

Dan slovenskega superračunalniškega omrežja, MREŽA ZNANJA
16. november 2023

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EURO



SLING

MAX: MAterials design at the eXascale



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Institut „Jožef Stefan“



DRIVING
THE EXASCALE
TRANSITION

Chemistry & materials science: a traditional way



Chemistry & computation



"Every attempt to employ mathematical methods in the study of chemical questions must be considered profoundly irrational and contrary to the spirit of chemistry. If mathematical analysis should ever hold a prominent place in chemistry – an aberration which is happily almost impossible - it would occasion a rapid and widespread degeneration of that science."

Auguste Comte, Philosophie Positive, 1830

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be solved."

Paul A.M. Dirac, Proc. Roy. Soc. (London) 123, 714 (1929)

Chemistry & computation



MAX: Materials design at the eXascale



materials

codes

HPC

Materials design at the e**X**ascale –
European Centre of Excellence



“MaX: *Materials Design at the Exascale*” has received funding from the European Union under grant agreement no. 101093374.



The project is supported by the Euro HPC Joint Undertaking and its members.

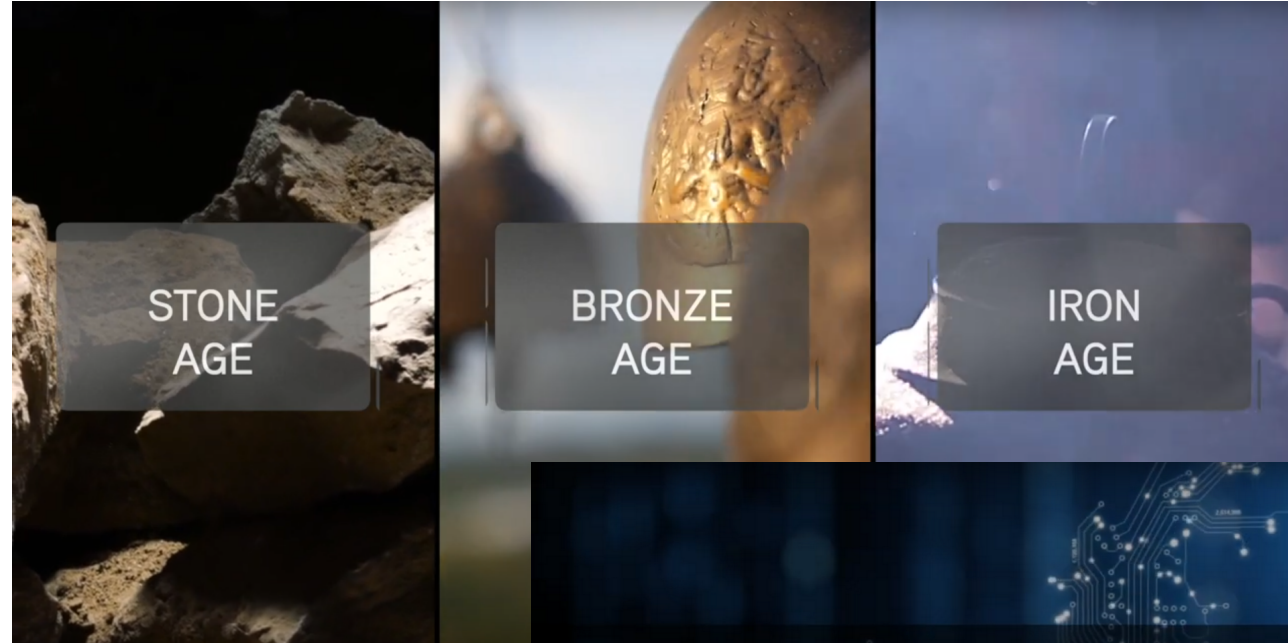
MAX: Materials design at the eXascale



materials

codes

HPC



MAX: MAterials design at the eXascale



materials

New materials discovery is the base of every technological revolution!

codes

New materials were usually discovered by serendipity or through painstaking search (e.g. Edison tried more than 1600 materials for over 14 months to find the best one for the light bulb).

HPC

A new way to design and test materials: **modeling & simulations**

Simulations require **scientific codes** and powerful **supercomputers**

Computational materials design



nature materials REVIEW ARTICLE
PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

Stefano Curtarolo^{1,2*}, Gus L. W. Hart^{2,3}, Marco Buongiorno Nardelli^{2,4,5}, Natalio Mingo^{2,6}, Stefano Sanvito^{2,7} and Ohad Levy^{1,2,8}

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. Bligaard¹, J. Rossmeisl¹ and C. H. Christensen²



LETTERS

Where are nature's missing structures?

GUS L. W. HART

Department of Physics & Astronomy, Brigham Young University, Provo, Utah 84602, USA
e-mail: gus.hart@gmail.com

Physics ABOUT BROWSE PRESS COLLECTIONS

VIEWPOINT

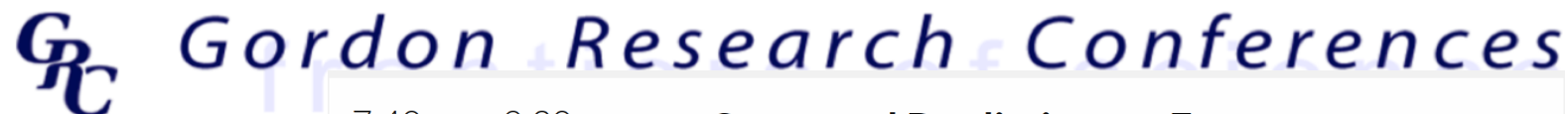
Materials Prediction Scores a Hit

Filip Ronning and John L. Sarrao

Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

October 7, 2013 • *Physics* 6, 109

Calculations predicting a new high-pressure superconductor are borne out by experiment.



7:40 pm - 9:30 pm

Structural Predictions at Extreme Conditions: Are Experiments Still Necessary?

