

Applications of high-performance computing in physics - Cases Lumi, LUMI AI Factory, Sweden AI Factory

Dr. Tomasz Malkiewicz

Director, NeIC
CSC - IT Center for Science, Finland

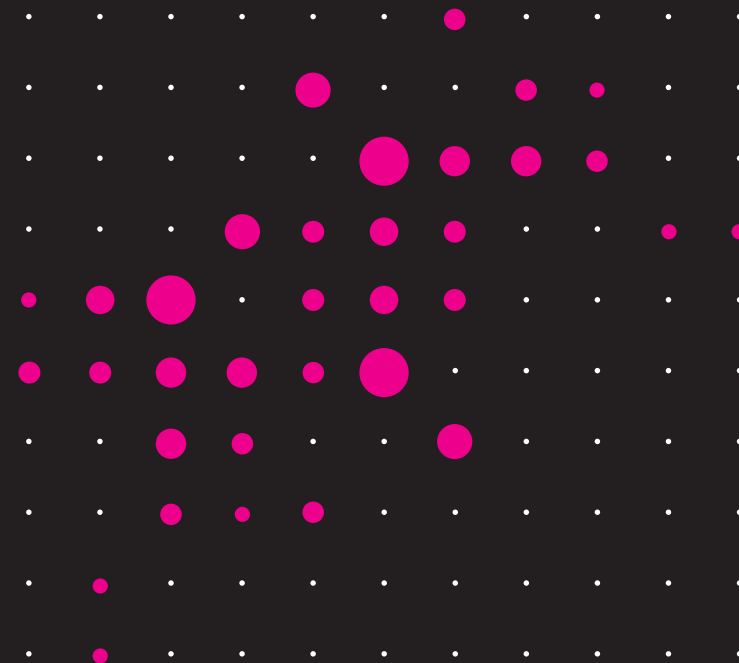


*Tomasz
Malkiewicz*

- 2017- **Nordic e-Infrastructure Collaboration (NeIC)**, *neic.no*
 - *Director* 01.2025-
 - Executive Team member 2017-2024, Executive Manager
- 2011- **CSC – IT Center for Science, Espoo, Finland**, *csc.fi*
 - *Management Group member* 10.2016- , Senior Applications Specialist
- 2009-2011 CNRS Postdoctoral Researcher, LPSC Grenoble, France
 - Ministère de l'Enseignement Supérieur et de la Recherche, Lecturer (Maître de Conférence), Nuclear and Particle Physics, 02.2011
- 2002-2009 University of Jyväskylä, Faculty of Mathematics and Science, Jyväskylä, Finland
 - Ph.D. in Physics, 09.2009
 - M.Sc. in Physics, 01.2004
- 1999-2004 Warsaw University of Technology, Faculty of Physics, Warsaw, Poland
 - M.Sc. Eng. in Physics, 04.2004

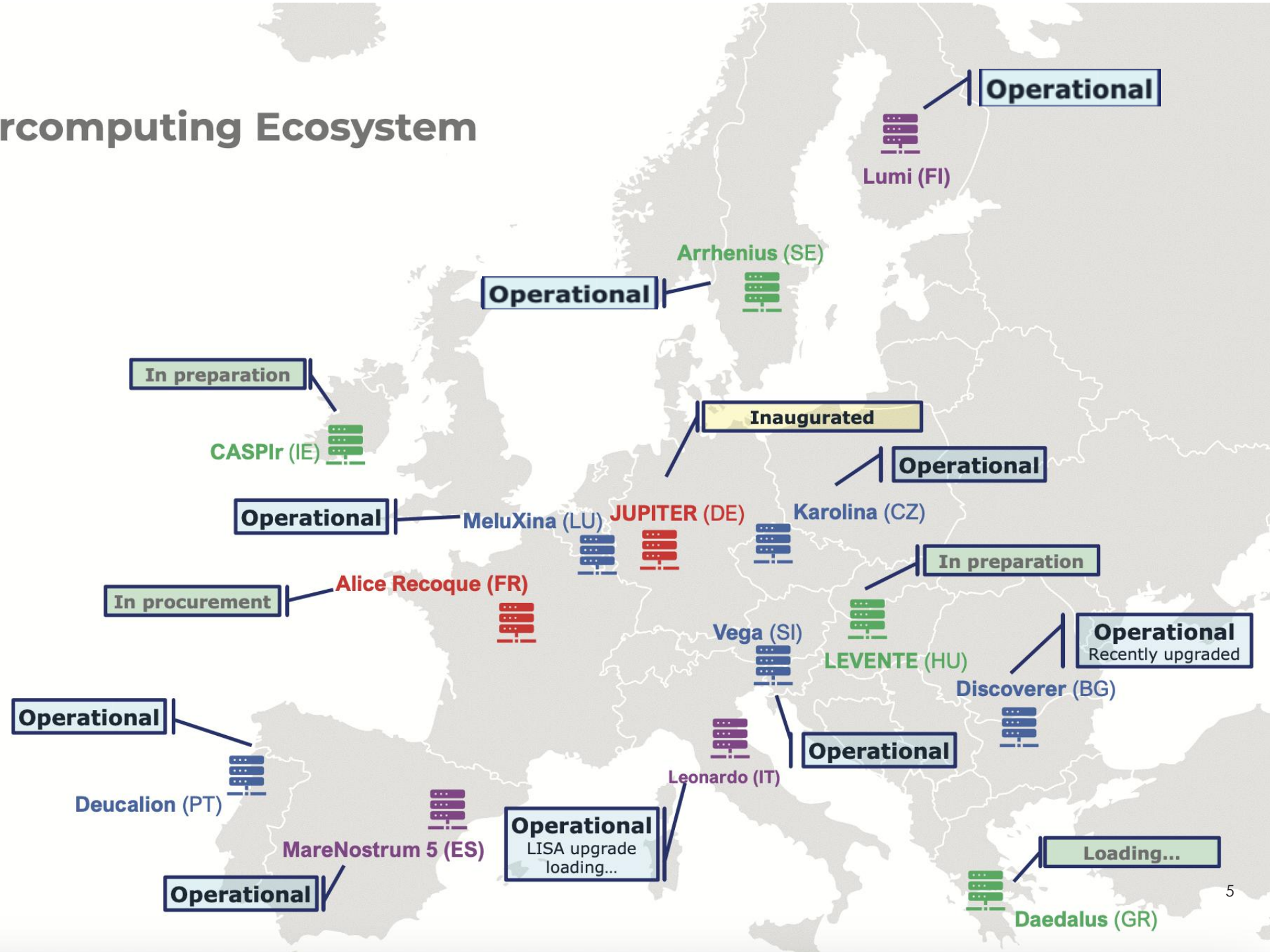
- EuroHPC JU supercomputers & AI Factories
- Lumi supercomputer, Lumi AI Factory and Lumi-AI, the next-generation HPC+AI+QC infrastructure
- Applications, physics applications on LUMI
- Sweden AI Factory
- Applications, physics applications on Sweden AI Factory
- Physics applications on HPC

Building Europe's digital sovereignty with EuroHPC JU



The EuroHPC Supercomputing Ecosystem

-  EXASCALE
-  PRE-EXASCALE
-  PETASCALE
-  MID-RANGE



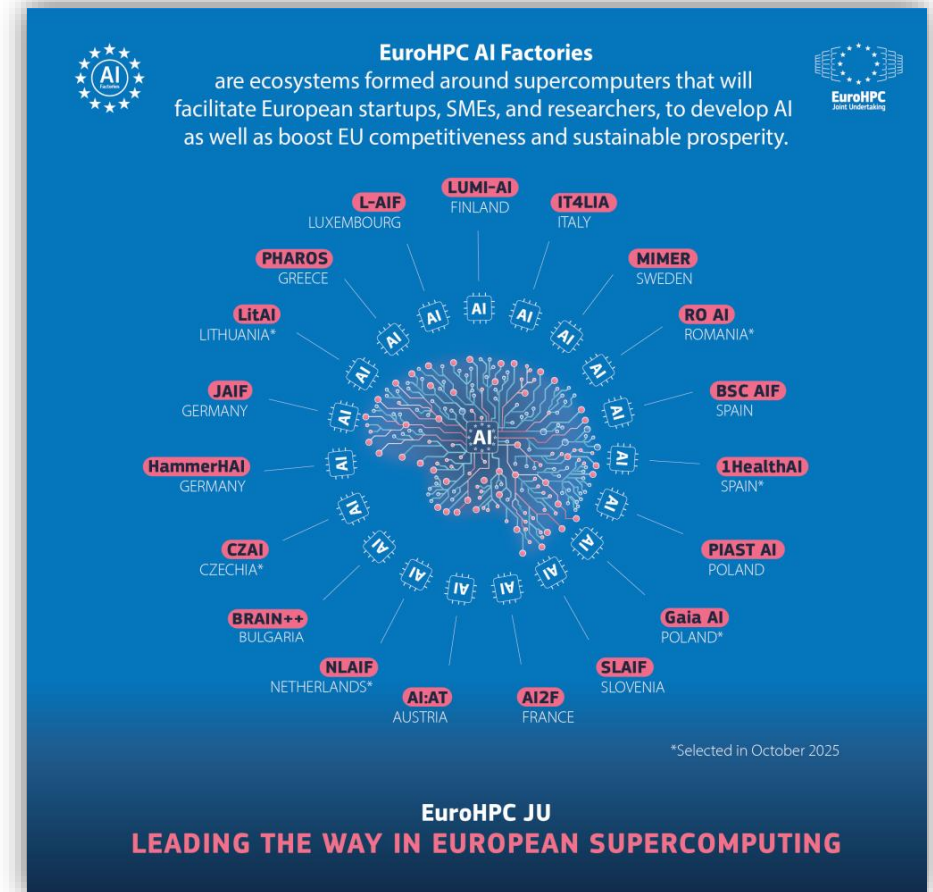
EU promotes AI innovation with AI Factories

The EuroHPC AI Factories

- Boost European competitiveness in AI
- Ecosystems formed around supercomputers to foster innovation
- Compute + Data + Talent
- 19 AI Factories + 13 AI Factory Antennas

LUMI AI Factory (LUMI AIF)

- CSC (Finland) coordinates consortium with participation from Czechia, Denmark, Estonia, Norway and Poland
- Four associated antennas: Belgium, Iceland, Latvia and Switzerland
- **Largest EuroHPC AI Factory investment** with total budget over 650 million euros



