future architectures** towards the exascale, develop new capabilities
- leverage the convergence of HPC with automated **high throughput computing** and high-performance **data analytics**
- hardware-software **codesign** in practice
- widen access to codes, engage & train **users communities** in industry and academia

How: codes, data, codesign, users

MAX DRIVING THE EXASCALE TRANSITION



- **6 flagship codes**
  - Quantum Espresso
  - Yambo
  - Fleur
  - Siesta
  - Cp2k
  - BigDFT

  + impact on other codes, interoperability

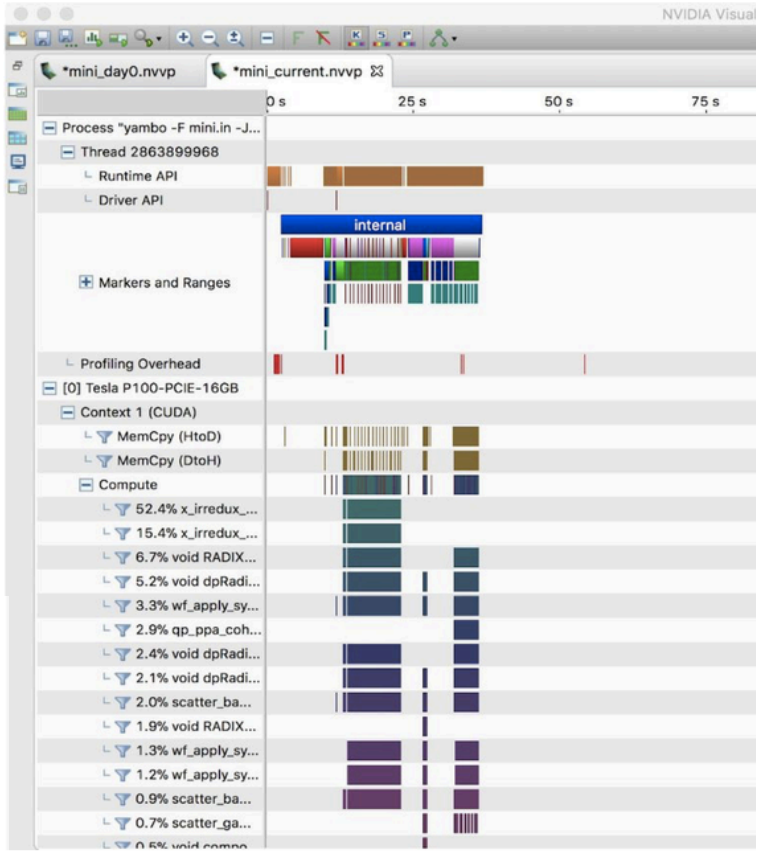
  - > 10 000 downloads
  - 2500 papers/yr

- a dedicated platform to enable **automated high-throughput** screening: workflows, turn-key solutions, curated data, analytics

- **users**: dedicated tools for automated simulations, training

Performance portability: GPU

- Porting of **Quantum ESPRESSO** & **Yambo on GPUs**
- In collaboration with **NVIDIA**



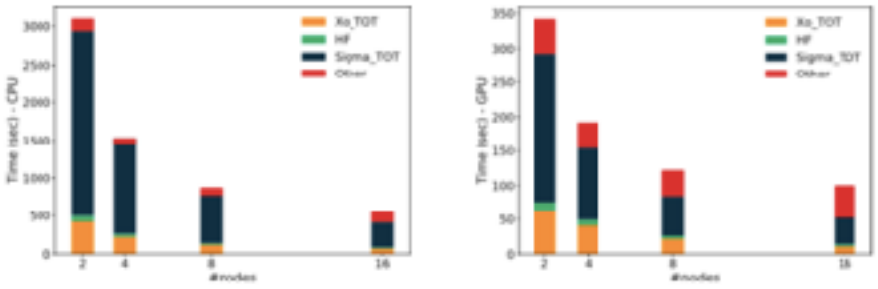
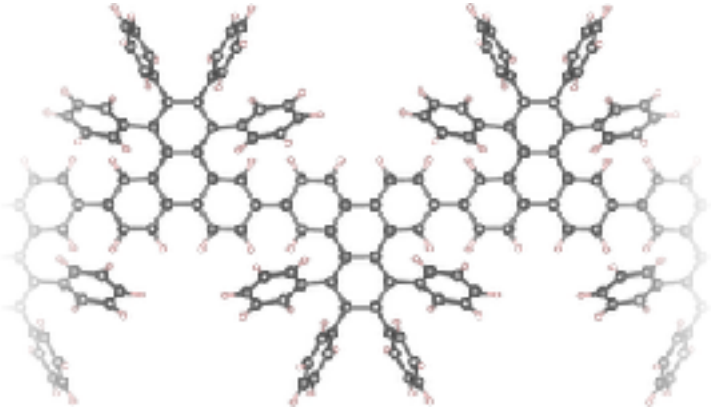