MAX: Materials design at the eXascale



materials

Quantum-mechanics based open-source community codes

codes



HPC



MAX: Materials design at the eXascale



materials

Quantum-mechanics based **open-source** community codes

codes



HPC

An integrated suite of codes for electronic-structure calculations and materials modeling at the nanoscale, based on density-functional theory (DFT), plane waves, and pseudopotentials.

www.quantum-espresso.org

MAX: MAterials design at the eXascale



materials

Quantum-mechanics based **open-source** community codes

codes



HPC

A code that implements first-principles methods to describe excited-state properties of materials (optical spectra, quasiparticle energies).

www.yambo-code.eu

MAX: Materials design at the eXascale



materials

Quantum-mechanics based **open-source** community codes

codes



HPC

A density-functional theory (DFT) code for efficient electronic-structure calculations and ab initio molecular dynamics simulations of molecules and solids.

departments.icmab.es/leem/siesta

MAX: Materials design at the eXascale



materials

codes

HPC

Quantum-mechanics based **open-source** community codes



A fast, precise, and flexible pseudopotential density-functional theory (DFT) code for ab initio atomistic simulation that employs Daubechies wavelets as a basis set.

bigdft.org

MAX: Materials design at the eXascale



materials

Quantum-mechanics based **open-source** community codes

codes

HPC



A program package for calculating ground-state and excited-state properties of materials, based on the full-potential linearized augmented-plane-wave method.

www.flapw.de

MAX: Materials design at the eXascale



materials

codes

HPC

Quantum-mechanics based electronic-structure methods

- highly accurate (predictive)
- computationally demanding
- a case for HPC
- the **exascale** opportunity

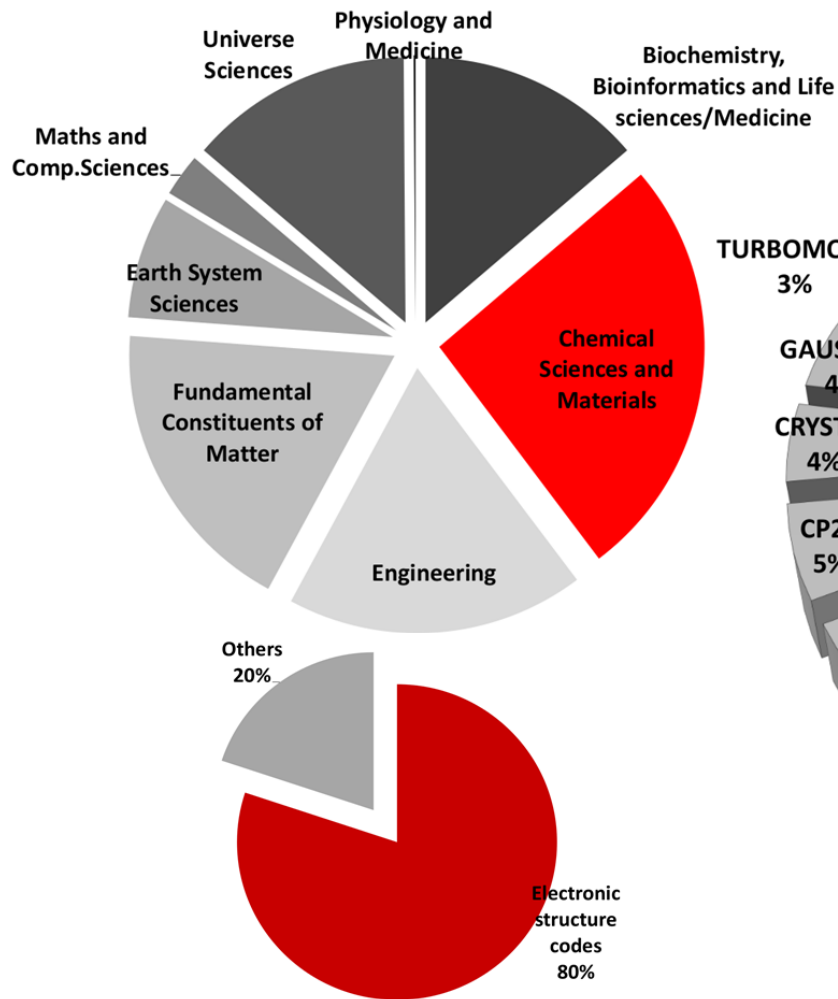


Higher accuracy

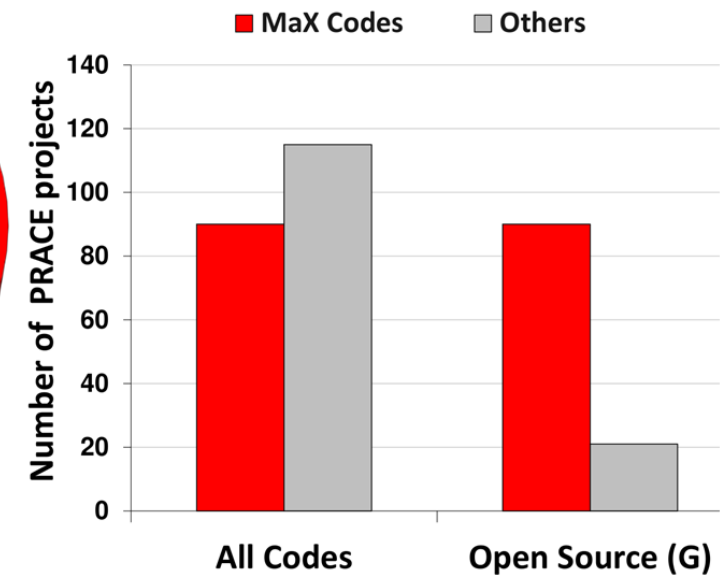
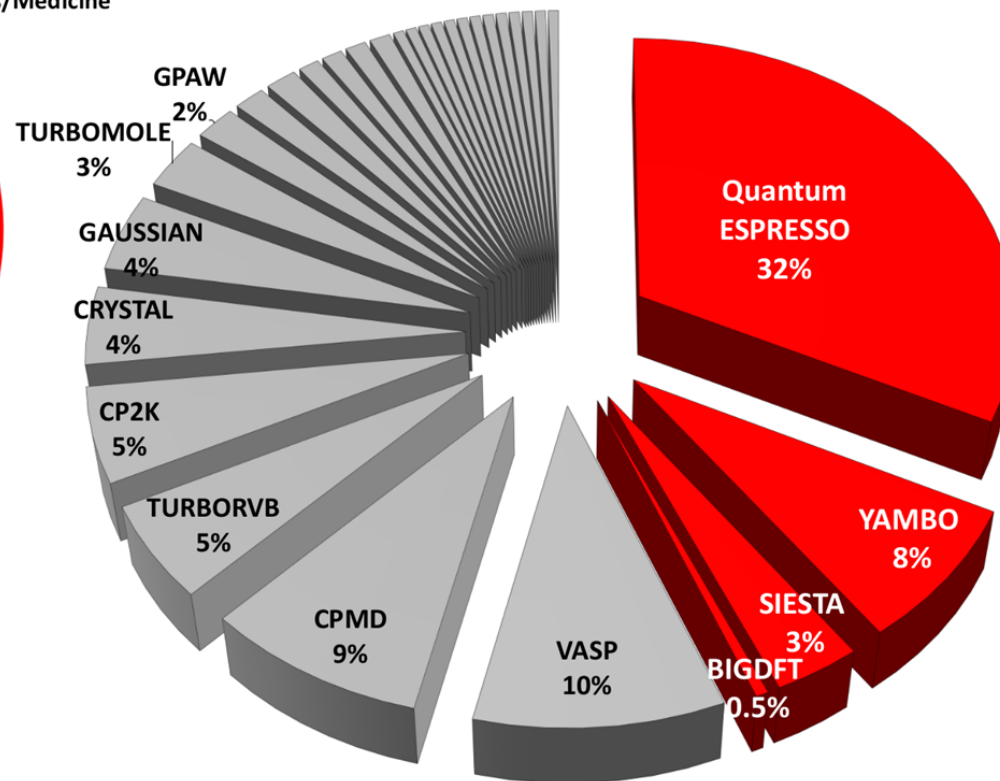
High throughput screening

