



EuroHPC
User Days

Dublin Ireland
22→24
September 2026



EuroHPC
Joint Undertaking



ÉIRE2026.EU
IRELAND2026.EU

Whole Sun simulations

Riding Exascale to the Core

The Sun: Features and Scales

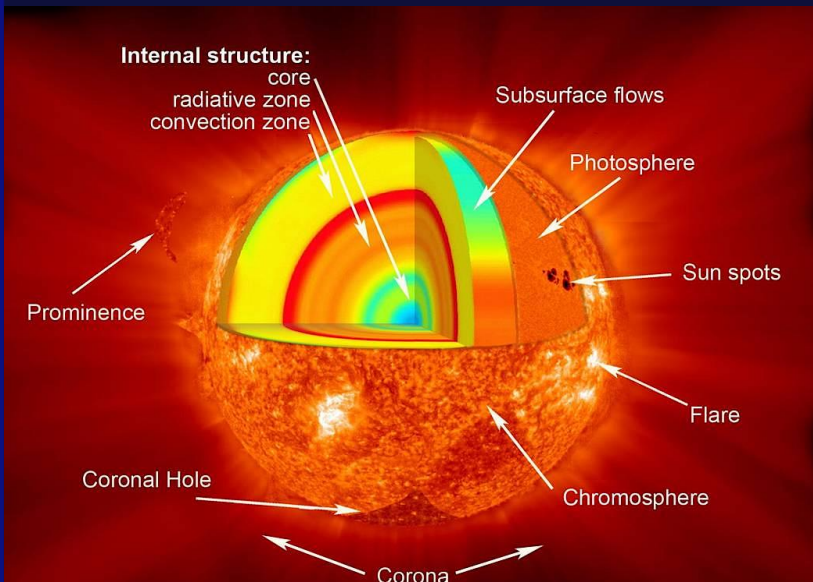
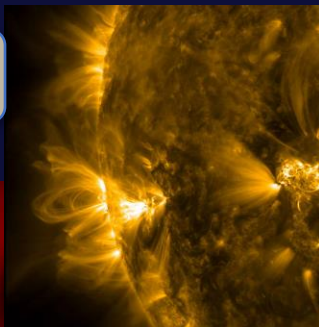


