MaX³
MAterials design at the eXascale

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MAX (MAterials design at the eXascale) is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current and future High Performance Computing (HPC), High Throughput Computing (HTC) and data analytics technologies.

QUANTUM ESPRESSO: a suite of applications for ab-initio electronic structure calculations using plane waves and pseudopotentials, supporting self-consistent energies, forces and stresses, structural optimization, molecular dynamics (PW and CP); search for transition path-ways (NEB)

YAMBO implements ground-state as well as excited-state properties in an ab initio context: MBPT, DFT and Non-Equilibrium Green's Function Theory (NEGF) allowing to calculate a wealth of physical properties: reliable band gaps, band alignments, defect quasiparticle energies, optical and non–equilibrium properties.

www.flapw.de

FLEUR is an all-electron density functional theory code based on the full-potential linearized augmented plane wave (FLAPW) method with a versatile DFT code for the ground-state properties of multicomponent one-, two- and three-dimensional solids supporting non-collinear magnetism, the determination of exchange parameters, spin-orbit related properties.

SIESTA is pseudopotential-based density functional theory software using atomic-like strictly-localised basis sets to achieve a given accuracy faster, and the finite support of the orbitals leads to sparsity in the Hamiltonian and overlap matrices in order to use reduced-scaling methods.

BigDFT uses Daubechies wavelets as a basis set for DFT using pseudopotentialsis achieving excellent flexibility, performance and precision. Beyond the traditional cubic-scaling DFT approach, the wavelet-based approach enables modelling DFT calculations of large systems containing many thousands of atoms with linear scalability.

AiiDA is a Python materials' informatics framework to manage, store, share, and disseminate the workload of high-throughput computational efforts, while providing an ecosystem for materials simulations where complex scientific workflows involving different codes and datasets can be seamlessly implemented, automated and shared.

LIGHTHOUSE CODES

DOMAIN EXPERTS & CODE DEVELOPERS

**HPC EXPERTS & DATA CENTRES**

TECHNOLOGY & CO-DESIGN PARTNERS

Partnership

- European leaders in the materials domain
- prominent European HPC centres
- Technology & co-design partners
- training & communication experts

First principles based flagship codes and workflows for materials design since 2018.

MAX coordination and management: Cnr – Modena, Italy

MaX — DRIVING THE EXASCALE TRANSITION

Geographic distribution of authors' affiliation in peer-reviewed publications citing MaX lighthouse codes in 2023