DARE – Digital Autonomy with RISC-V in Europe

LUMI AI Factory

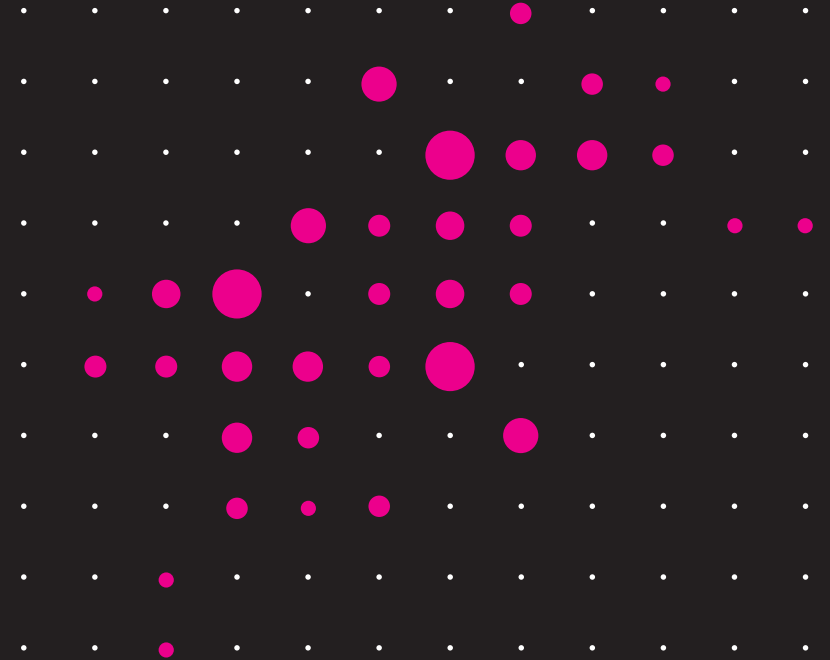


- Mission: Build a fully European supercomputing hardware and software stack - designed and developed in Europe
- Open ecosystem based on the RISC-V instruction set architecture
- 45 partners and affiliated entities in 15 countries
- Three RISC-V based chiplets
 - General-purpose processor optimized for HPC workloads
 - Vector accelerator for high-precision HPC
 - AI processing unit for inference acceleration in HPC applications
- First prototypes hosted at BSC (Barcelona) and CSC (Kajaani) in early 2028



EuroHPC
Joint Undertaking

Lumi supercomputer, the story so far



LUMI



- LUMI - one of the fastest supercomputers in the world since 2022
- ClimateDT
- Physics applications
- (Ice modelling)



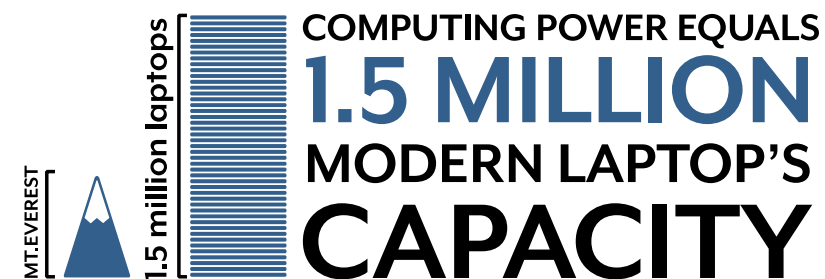
LUMI is one of the fastest supercomputers in the world

LUMI

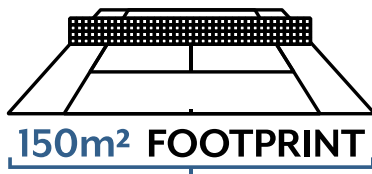
SUSTAINED PERFORMANCE

380 PETAFL0P/S

= performs 380×10^{15} calculations per second



2 x



High-
performance
computing

AI

Data
analytics

What does using a supercomputer look like?



Connect to a login node



Prepare Software & Data



Customize batch job template
(specify resources, load
modules, run program)



Submit job from the login node to
a compute node



View and analyze results on
supercomputer or locally

A terminal window with a dark purple background. The title bar shows 'prediger@notvacka: ~'. The terminal content shows a successful SSH connection to a LUMI node. It displays the LUMI logo in large white letters, followed by the text 'The Supercomputer of the North'. Below this, it provides user guides and support links: 'https://docs.lumi-supercomputer.eu' and 'https://lumi-supercomputer.eu/user-support'. The prompt changes from '(base) :~\$' to 'lukaspre@uan01:~>'.

```
(base) :~$ ssh lumi
Last login: Wed Apr 24 17:05:55 2024 from 195.148.17.138
*
*  L U M I  *
*
*  The Supercomputer of the North  *
*
*****
|User guide and support|
|https://docs.lumi-supercomputer.eu|
|https://lumi-supercomputer.eu/user-support|
*****
lukaspre@uan01:~>
```

Access to LUMI: PLGrid example

 Portal PLGrid 

 [Zaloguj się](#)  [Utwórz konto](#) 

Dołącz do nas w tworzeniu **innowacyjnych badań**:

Grant właściwy PLGrid

Predefiniowany grant zawierający określone zasoby dostępne w ramach infrastruktury PLGrid.



[Aplikuj](#)

Grant pilotażowy PLGrid

Grant pilotażowy służący do testowania potrzeb użytkownika w zakresie korzystania z Infrastruktury PLGrid.



[Aplikuj](#)

Grant LUMI

Granty są obecnie nieaktywne

Granty obliczeniowe realizowane na superkomputerze LUMI. Wnioski przyjmowane zgodnie z harmonogramem konkursu. Nabór wniosków odbywa się 2 razy do roku. Więcej na: <https://guide.plgrid.pl/grants/lumi/>



[Aplikuj](#)

Grant testowy LUMI

W ramach dostępu testowego użytkownik może korzystać z zasobów LUMI CPU przez 1 miesiąc (30 dni). Dostęp testowy zapewnia 10 000 godzin obliczeniowych na CPU które użytkownik może wykorzystać.



[Aplikuj](#)

Modern architecture

LUMI-C:
x86 Partition
Supplementary CPU partition:
over **262,000**
AMD EPYC CPU cores.

LUMI-K:
Container Cloud Service

LUMI-O:
Object Storage Service
30 PB
encrypted object storage
(Ceph) for storing, sharing
and staging data.

LUMI-Q:
Quantum Computing

High-speed interconnect

Possibility for combining
different resources within
a single run. HPE
Slingshot technology.



LUMI-G:
GPU Partition
Sustained performance
380
Pflop/s powered by AMD
Radeon Instinct™ MI250X GPUs.



LUMI-D:
Data Analytics Partition
Interactive partition with
32 TB
of memory and graphics GPUs for
data analytics and visualization.



LUMI-F:
Accelerated Storage
10 PB
Flash-based storage layer with
extreme I/O bandwidth of
2 TB/s and IOPS capability.



LUMI-P:
Lustre Storage
80 PB
parallel file system.



Large models trained on LUMI

LUMI

Uutinen

A New Foundation for AI Is Being Built in Finland – Offering an Alternative to American Giants

Antti Leikas 6.12.2023 09:45 | päivitetty 8.12.2023 15:07 TIVI IN ENGLISH ARTIFICIAL INTELLIGENCE

The development of the Poro language model utilizes Lumi, the fastest supercomputer in Europe, located in Kajaani.



Artificial Intelligence. According to Peter Sarlin (center), the development of the Poro language model aims at democratizing AI technology and ensuring equal treatment of European languages. TIINA SOMERPURO

Uutinen

Silo AI has released an artificial intelligence model designed for Nordic languages – Particularly suitable for coding

Joona Komonen 13.6.2024 12:22 ARTIFICIAL INTELLIGENCE TIVI IN ENGLISH

The Viking language model is a continuation of the Poro model specialized in the Finnish language.

Source: tivi.fi

AI2 OLMo

Open Language Model

News

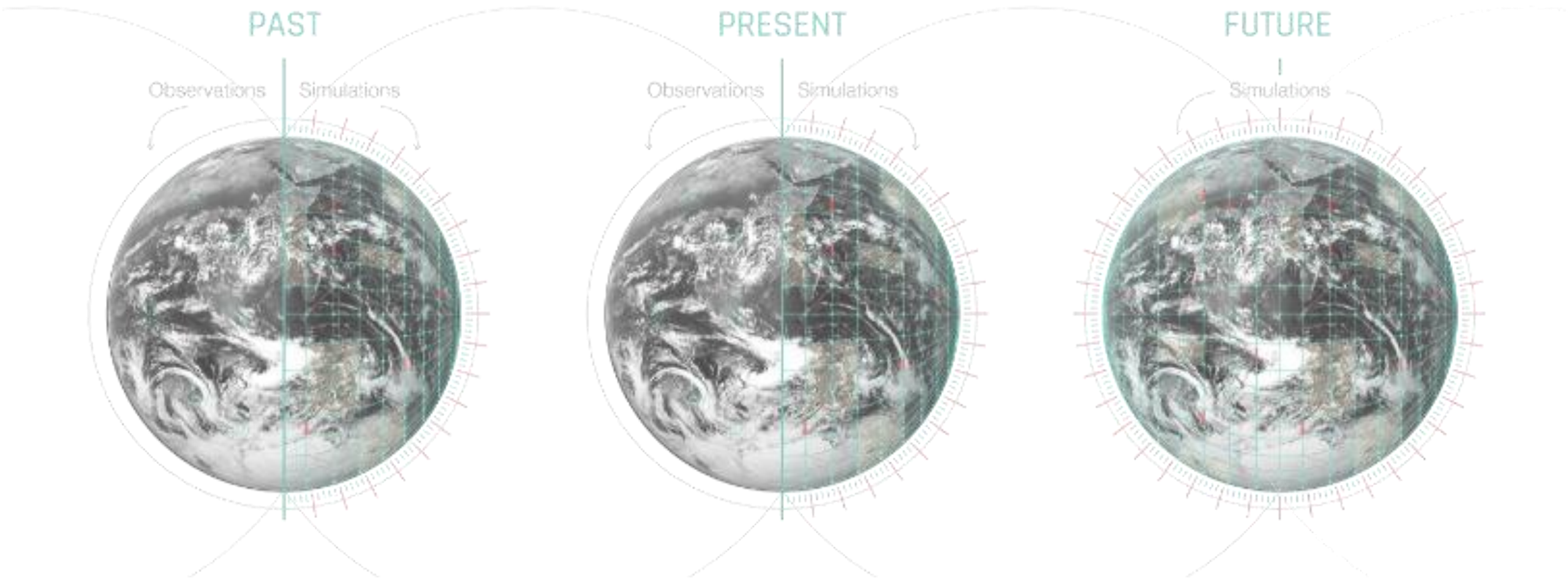
2.2.2024

A truly open large language model released, developed with LUMI

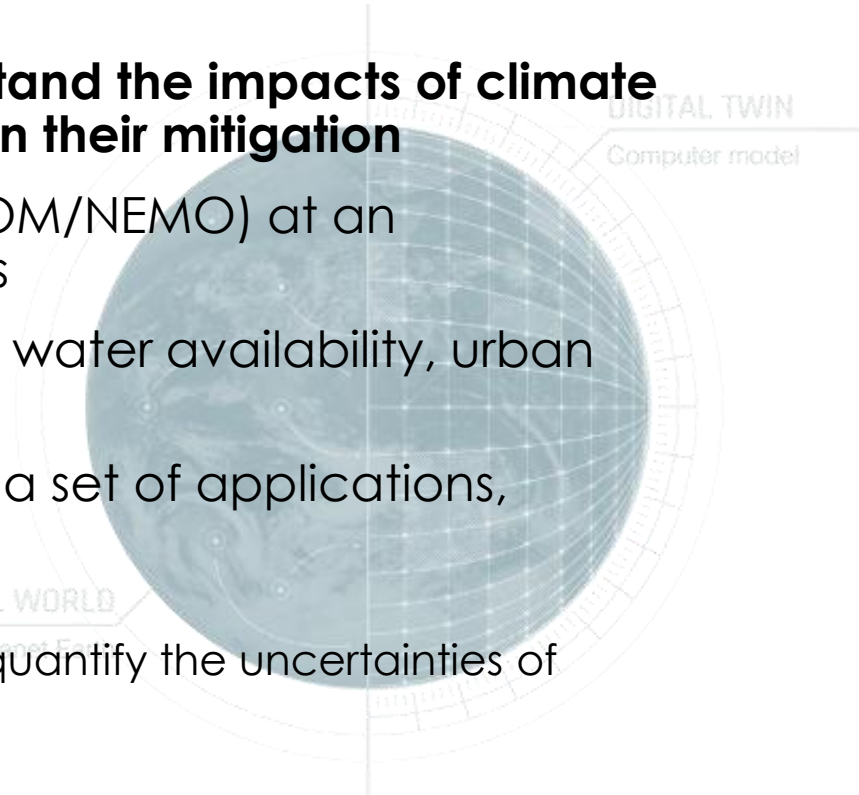
The Allen Institute for AI (AI2) has released OLMo 7B, a truly open, state-of-the-art large...