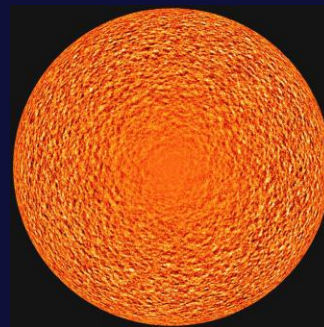
Image credit: NASA/Goddard



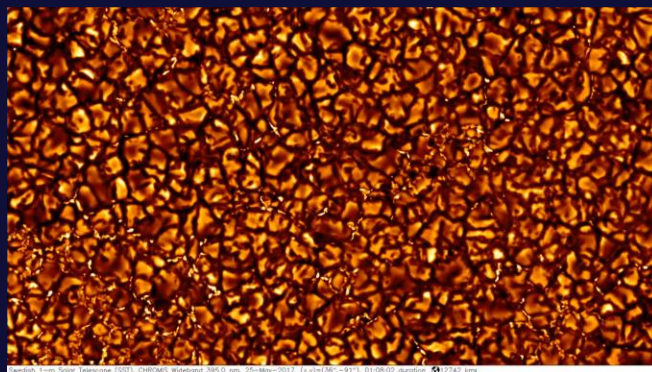
100 Mm



10 - 100 Mm



30 - 50 Mm



~ 1Mm

Image credit: NASA/SDO, SOHO/MDI/ESA, Luc Rouppe van den Voort

Previous Simulations

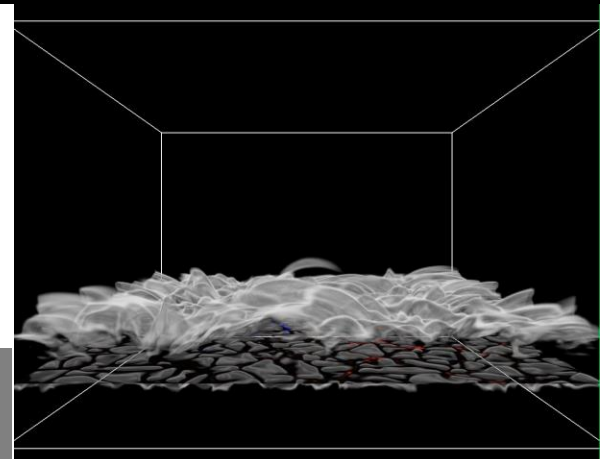
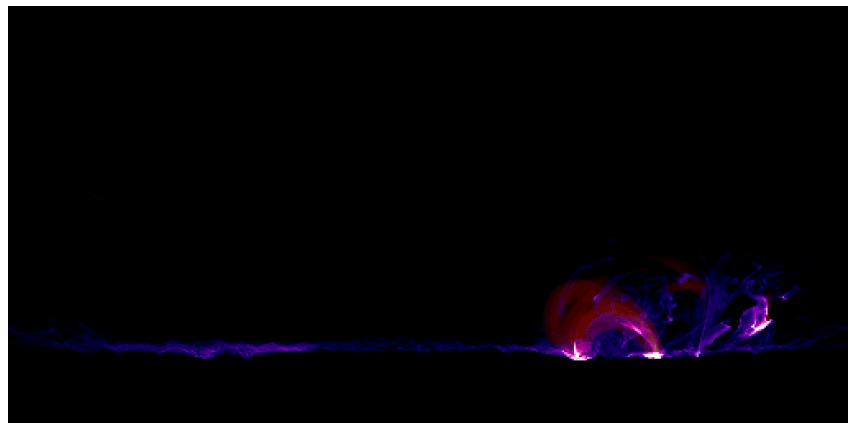
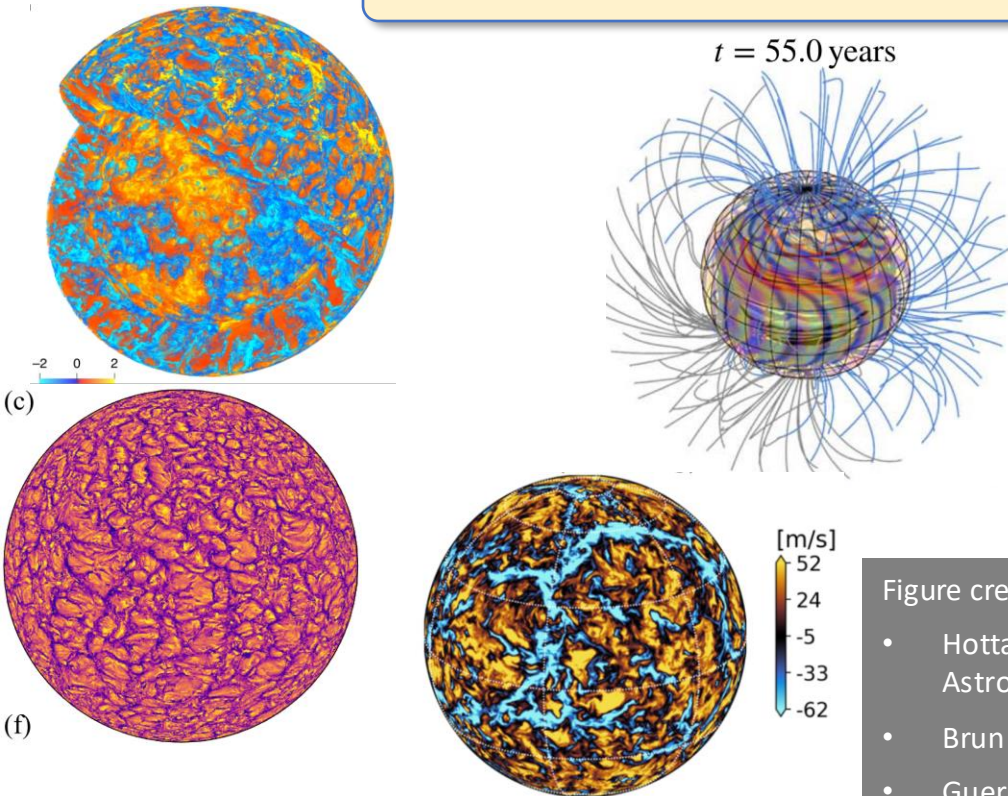


Figure credit:

- Hotta & Kusano (Nature Astronomy, 2021)
- Brun et al. (AJ 2022)
- Guerrero et al. (ApJ, 2022)

Video credit:

Carlsson et al. (2016)
Cheung et al., Nature Astronomy (2019)