MaX Lighthouse Codes - Total Citations
Source Web of Science

FLEUR BIGDFT YAMBO SIESTA QE
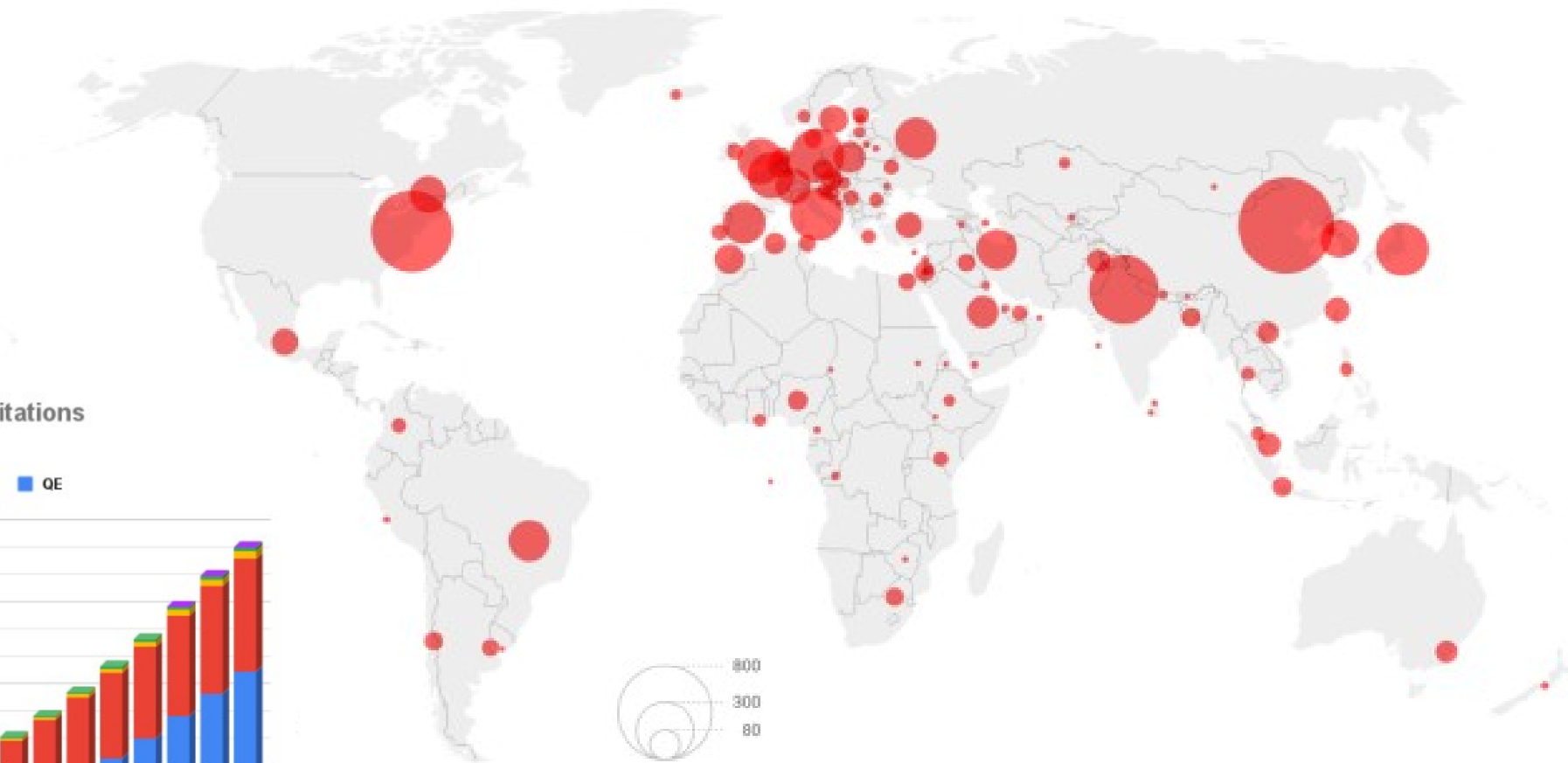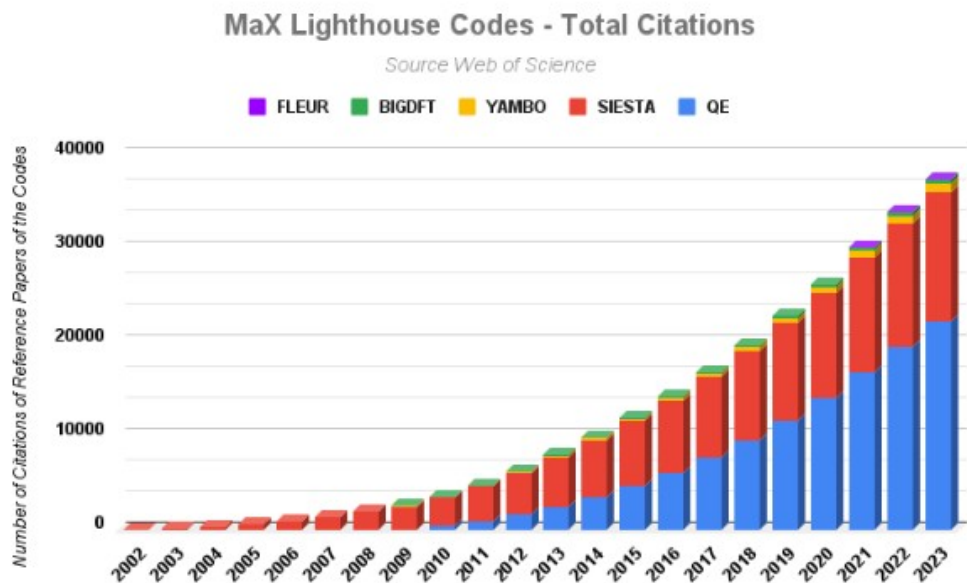
44% of PRACE calls in within the "Chemical Sciences and Materials"

Challenges

- Increased CI/CD, GIT requirement
- Build and benchmark on all HEs
- HE build/module requirements
- Getting HEs to deploy

Technical or Administrative?

- No dedicated access: calls
- No technical access: 2FA
- No services for gitrunners
- Making CD a reality

Getting to KPIs

- Access mode campaign
- Direct access and optimization
- EESSI and EasyBuild
- Buildchain testing
- Getting HEs to deploy

Beyond KPIs

- Access to new hardware
- Testing with miniapps
- Profiling, energy reports
- Security, code quality
- Containers