Source: tivi.fi

BioDT and ClimateDT on LUMI

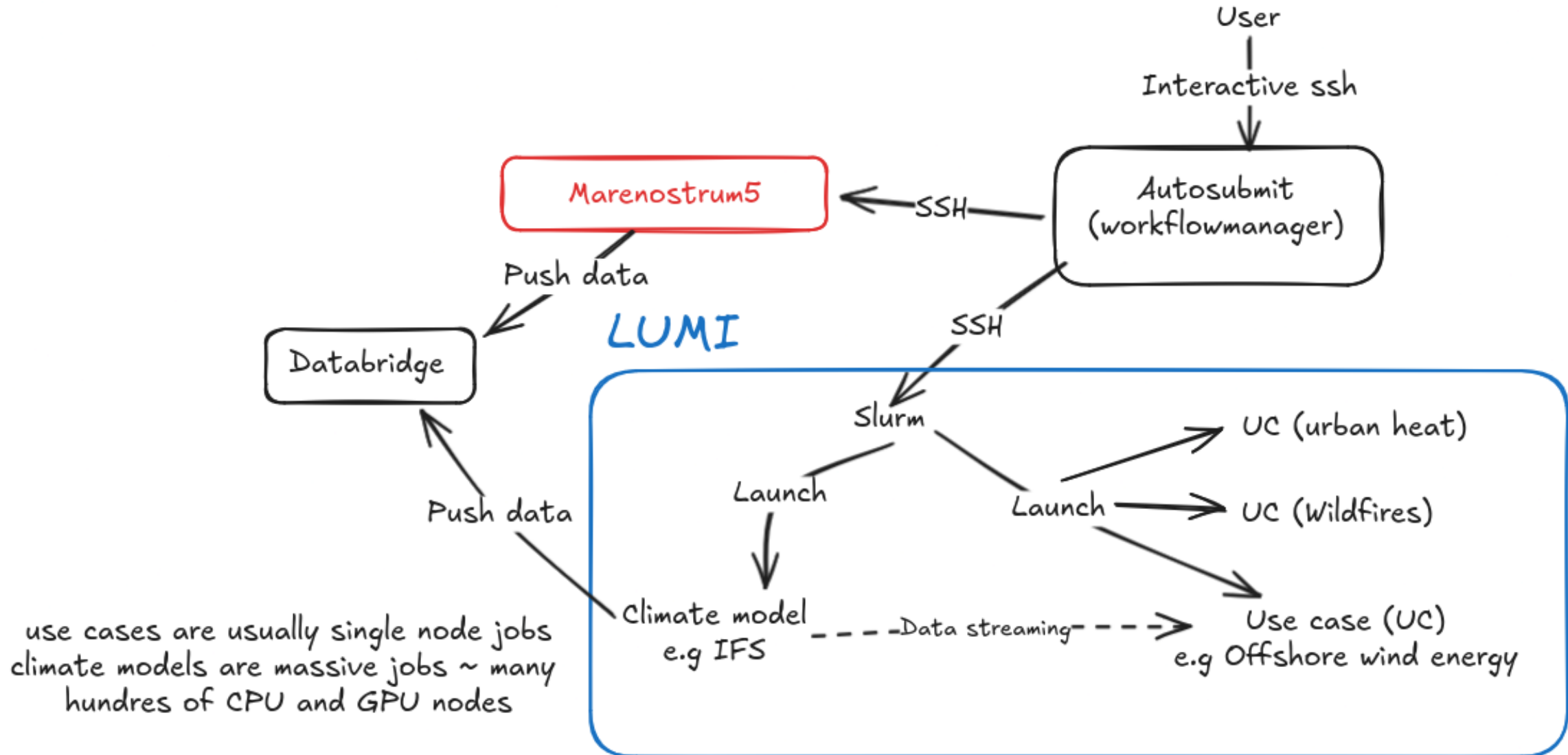


- **Objective: To build a digital twin of Earth's climate to understand the impacts of climate change and help in making data-driven political decisions in their mitigation**
- Global climate simulations with two ESMs (ICON and IFS-FESOM/NEMO) at an unprecedented resolution (5 – 10 km) over multiple decades
- Six prototype impact models: Wind energy, river floods, fresh water availability, urban heat waves, wild fire risk and emissions
- With a novel approach, output of ESMs can be streamed to a set of applications, including impact models
 - Timely delivery of climate information to users and interactivity
 - Earth observation data will be used to ensure model quality and quantify the uncertainties of impact assessments.
- Deployment on LUMI and MareNostrum 5



ClimateDT workflow

LUMI

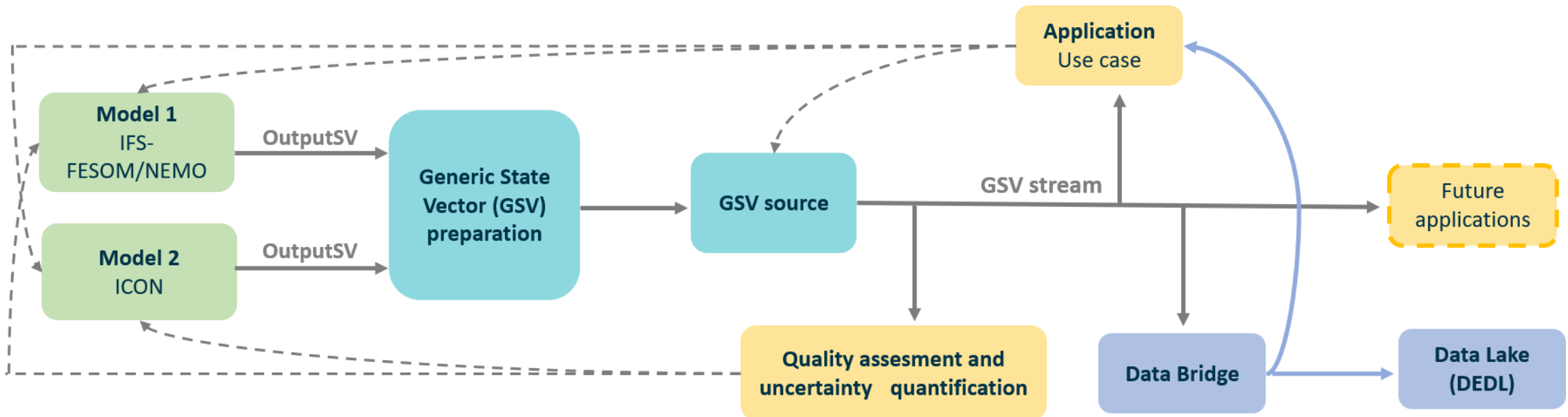


use cases are usually single node jobs
climate models are massive jobs ~ many
hundreds of CPU and GPU nodes

CLIMATE DT WORKFLOW COVERS THE FULL CHAIN FROM CLIMATE MODELS TO IMPACTS

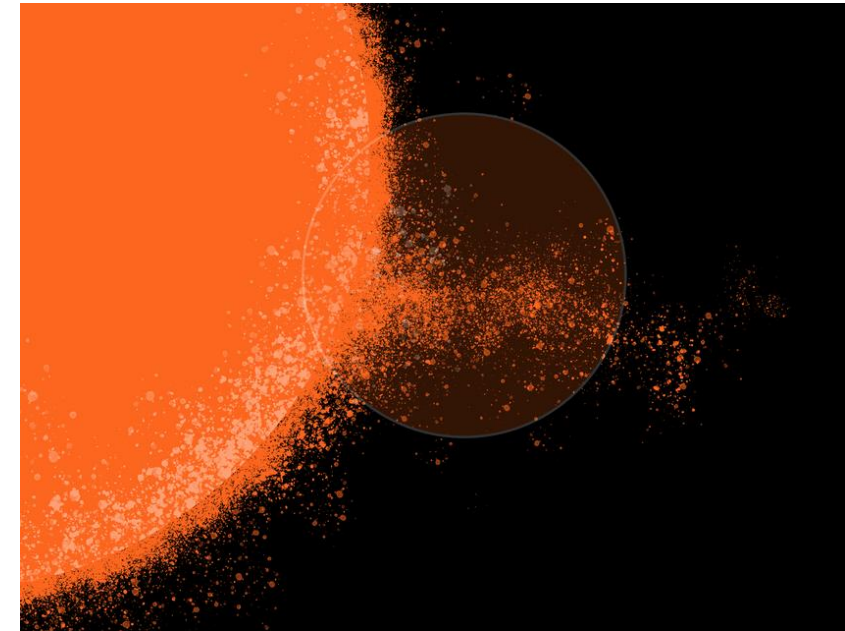
Streaming of model output in a standardized form (*generic state vector, GSV*) enables

- **Data consumers have access to the full model state** as soon as it is produced
- **Scalability** - new applications and requirements can be added
- **On-demand production** – provision of simulations and variables based on user requests



LUMI early showcase: Solar Astrophysics

- **Objective: Understand subsurface solar physics to improve forecasting of solar storms and therefore space weather**
- LUMI pilot project verified the existence of the fluctuating dynamo mechanism in the Sun