Improved modelling (complexity)

Materials modeling & MAX codes in HPC



PRACE PROJECTS: CODE BREAKUP (calls 1 – 23)



MaX: codes and partners



LIGHTHOUSE CODES



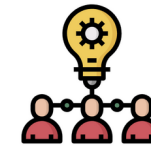
DOMAIN EXPERTS & CODE DEVELOPERS



HPC EXPERTS & DATA CENTRES



TECHNOLOGY & CO-DESIGN PARTNERS



16 Partners with unique expertise in:

- Materials Science
- Software Development
- Code Validation
- System & Data Management
- Technology development & co-design
- Communication & Outreach

Countries:

- Italy, Spain, Germany, France, Czech, Slovenia

MAX coordination and management: Cnr – Modena, Italy



MAterials design at the e**X**ascale
European Centre of Excellence



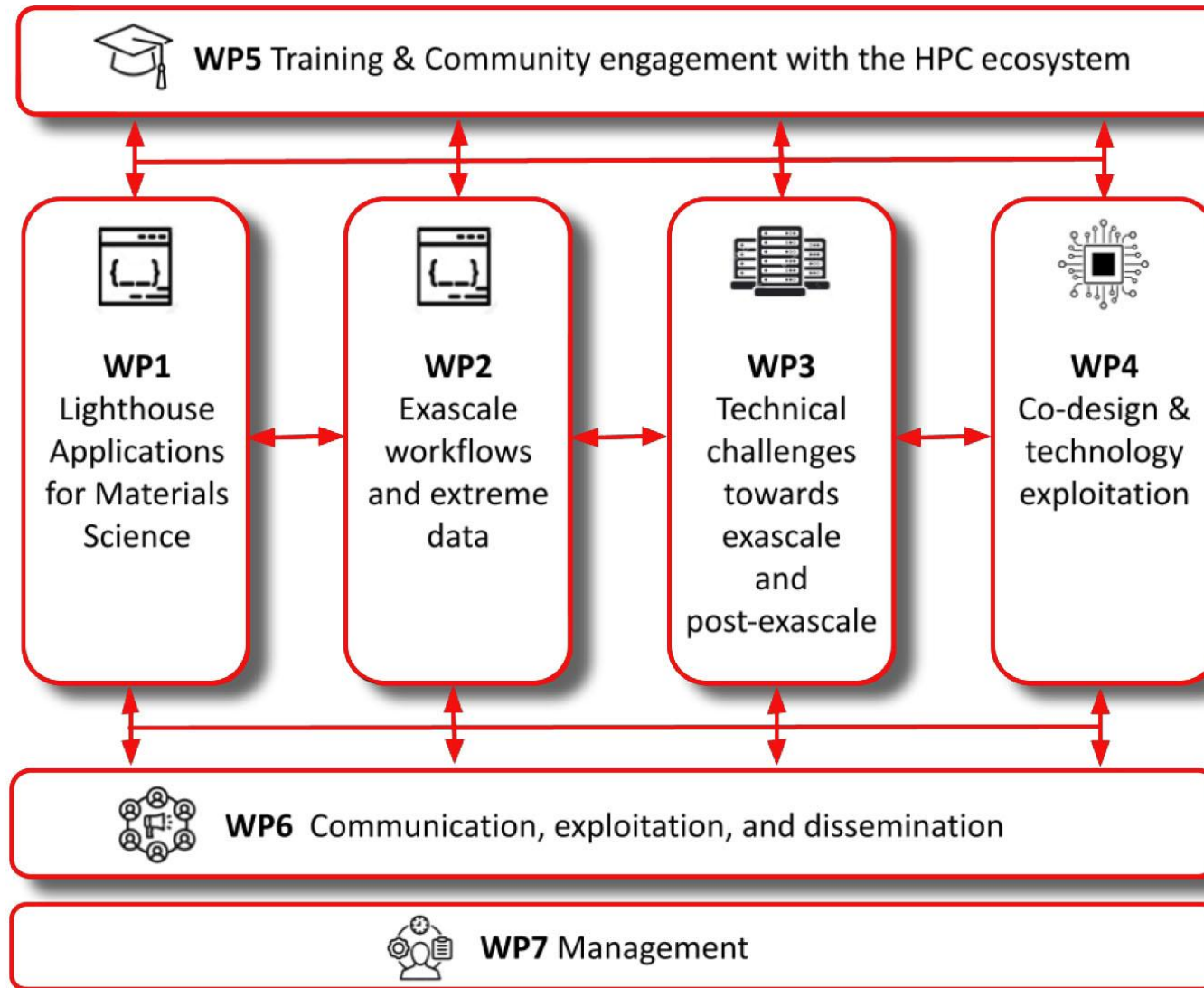
48 Months Project (Jan 2023 – Dec 2026)

4 Key Actions:



- Restructure the MAX flagship codes in **quantum simulation** of materials towards **exascale** and extreme scaling performance;
- Co-design activities to ensure that **future HPC architectures** are well suited for the materials domain applications and *vice versa*;
- Develop a broader ecosystem enabling the convergence of **HPC** and **HTC** with high-performance data analytics in the materials domain;
- Widen the **access to codes** and foster transfer of know-how to broader and diverse user communities and developers.