Uncertain Future

- JU management of grants and reviews
- CASTIEL central services
- European Commission's strategic decisions
- Concept Paper on the EuroHPC R & I funding programme for HPC applications
- RIAG + INFRAG + External Experts Feedback on the Concept Paper
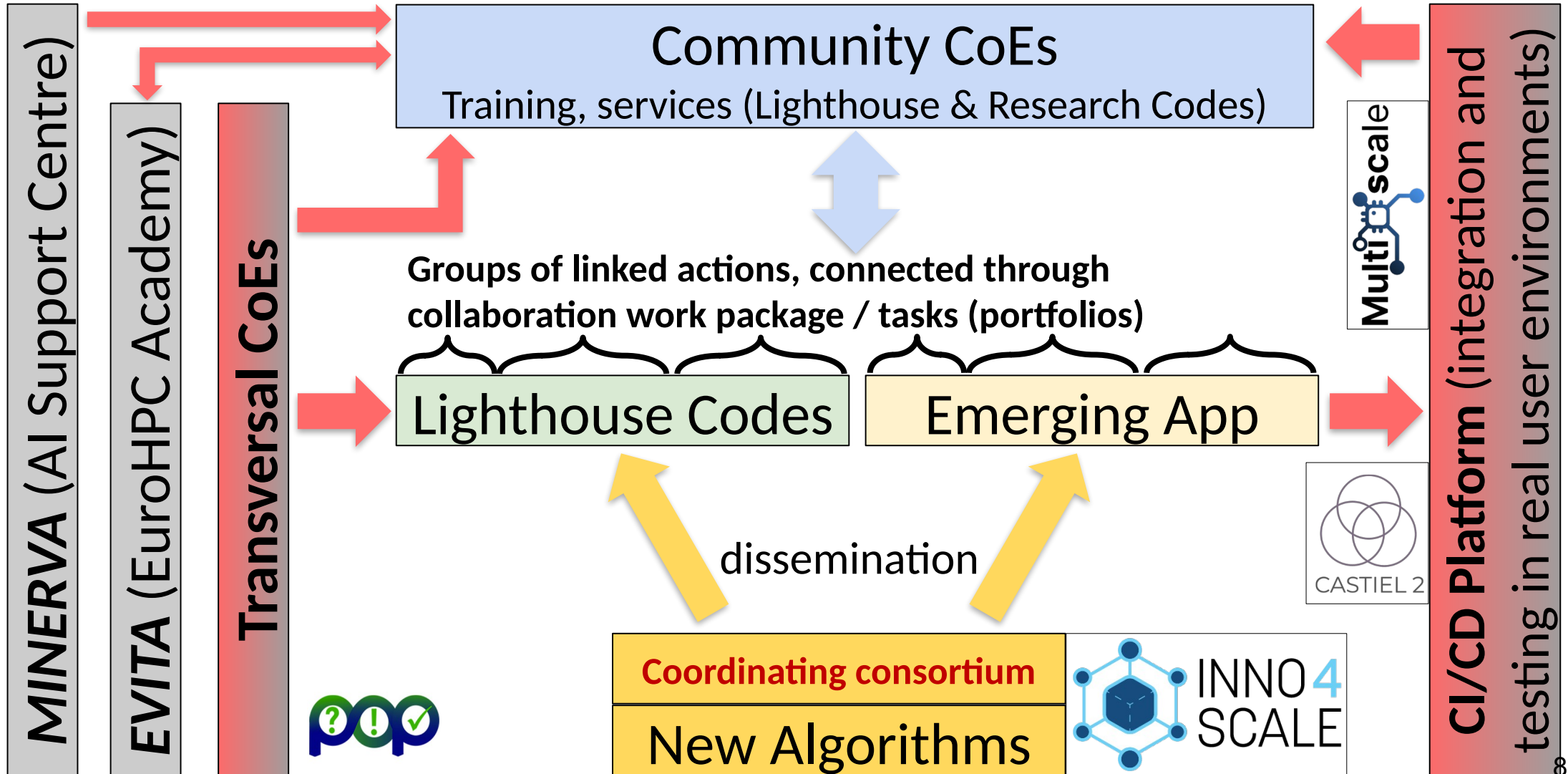- Governance Board Decisions

Avoiding the "closed club" effect, break up multiple structures but with limited number of organizations, member states and participants.

MINERVA (AI Support Centre)

EVITA (EuroHPC Academy)

Transversal CoEs

Community CoEs
Training, services (Lighthouse & Research Codes)

Multiscale

CI/CD Platform (integration and testing in real user environments)

Groups of linked actions, connected through collaboration work package / tasks (portfolios)

Lighthouse Codes

Emerging App

dissemination

Coordinating consortium

New Algorithms

INNO4SCALE

CASTIEL 2

8

Different instruments for distinct objectives

| Applications Support	Proposed action (Work Programme)	Driven by
Use Cases	EuroHPC Access Calls	Users
Workflows	Community CoEs (WP25)	Users
Application Codes	Lighthouse Codes (WP25)	Developers
Libraries	Emerging Technologies (WP24)	Developers
Algorithms	New Algorithms (WP25)	Researchers/Scientists
Tools	Transversal CoEs (WP25) and CI/CD platform (WP24)	Developers

