

ANTWERP

Centres of Excellence

Deploying Flagship Codes on EuroHPC Supercomputers



HiDALGO2 – Overall status

Marcin Lawenda

Centres of Excellence: Deploying Flagship Codes on EuroHPC Supercomputers

EuroHPC Summit 2024, March 19th, 2024, Antwerp, Belgium



EuroHPC
Joint Undertaking

Grant number: 101093457

Mission

- Bring together advanced solutions (HPC, HPDA, AI) to provide stakeholders and decision-makers tools that would mitigate tragic consequences of climate and civilization phenomenon by delivering necessary knowledge

Vision

- Extend the possibilities of the world's leading scientific applications in the field of environmental protection to effectively analyse phenomena, on a large scale and with high precision, that threaten human life and health.

Consortium composition

9 partners from 7 countries:

- **Instytut Chemii Bioorganicznej Polskiej Akademii Nauk (PSNC)** – Poland – Coordination, Use case owner
- **University Of Stuttgart (USTUTT)** – Germany – Technical Coordination
- **ATOS Spain SA (ATOS)**– Spain – Quality Manager
- **Szechenyi Istvan Egyetem (SZE)** – Hungary – Use case owner
- **Meteogrid SL (MTG)** – Spain – Use case owner
- **Universite De Strasbourg (UNISTRA)** – France – Use case owner
- **Friedrich-Alexander-Universitaet Erlangen-Nuernberg (Fau)** – Germany – Use case owner
- **Erevnitiko Panepistimiako Institouto Systimaton Epikoinonion Kai Ypolgiston-EMP (ICCS)** – Greece – Data analytics and AI support
- **Future Needs Management Consulting LTD (Future Needs)** – Cyprus - Dissemination



Use cases



Urban Air Project

Evolution of the air in the urban areas considering pollution, wind, comfort and planning.



Urban Buildings

Advanced building models for better integration with urban architecture. Providing a source term for heat and air pollutants (CO₂ and NO_x) to the urban air pollution model.



Renewable Energy Sources

Energy production from renewable sources like wind and solar panels. Solution accustomed to urban and rural areas



Wildfires

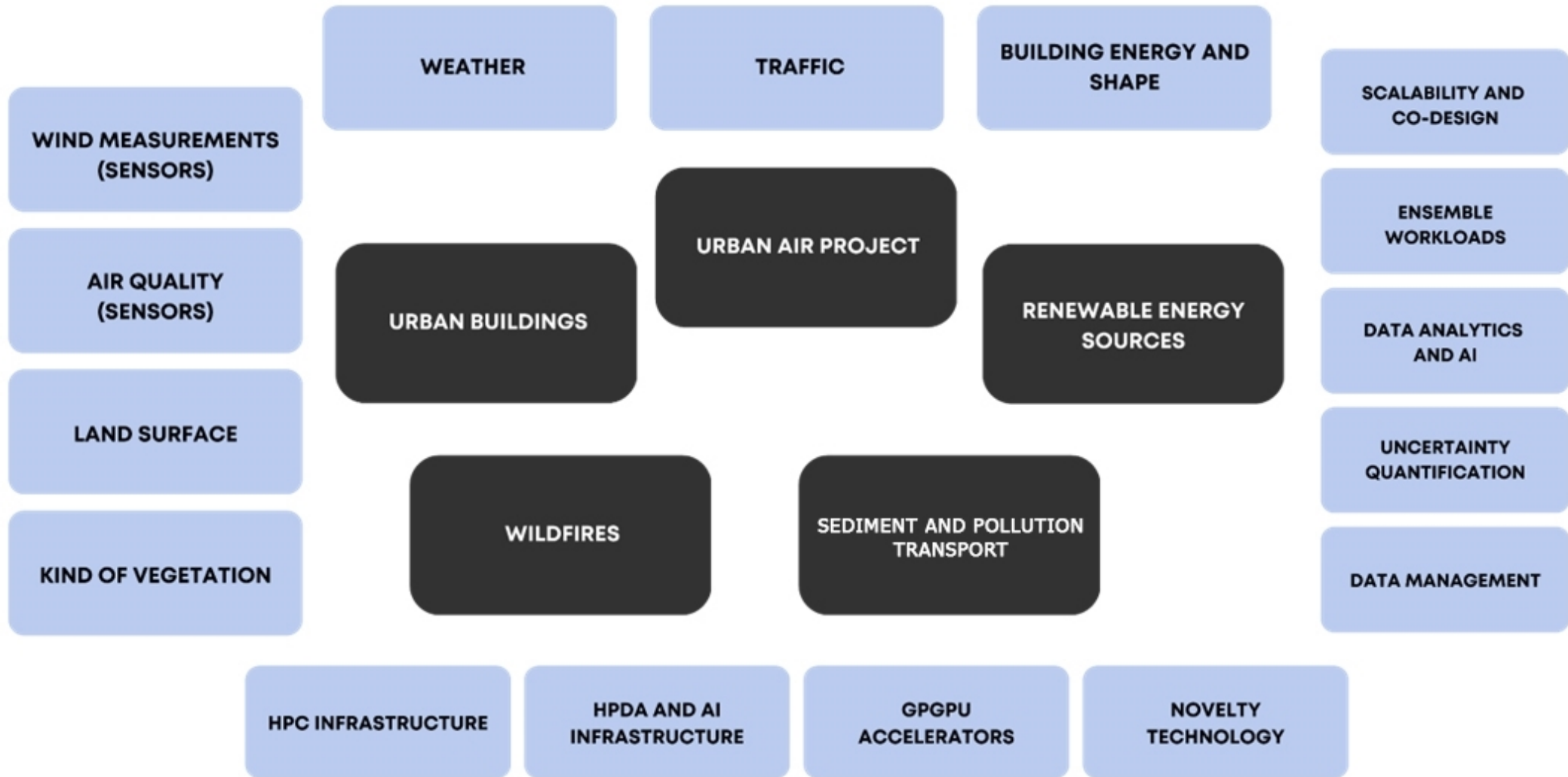
Simulation of wildfire atmosphere interactions and smoke dispersion in forest and urban areas.