MaX: project structure



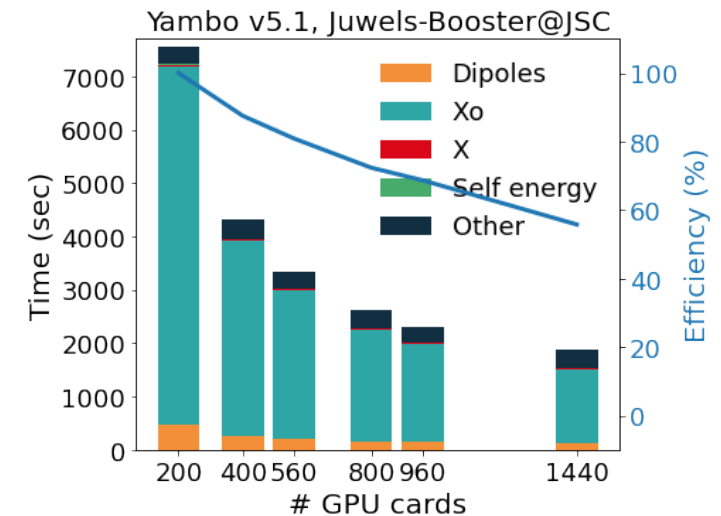
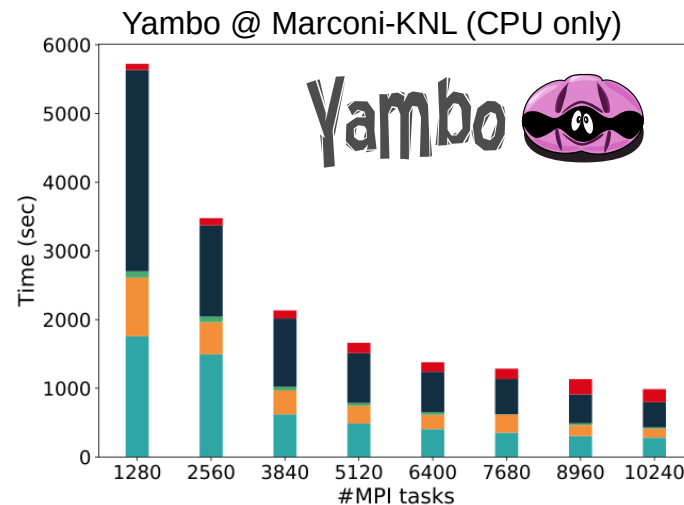
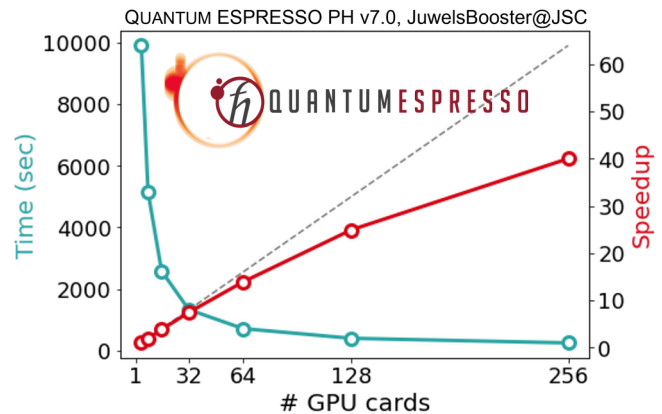
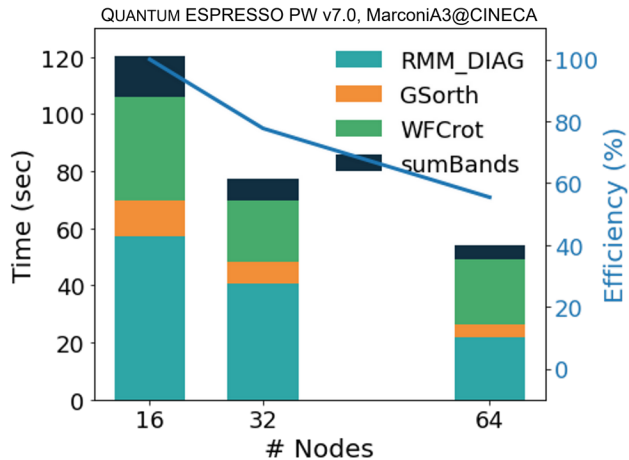
WP1: lighthouse codes for materials science



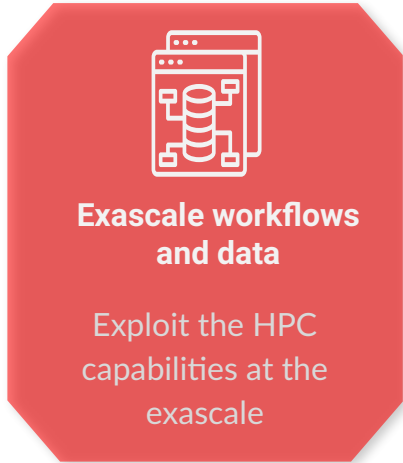
GOAL:

turn the MAX flagship codes into exascale-enabled applications:

- **large scale MPI** parallelism (order of 10000 tasks)
- combined with **GPU awareness**



WP2: exascale workflows & data



Materials properties are usually not obtained with a single calculation but rather as chains of interdependent calculations → **workflows**

GOAL: map complex materials properties into **workflows**

Workflow types:

- **single or a few exascale runs of flagship codes:** individual runs of MAX codes may require exascale computational resources;
- **exascale workflows with heavy data dependencies:** a series of petascale calculations with strong dependency on extensive data exchange embodied in the workflow that requires exascale computational resources;
- **typical high-throughput computing:** state-of-the-art materials screening where a large number of independent or loosely coupled calculations are performed under the supervision of a workflow engine.

