# From PRACE to EuroHPC

Luigi Del Debbio

The University of Edinburgh

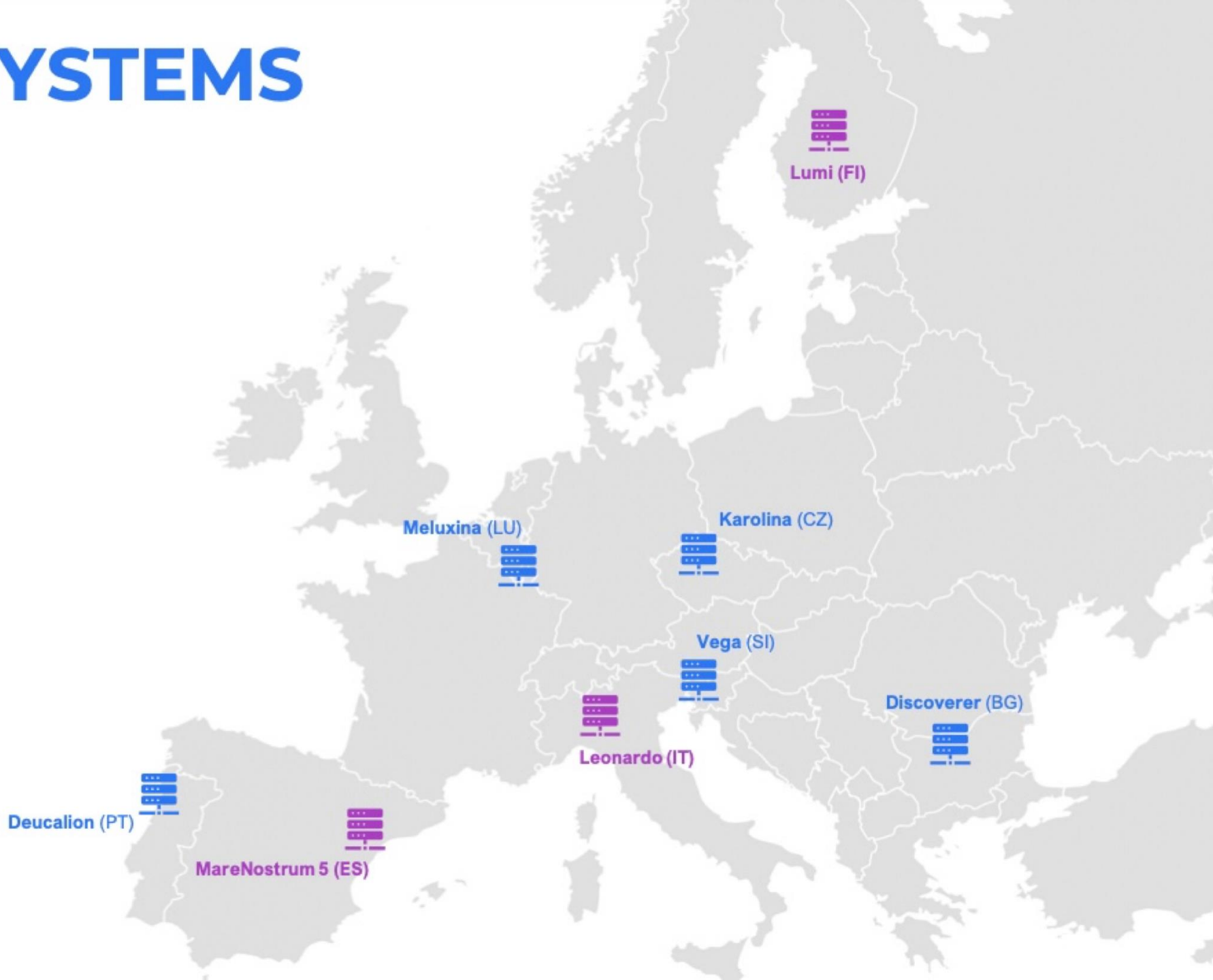
# Computing: an on-going revolution

- My personal *visions* of the field, shaped by my own work
    - Research in high-energy theoretical physics
    - Chair of Resource Allocation in EURO-HPC
    - Scientific Advisory Committee of CSCS (Switzerland)
    - Chair of DiRAC Board (UK)
    - SIAB for UK Exascale project
- I hope I can provide a broad overview
- Do ask questions!