Global simulations

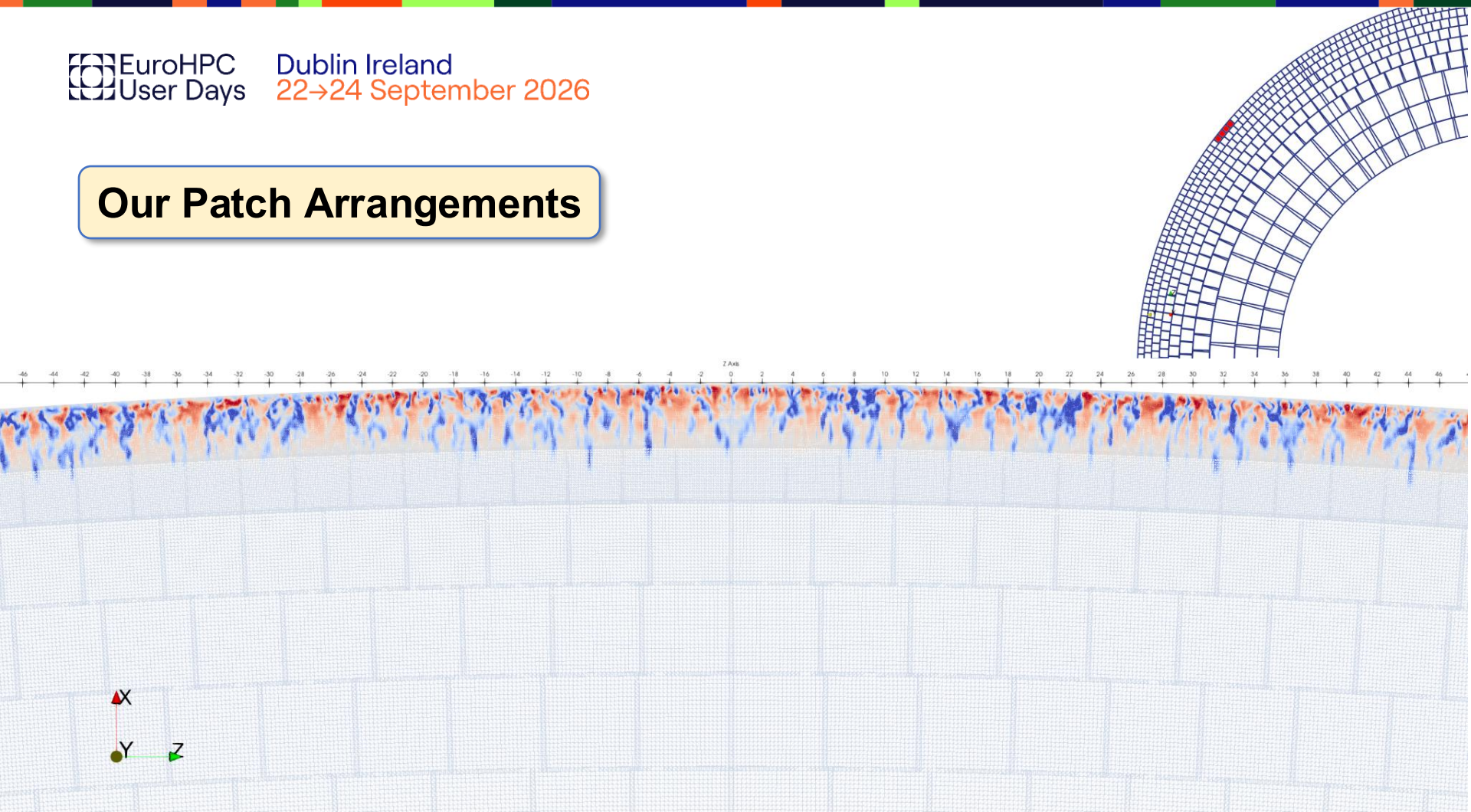
Connecting the interior to the surface

- DISPATCH framework (Nordlund et al., 2018)
- Tabular FreeEOS (Irwin A, W, 2012)
- Entropy-based HLLD Riemann solver (Popovas, A&A 2025.)
- Surface cooling driven convection
- Blue opacity package (Amarsi et al., 2016) + OP opacities
- Coriolis and centrifugal forces
- Radially dependent gravity
- Simulation domain $0.655\text{--}0.998 R_{\odot}$ (**$0.655\text{--}1.0 R_{\odot}$**)
- 600k patches (**5.8M at currently highest resolution**),
24³ cells per patch, 300 GB (**2.3TB**) snapshots
- 194 km (**71 km**) smallest cell size at $0.998 R_{\odot}$ (**$1.0 R_{\odot}$**)



Our Simulation Features

Our Patch Arrangements



Convection in observations

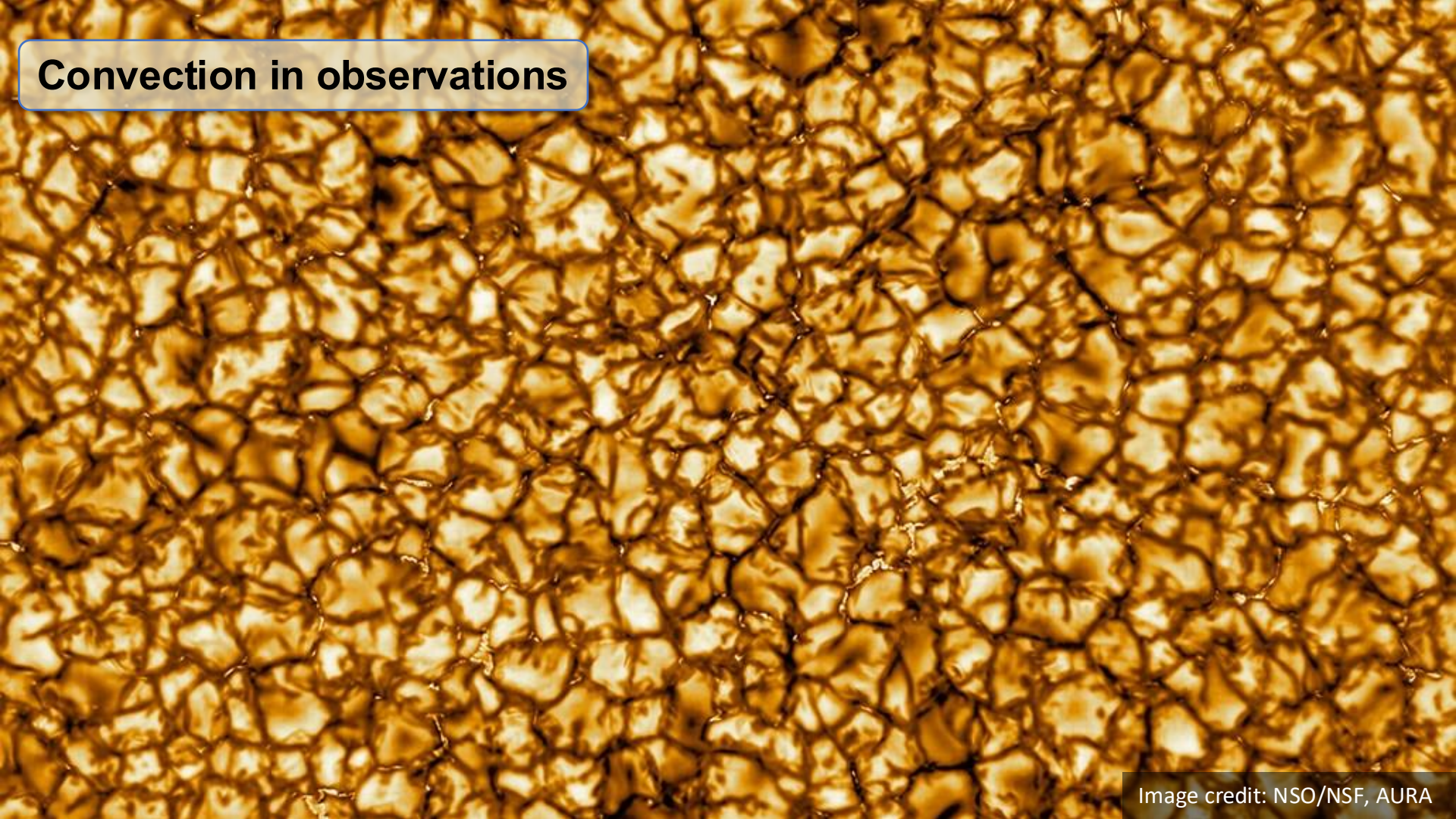
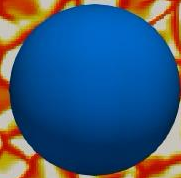