Sediment and Pollution Transport

Direct numerical simulation of environmental multiphase flows including phase transitions of sediment transport and the spread of pollutants in water











Project components



Service Support

	Service	Description
	Website	Project Website
	Askbot	User Forums
	Zammad	User Support
	Wiki	Knowledge Management
	Moodle	Learning Platform
	Open Project	Project Management
	Bitbucket	Git Repository
	Gitea	Git Repository

Development Support

	Service	Description
	MathSO Portal	Workflow Orchestrator
	QCG Portal	Workflow Orchestrator
	Prototype	Compute Cluster
	JupyterHub	Jupyter Notebooks
	Keycloak	Identity Management
	Zabbix	Monitoring Infrastructure
 	CKAN/Hadoop	Data Management System
 	Kafka/ElasticSearch	Streaming Data Services

EuroHPC System Access Coverage

System	Partition	RES	UAP	UB	WF	Benchmarking
Discoverer	CPU	Yellow	Green	Yellow	Yellow	Green
Karolina	CPU	Green	Red	Yellow	Green	Green
	GPU	Red	Green	Red	Red	Green
LUMI	CPU	Green	Green	Yellow	Green	Green
	GPU	Red	Yellow	Red	Yellow	Green
Meluxina	CPU	Green	Green	Yellow	Green	Green
	GPU	Red	Yellow	Red	Green	Green
	FPGA	Red	Red	Red	Red	Red
Vega	CPU	Yellow	Yellow	Yellow	Green	Green
	GPU	Red	Green	Red	Green	Green
Leonardo	CPU	Yellow	Yellow	Yellow	Yellow	Green
	GPU	Red	Yellow	Red	Red	Green
MareNostrum5		<i>System not available yet</i>				
Deucalion		<i>System not available yet</i>				

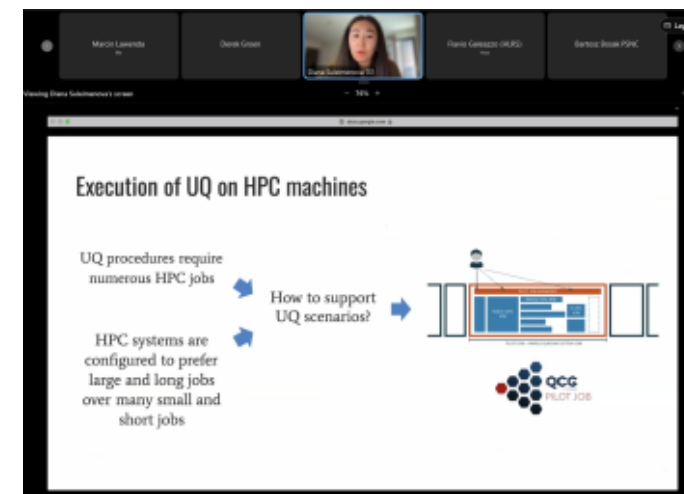
- **green cell** indicates that access has been awarded
- **yellow cell** indicates that a partner is waiting for or intends to request access
- **red cell** denotes a system that we are not yet targeting

Access methods:

- Public repositories
- CASTIEL2 repository
- HiDALGO2 portal (MathSO and QCG Portal)

Pilot	Partner	Applications	Code repositories
UAP	SZE	<ul style="list-style-type: none"> • UAP-Foam • RedSim • Xyst 	<ul style="list-style-type: none"> • Internal SZE repository • Internal SZE repository • https://codeberg.org/xyst/xyst.git
RES	PSNC	<ul style="list-style-type: none"> • RES (WRF+EULAG) 	<ul style="list-style-type: none"> • Internal PSNC repository
UB	UNISTRA	<ul style="list-style-type: none"> • Ktirio Urban Building • Feel++ 	<ul style="list-style-type: none"> • Internal UNISTRA repository • https://github.com/feelpp/feelpp
Wildfires	MTG	<ul style="list-style-type: none"> • WRF-Sfire 	<ul style="list-style-type: none"> • Internal MTG repository
SPT	FAU	<ul style="list-style-type: none"> • waLBerla • HyTeG 	<ul style="list-style-type: none"> • https://i10git.cs.fau.de/walberla/walberla • https://i10git.cs.fau.de/hyteg/hyteg

- Collaboration on urban air pollution simulations with **NCC Sweden**
- Collaboration on the prediction of the spreading of wildfires with **NCC Spain**
- Workshop with **exaFOAM** and **EXCELLERAT P2** in Computational Fluid Dynamics focusing on OpenFOAM
- **HiPEAC 2024 Workshop** about topics related to uncertainty quantification, orchestration platforms, and visualisation techniques
- Workshop to identify synergies on Uncertainty Quantification with **SEAVEA** and **CIRCE** (June 2024)



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Disclaimer

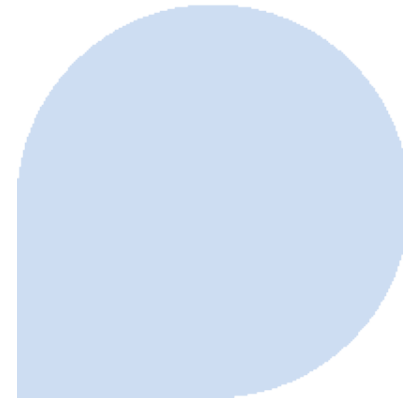
Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European High Performance Computing Joint Undertaking (JU) and Poland, Germany, Spain, Hungary, France, Greece. Neither the European Union nor the granting authority can be held responsible for them.