# EUROHPC SYSTEMS
## 2019 → 2023

PRE-EXASCALE

PETASCALE



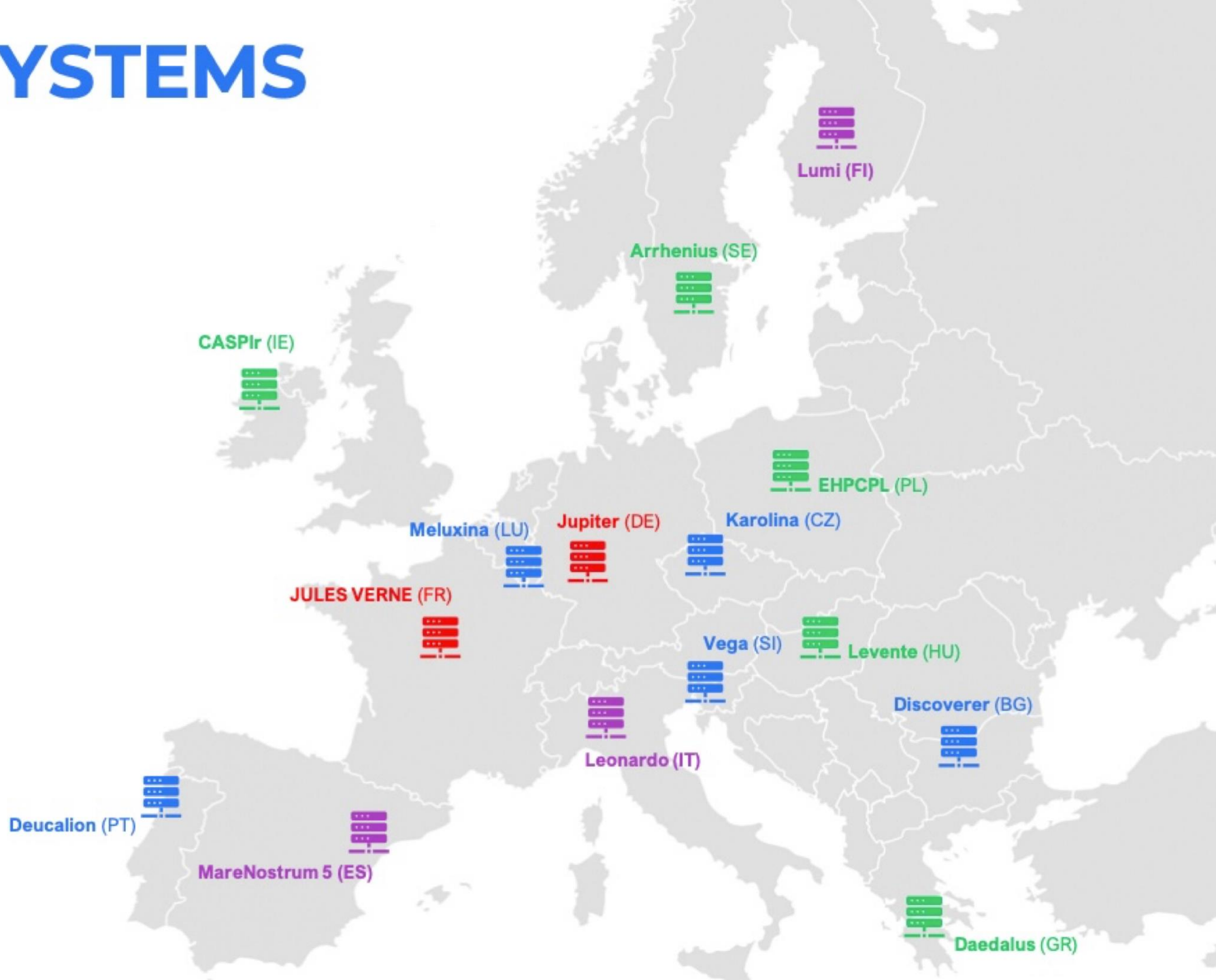
# EUROHPC SYSTEMS
## 2024 → 2026

EXASCALE

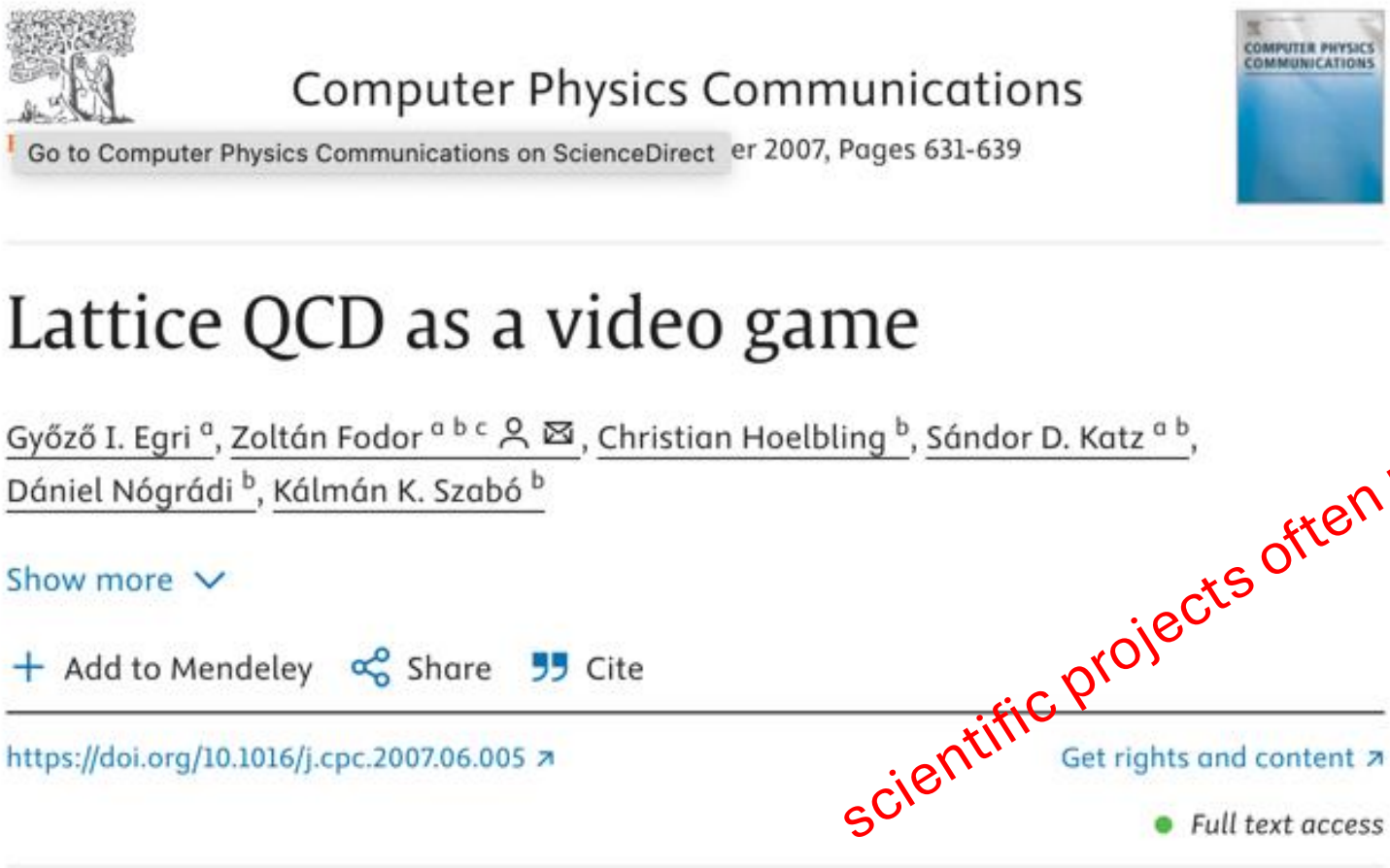
PRE-EXASCALE

PETASCALE

MID-RANGE



# early GPU adopters... (2007)



Computer Physics Communications

Go to Computer Physics Communications on ScienceDirect er 2007, Pages 631-639

## Lattice QCD as a video game

Győző I. Egri [a], Zoltán Fodor [a b c], Christian Hoelbling [b], Sándor D. Katz [a b], Dániel Nógrádi [b], Kálmán K. Szabó [b]

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https://doi.org/10.1016/j.cpc.2007.06.005

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Full text access

scientific projects often push the boundaries

# Scaling Lattice QCD beyond 100 GPUs


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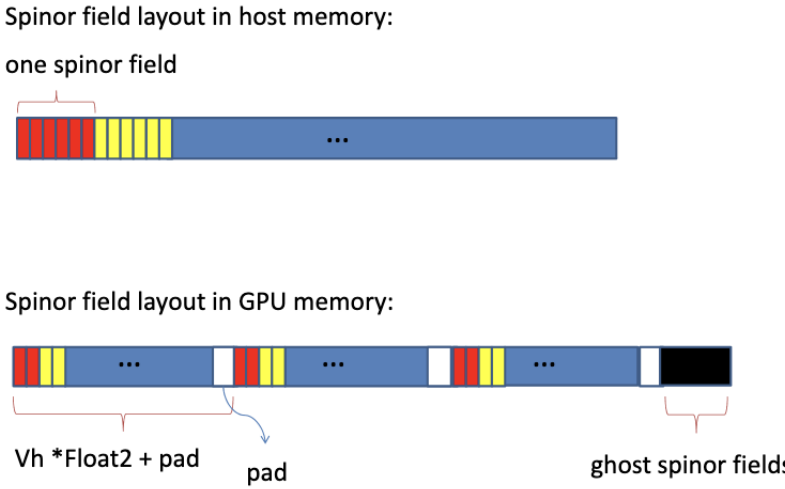
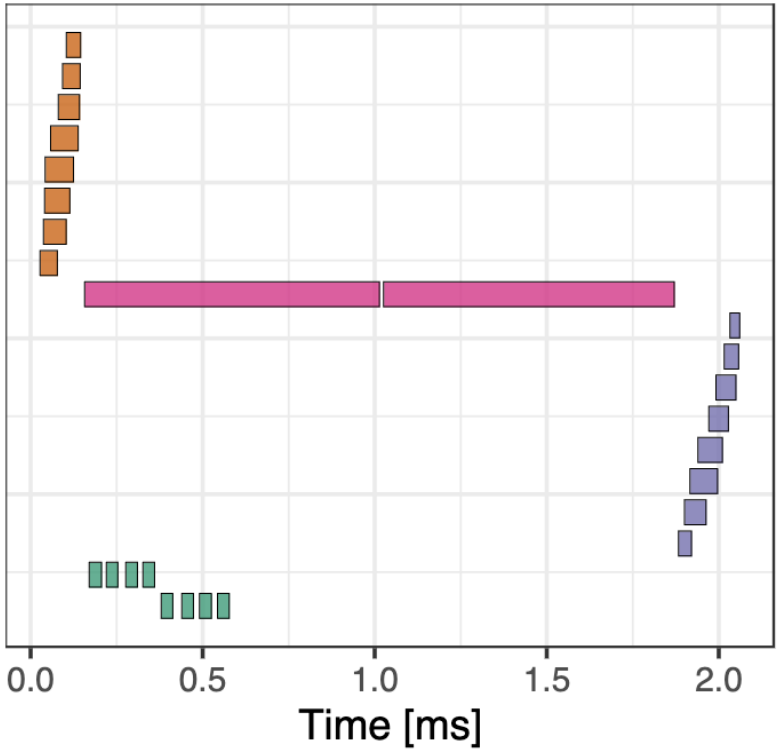
2011