Image credit: NSO/NSF, AURA

Full Scale Range



DISPATCH simulations of the Sun

- Convection morphology
 - Small and large scale flows
 - Magnetic field topology and flux emergence (active regions / sunspots)
 - Helioseismology applications
-
- 2 week runtime with 30s cadence $\Rightarrow$ 93 PB of data!
 - In-transit data analysis is needed (WIP)

Low Entropy “Rain”

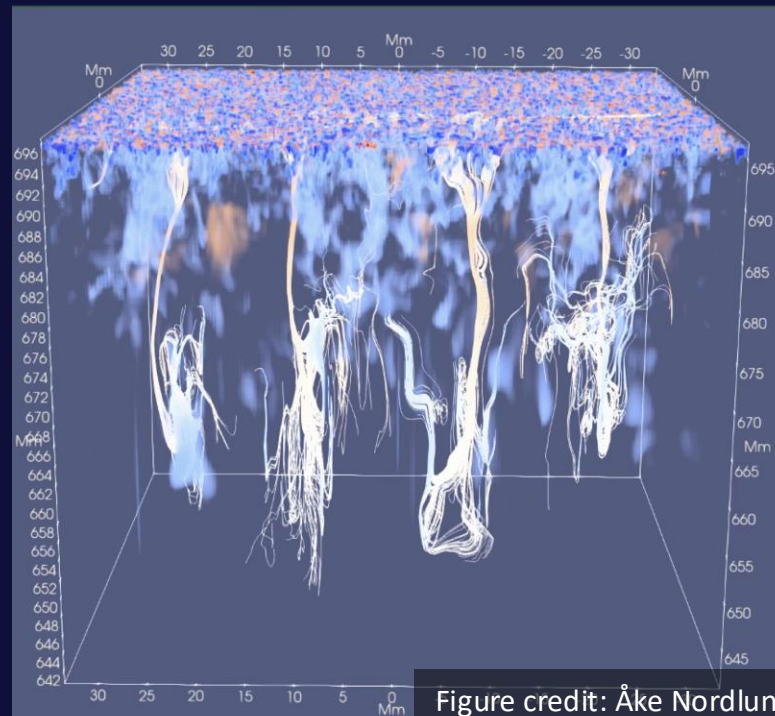
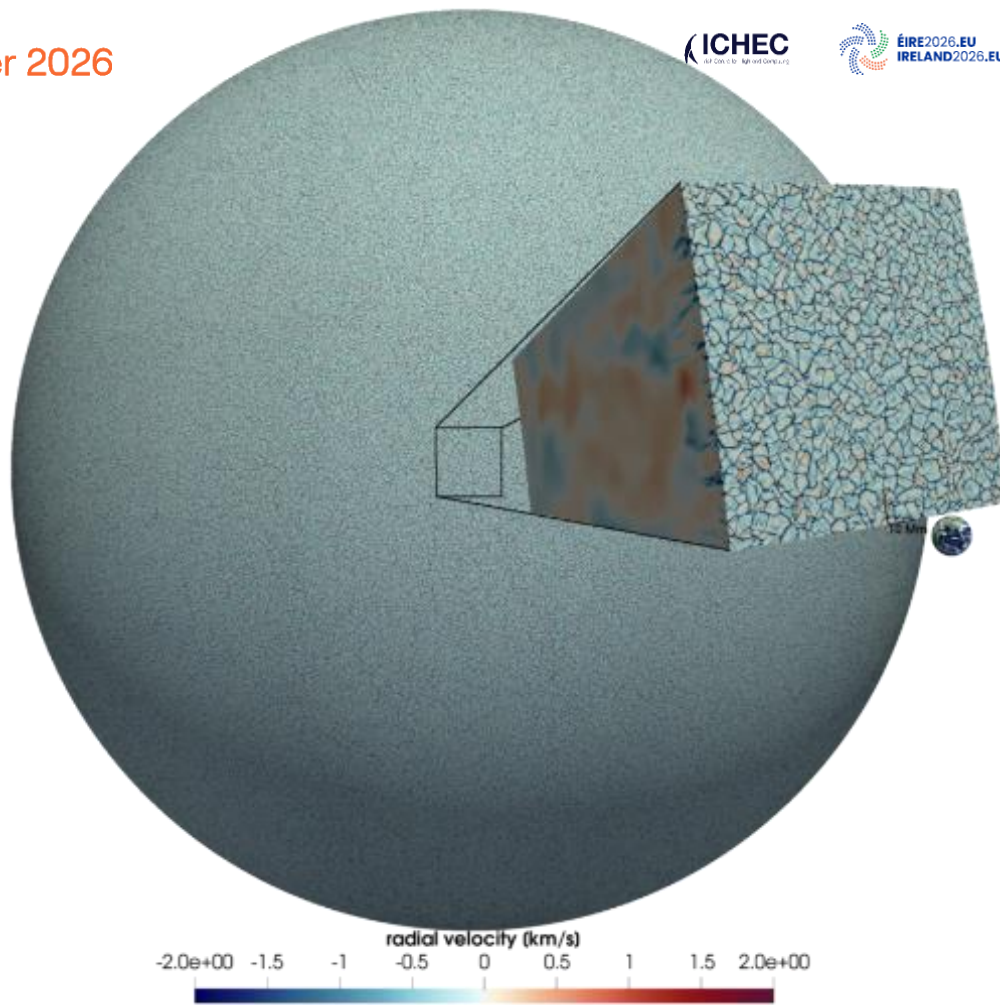