WP3: technical challenges

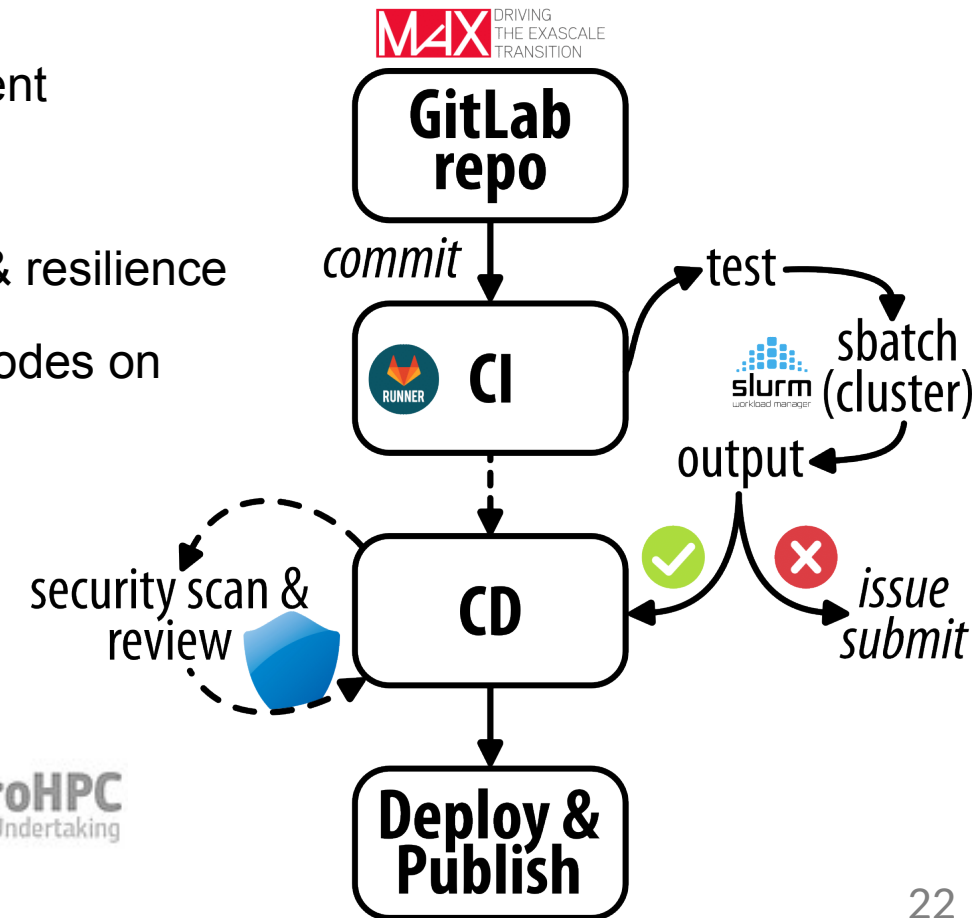
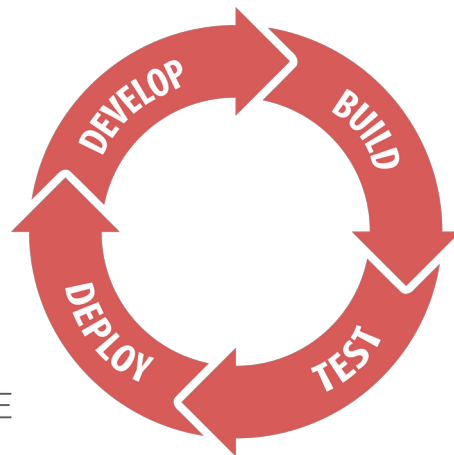


HPC EXPERTS
& DATA CENTRES



GOAL: provide technical support aimed at exascale machines to the MaX flagship codes

- Performance analysis and scalability assessment
- Test and exploit different programming models
- Asses middleware technologies for workflows & resilience
- Continuous integration & deployment of MaX codes on EuroHPC machines



EuroHPC
Joint Undertaking

WP4: co-design & technology exploitation



TECHNOLOGY & CO-DESIGN PARTNERS

Atos

SIPEARL
The Silicon Pearl

E4
COMPUTER
ENGINEERING

LEONARDO

GOALS:

- provide technology developers with **realistic data & requirements of MaX codes**
- prepare MaX codes for future hardware
- explore the use of prototype hardware with MaX codes
- evaluate and optimize energy efficiency of MaX codes

WP5: training



GOALS:

Training new generations of developers

- Hackathons on MaX codes with dedicated training to developers

Supporting and expanding the users base of MaX code

- Hands-on training on MaX codes, including virtual events
- availability of training material

Transverse training initiatives

- coordinate with nCC, CoEs, HPC Centres, EuroHPC initiatives...