# Scaling SU(2) to 1000 GPUs using HiRep

2024


**Sofie Martins,**[a,b,*] **Erik Kjellgren,**[a] **Emiliano Molinaro,**[a] **Claudio Pica**[a,b] **and Antonio Rago**[a,b]

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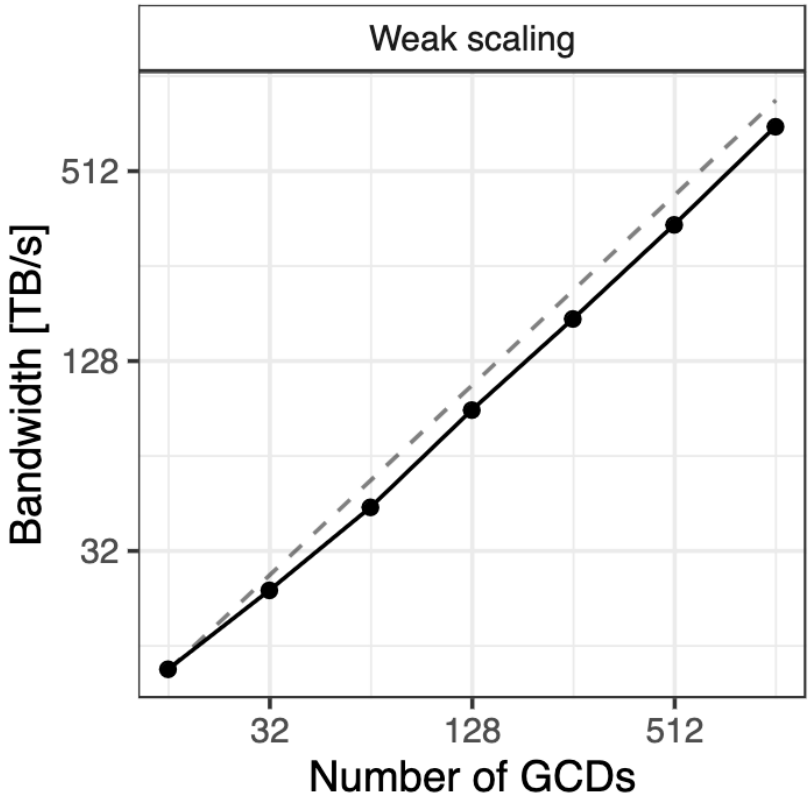
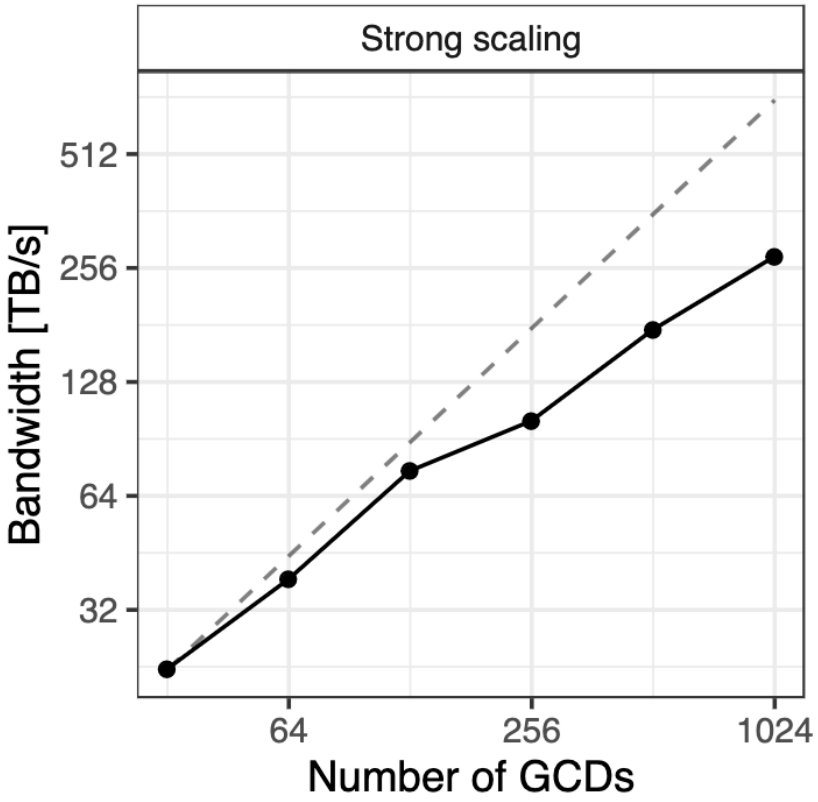
- weak and strong scaling (not easy on current architectures!)
- non optimized codes waste energy and money!




[Martins et al 2024]

# AI factories

- increased focus on AI hardware
- right now, it’s good for lattice
- not sure about future hardware
- keep flexible boundaries

# First Global Gyrokinetic Simulations of Multi-Scale Plasma Turbulence in Tokamaks

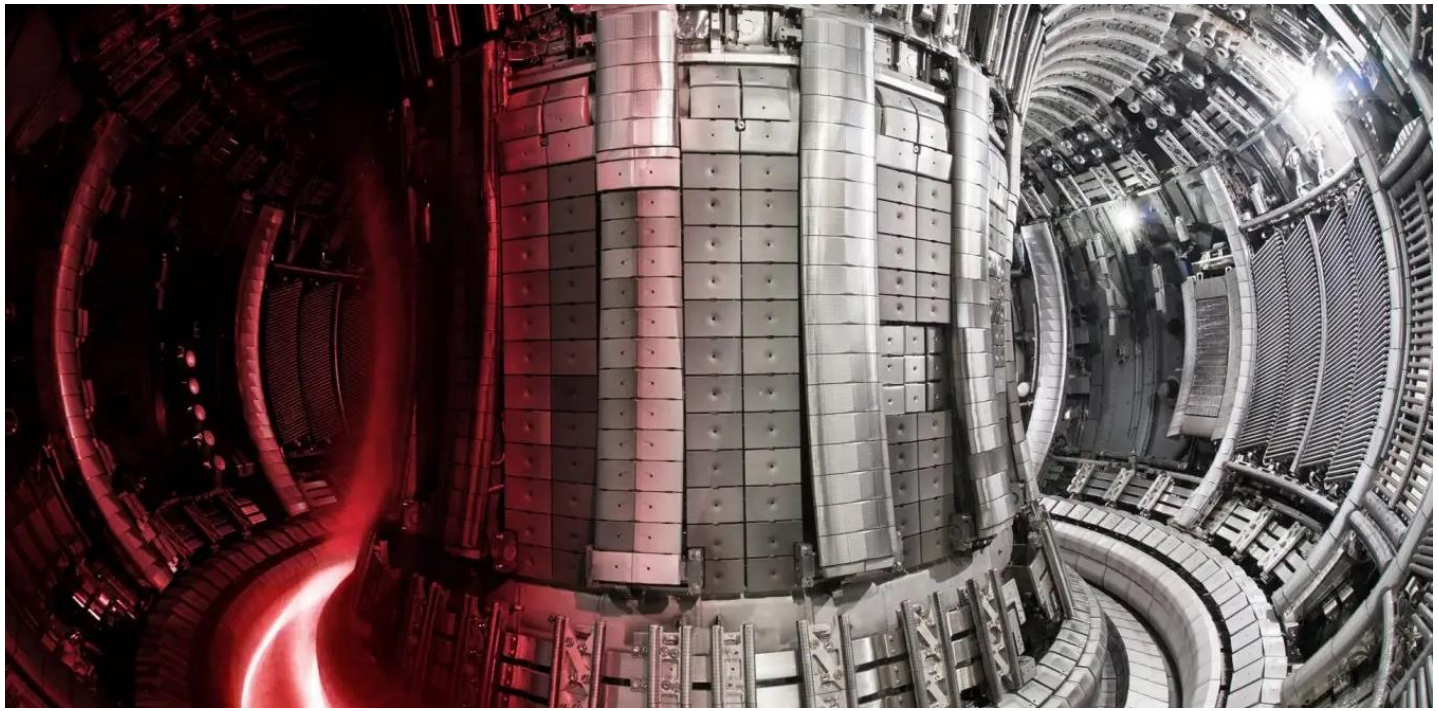
1,520,000
Awarded Resources (in node hours)