Figure credit: Åke Nordlund

Thank you



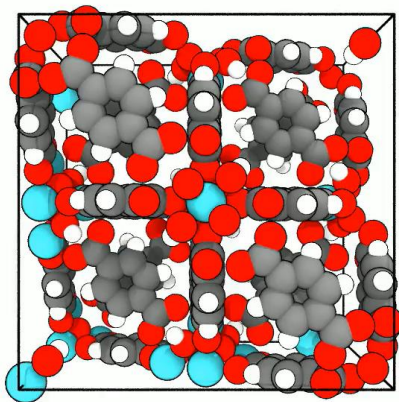
Bridging the Gap from the Nano- to the Mesoscale:

The Machine Learning Revolution in Materials Modelling

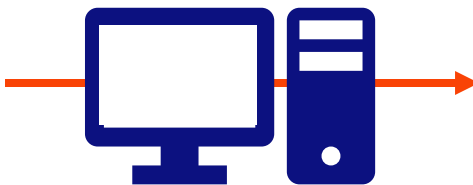
Massimo Bocus

Ghent University, Center for Molecular Modeling

massimo.bocus@ugent.be



Atomistic structure
of the material



Computer
simulation

$$\hat{H}\psi = E\psi$$

e.g., Density Functional Theory (DFT)

How much CO₂ it stores?

At which temperature does it degrade?

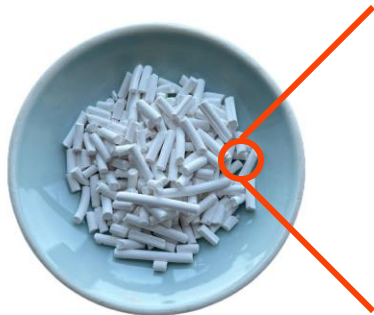
Can it break down NO_x?

...

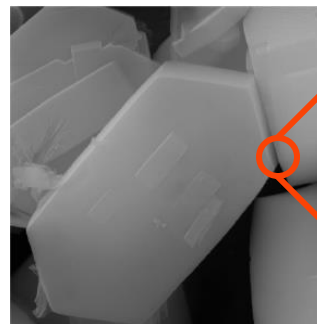


Methanol-to-olefins
industrial plant (China)

http://english.dicp.cas.cn/news/headline/201604/t20160420_314717.html

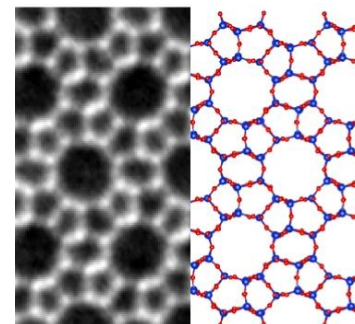


Catalyst pellets



Catalyst crystals

Qin et al. *Chem. Mater.* 2013



Catalyst atomistic structure

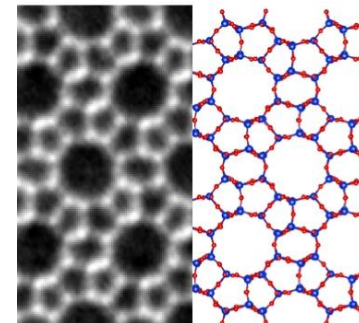
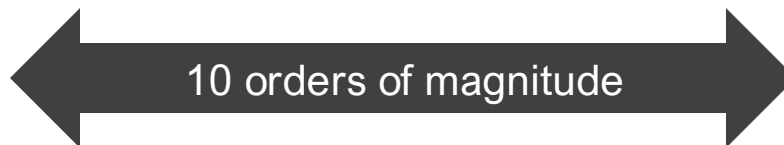
Shen et al. *Nature* 2022





Methanol-to-olefins
industrial plant (China)

http://english.dicp.cas.cn/news/headline/201604/t20160420_314717.html



Catalyst atomistic structure

Shen et al. *Nature* 2022

10^1 m

10^{-1} m

10^{-3} m

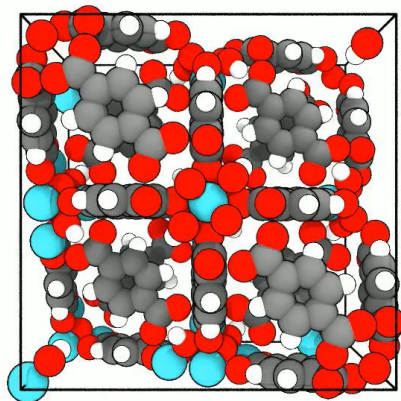
10^{-5} m

10^{-7} m

10^{-9} m

What we would
like to simulate

What we
can simulate



Atomistic structure
of the material



How much CO₂ it stores?