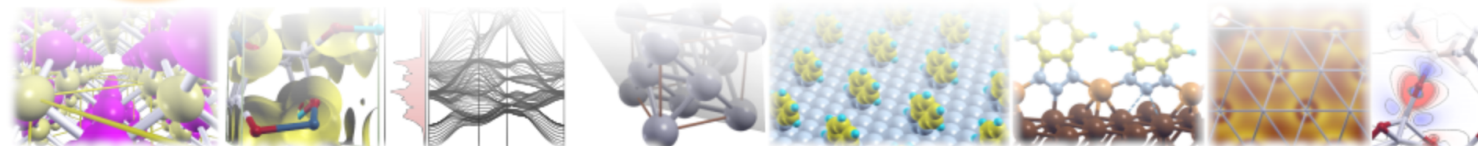


qe2019.ijs.si

September 16–20, 2019
Ljubljana, Slovenia



Summer School on Advanced Materials and Molecular Modelling



Our examples of software development @ IJS



www.xcrysden.org

PW
TK

```
# load data from pw.x input file
load_fromPW relax.in

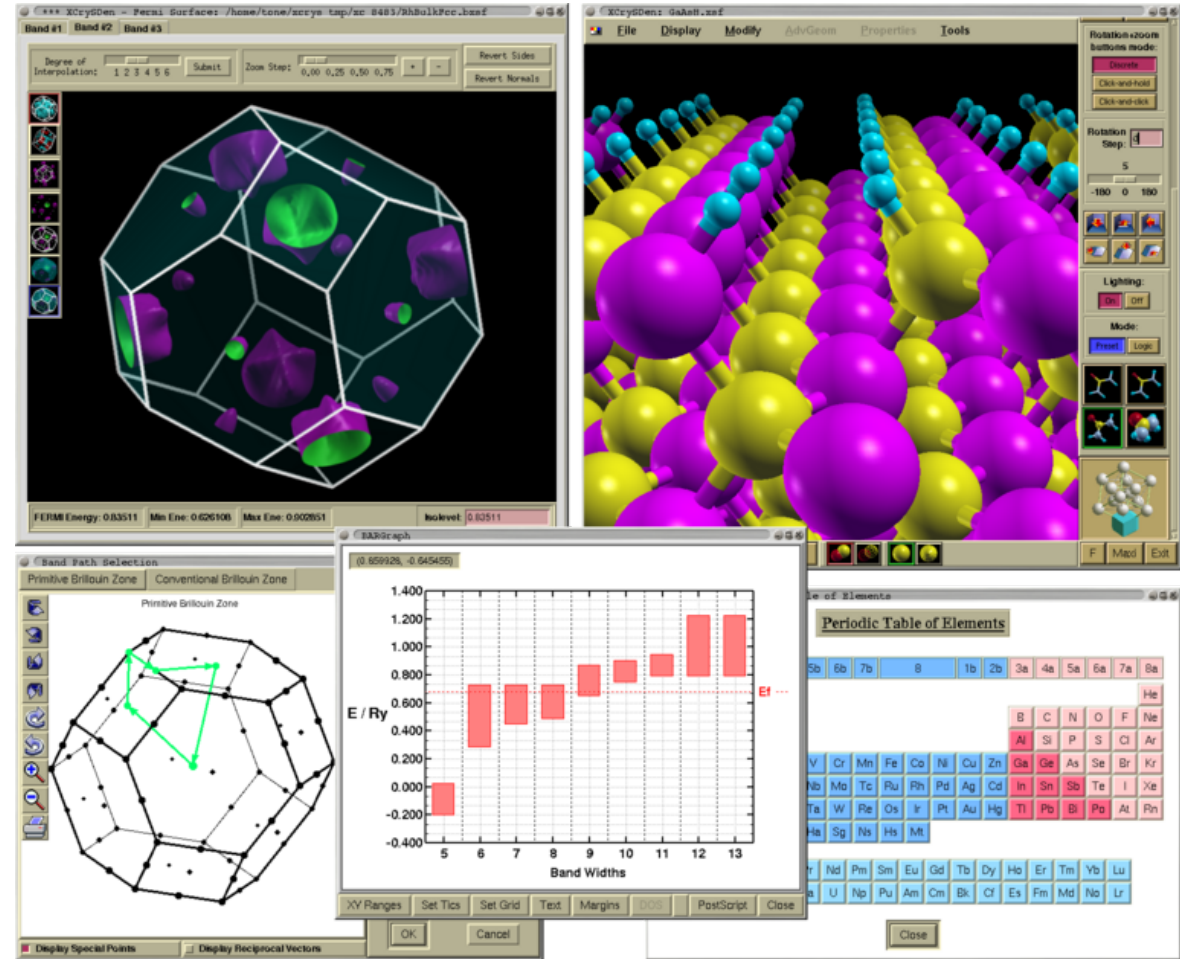
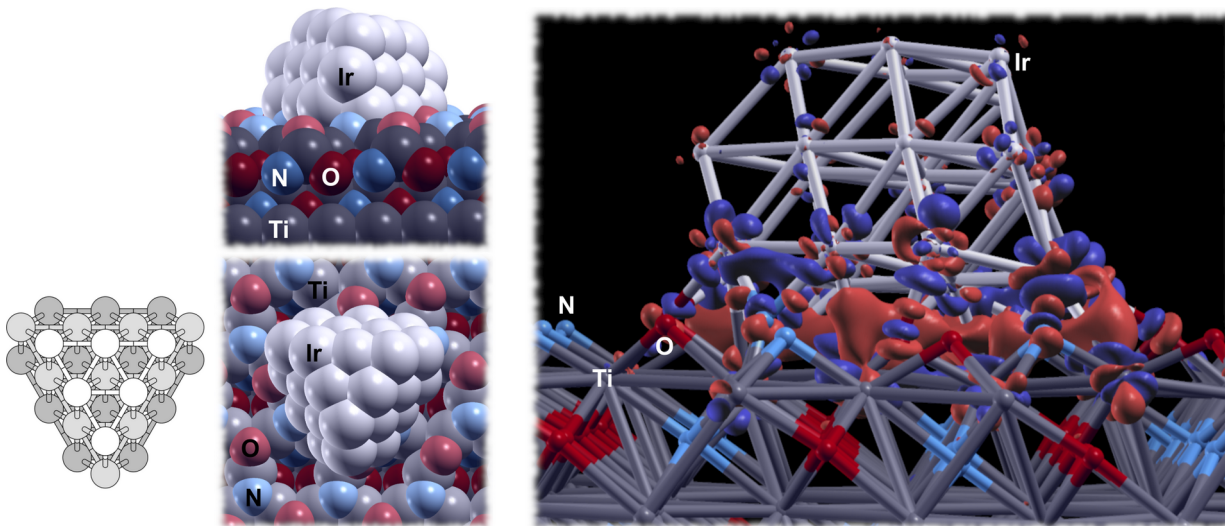
# load optimized coordinates from pw.x output file
ATOMIC_POSITIONS_FROM_PWO end relax.out

# change some input data
SYSTEM {
  ecutwfc = 35, ecutrho = *8
  ...
}

# run pw.x with new parameters
runPW relax.e35_k6
```