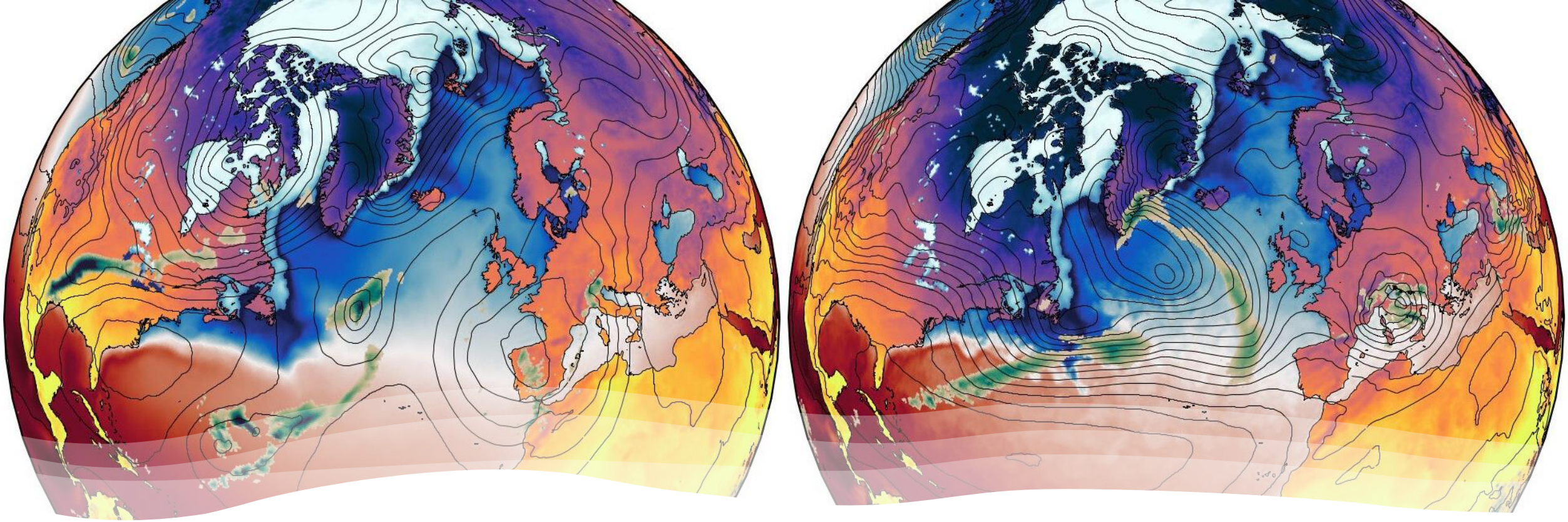
LUMI-G
System Partition

1 May 2024 - 30 April 2025
Allocation Period

# Nuclear Fusion

- GENE codebase
- international collaboration
- GPU-enabled
- Potentially huge societal impact





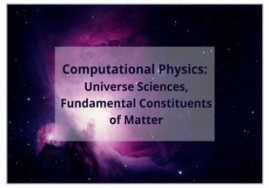
EERIE project: https://eerie-project.eu/

# Weather simulations

# More EuroHPC projects

### Cloud-Circulation Coupling in a Changing Climate (C5)

For the first time in the history of climate modelling, it is becoming possible to run multi-year climate simulations with a global atmospheric model that has a horizontal resolution of a few kilometers.




### Forward-Modeling the First Billion Years

The birth of the first stars, galaxies and black holes heralded the beginning of the Cosmic Dawn (CD).

### FemtoDose

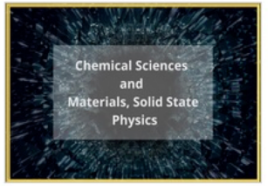
FLASH radiotherapy (RT) consists in delivering a therapeutic dose over much shorter times than in conventional treatment protocols.

### Large Scale and High Resolution CFD Simulations for Wave Energy Farms

The project aims to perform the first simulation of a wave energy farm using high-fidelity numerical modelling to anticipate the effects of arraying wave energy converters (WECs) within the same sea stretch.

### The continuum limit of lattice QCD for high-precision tests of the standard model of particle physics from domain wall fermions

Exploring the standard model of particle physics and finding new physics beyond is in many cases limited by the lack of high-precision knowledge of low-energy QCD effects.




### Universal Machine Learning Potential for Complex Metal Alloys

Atomistic modeling can provide mechanistic insights and improved design principles, but it is limited by the complexity of modern alloys that involve up to a dozen carefully tuned components.

Just a few examples…

# Short Summary

- Heterogeneous ecosystem
- Porting & efficiency are tricky
- … or rather they require a lot of work (and collaboration)!

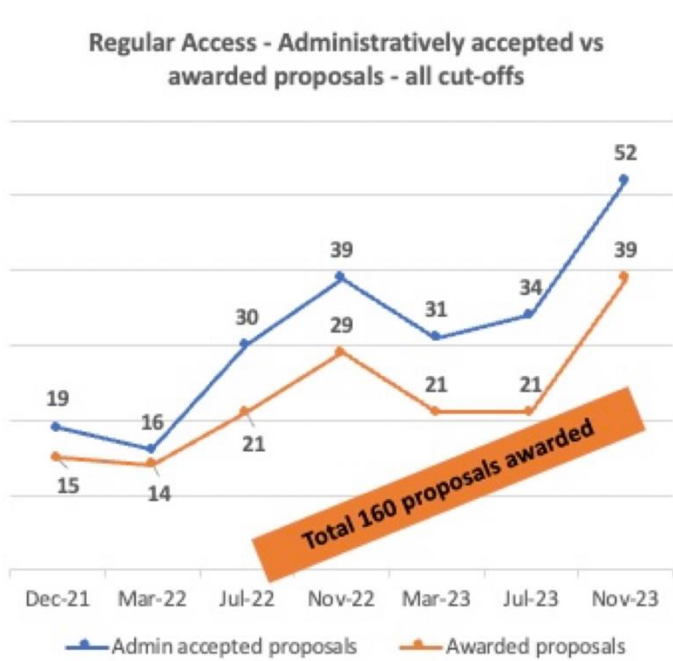
- Need  adequate human resources
- Highly-specialised workforce
- Training/careers/retention

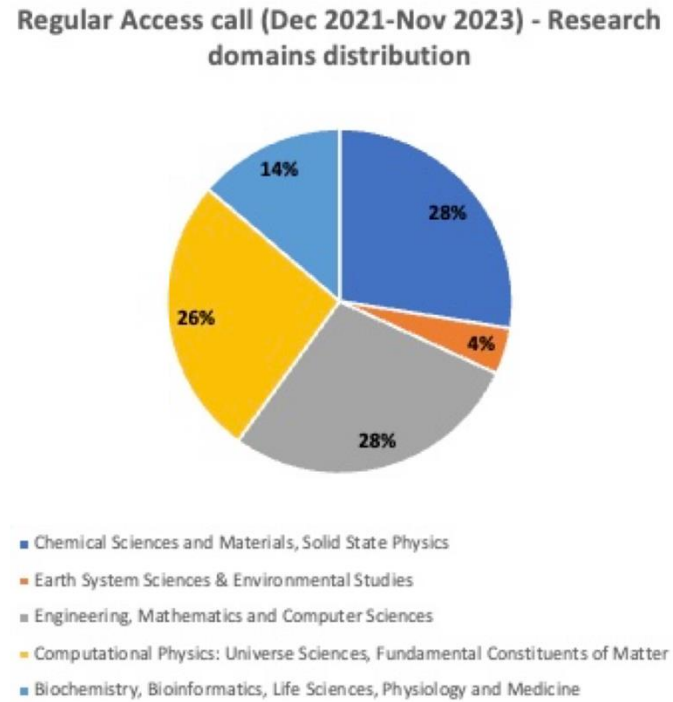
Who is using these machines? How do we access them?