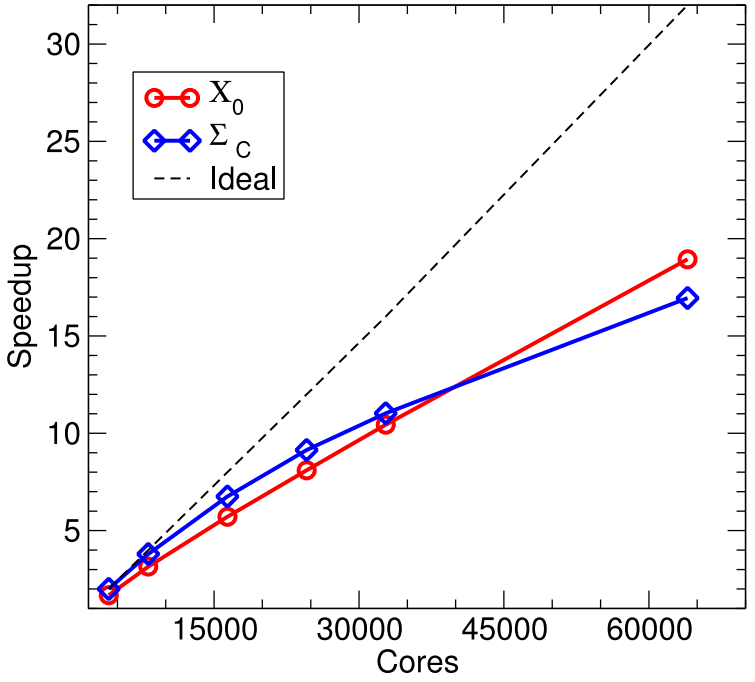
Figure 12: Full socket (left panel) vs GPU (right panel) timing for poly-acetylene on Piz Daint (XC50 partition). The time for each of the main tasks of the code is given separately. The total time taken to perform other tasks is labeled as "Other".

Performance portability: KNL

Putting all together:

- Yambo **single GW calculation** scaling up to 1000 KNL nodes (~ 3 PFl/s, 16 k MPI)
- Calculations relevant for an active research field (**flexible optielectronics**)
  R. Denk et al, Nanoscale 9 (2018)
- Performed on a **many-core architecture** (Intel KNL, Marconi @ CINECA)