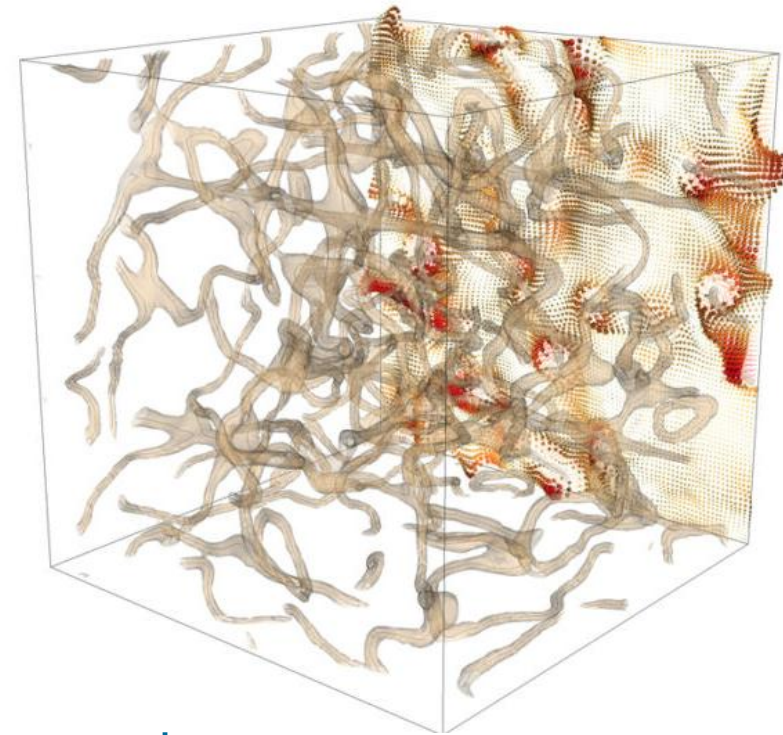


<https://www.lumi-supercomputer.eu/researchers-discovered-information-from-under-the-suns-surface-about-the-emergence-of-solar-storms-using-the-lumi-supercomputer/>

LUMI early showcase: Turbulent Dynamics in Superfluid Fermi Systems



- Fermionic superfluids important in e.g. understanding neutron stars
- To model a fermion superfluid, one needs to track all quantum states
- A pilot project on LUMI performed eigenvalue problem solutions with matrix sizes of 3M
 - The largest direct eigenvalue solution to date



<https://www.lumi-supercomputer.eu/successful-polish-lumi-pilot-project-in-the-field-of-quantum-mechanics/>

Machine-learning predictions of materials across the periodic table

Computational Materials Science | EPFL, Switzerland

LUMI

Project description

- We create a general-purpose **machine learning model** capable of simulating almost **all possible inorganic crystals** at various conditions based on near 100'000 quantum-mechanical calculations done within LUMI framework.

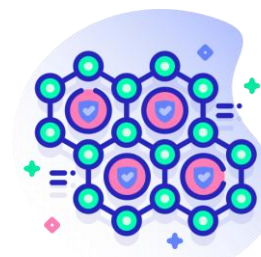
Objectives & Outcomes

- Quantum-mechanical calculations of materials remain one of the most popular yet extremely expensive approach for the computational designing of new materials. **ML models allow increasing the time and length scales accessible to simulations, while reducing their cost.**
- ML models require large amounts of precise reference calculations.** These are particularly lacking when it comes to design broadly-applicable models that span the entire periodic table and many crystal structures. **We target to achieve DFT accuracy for all possible inorganic bulk structures.**
- The infrastructure of LUMI HPC allows to run **thousands of quantum-mechanical calculations of inorganic crystals** in a fast and convenient way, providing **near 10x speedup** in building a training database for our model compared to other HPC solutions



**Database construction
within LUMI resources**

**A universal machine
learning model for
inorganic materials**

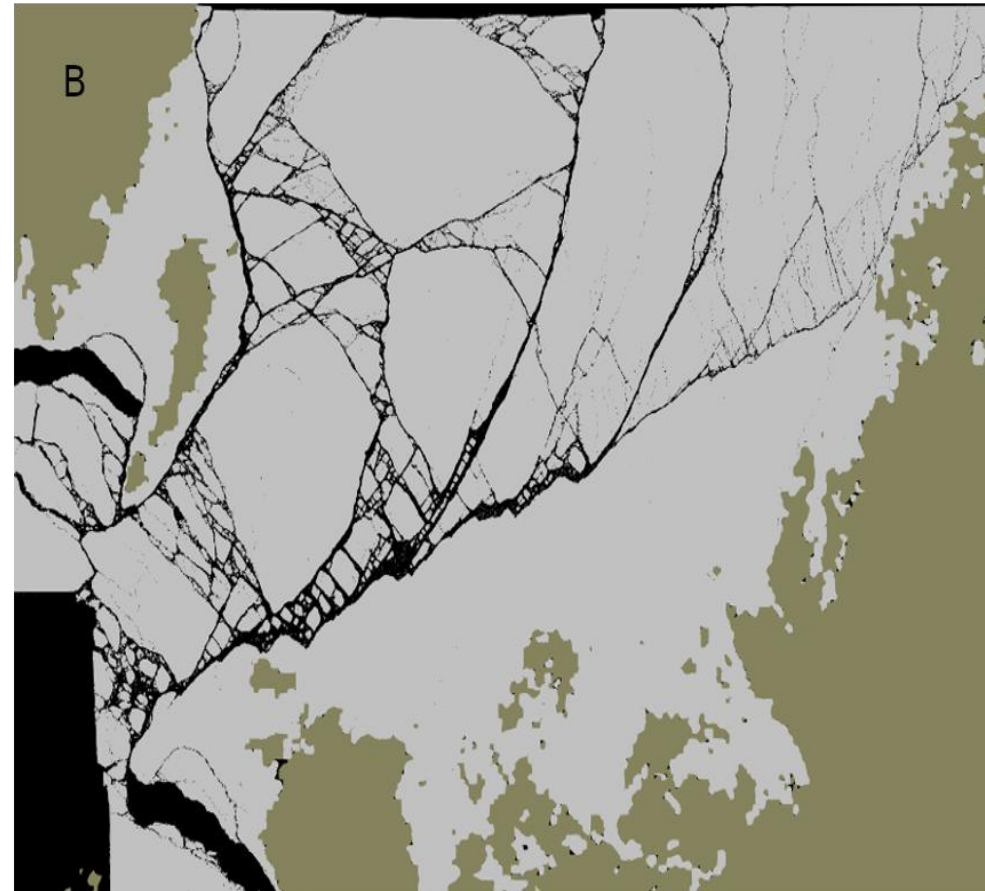
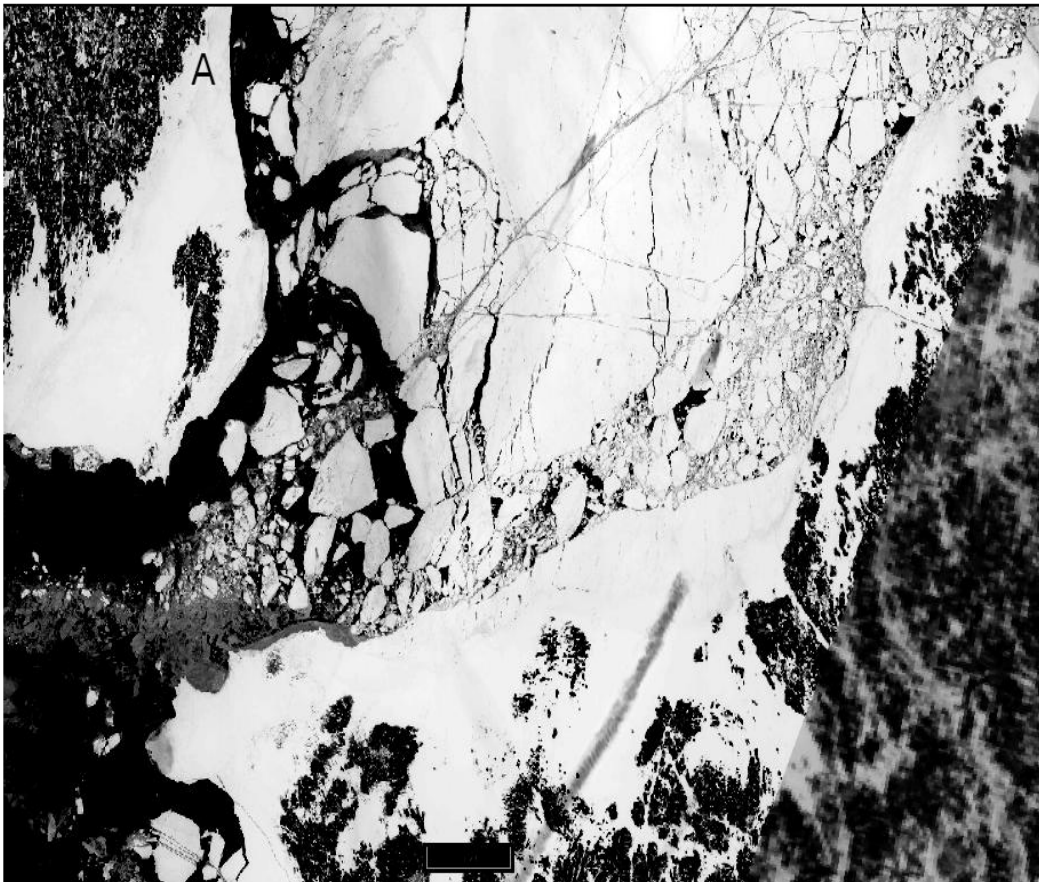


**Materials' design and
properties optimization**

Sea ice breakup and glacier calving simulations



Satellite (left) and simulated (right) image of sea ice breakup in the Kvarken region of the Baltic sea