# resource allocation

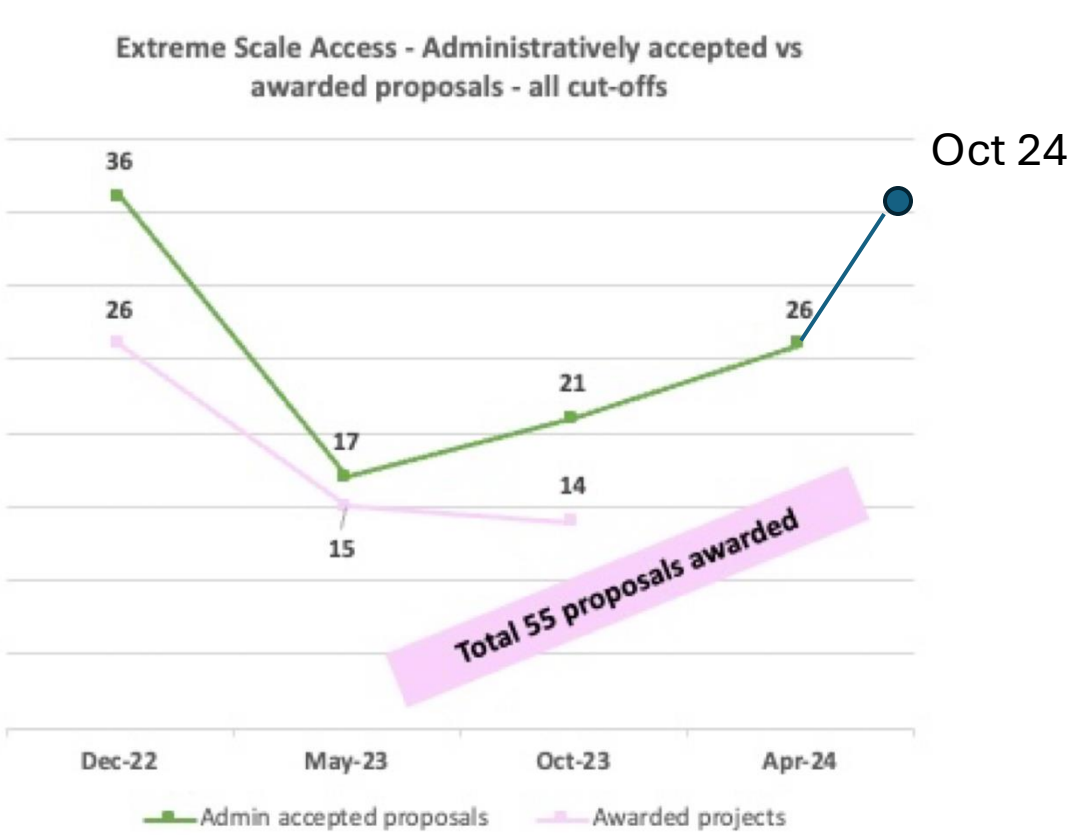
- A single panel across *all* domains – one-year **focused** applications
- Raises the bar for ***all*** domains
- Quality of applications has improved – frequency of calls
- Very expensive in terms of human resources (thank you !)

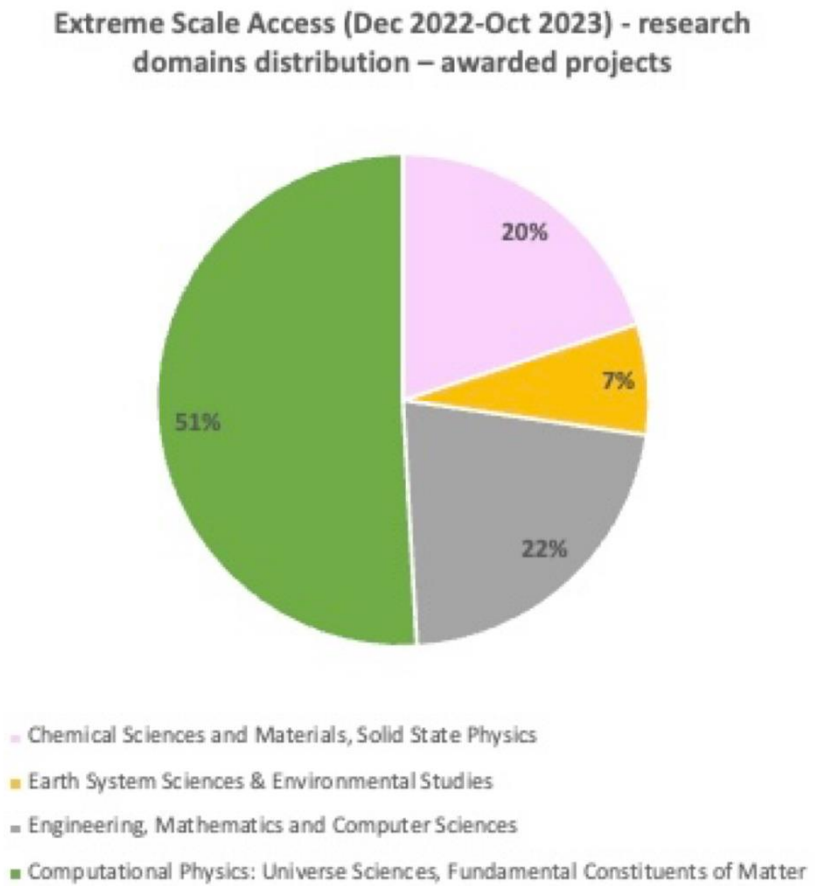
# Regular Access statistics – proposal numbers



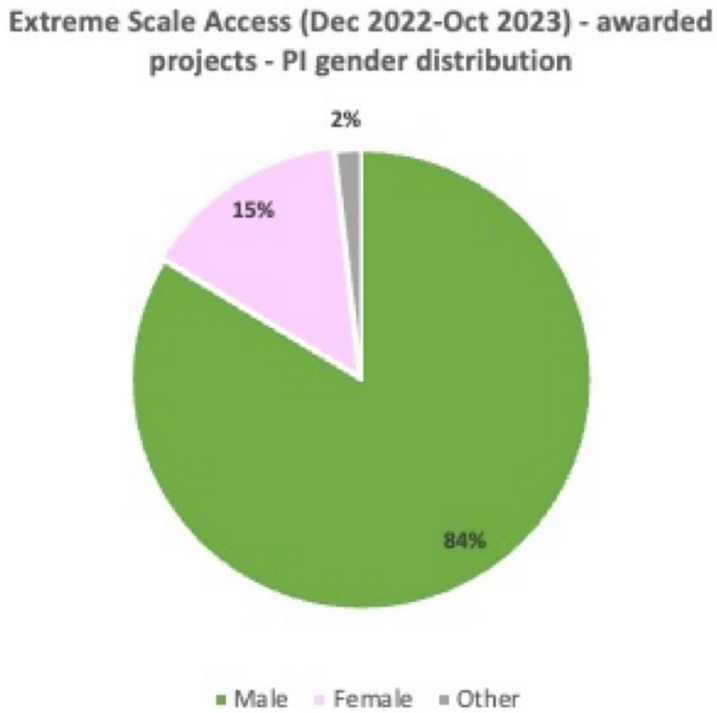
# Extreme Scale Access statistics – proposal numbers