At which temperature does it degrade?

Can it break down NO_x?

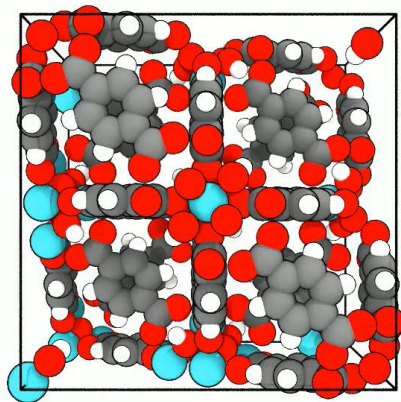
...

Computer
simulation

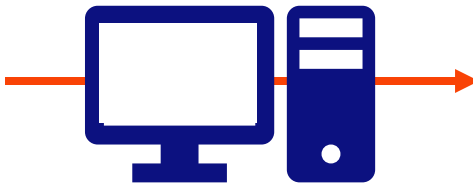

$$\hat{H}\psi = E\psi$$

e.g., Density Functional Theory (DFT)

Very
expensive



Atomistic structure
of the material



How much CO_2 it stores?

At which temperature does it degrade?

Can it break down NO_x ?

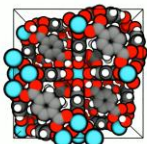
...



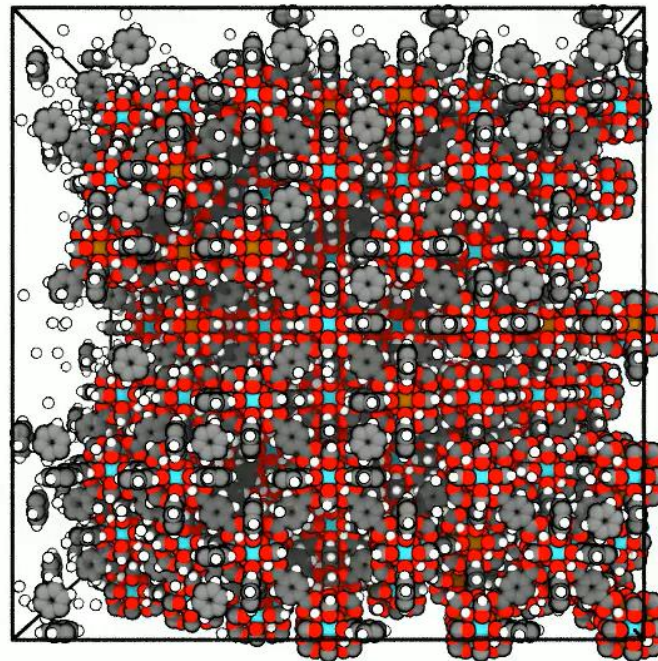
Machine learning
interatomic potentials

Density functional theory

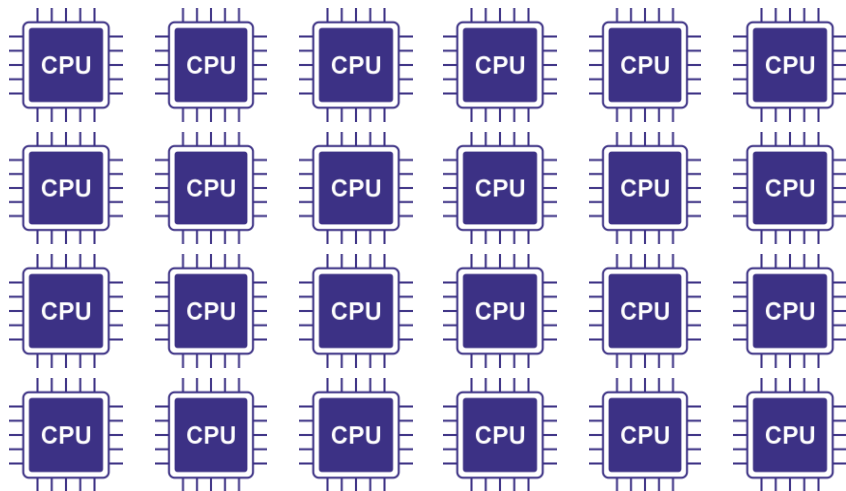
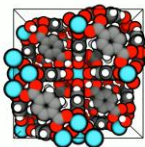
~ 100 atoms, ps long simulations

Comparable
accuracy!**Machine learning interatomic potentials**

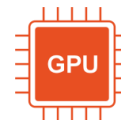
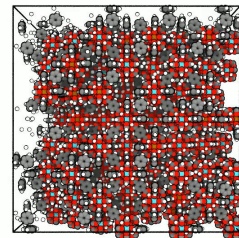
~ 20,000 atoms, ns long simulations