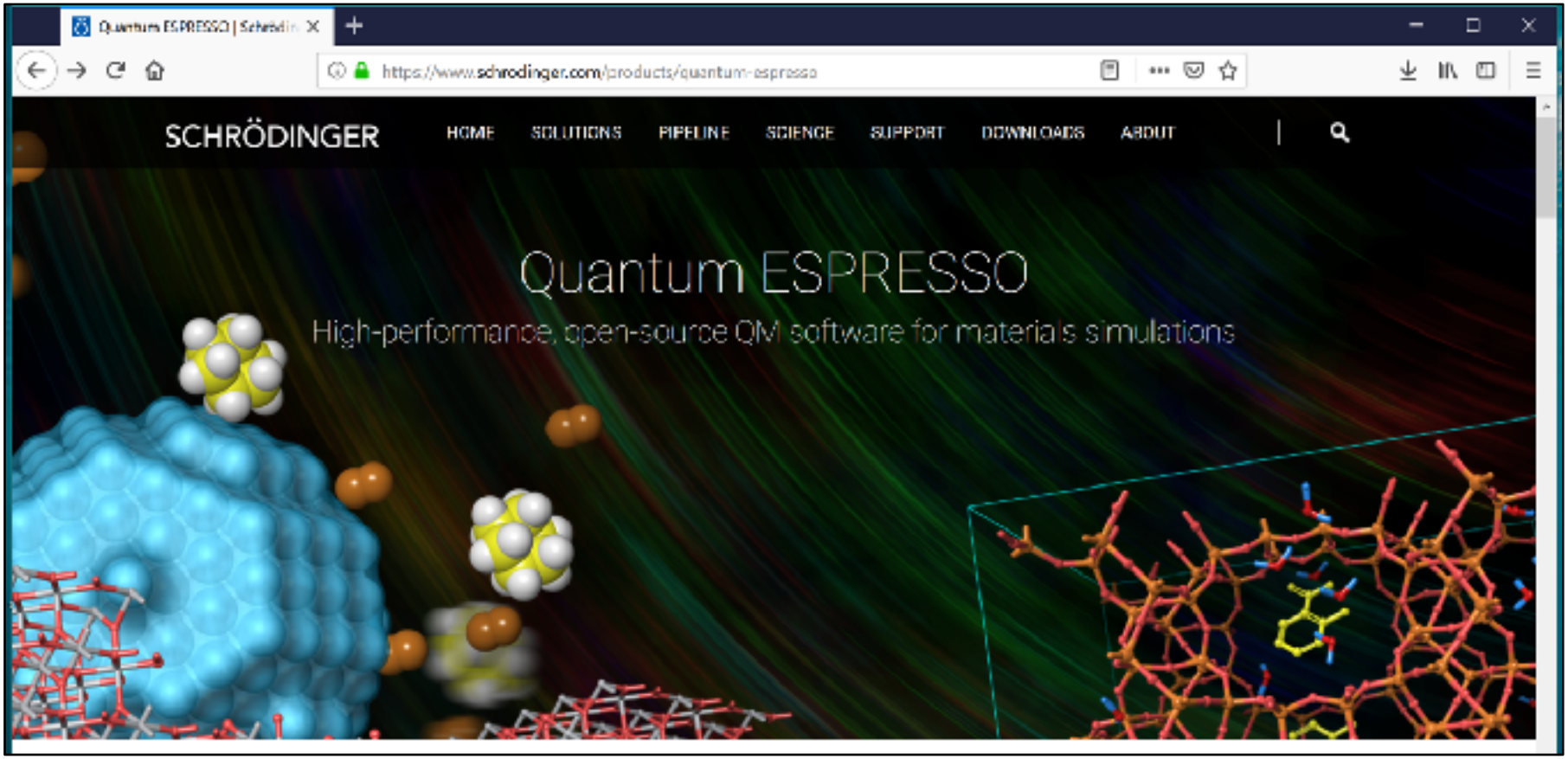




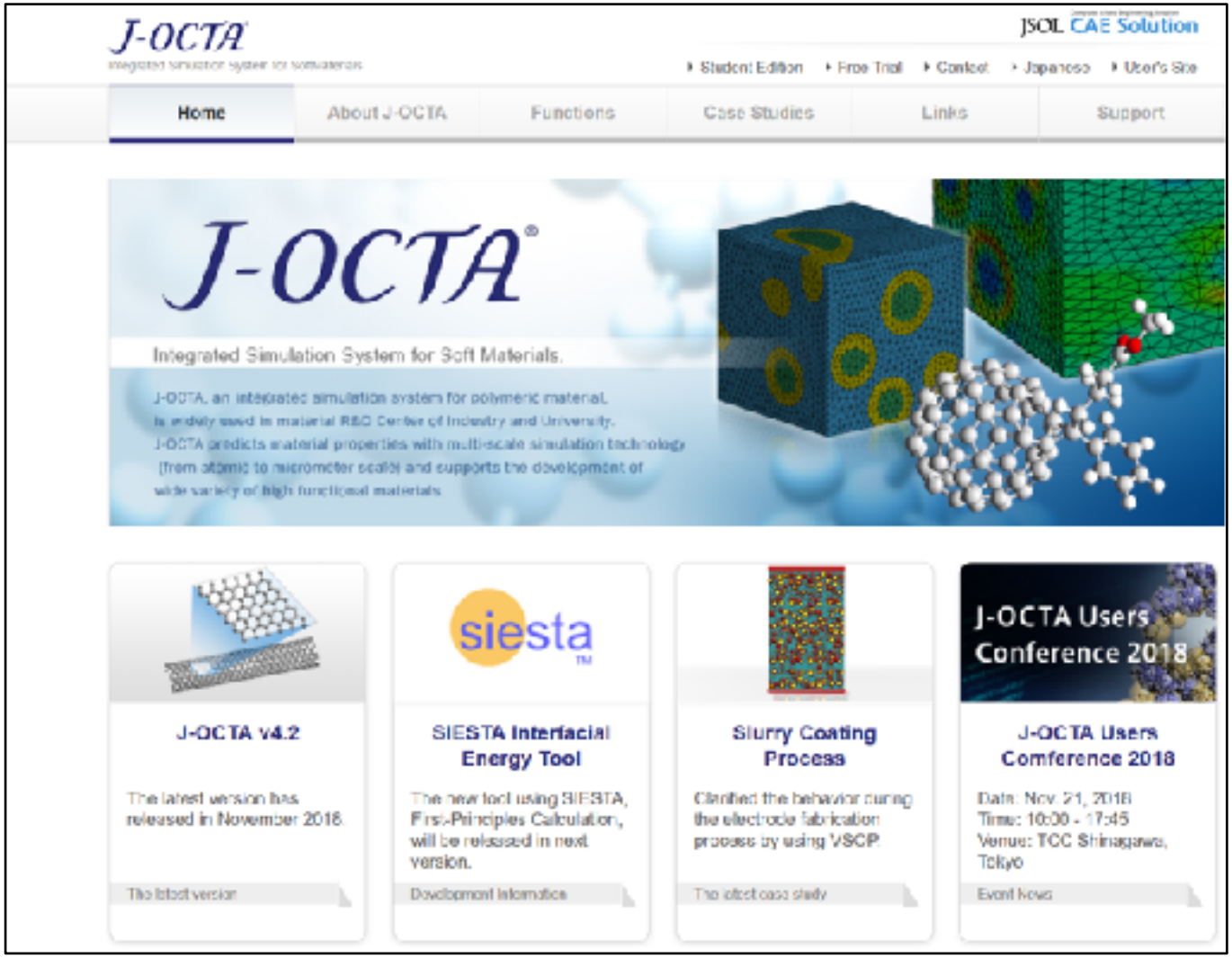
independent software vendors

MAX DRIVING THE EXASCALE TRANSITION

open source codes: what business models



independent software vendors

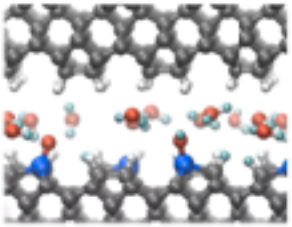


industrial success stories

MAX DRIVING THE EXASCALE TRANSITION

TOTAL

TOYOTA

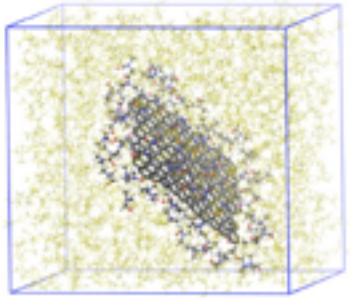


Friction - Tribochemistry

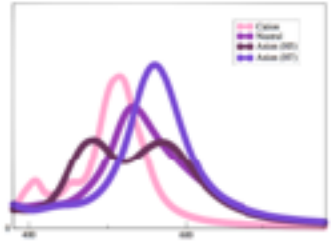
ABENGOA RESEARCH

ICN2

Institut Català de Nanociència i Nanotecnologia



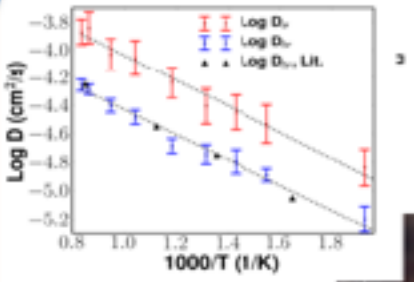