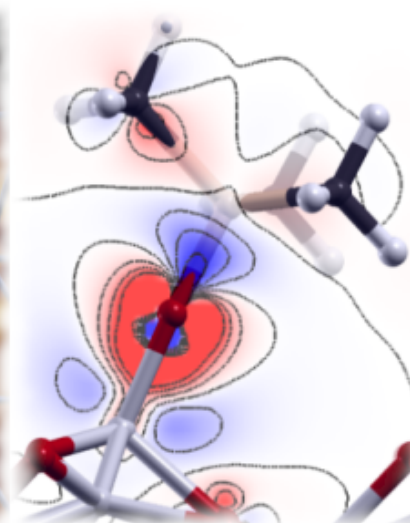
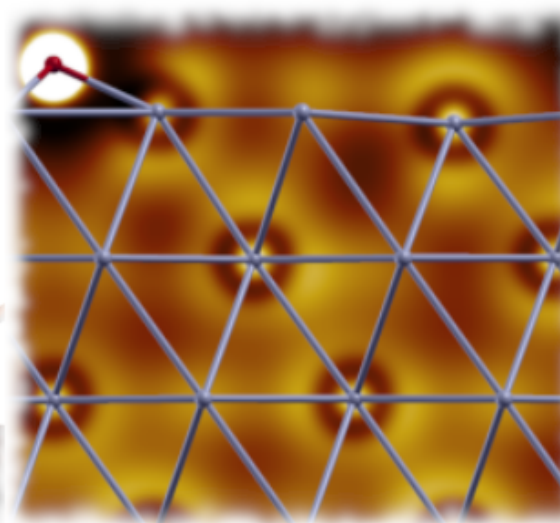
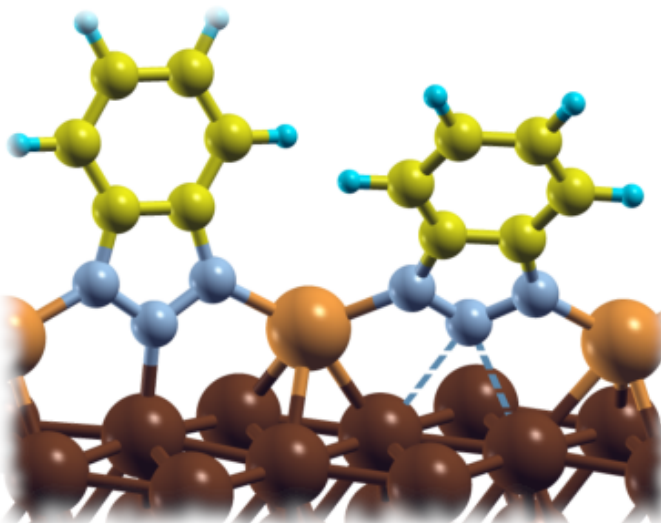
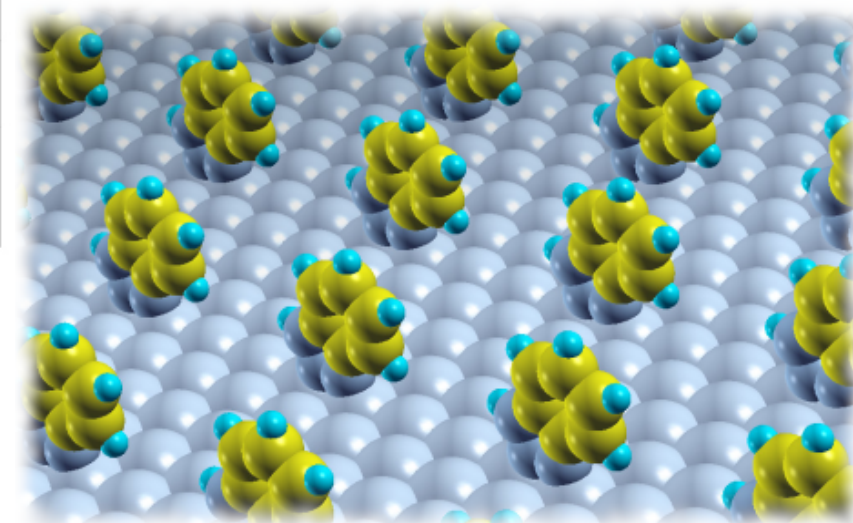
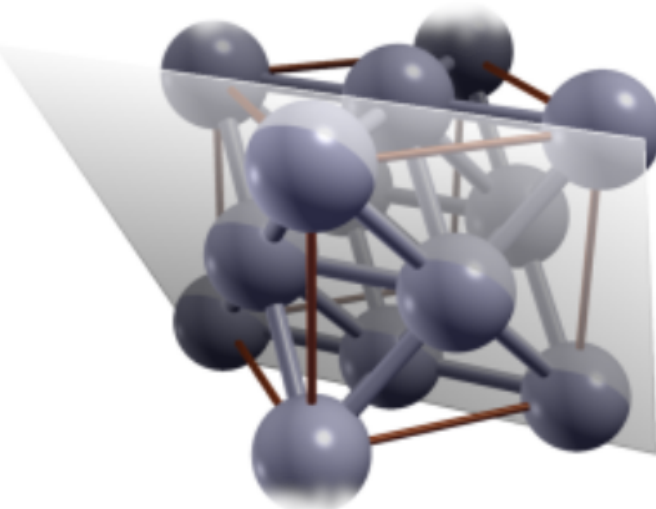
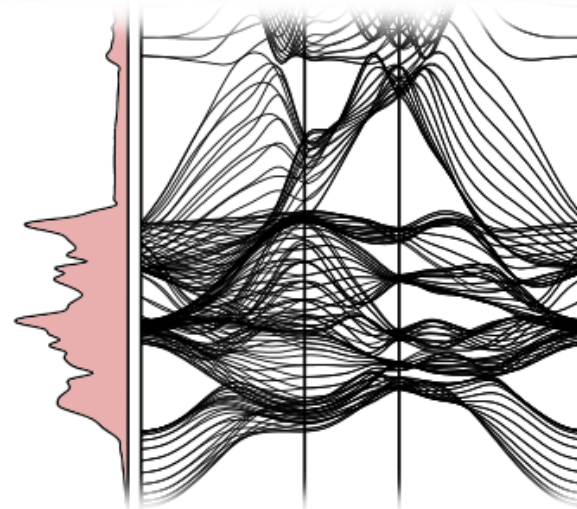
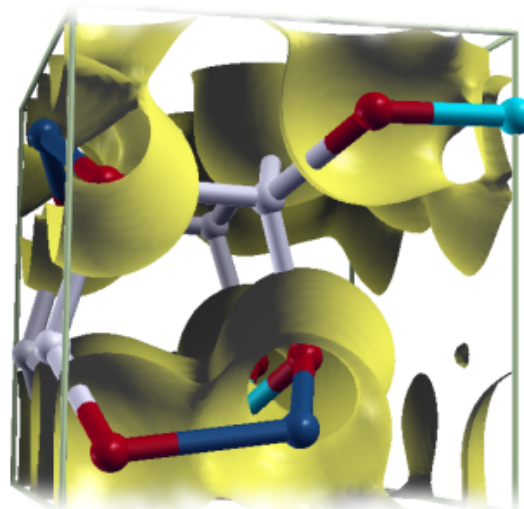
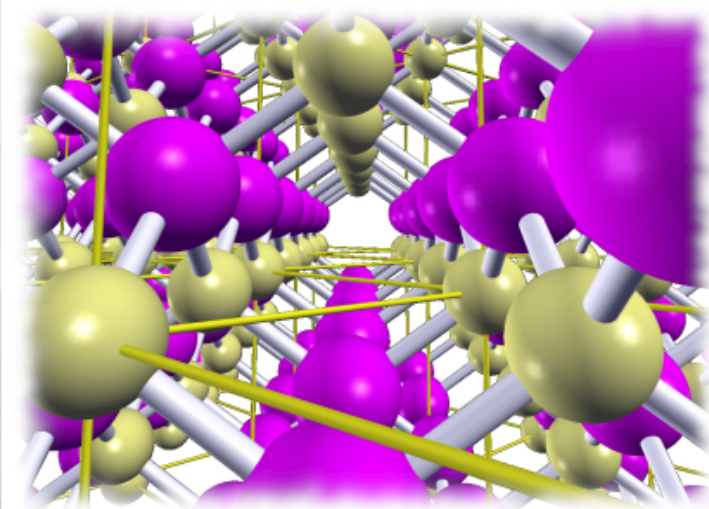
PWscf ToolKit
pwtk.ijs.si