Density functional theory



Machine learning interatomic potentials





More realistic models



Better predictions



Towards computer-aided design of
materials with industrial applications





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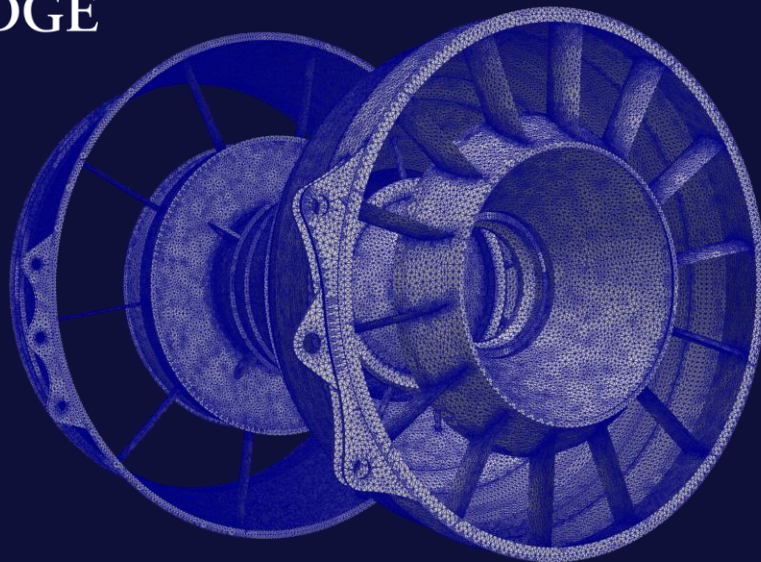
EuroHPC User Forum

Chris Richardson, chair
cnr12@cam.ac.uk

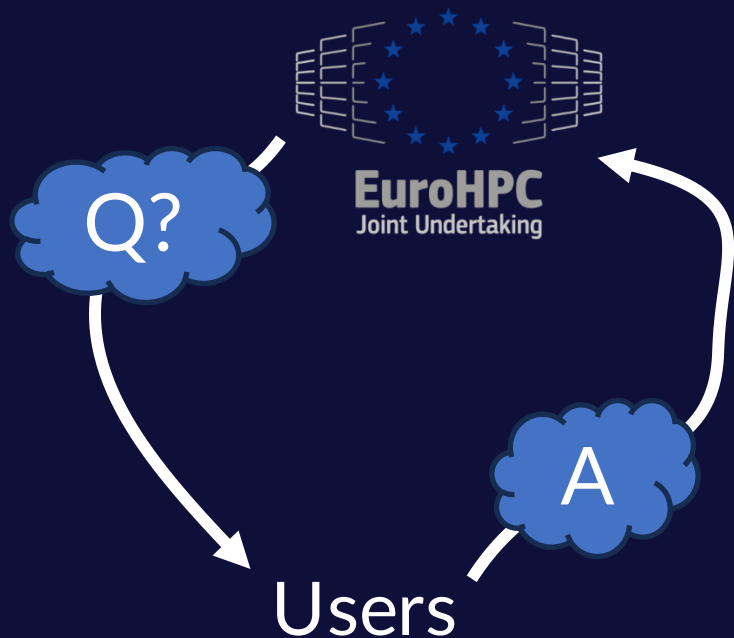
About me... very briefly...



fenicsproject.org

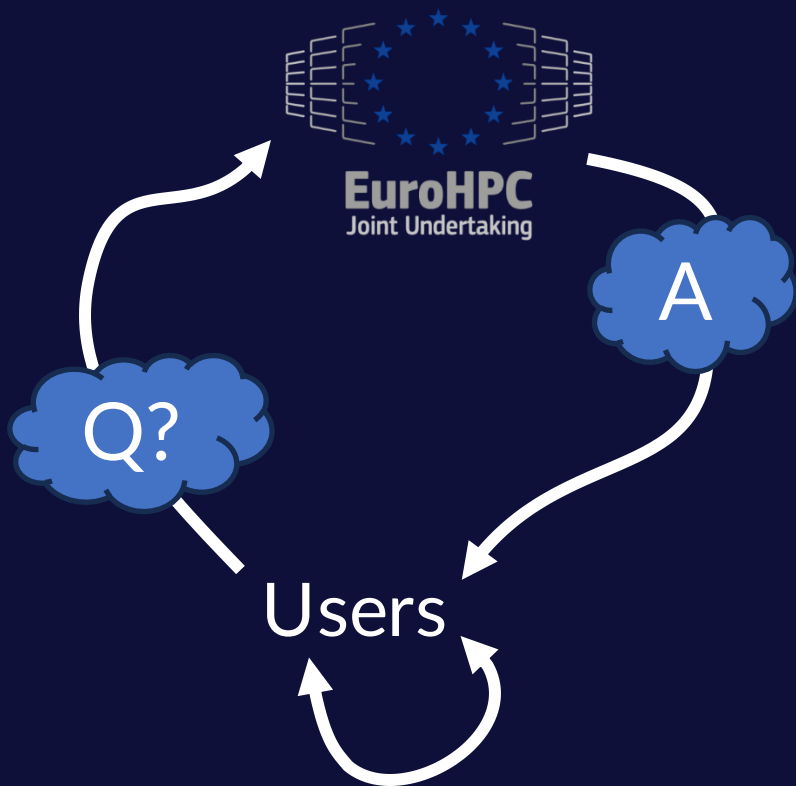


User Forum: aims



- The aim of the User Forum is to foster structured, coherent, and regular **communication and exchange** with all user communities and stakeholders.
- The User Forum facilitates open consultation with user and scientific communities that also serves to highlight the EuroHPC vision.
- The User Forum has administrative support from the JU
- The JU has oversight of the Forum's activities and collates and communicates **feedback on user requirements** to the Advisory Groups of EuroHPC as necessary;
- See the EuroHPC MASP online!