**Thank you for your
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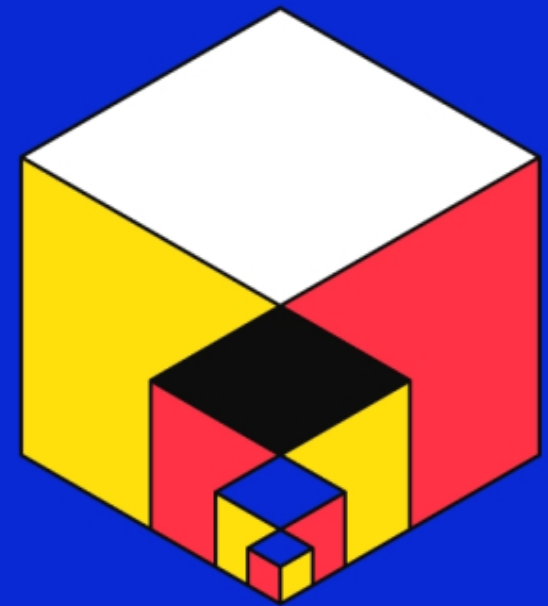
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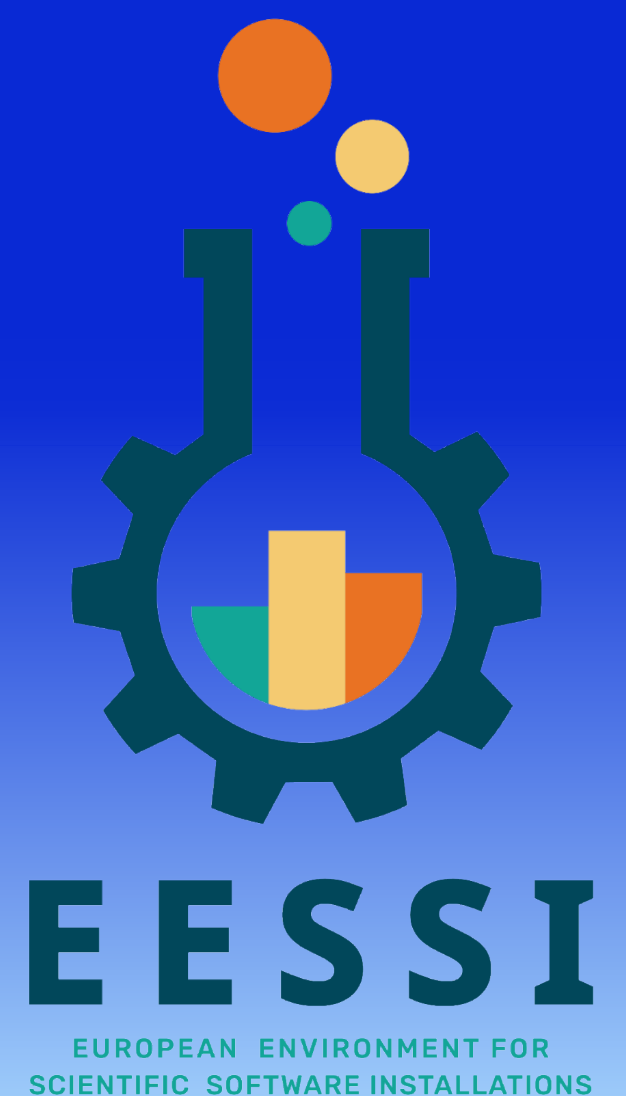
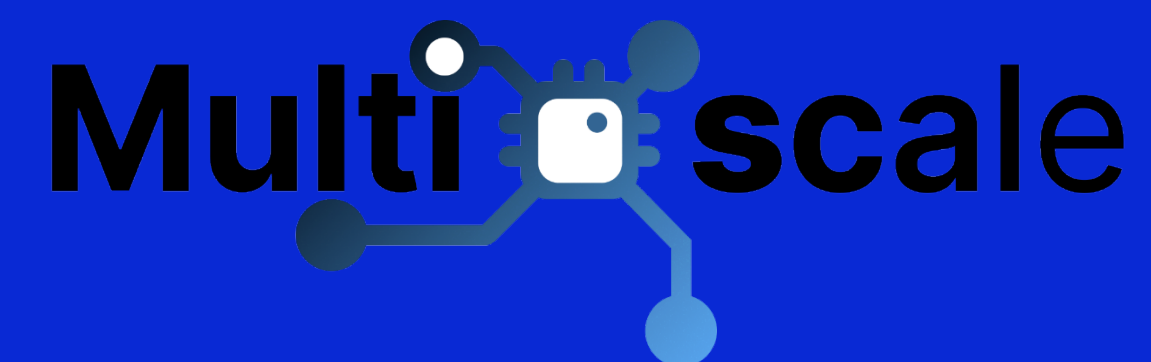


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European Environment for Scientific Software Installations:
Streaming **optimized** scientific software