scripting interface for Quantum ESPRESSO

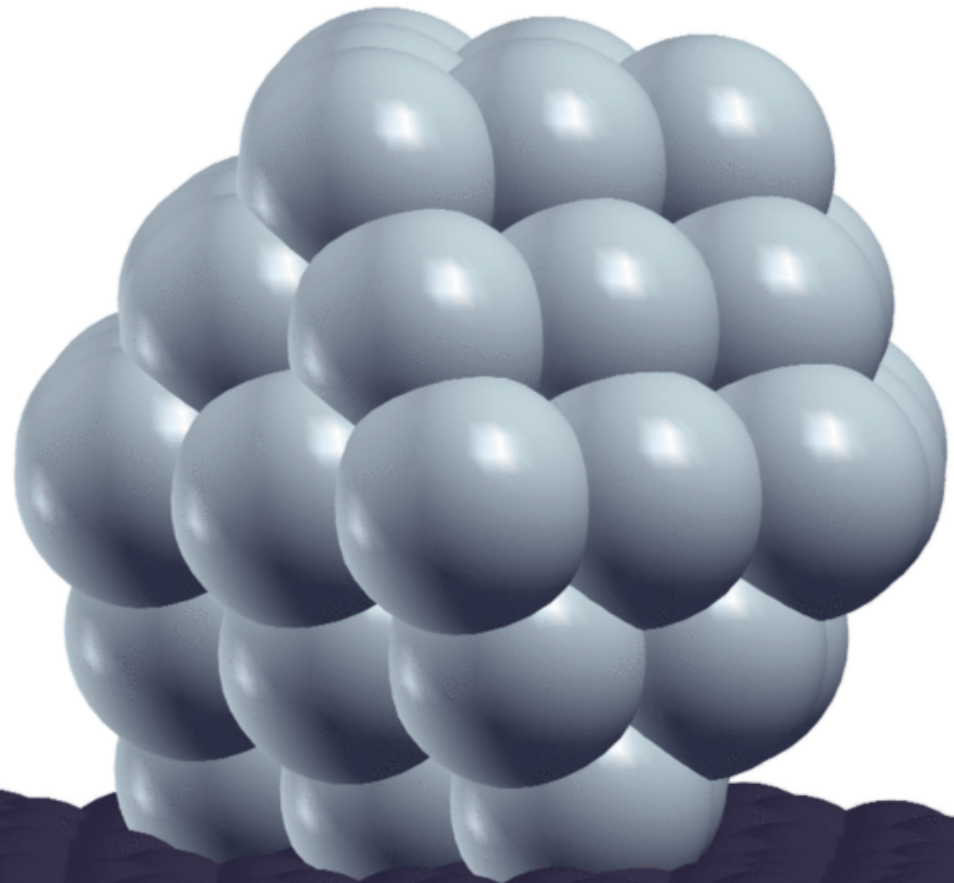


crystalline and molecular structure visualization program

Our examples of materials modeling @ IJS



Animation by Lea Gašparič



INFO:
in 2024 we will organize a
Quantum ESPRESSO school



Thank you for
your attention!

Projekt EuroCC 2 financira Evropska unija. Financiran je s sredstvi Skupnega evropskega podjetja za visokozmogljivo računalništvo (EuroHPC JU) ter Nemčije, Bolgarije, Avstrije, Hrvaške, Cipra, Češke republike, Danske, Estonije, Finske, Grčije, Madžarske, Irske, Italije, Litve, Latvije, Poljske, Portugalske, Romunije, Slovenije, Španije, Švedske, Francije, Nizozemske, Belgije, Luksemburga, Slovaške, Norveške, Turčije, Republike Severne Makedonije, Islandije, Črne gore in Srbije v okviru sporazuma o dodelitvi sredstev št. 101101903.



Funded by
the European Union



DRIVING THE EXASCALE TRANSITION

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[youtube/channel/MaX Centre eXascale](https://youtube/channel/MaX%20Centre%20eXascale)



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