User Forum: aims



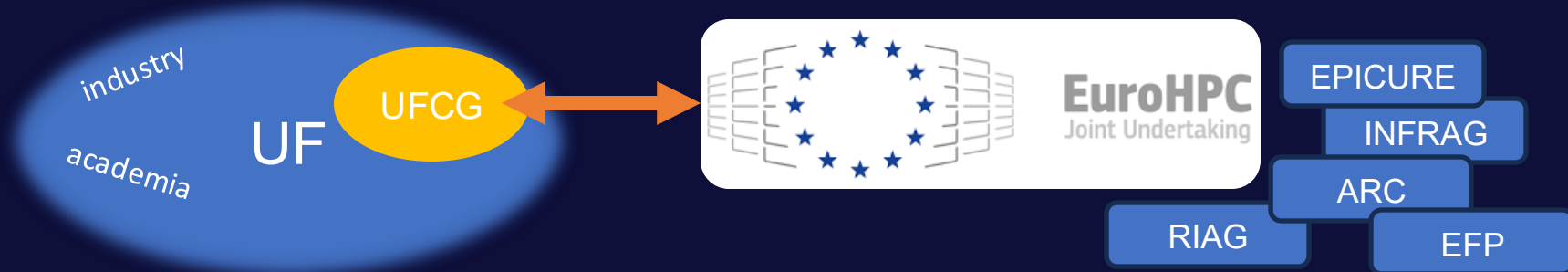
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Code of Conduct

- **Maintain professionalism in all interactions**—whether in-person at conferences/workshops, related social events, or in virtual and social media spaces.
- **Respect others by avoiding offensive comments or behaviors**, including harassment, intimidation, or exclusionary remarks based on gender identity, sexual orientation, disability, physical appearance, race, nationality, religion, or any other personal characteristic.
- **Engage in constructive scientific discussions** without personal attacks, insults, or belittling remarks. Critical feedback should be professional and focused on ideas rather than individuals.
- **Respect privacy when sharing content**. If recording online talks or posting speaker photos on social media, obtain permission beforehand. Content from presentations may be shared unless the speaker has requested otherwise.

Forum & Coordination Group in practice

- UFCG Monthly meeting on Teams including some EuroHPC staff
- Independent – a group of **Users**
- Limited term – keep fresh with new members
- Slack channel (see later)
- Two-way communication from users to EuroHPC
- Connection to RIAG/INFRAG/EPICURE
- Provide feedback to documents and reports from EuroHPC JU



Who is in the Coordination Group?



Chris Richardson (chair) Cambridge UK,
Physics/Engineering finite element
software development



Maria Girone (vice chair) High Energy Physics,
CERN, Switzerland, Head of CERN openlab



Andrius Popovas (University of
Oslo, Norway) HPC users for
computational astrophysics



Ivan Carnimeo (CNR-IOM, Italy): Materials
science/Chemistry/Physics developer of Quantum
ESPRESSO



Alessio Roccon – Fluid Mechanics
University of Udine, Italy



Massimo Bocus – Molecular dynamics
University of Ghent, Belgium



Eleni Briola – Danmarks Meteorologiske Institut,
Denmark: AI for weather forecasting



Lara Peeters (VSC - HPC in Flanders, Belgium) - Digital
Humanities



Sinéad Ryan (Trinity College Dublin, Ireland) –
Lattice Quantum Chromodynamics



Zoe Cournia - Biomolecular simulations and drug discovery
Academy of Athens, Greece



Matthias Meinke - Institute of Aerodynamics
RWTH Aachen, Germany

Activities: Webinars

- Access Webinar May 2026
- Organised by Ivan Carnimeo and Zoe Cournia
- 366 participants online
- General info, peer review, tech evaluation, case study
- Upcoming Webinar planned for 5 November 2026
- AI Factories
- Eleni Briola and Alessio Roccon

Electing new members of UFCG

- “Members of the UFCG should be geographically distributed and cover wide range of disciplines as well as strive for gender balance. They should also represent different types of experience in applications related to HPC, Quantum and AI computing. ”
- Nominations: **put yourself forward**



Join in.

- Informal slack “chat” application
- Helps to start conversations
- Not “high security”
- Not archived
- Real people...



User Requirements for Grand Challenge Science

Sinéad Ryan, Dean of Research, Trinity College Dublin, MODERATOR

Alan O'Cais, Coordinator, EESSI

Maïke Gilliot, Chair, RIAG

Walter Lioen, Chair, INFRAG

Maria Girone, Vice-Chair, UFCG and Head of CERN openlab

Mark Parsons, Director, EPCC and Dean of Research Computing, University of Edinburgh

Irene Lopez de Vallejo, Head of Business Development, Tecnalia/QTAG

Alberto Ramos Martínez, ARC Committee, Researcher CISC and University of València

Massimo Bocus

Inspiring User Presentation

"Bridging the Gap from the Nano- to the Mesoscale: The Machine Learning Revolution in Materials Modelling"

MADONNA at the Table