Alan O'Cais, Technical Manager of MultiXscale



UNLEASHING THE
POWER OF EUROPEAN
HPC AND QUANTUM
COMPUTING

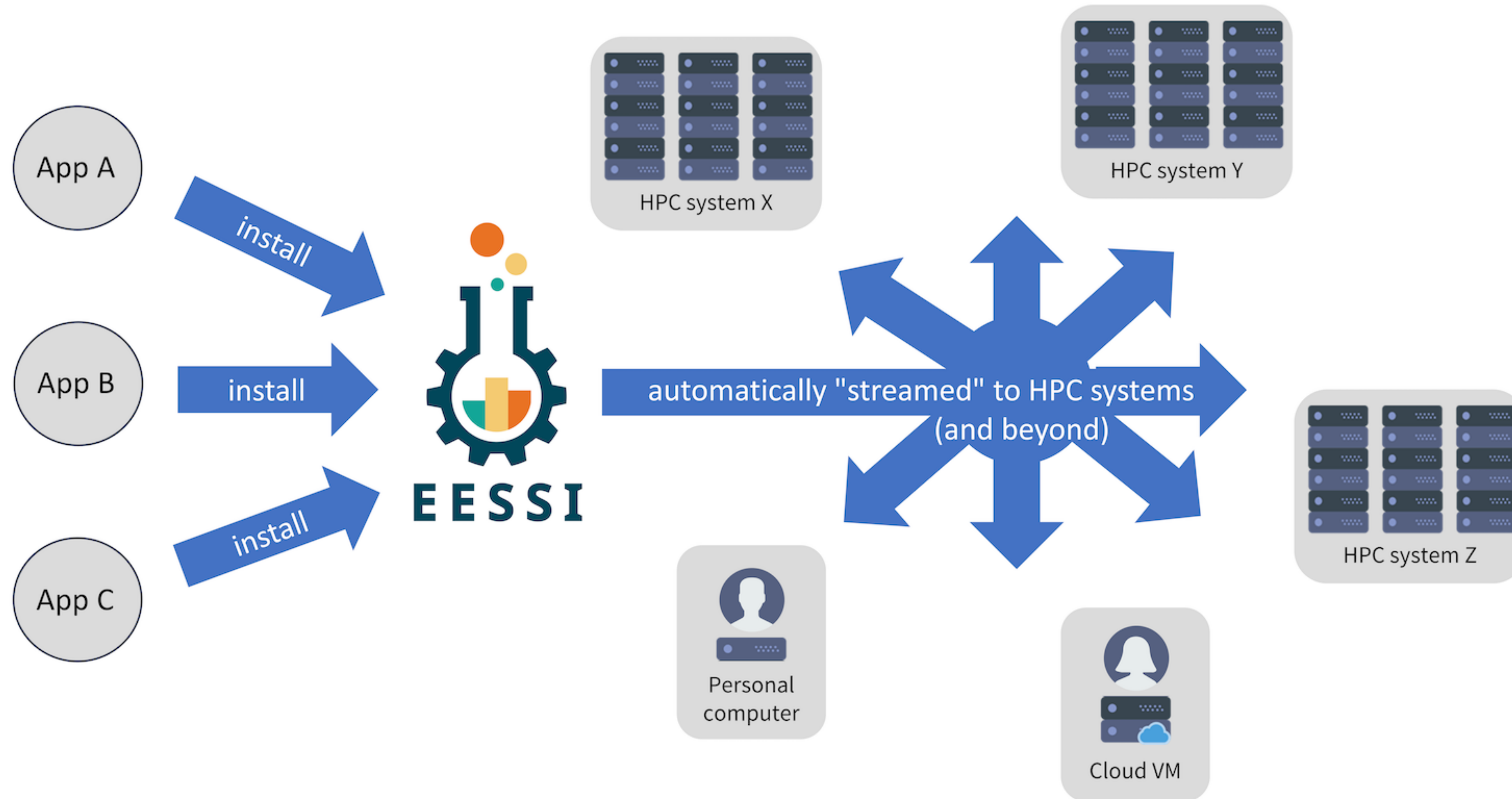


MultiXscale in a Nutshell





MultiXscale after one year



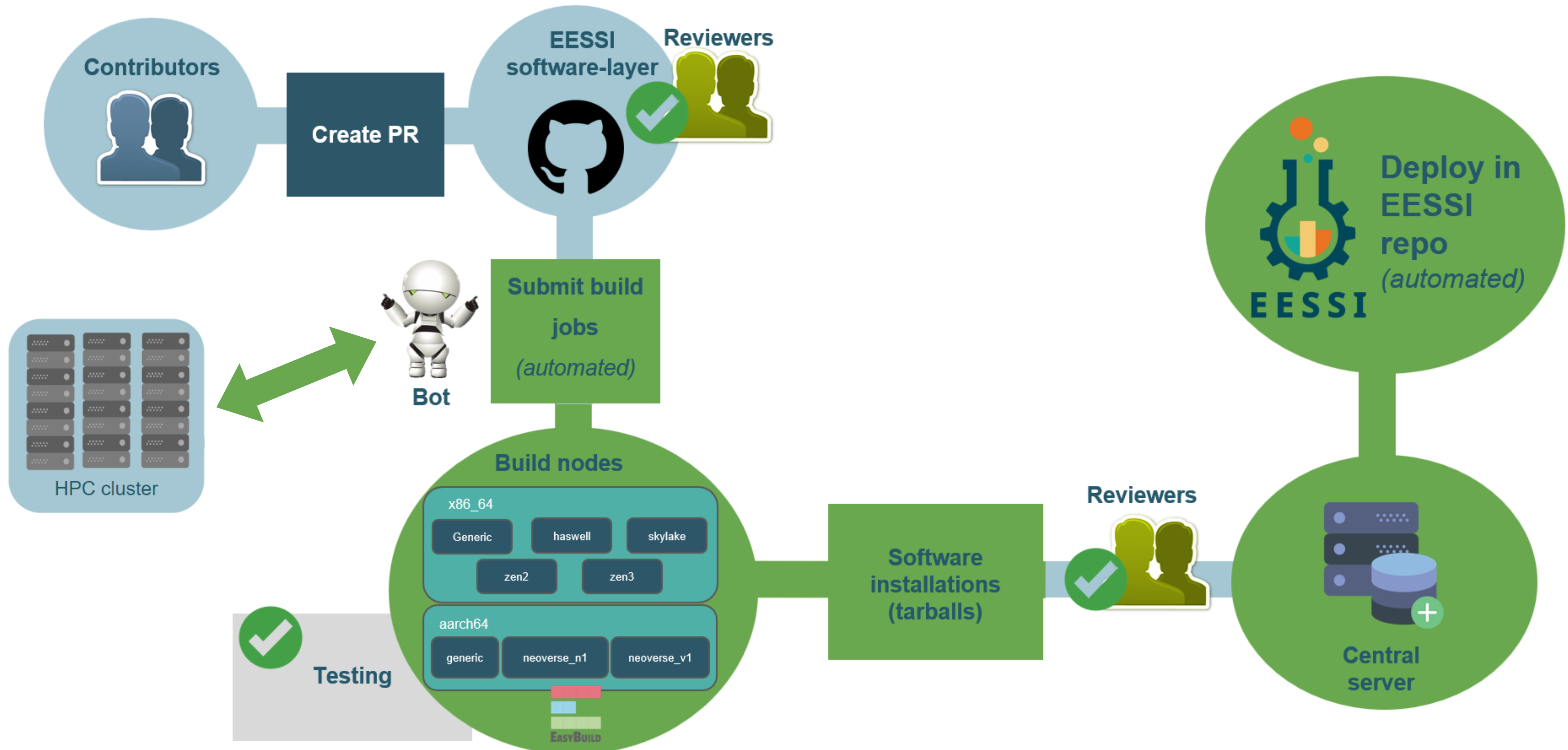


Use cases enabled by EESSI

- A **uniform software stack** across HPC clusters, clouds, servers and laptops
- Significantly facilitates setting up infrastructure for **HPC training**
 - Participants can easily get access to same software environment "at home"
- Enhanced **collaboration with software developers** and application experts
- **Community software and portable workflows**
- Sharing the burden of installing software across HPC sites