Credit:
Jan
Åström
/CSC

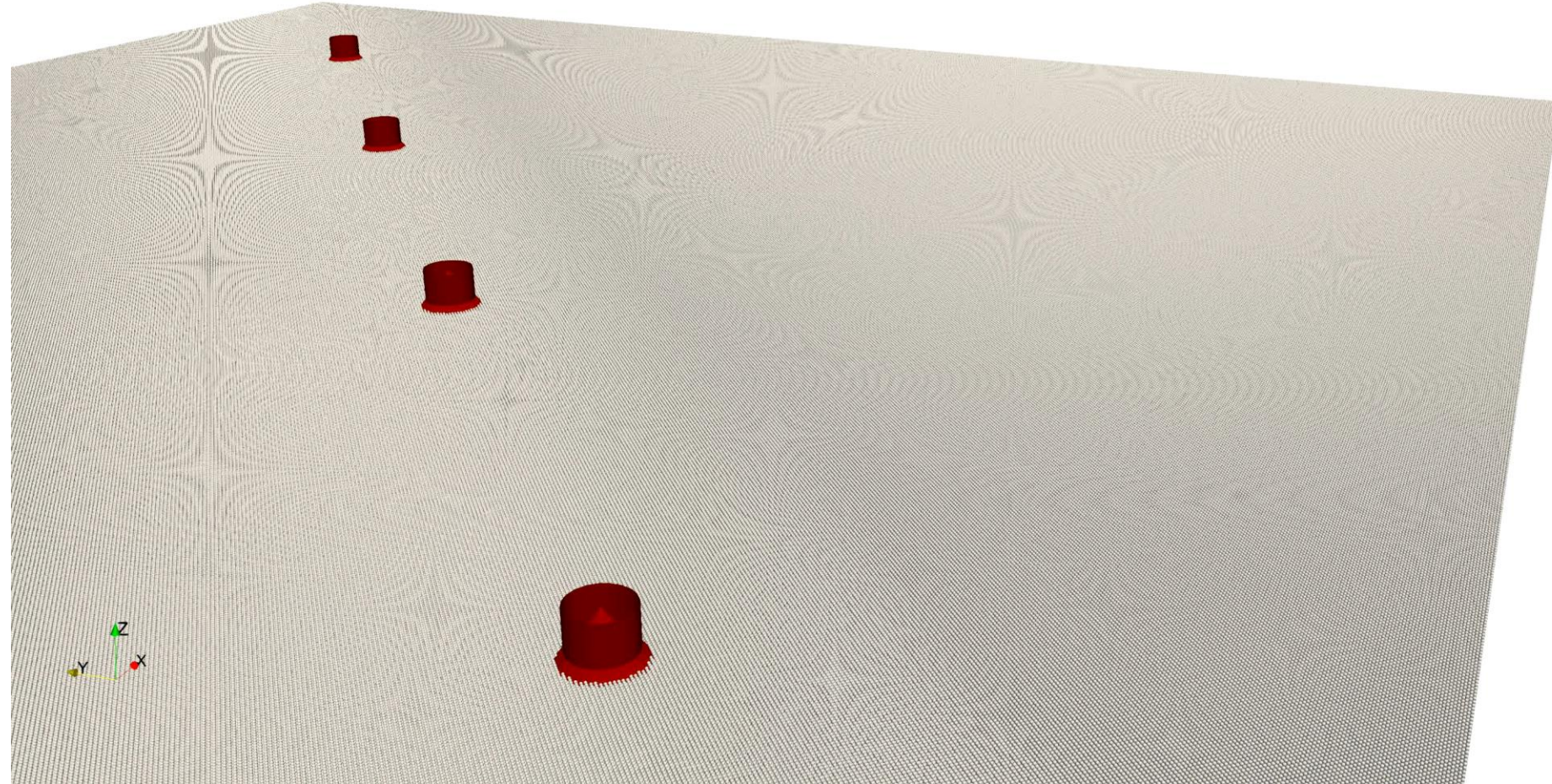
Windpower park simulation



An array of foundations of power generators (red) interacting with Sea ice.

[A large-scale high-resolution numerical model for sea-ice fragmentation dynamics](#)

Åström, F Robertsen, J
Haapala, A Polojärvi, R
Uiboupin, I Maljutenko
The Cryosphere 18 (5), 2429-
2442, 2024



Credit: Jan Åström /CSC

LUMI AI Factory

Empowering Europe's AI innovation

The three pillars of LUMI AI Factory

1. AI-optimised supercomputer **LUMI-AI**
2. Expert support by **LUMI AI Factory Services**
3. Experimental quantum-computing platform **LUMI-IQ**

Boosting European AI research and innovation

LUMI AI Factory



- Largest AI supercomputers in Europe
- Different sized packages for AI computing
- Supercomputing environment & Kubernetes
- Scalable AI training up to foundation model range



- Access to high value data (Datasets as a Service)
- Integration of data streams
- Confidential and secure data environment
- LUMI hosting is ISO 27001 certified

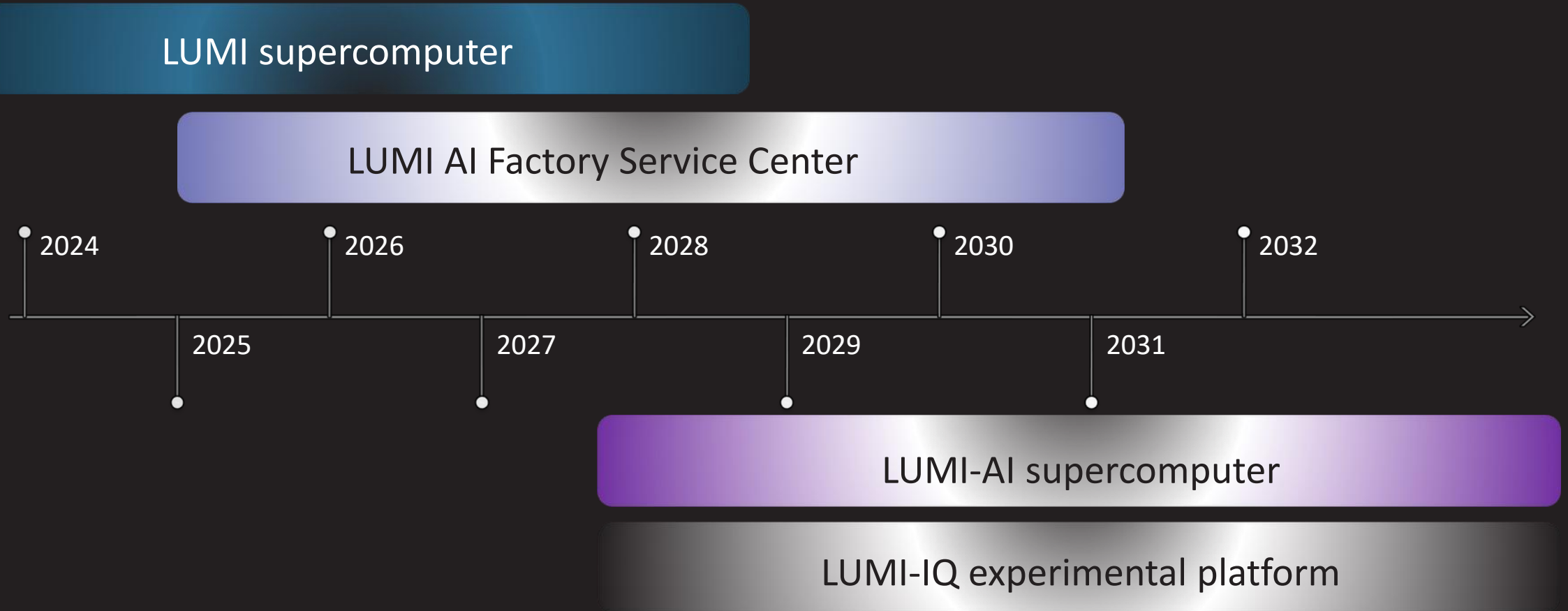


- AI expertise from a consortium of 200+ specialists
- Consultation for all phases of AI development
- Special skills in large scale AI and code optimization
- Tailored training in AI and high-performance computing

Services are free of charge for academic research, public sector and startups & SMEs.

LUMI AI Factory timeline

LUMI AI Factory



Introducing LUMI-AI

HPC

AI

**Build a supercomputing infrastructure
that could serve both worlds – and workloads mixing them**

- ✓ Need to harness the full system for a
- ✓ Need for 64-bit precision
- ✓ Big collection of (legacy)apps
- ✓ Write-dominant I/O
- ✓ Fair sharing of resources (jobs & scheduling)
- ✓ Shared environment
- ✓ Advanced support by humans

Support emerging needs

– sensitive data, quantum computing, Agentic AI

- ✓ Partitioning of the system, small
- ✓ Low fp precision
- ✓ AI frameworks, MLOps
- ✓ Read-dominant I/O
- ✓ Interactivity and immediate access
- ✓ Private enclaves
- ✓ Compute (GPU) cycles

LUMI-AI: the most advanced HPC+AI+QC platform in the world



LUMI-AI supercomputer

Liquid-cooled supercomputer delivered by **Bull**, based on **BullSequana XH3500** architecture.

AMD's next-generation MI430X GPUs alongside AMD's Venice 256-core processors, providing flexibility across diverse computing workloads.

Ambitious storage solution based on **IBM's Storage Scale** technology.

BXI interconnect by Bull, complemented by a storage network by **Nokia**.



LUMI-IQ brings Europe to the forefront of hybrid computing and boosts European technology

LUMI-IQ quantum computer will bridge **high-performance computing** and **AI** capabilities with emerging **quantum technologies** for academic and industrial use across Europe.

The system will be delivered by **IQM Quantum Computers**. First installation in 2027 with **150 physical qubits**, followed by two upgrades towards fault tolerance.

Tightly integrated to the LUMI-AI supercomputer.

LUMI-AI and LUMI-IQ facility

LUMI AI Factory

100% hydroelectric energy (23 MW IT capacity)

Waste heat reuse in the city district heating

Constructed of Finnish cross-laminated timber



Visualization: NOAR - Nordic Architects

Physics applications examples from Sweden AI Factory





FUNDED BY



EuroHPC
Joint Undertaking

VINNOVA
Sweden's Innovation Agency



Swedish
Research
Council



Co-funded by
the European Union

 **Sweden
AI Factory**

A strong national collaboration – part of the European AI ecosystem



Sweden AI Factory

From idea to impact

We help SMEs, startups, the public sector and researchers develop and deploy AI solutions. We combine world-class compute with expert support to turn ideas into real-world impact.

WHAT WE OFFER



Support

Hands-on guidance for AI development and scaling



Skills

Training and workshops in AI and HPC



Access

AI-optimised compute and data infrastructure



Trustworthy AI

Reliable, ethical and compliant AI

OUR SPECIFIC FOCUS AREAS



Life Sciences

AI for medical imaging, drug discovery, and precision medicine



Materials Science

AI for materials discovery, simulation, and industrial scale-up



Gaming

AI for real-time simulation, player behaviour, and content generation



Autonomous Systems

AI for robotics, vehicles, and intelligent physical systems



Awareness



Use case definition



Prototype



Pilot



Scale

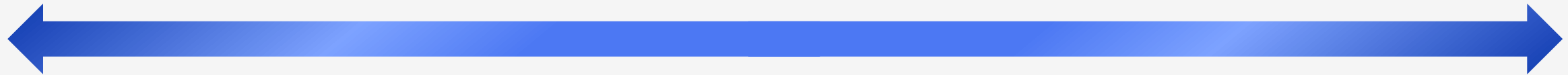
★★★ Impact

Supporting your AI journey, every step of the way

User engagement spectrum

**Emerging Users:
High Support Need**

**Advanced Users:
Low support need**



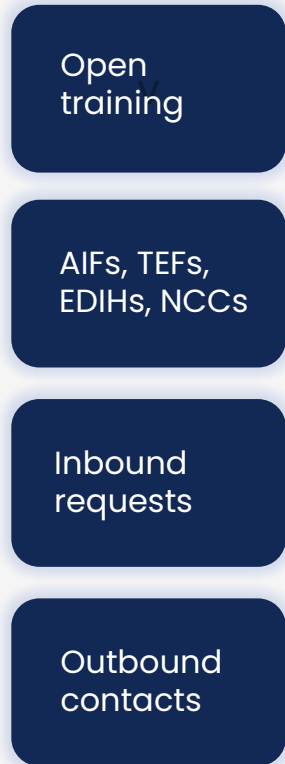
Full Co-Development	Collaborative PoCs	Tech Guidance & Tools	Compute Access Only
Low AI maturity users (often SMEs, startups) • SEAIF experts embedded in project teams • End-to-end support from scoping to deployment	Co-development with SEAIF experts • Implementation of models or data pipelines • Knowledge transfer and capacity building	Moderately advanced users needing help integrating AI/HPC • Tool selection, workflow optimisation • Short consultations or mentoring	Experienced users, self-sufficient in AI workflows • Access to HPC • Minimal support – helpdesk/onboarding only