**fantastic resource for European research & leadership**

# Extreme Scale Access statistics – gender distribution




| PI GENDER DISTRIBUTION – AWARDED PROJECTS | | |
|---|---|---|
| **GENDER** | **Number of proposals** | **%** |
| Male | 46 | 84% |
| Female | 8 | 15% |
| Unspecified | 1 | 2% |
| **TOTAL** | **55** | **100%** |

| PI GENDER DISTRIBUTION – SUBMITTED PROPOSALS | | |
|---|---|---|
| **GENDER** | **Number of proposals** | **%** |
| Male | 64 | 80% |
| Female | 15 | 19% |
| Unspecified | 1 | 1% |
| **TOTAL** | **80** | **100%** |

# anectodes: peer review is hard! (but the best)

- a good proposal needs to have
- … solid motivations
- … ambitious goals
- … performant software
- … requests that are justified by milestones

- all of this needs to be **in the application!**
- … needs to be **clearly stated** for external reviewers
- … and for a majority of panel members

# more anecdotes

- economics is the management of insufficient resources
  - what could you do with half of the requested time?
- I would love to allocate **all** proposed projects

# more anecdotes

- economics is the management of insufficient resources
  - what could you do with half of the requested time?
- I would love to allocate **all** proposed projects

- … actually, **NO**, I would only allocate the good ones!
- there are **two** calls per year, this allows rejected projects to improve and resubmit quickly
- this is a great resource, projects do improve

# a financial curiosity

- try buying computer time?
- cloud providers charge for 250k node-hr…

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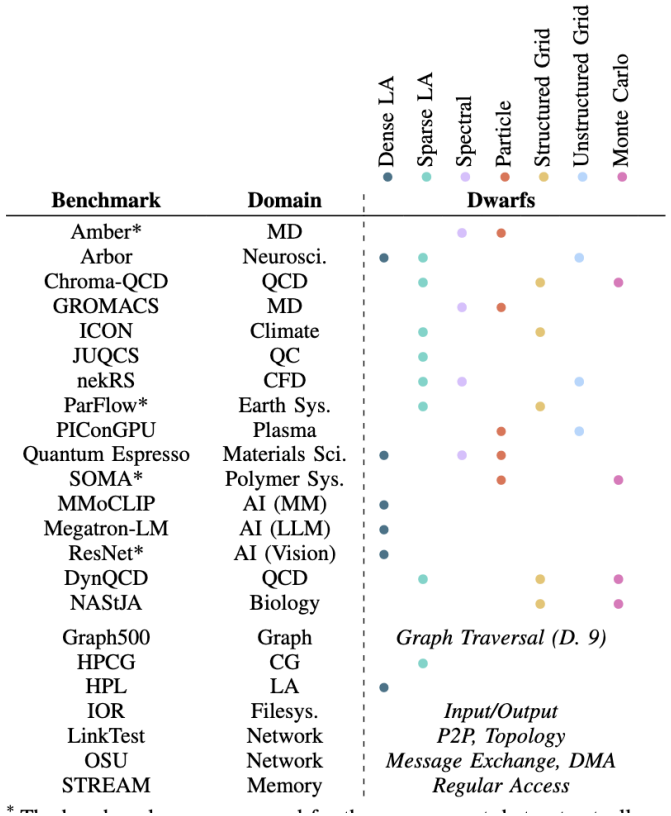
- try buying computer time?
- cloud providers charge for 250k node-hr…  M€

- EuroHPC is a fantastic research infrastructure
- it is our duty to make the best use of it
- help the ARC: keep submitting strong proposals
- make sure fundamental research remains a core priority!
- invest in creating a proper interface with industry

# procuring new systems



| Benchmark | Domain | Dense LA | Sparse LA | Spectral | Particle | Structured Grid | Unstructured Grid | Monte Carlo |
|---|---|---|---|---|---|---|---|---|
| Amber* | MD | | | ● | ● | | | |
| Arbor | Neurosci. | ● | ● | | | | ● | |
| Chroma-QCD | QCD | | ● | | | ● | | ● |
| GROMACS | MD | | | ● | ● | | | |
| ICON | Climate | | ● | | | ● | | |
| JUQCS | QC | | ● | | | | | |
| nekRS | CFD | | ● | ● | | | ● | |
| ParFlow* | Earth Sys. | | ● | | | ● | | |
| PIConGPU | Plasma | | | | ● | | ● | |
| Quantum Espresso | Materials Sci. | ● | | ● | ● | | | |
| SOMA* | Polymer Sys. | | | | ● | | | ● |
| MMoCLIP | AI (MM) | ● | | | | | | |
| Megatron-LM | AI (LLM) | ● | | | | | | |
| ResNet* | AI (Vision) | ● | | | | | | |
| DynQCD | QCD | | ● | | | ● | | ● |
| NAStJA | Biology | | | | | ● | | ● |
| Graph500 | Graph | *Graph Traversal (D. 9)* | | | | | | |
| HPCG | CG | | ● | | | | | |
| HPL | LA | ● | | | | | | |
| IOR | Filesys. | *Input/Output* | | | | | | |
| LinkTest | Network | *P2P, Topology* | | | | | | |
| OSU | Network | *Message Exchange, DMA* | | | | | | |
| STREAM | Memory | *Regular Access* | | | | | | |

Dwarfs

## Application-Driven Exascale: The JUPITER Benchmark Suite

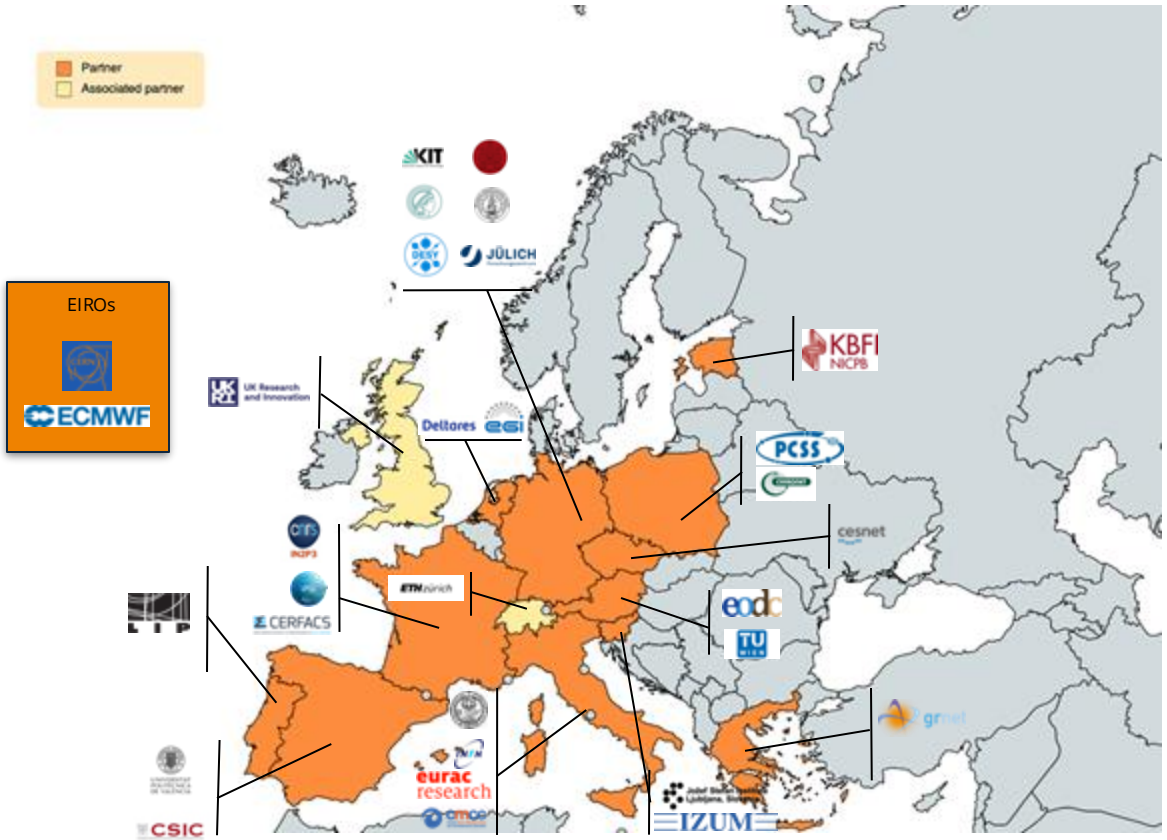
Andreas Herten, Sebastian Achilles, Damian Alvarez, Jayesh Badwaik, Eric Behle, Mathis Bode, Thomas Breuer, Daniel Caviedes-Voullième, Mehdi Cherti, Adel Dabah, Salem El Sayed, Wolfgang Frings, Ana Gonzalez-Nicolas, Eric B. Gregory, Kaveh Haghighi Mood, Thorsten Hater, Jenia Jitsev, Chelsea Maria John, Jan H. Meinke, Catrin I. Meyer, Pavel Mezentsev, Jan-Oliver Mirus, Stepan Nassyr, Carolin Penke, Manoel Römmer, Ujjwal Sinha, Benedikt von St. Vieth, Olaf Stein, Estela Suarez, Dennis Willsch, Ilya Zhukov
*Jülich Supercomputing Centre*
*Forschungszentrum Jülich*
Jülich, Germany