EESSI as a community software stack





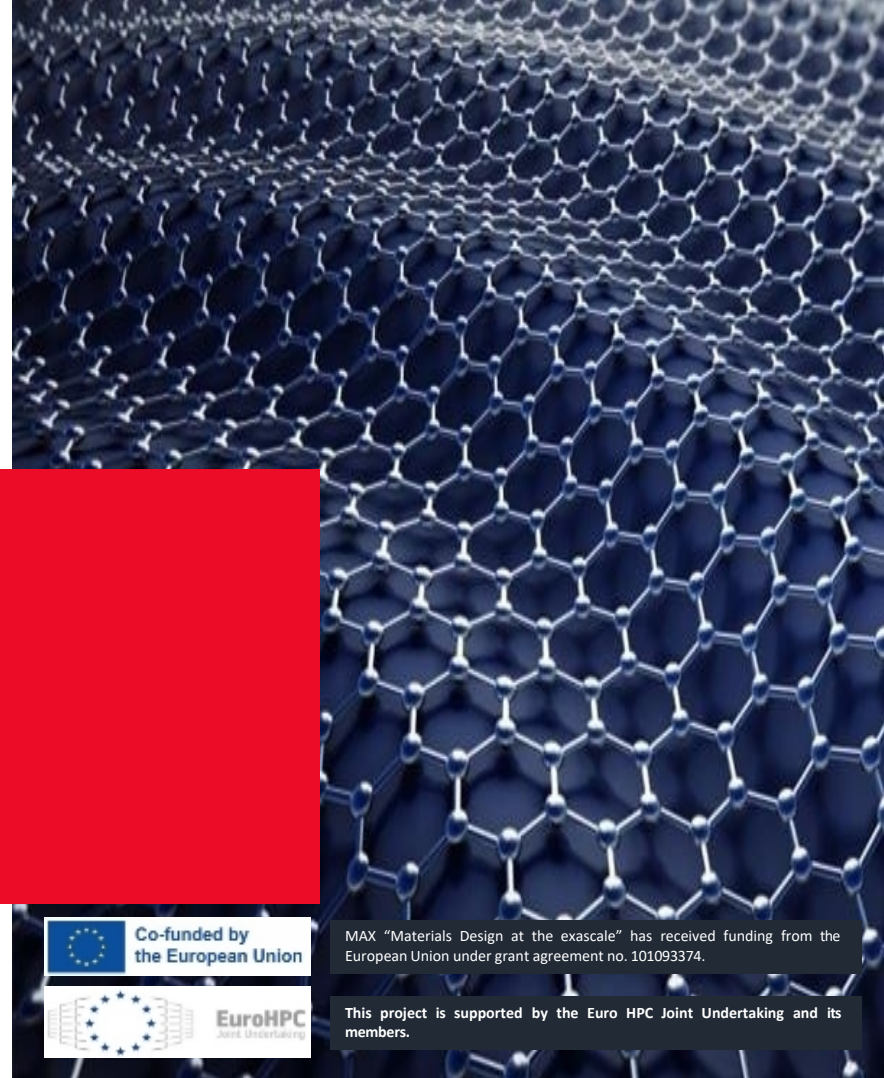
Facilitating CI/CD through EESSI

- Continuous integration and continuous deployment
 - CI is developer-centric and driven by source code
 - Deployments are a broader collaboration driven by artifacts and **environments**.
- EESSI right now is a **continuous deployment solution**
 - Interest from SKA observatory in adopting EESSI
- EESSI is being leveraged in CI use cases
 - EESSI has a GitHub Action
 - Already being done in applications that rely on MultiXscale software
- Scope of services EESSI can support for CI/CD could be greatly expanded

MaX – Materials design at the eXascale

Elisa Molinari and Andrea Ferretti

CNR & UniMoRe, Modena, Italy
MaX Coordinator



MAX "Materials Design at the exascale" has received funding from the European Union under grant agreement no. 101093374.



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

"Centres of Excellence: Deploying Flagship Codes on EuroHPC Supercomputers"
EuroHPC Summit, 19 March 2024

Codes and team

MaX

LIGHTHOUSE
CODES



DOMAIN EXPERTS &
CODE DEVELOPERS



HPC EXPERTS &
DATA CENTRES



TECHNOLOGY &
CO-DESIGN
PARTNERS

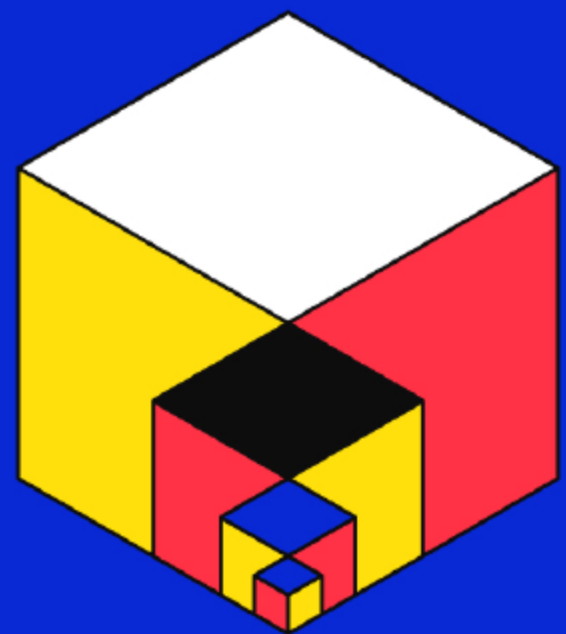


MaX coordination and management – CNR Modena, Italy

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ANTWERP

The Center of Excellence for Exascale in Solid Earth (ChEESE-2P)

EuroHPC Summit Week
Antwerp, 18-21 March 2024

Prof. Arnau Folch
Geociencias Barcelona (GEO3BCN-CSIC)



ChEESE

UNLEASHING THE
POWER OF EUROPEAN
HPC AND QUANTUM
COMPUTING



Project funded by EuroHPC under the grant agreement No 101093038.