- Actions must **align with the objectives of the relevant community** to be successful and sustainable
- Actions typically overlap with other layers and need **involvement of different target groups**

MAX DRIVING THE EXASCALE TRANSITION
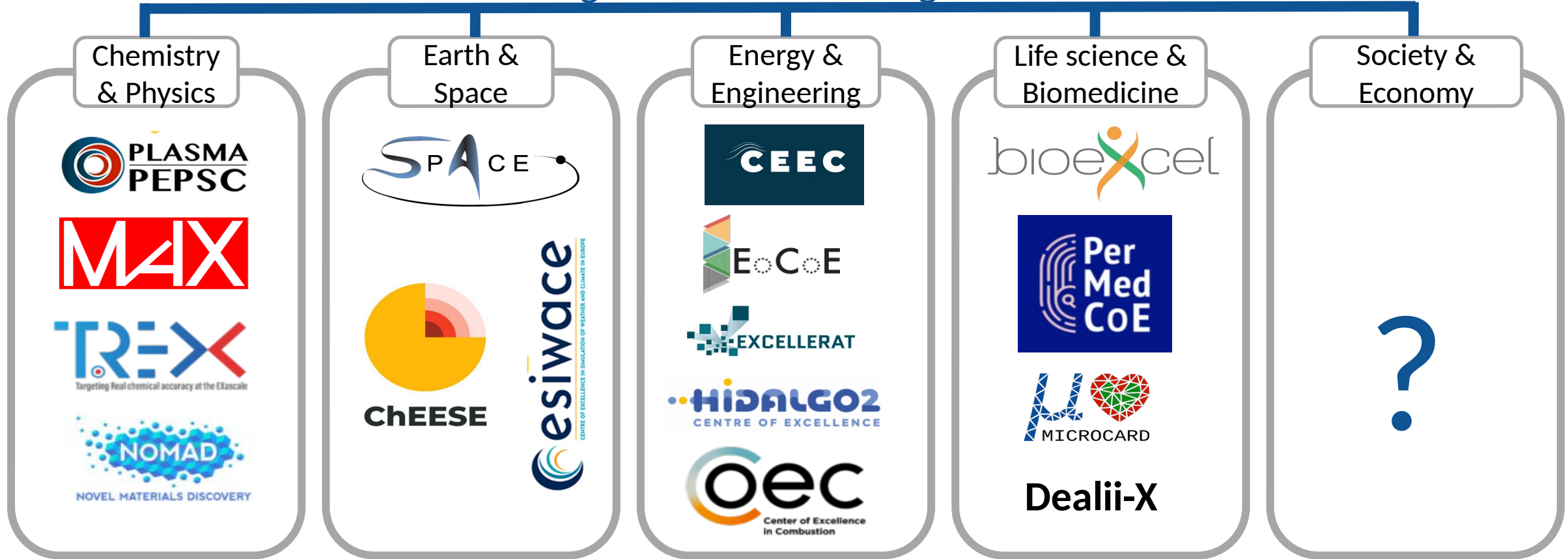
lighthouse code vs. research code: TLR, impact codes/packages, libraries, algorithms

| Use Cases |
| Workflows |
| Applications |
| Libraries |
| Algorithms |
| Tools |

Applications - Call on Lighthouse Codes
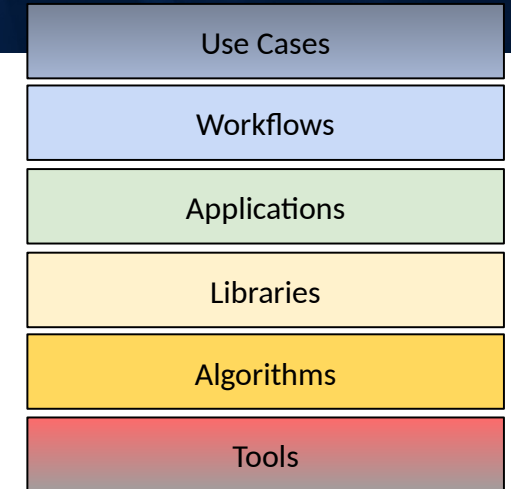## Simple, competitive, fair and transparent and easy to access

Simplified proposals due to technical focus on software development and limitation to one software product per proposal

- Reduced proposal complexity (e. g. page limit) compared to CoEs
- High Technology Readiness Level - Innovation Action to enable private investments
- Small consortia of ca. 5 partners in line with industrial working arrangements

Portfolio approach

- Combine benefits of grants for individual applications (simple and fair evaluation on individual merits) with the coordinated implementation of a grant aggregating multiple applications
- Mandatory collaboration work package/tasks to engage with complementary grants
- JU will adopt a coordinated approach to manage portfolios (small groups of grants)

Not limited to one domain?
Allow up to 3 codes?
Work with community CoEs?