Nanofluids for Thermal Storage



Mars

SISSA

Natural food colorings



BOSCH

EPFL

Solid State Electrolytes

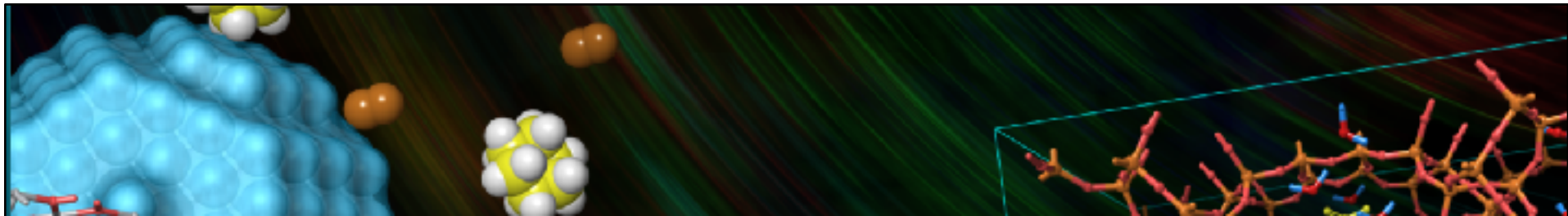
what can we do for you ?

MAX DRIVING THE EXASCALE TRANSITION

1. codes

open source, **powerful, green**
matching industry **standards**
ready to go **modules & libraries**
come with automated **workflows**

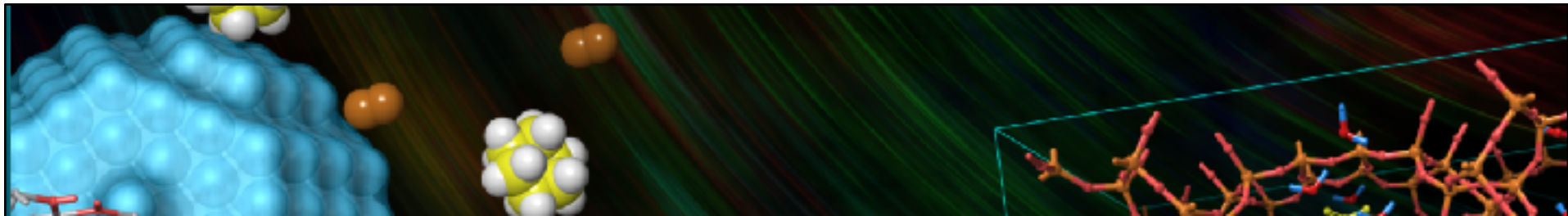
www.max-centre.eu



2. consulting and support

consulting:	problem → HPC solution including dedicated code development / evolution
training:	hands-on schools, tutorials, hackatons training through research in MaX labs dedicated training for industry materials for academic training
support:	code and documentation download basic and advanced support containers
EU call participation:	Prace, H2020, HEurope: support or joint consortia EuroHPC, HEurope → e.g. next EuroHPC calls for SMEs, industrial software, R&I

www.max-centre.eu



MATERIALS DESIGN AT THE EXASCALE

www.max-centre.eu

Ask your question now!

Q&A

Thank you!

DRIVING THE EXASCALE TRANSITION

JOIN THE COMMUNITY NOW!

Follow us on:

@max_center2

http://www.max-centre.eu/

company/max-centre/

youtube/channel/MaX Centre eXascale