ChEESE in a nutshell

ChEESE covers 3 approaches to exascale

1

Capability computing

Solve large monolithic problems that traditionally have been parameterised because are unaffordable with current hardware

2

Capacity computing

Solve ensembles of single problems affordable with petascale-range machines but that can aggregate into an exascale workflow (e.g. data inversion, model data assimilation, uncertainty quantification, etc)

3

Urgent computing

Solve capability/capacity problems under strict time constraints in terms of time-to-solution (emergency situations)

ChEESE sustains on 3 pillars

11

Flagship codes

Open source community codes on seismology, tsunamis, volcanoes, geodynamics, magnetohydrodynamics, and glaciers

9

Pilot Demonstrators

Workflows that address underpinning capability/capacity/UC exascale computational challenges

15

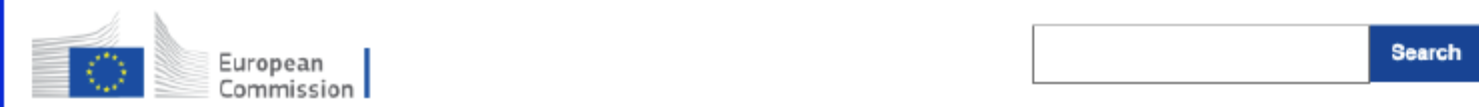
Simulation cases and services

Enabling of services on socially-relevant aspects of geohazards like urgent computing for disaster response, early warning and hazard assessment



Success stories of users (using supercomputers to save lives)

- ChEESE builds on top of consolidated relationships with:
 - **Public sector**, e.g. National-level and European civil protection agencies, governments (decision makers)
 - **Private sector**, e.g. insurance, ATM, reservoir prospection



Home > Research and Innovation > Projects > Success stories > All success stories > Supercomputers help save lives during natural disasters

Supercomputers help save lives during natural disasters

Natural disasters threaten citizens around the world with disruption to essential services, damage to property and infrastructure, and the loss of life. The EU-funded ChEESE project uses supercomputing to help forecast accurate disaster scenarios. As a result, authorities in La Palma were able to make informed decisions and save lives when the Cumbre Vieja volcano erupted.



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Shaping Europe's digital future

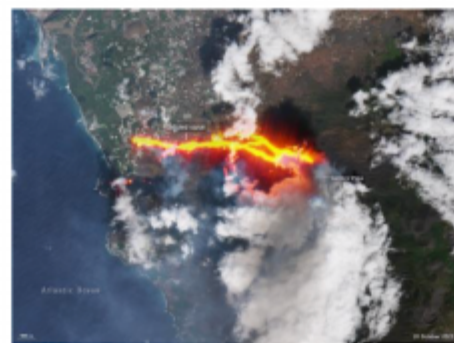
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Home > News & Views > EU Centre of Excellence in High Performance Computing: ChEESE's urgent computing in the service of Cumbre Vieja volcanic eruption