Training & Upskilling Pathways (cross-cutting)

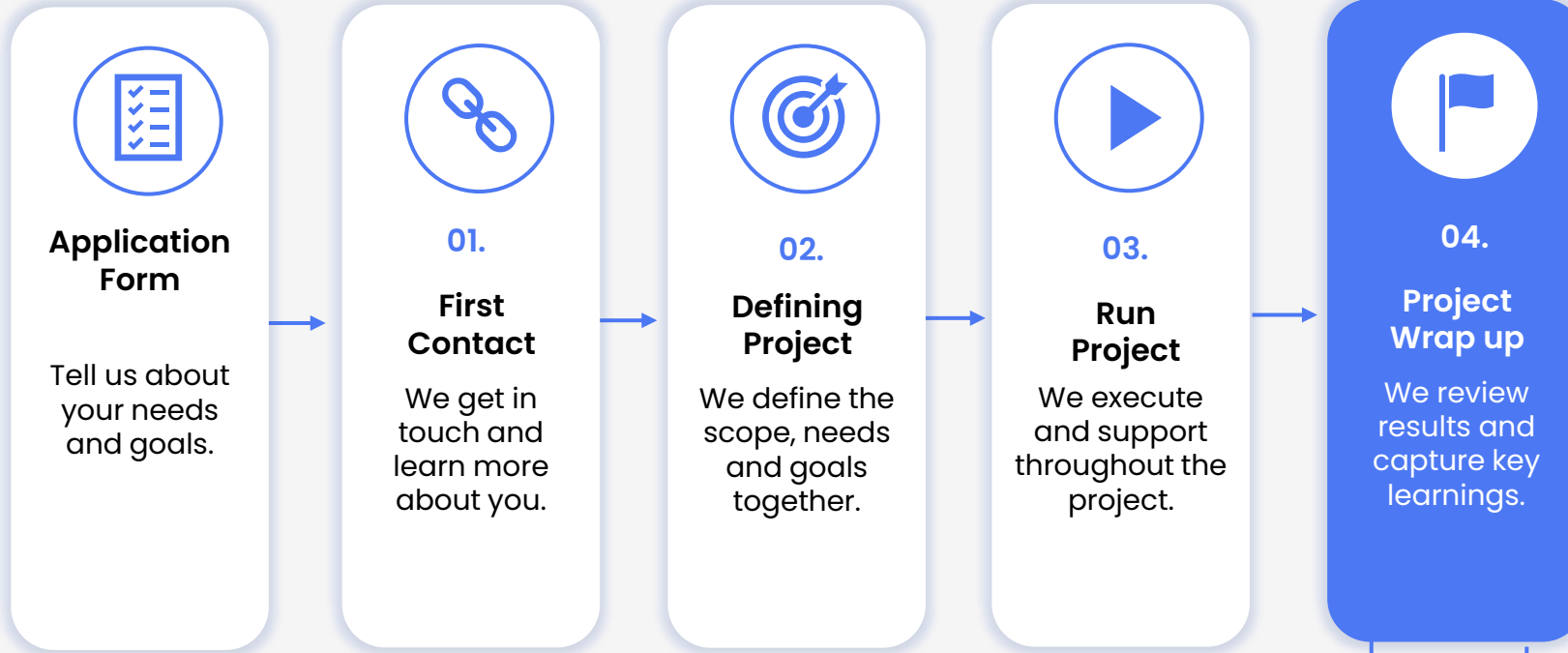
All users can engage in training, workshops, or “train-the-trainer” sessions

Sweden AI Factory Customer Journey

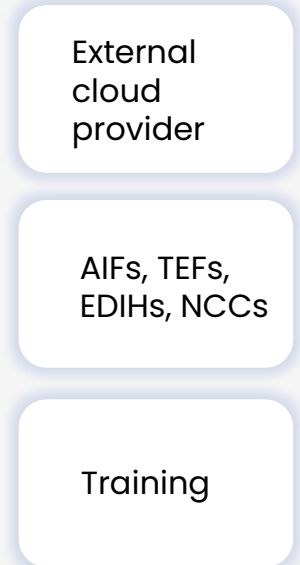
HOW YOU CONNECT



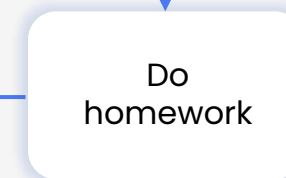
OUR JOURNEY TOGETHER



WHERE WE CAN TAKE YOU



Start your journey
Scan the QR code to fill in our contact form.



Trustworthy AI

Prototype (off-boarded)



Applied AI
Sweden

Presented by: Laurynas Adomaitis

Image source: Press release

The Company:

Applied AI Sweden AB

The Problem:

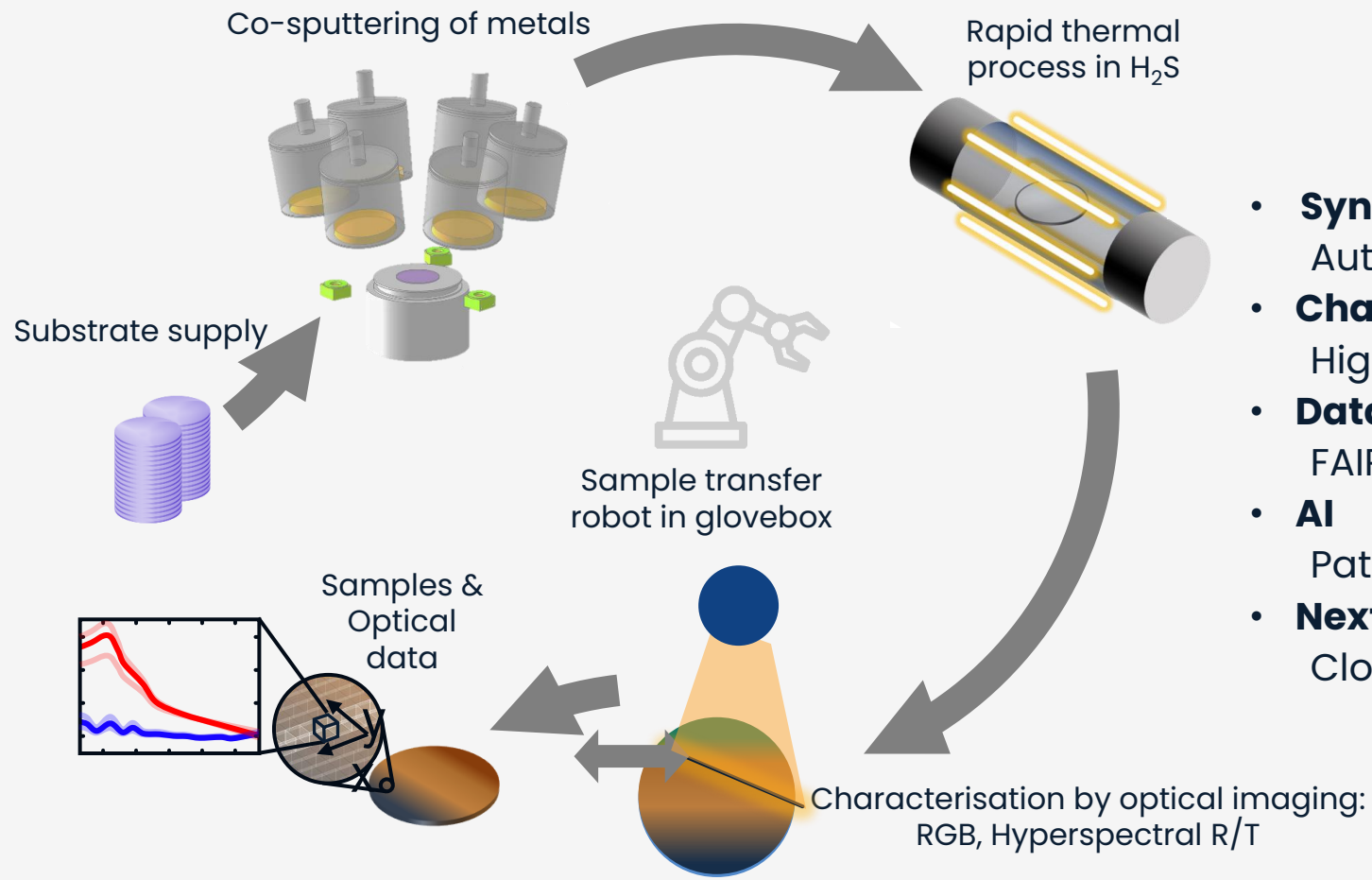
The company wants to evaluate the ethics readiness level of their agentic AI elderly care application. They approached Mimer looking for help into the ethics evaluation among others.

How Mimer Helped:

Mimer Team (Laurynas Adomaitis) went through the process of ethics readiness evaluation of their Agentic AI application prototype with the representative from Applied AI Sweden, and also made them aware of the ethics evaluation results. The evaluation was provided with an exit report. They are now able to apply the learning, with opportunity to come back to Mimer for follow-up if necessary.

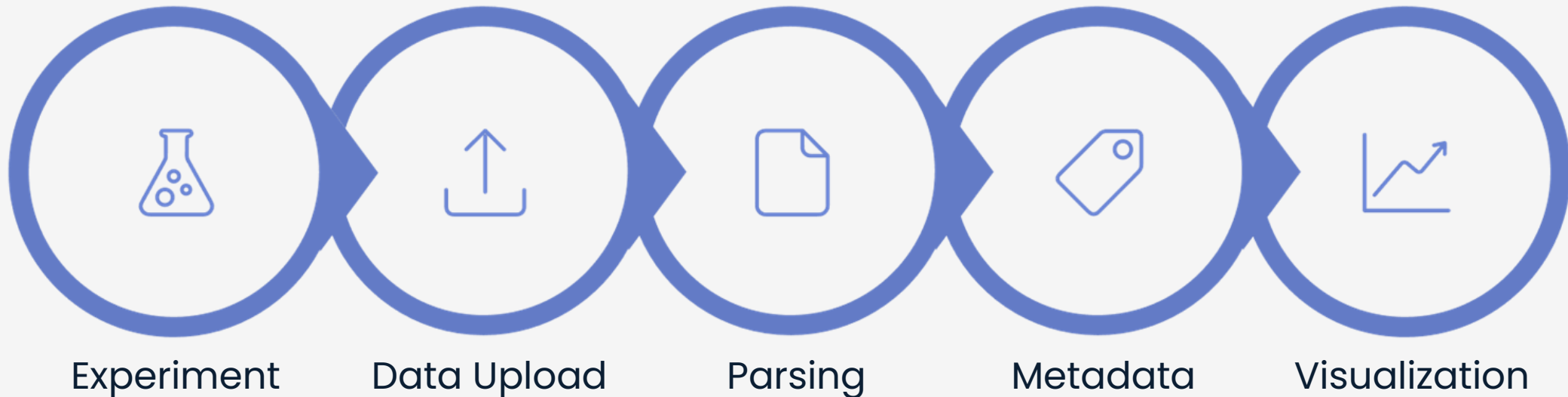
“It was genuinely helpful to discuss the solution design at this depth”

Autonomous Research Loop



- **Synthesis**
Automated deposition of combinatorial samples
- **Characterization**
High-throughput imaging and spectroscopy
- **Data**
FAIR storage with rich metadata
- **AI**
Pattern discovery and experiment recommendation
- **Next Experiment**
Closed-loop autonomous decisions

Autonomous Research Loop – Data Governance



- Each step is triggered automatically, ensuring data integrity and full provenance from instrument to repository.