Aug 2024

***Abstract*—Benchmarks are essential in the design of modern**

This paper introduces the *JUPITER Benchmark Suite*, a

# Intertwin at a glance




8 Infrastructure Providers Cloud, HTC , HPC resources

11 Technol Providers delivering the infrastructure a horizontal capab

14 Community representants from 5 domains developing DT applications and thematic modules

Co-designs and implements the prototype of an **interdisciplinary Digital Twin Engine for Science**

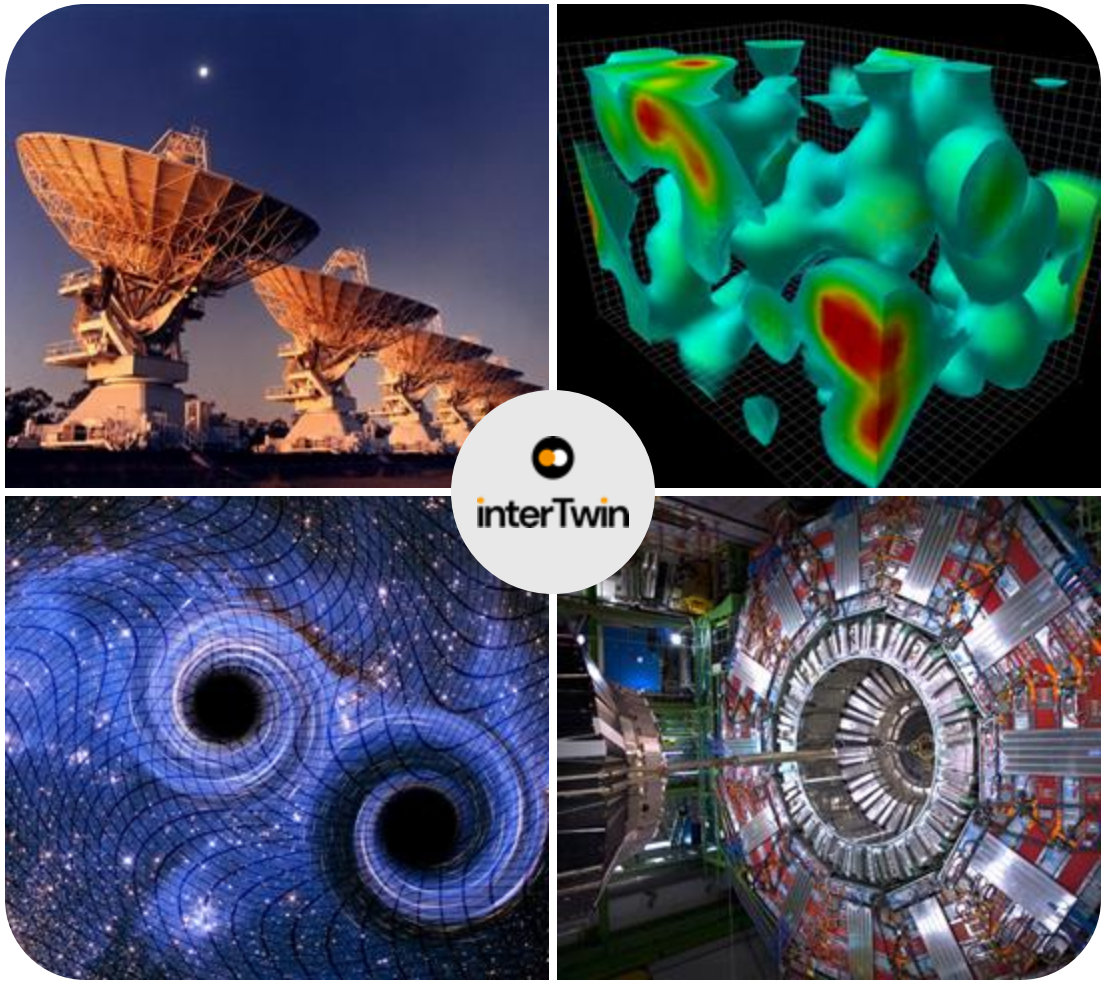
Piloted by a large spectrum of **diverse use cases** from **physics** and **environmental** sciences

**Open-source** platform based on **open standards** offering the capability to develop **application-specific Digital Twins (DTs)**

Lattice QCD as part of Digital Twin of HEP

# So have Physics use Cases, among them Lattice QCD

**Radio Astronomy Noise simulation**
Univ. of Heidelberg, Max Planck Society




**Lattice QCD Simulation**
CSIC, ETHZ, CNRS
Led by Isabel Campos / Marina Marinkovic / Benoit Blossier

**VIRGO Gravitational Wave Interferometer Noise Simulation**
INFN

**High Energy Physics Detector Simulation**
CERN, CNRS

https://www.intertwin.eu/us

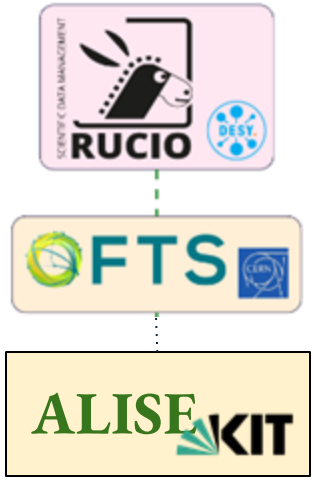
# Managing data in the same way large HEP experiments do (bringing LatticeQCD data management to the XXIst century)