NEWS ARTICLE | Publication 15 November 2021

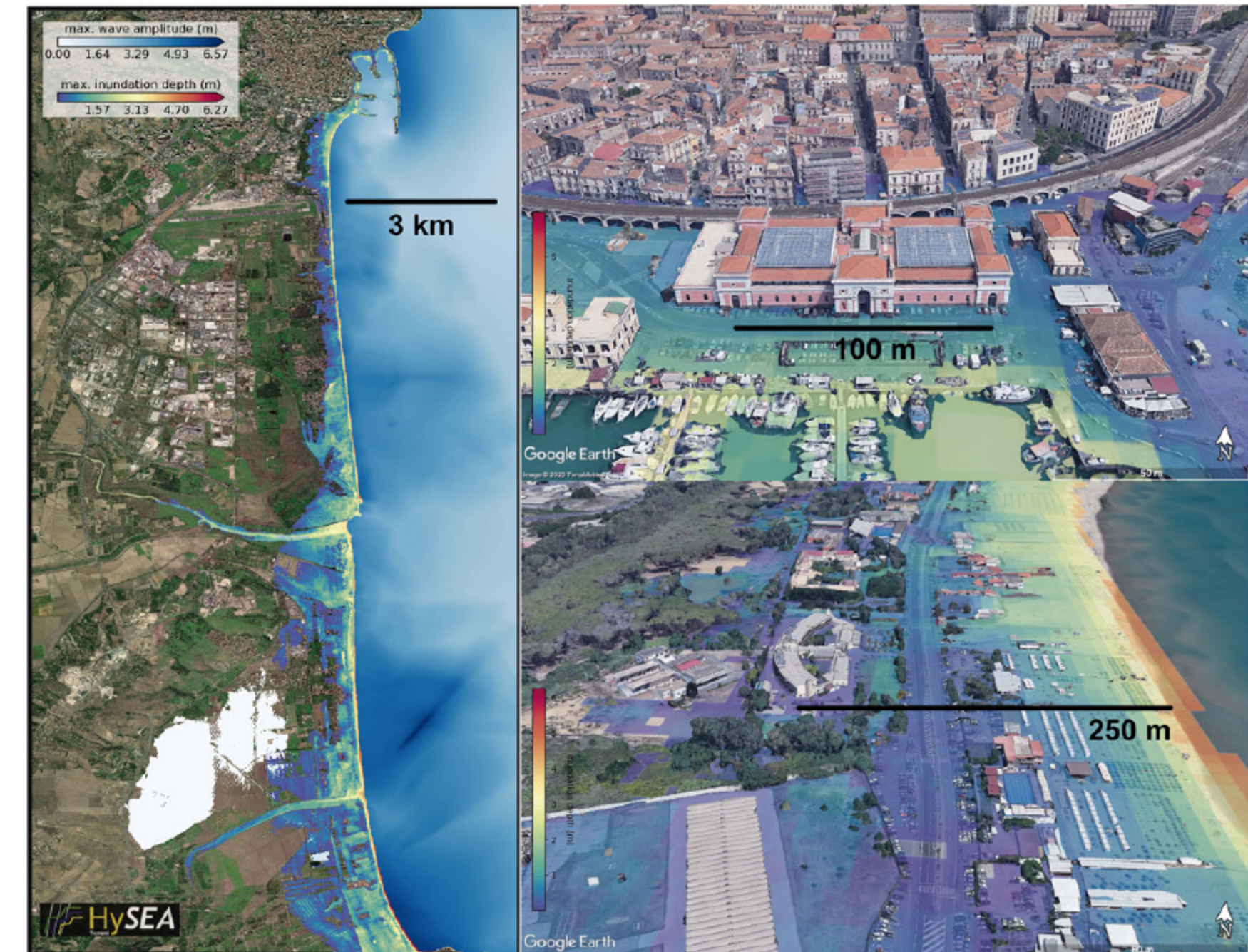
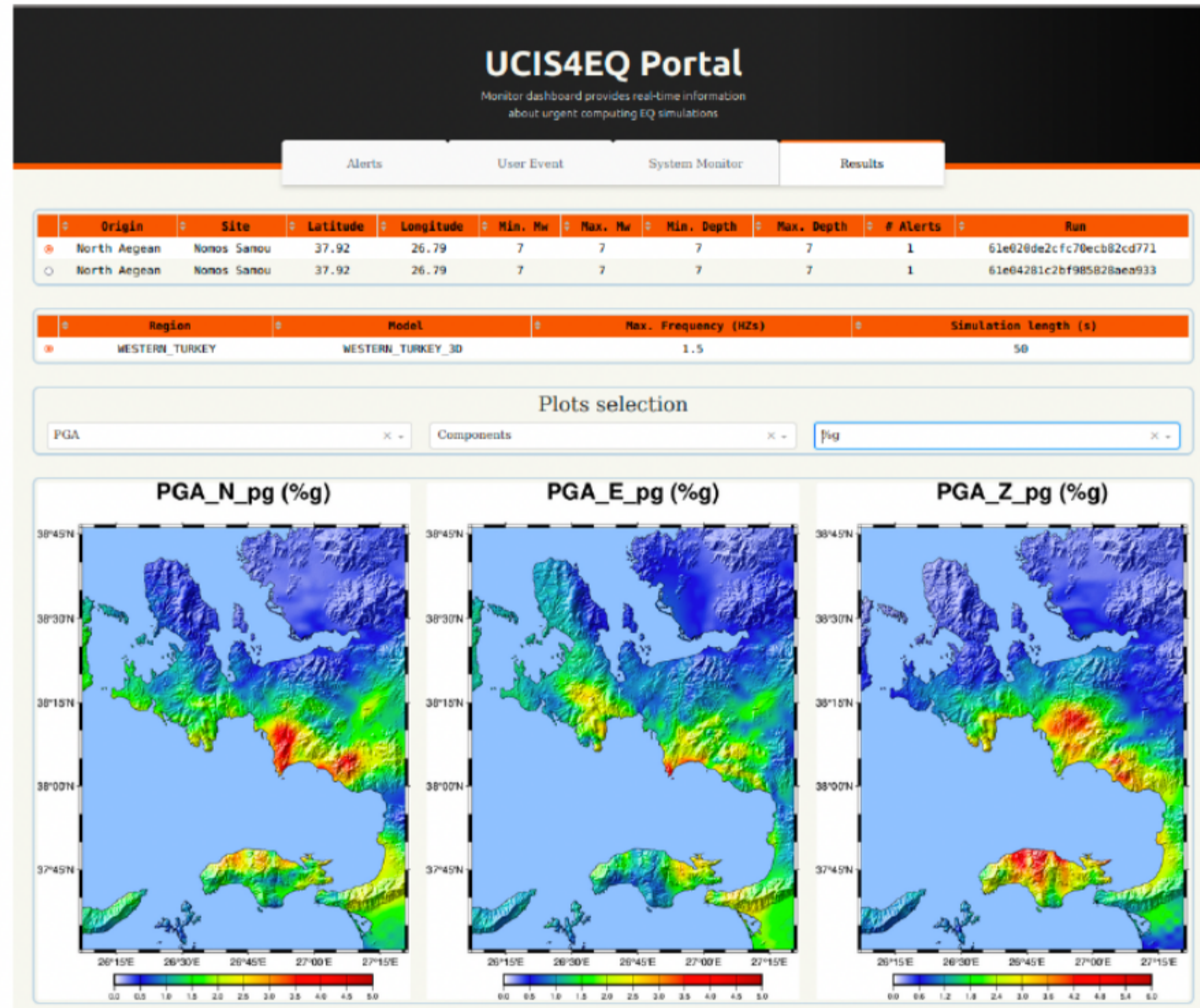
EU Centre of Excellence in High Performance Computing: ChEESE's urgent computing in the service of Cumbre Vieja volcanic eruption

The EU-funded ChEESE Centre of Excellence uses supercomputers to predict the behaviour of volcanic ash clouds and aerosols, helping crisis management of the Cumbre Vieja eruption in La Palma, Canary Islands