Custom Software Bridges Experiment and FAIR Infrastructure

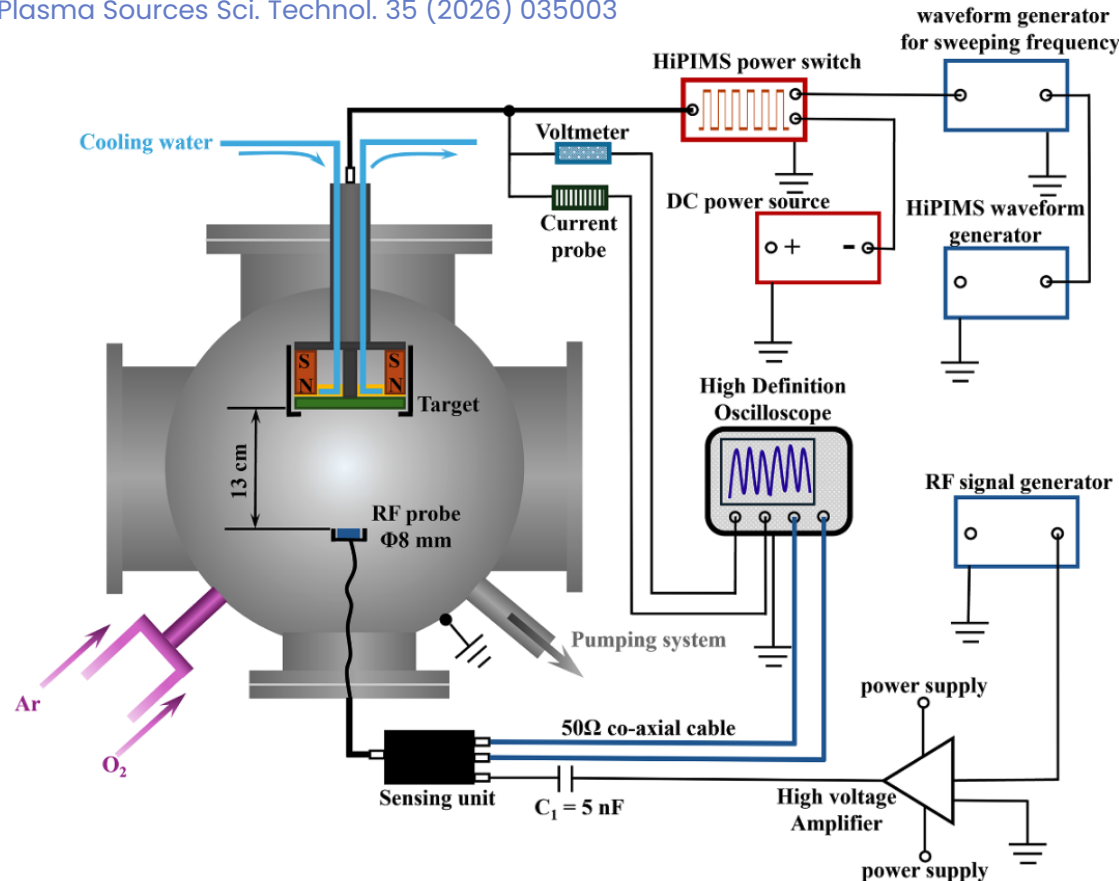
- To connect experimental instruments with NOMAD Oasis, we support developing custom parsers and visualization tools that automatically structure raw data into FAIR-compliant records.

Autonomous Research Loop – Optical Property Inference



Non-invasive High-Power Impulse Magnetron Sputtering Monitoring

Plasma Sources Sci. Technol. 35 (2026) 035003



Schematic diagrams of the radio frequency Sobolewski plasma characterization setups at the substrate side

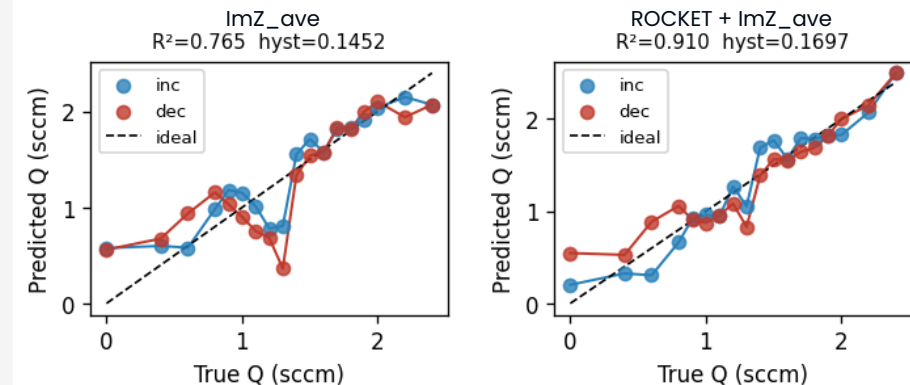
Project Objectives:

To Identify a monitored signal that exists:

- Monotonous trend as a function of the reactive gas flow rate
- Diminishing hysteresis
- Weakening scattering character

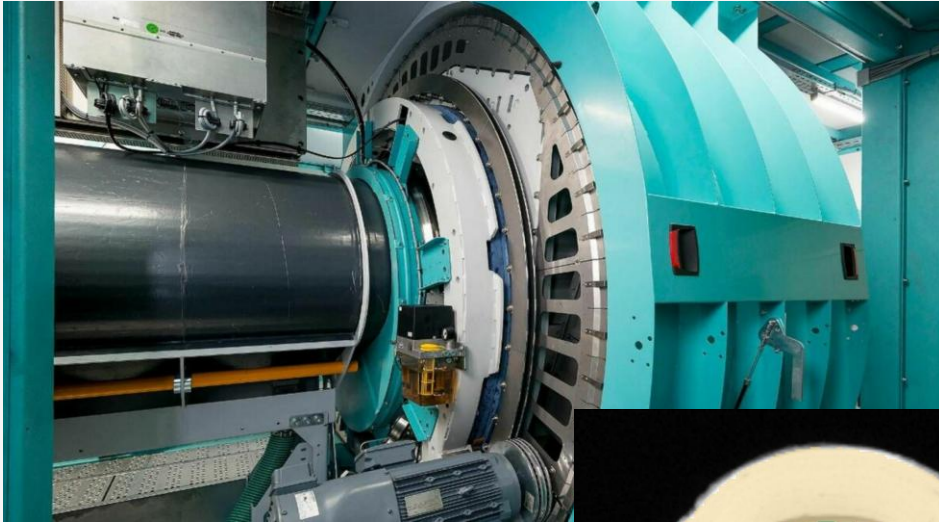
Machine learning techniques:

- RandOm Convolutional KErnel Transform (ROCKET) feature extraction and regression