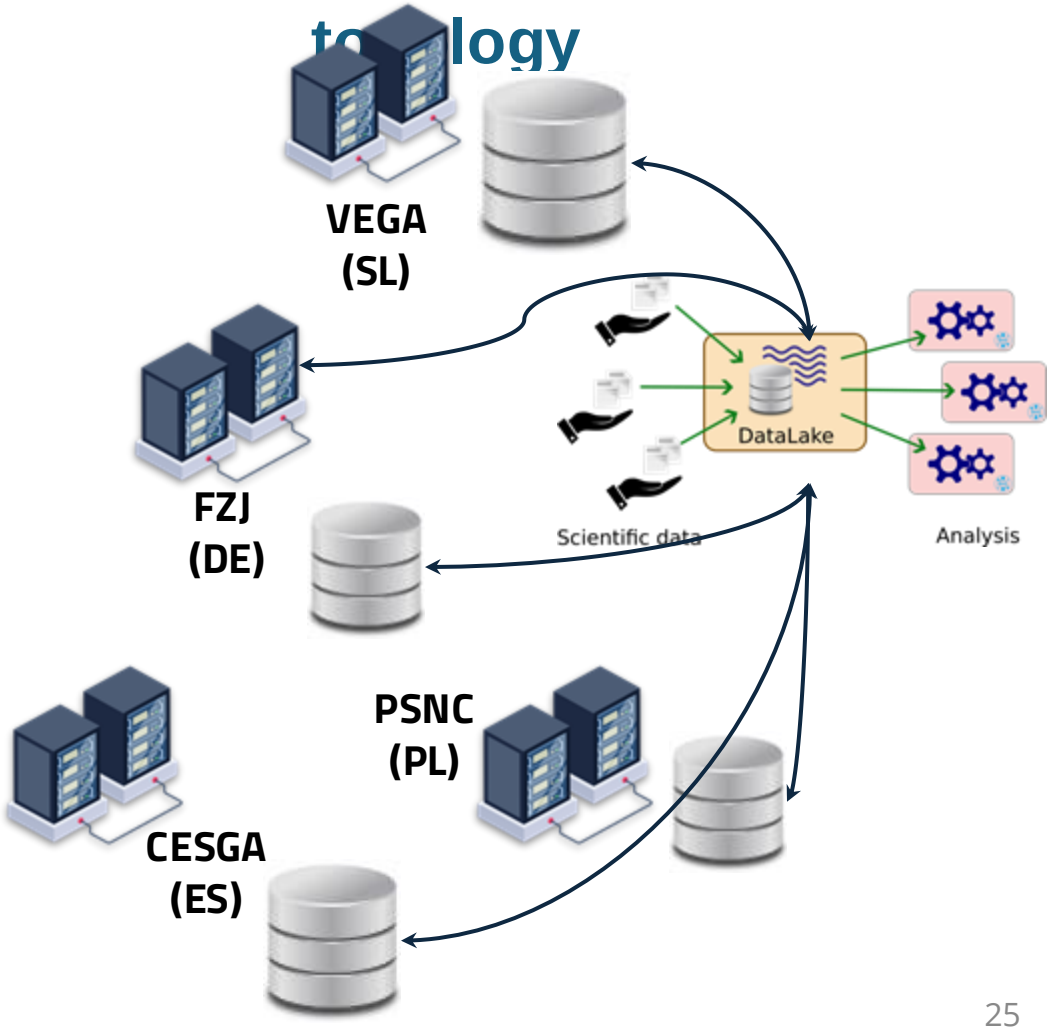
## Data Lake prototype for Lattice QCD

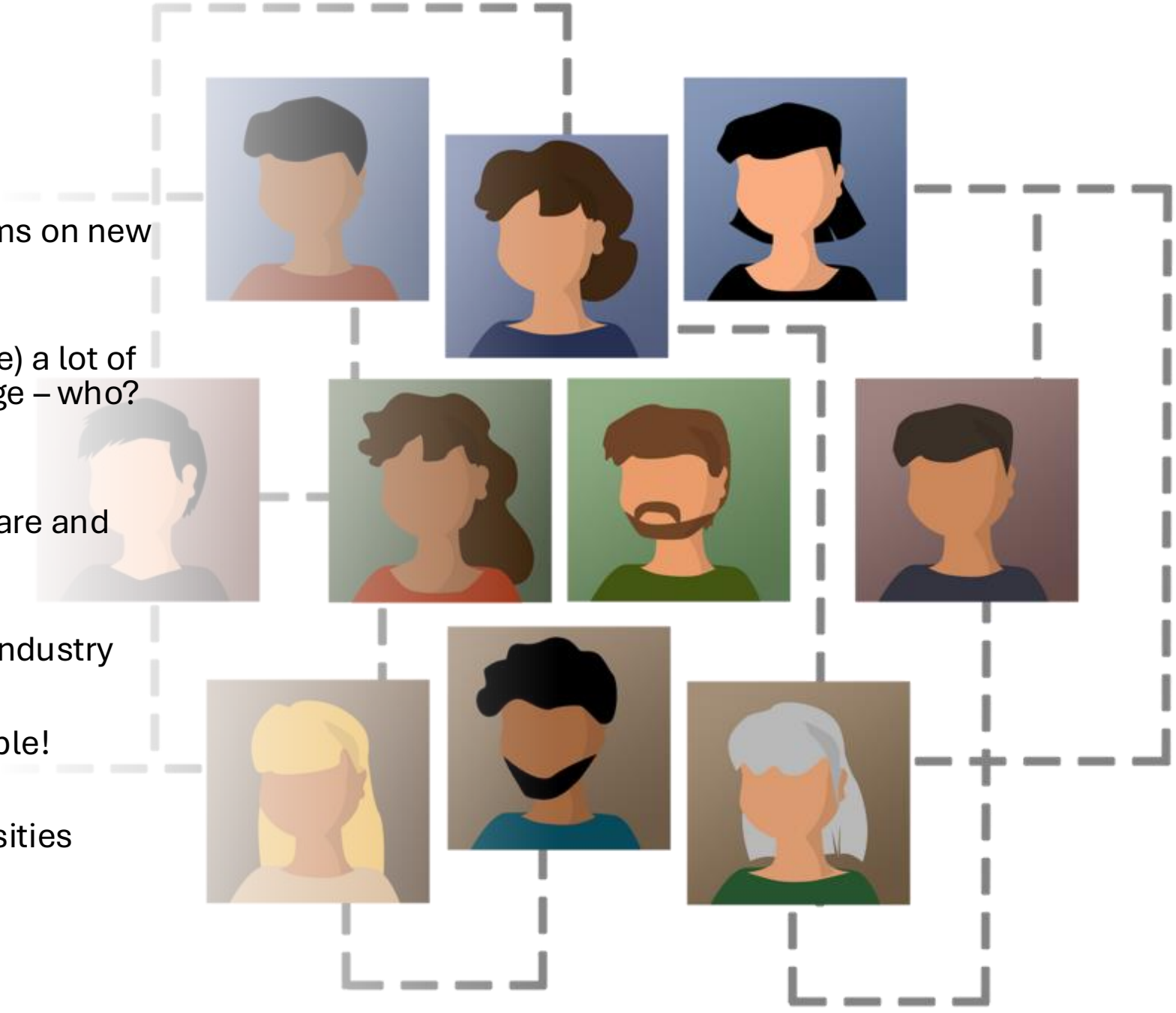
**RUCIO** service provided by DESY-HH
- manage large volumes of data spread across facilities at multiple institutions
- continuously extended to support the LHC experiments and others (SKA)

**FTS** service provided by CERN
- File Transfer Service used at LHC
- **TODO**: develop an *API* to use it as experimentals do (commandline cumbersome)

**ALISE** developed and provided by KIT
- Link local Unix account with <u>any</u> federated identity OIDC compliant
- Expects the local account to exist - these are created following HPC policies
- Towards the dream of having a single account everywhere
- **TODO**: get in touch, and try it https://alise.data.kit.edu/



# People!

- Develop efficient algorithms on new architectures
- Requires (in my experience) a lot of domain-specific knowledge – who? where?
- Porting on multiple hardware and benchmarking, data (!)
- Engage in co-design with industry
- Career path for these people!
- Work together with universities