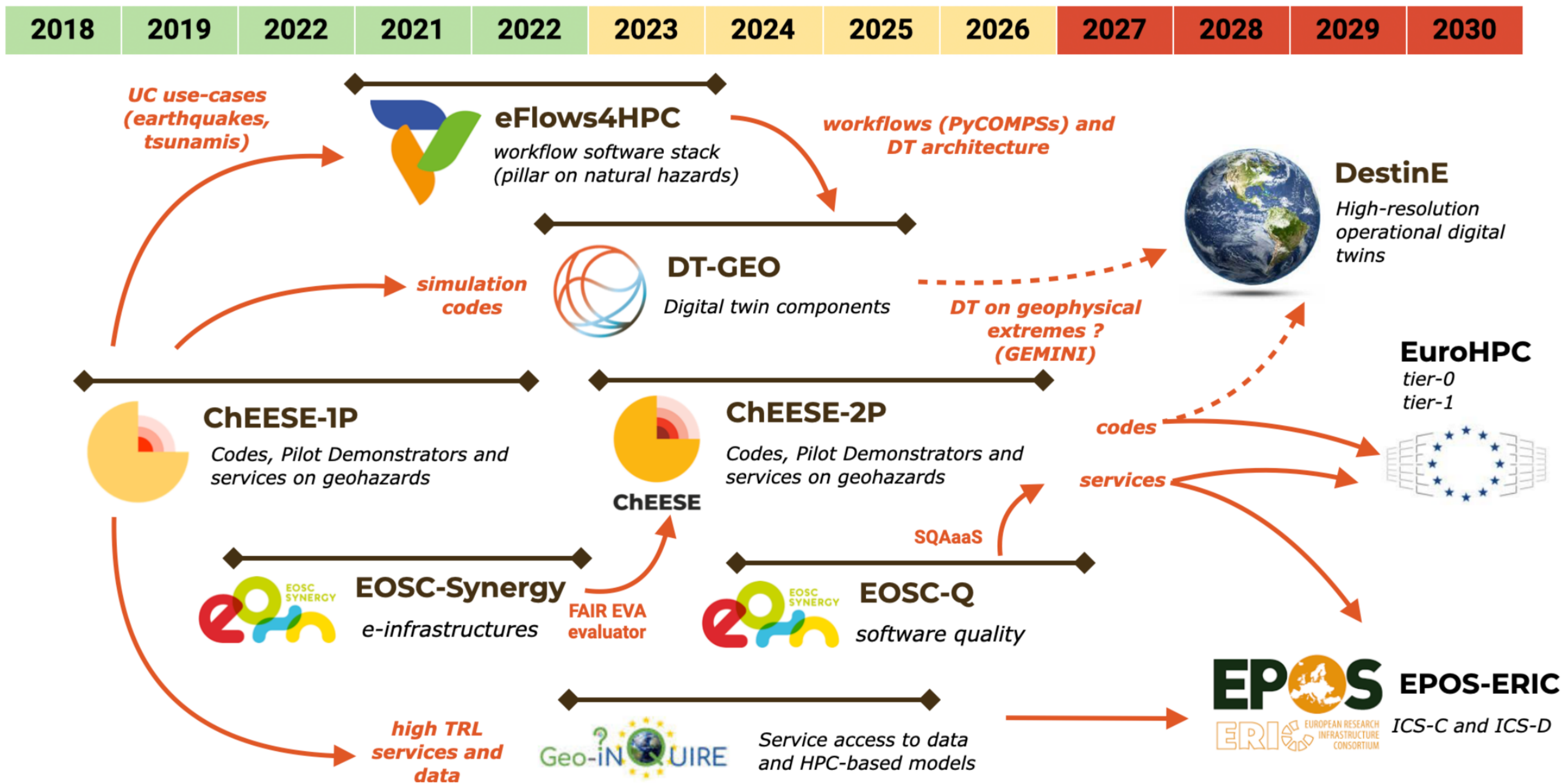
©Copernicus Sentinel-2

The Cumbre Vieja's eruption, which began in September 2021, has produced devastating lava flows and emissions, resulting in the evacuation of more than 6000 people, the destruction of dozens of houses, and the disruption of aerial navigation. In response to this, the "urgent computing" capacities (emergency use of computing resources to deal with disaster situations) of the ChEESE EU Centre of Excellence at the Barcelona Supercomputing Center have been vital. ChEESE scientists have been running simulations of the ash clouds and aerosols triggered by the ongoing volcanic activity, using the MareNostrum-4 pre-exascale supercomputer. These simulations provide forecasts for the eruption's evolution and cover the Canary Islands at a 1 km resolution and the wider region at a 5 km resolution. As a result, the PEVOCLA committee composed of





Community building (binding a scientific community around HPC)





Recent progress (2023 highlights)

- ChEESE code repositories
 - All 11 codes available in open GitLab/GitHub repositories
 - SQAaaS (quality badges): 1 Gold, 7 Silver, 3 Bronze
 - 7 mini-apps for co-design (EuPex/EuPilot)
 - Unity and scalability tests with metadata (FAIRness)
 - Codes mirrored to CASTIEL2 centralised repositories
- Code preparation
 - First audit campaign with POP3 (baseline metrics)
 - Porting/Tuning in the accelerators arena (NVIDIA/AMD)

FALL3D suite

Subgroups and projects Shared projects Archived projects

Q Search

Name

Tests

- Leonardo
 - Audit
 - Constant
 - Scalability
- LUMI
 - audit
 - constant
 - scalability

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6     "comment": "Baseline version without Extrae instrumentation. At M89 of ChEESE-2P project"
7   },
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14    "commitDate": "Mon Nov 06 09:15:29 2023 +0100"
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21    "nodeRAM": "512 GB"
22  },
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41  }
42 }
```




What is needed? (wish list)

- Dedicated access mode
 - CI/CD: mapping 11 codes in 12 partitions is unfeasible (132 development projects?)
 - By-passing the 2FA and limiting security aspects in hosting institutions
- Urgent computing
 - Need for establishment/regulations (joint goal with ESiWACE and DestinE)
- Transversal gluing projects (CoEs are thematic pillars)
 - workflows, AI, solvers, software engineering, services (HPCaaS, WaaS), data analytics, pre and post-process (including data streams), metadata standards and automatic FAIRness, etc.



ANTWERP
18-21 MARCH

TO EXASCALE
AND BEYOND

THANK YOU!