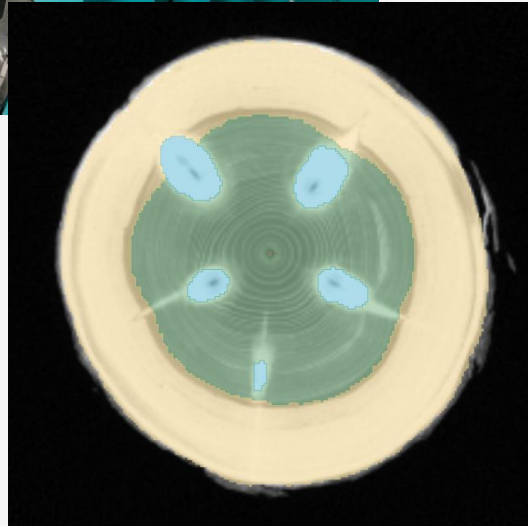
Imaginary part of sheath impedance

Sawmill: Automated Knot Detection



Neural network

automatically detects
internal features (knots)
in X-ray scans of timber



Optimization of sawing pattern

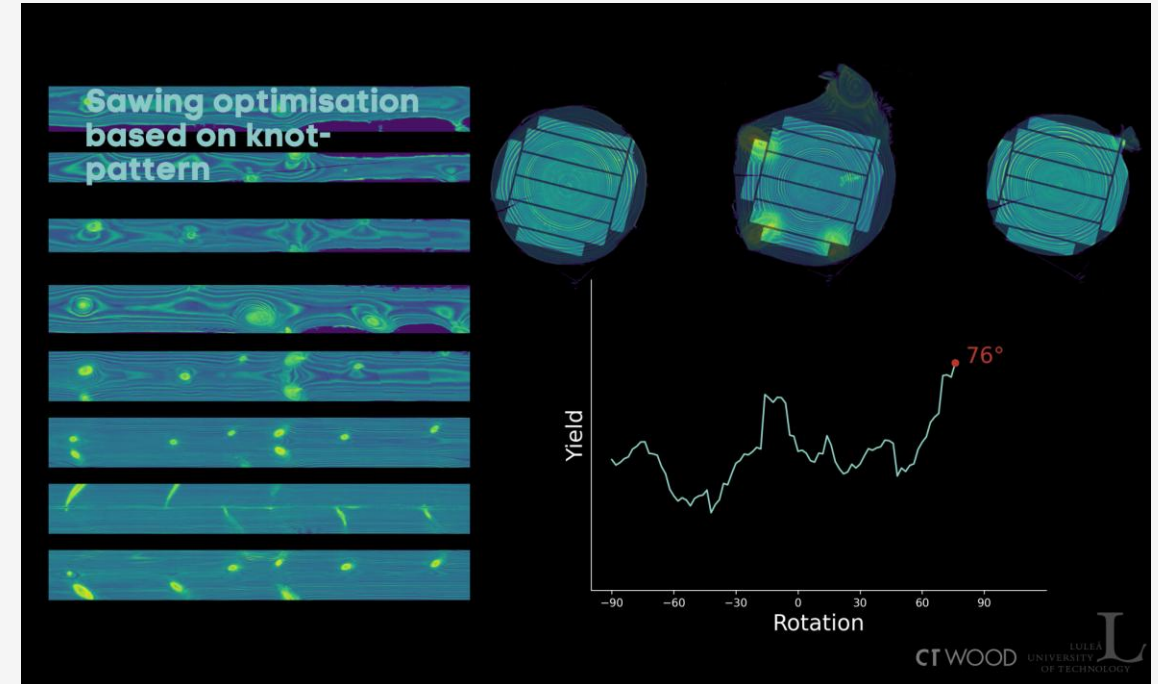
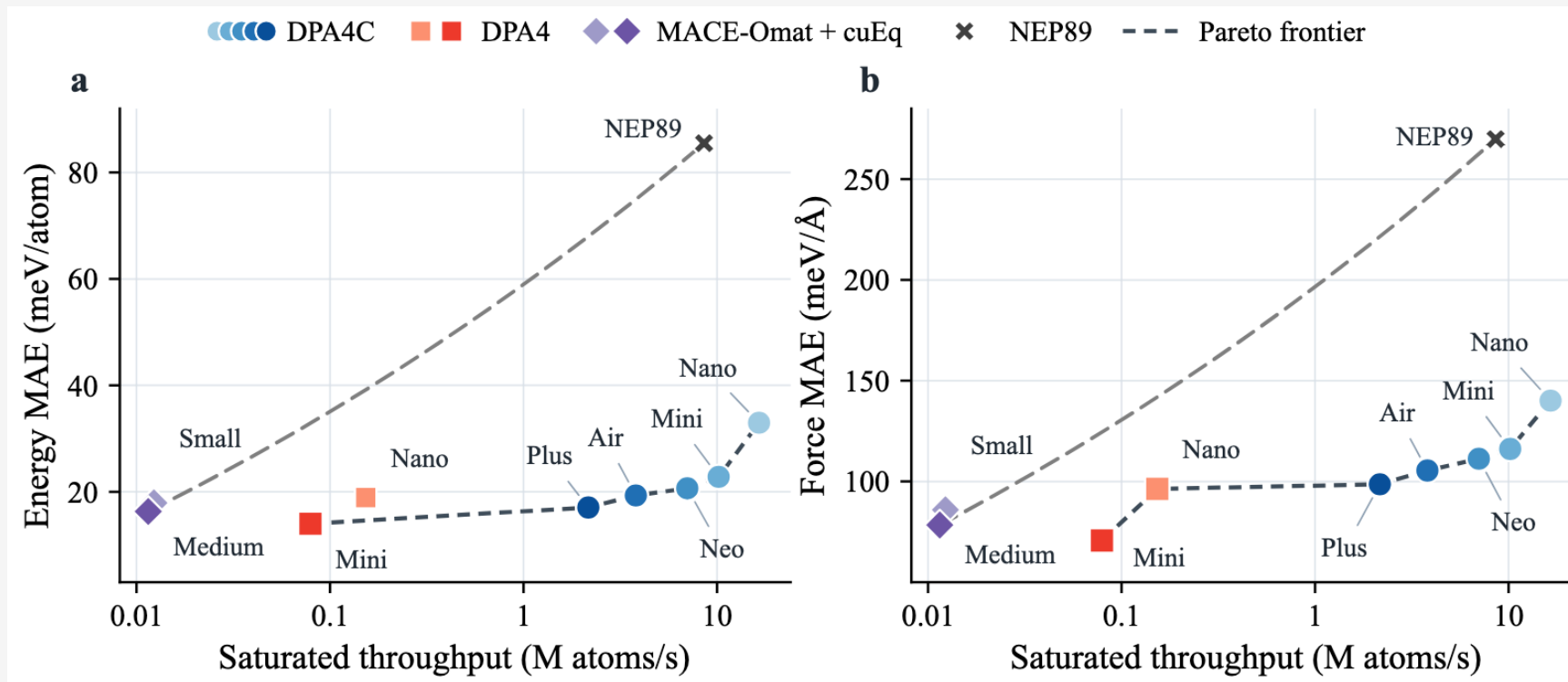


Figure: Yunbo Huang, Luleå University of Technology

Performance Benchmarking and Optimization of Machine-learning Interatomic Potential (MLIP)

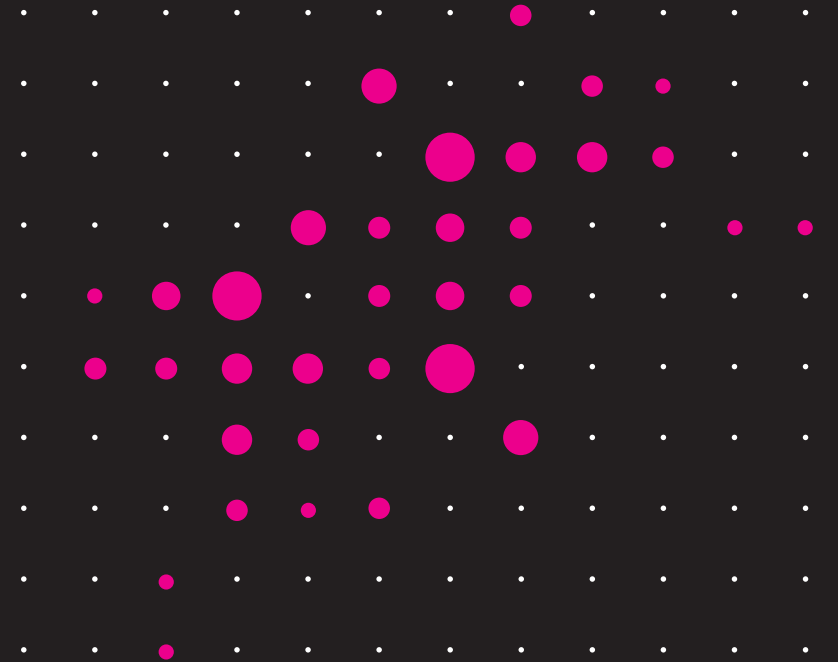


arXiv:2608.19041v2

Accuracy and saturated of throughput on OMat24 (on one NVIDIA H20)

- MLIP training and fine tuning for metastable metallic precipitate phase
- GPU acceleration to allow contributing thermodynamic models of those metastable phases to OpenCalphad community

Physics and supercomputers



Physics and supercomputing - examples (1)

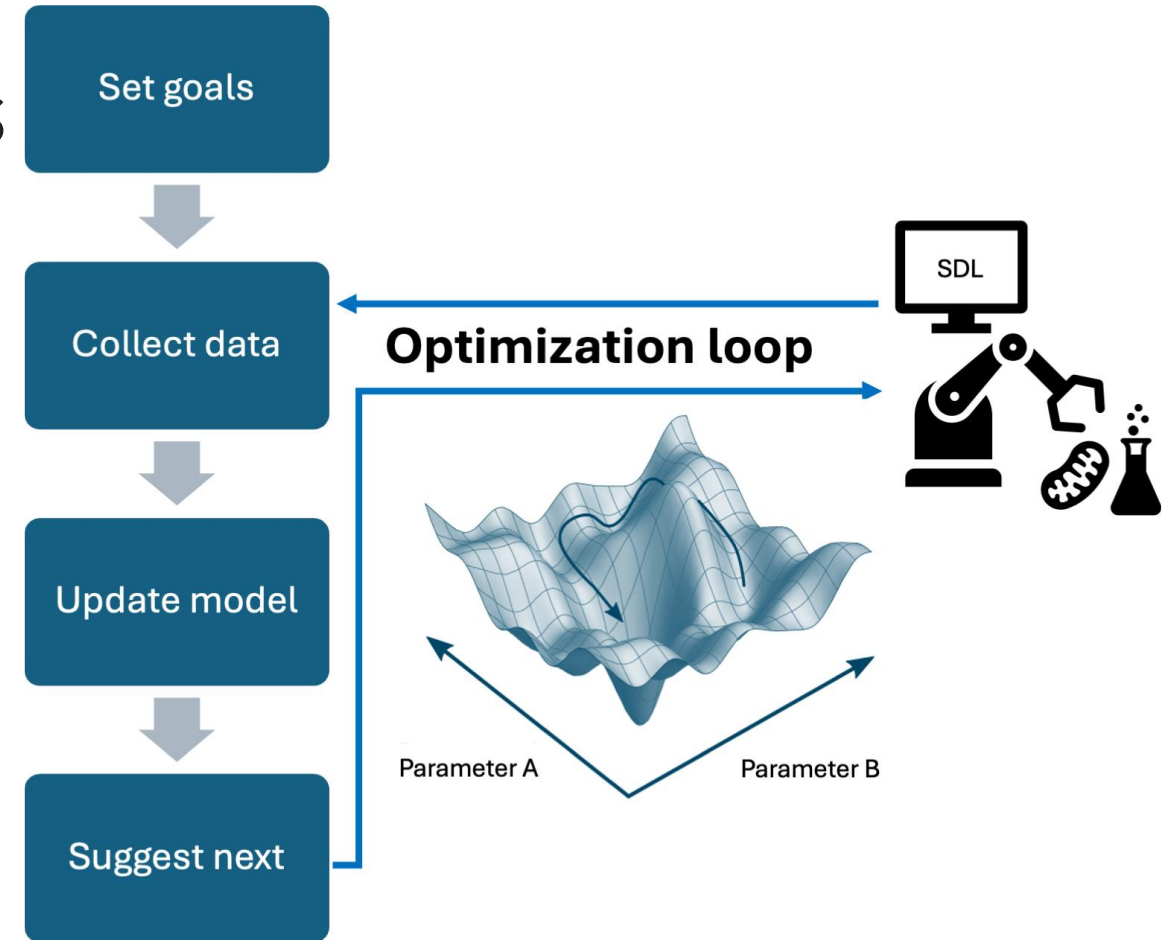
- Theoretical models have been run on supercomputers for decades
 - Example: calculations on Frontier
- Linking Detectors to Supercomputers for Real-Time Nuclear Physics Analysis at Berkeley Lab [1]
- AI aided tuning of accelerators at Argonne National Laboratory

[1] <https://www.hpcwire.com/off-the-wire/berkeley-lab-links-detectors-to-supercomputers-for-real-time-nuclear-physics-analysis/>

Nuclear physics and supercomputing LUMI AI Factory

- examples (2)

- One of the fastest computers in the world: El Capitan
 - Primary purpose is to support the stockpile stewardship program of the US National Nuclear Security Administration
- Future:
 - AI & quantum
 - Self-driving labs [2]



[2] Tobias AV, Wahab A. 2025, Autonomous 'self-driving' laboratories: a review of technology and policy implications. R. Soc. Open Sci. 12: 250646

Concluding remarks



- **LUMI** – available since 2022 for academia/research, public and private sector
- **LUMI AI Factory** empowers Europe's aspirations in AI, high-performance computing and "AI for X" with an advanced HPC+AI+QC platform, together with an unprecedented set of services
- **Sweden AI Factory** - from learning and expert guidance, to access to AI-optimised supercomputing resources
- **Physics applications** – plenty of opportunities not only for material science