DIGITAL-EUROHPC-JU-2022-NCC-01





Centres of Excellence (CoEs) Industry topics [Public tables]

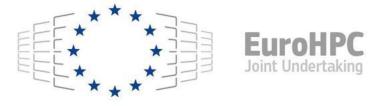
October 2023

Information collected by WP4 of CASTIEL (Industrial Interaction and Business Development) in interaction with the people in charge of industry in the CoEs

Project 101102047

Coordination & Support for National Competence Centres on a European Level Phase 2 Project Number: 101102047





This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101102047. The JU receives support from the Digital Europe Programme and Germany, Italy, Spain, France, Belgium, Austria.

CoEs - Industry topics October 2023 © 2023 Members of the CASTIEL 2 Consortium

List of abbreviations

CASTIEL2 Phase 2 of CASTIEL
CoE Centre of Excellence
EuroCC2 Phase 2 of EuroCC

EuroHPC JU The European High Performance Computing Joint Undertaking

HPC High-Performance Computing

JU Short version of EuroHPC Joint Undertaking

NCC National Competence Centre PMT Project Management Team

PoC Proof of Concept

SME Small and Medium-sized Enterprise

WP Work Package

CoEs - Industry topics October 2023 © 2023 Members of the CASTIEL 2 Consortium

Table of Contents

1	Introduction	6
2	Main goal, structure	6
3	Objectives regarding Industry outreach and provision of services	8

CoEs - Industry topics October 2023 © 2023 Members of the CASTIEL 2 Consortium

List of Tables

Table 1: Goals and structure	6
Fable 2: Provision of services & Services portal	8

1 Introduction

The following information was gathered by WP4 of CASTIEL in interaction with the CoEs between April 2023 and October 2023. The information in this document is public, and can be shared through the NCCs or CoEs websites, social media and other channels when relevant.

2 Main goal, structure

The CoEs are structured in different ways, therefore their interaction with industry can take several shapes. A summary of their goals and structure is gathered in Table 1 below.

Table 1: Goals and structure

СоЕ	Complete name/topic	Goal	Structure
EXCELLERAT-	CoE for supporting supercomputing engineering applications from large scaling to the exascale	To enable the use of simulations workflow at a large scale to exascale computing challenges	7 WPs: -1 PM -3 technical WPs -3 outcome WPs: WP5 center implementation, WP6 Market context & business development, WP7 Awareness, impact creation & outreach
ChEESE2	Center of Excellence (CoE) in the domain of Solid Earth	Identification of exascale computational challenges in geophysics (natural hazards) in term of capability computing, capacity computing, urgent computing	3 pillars: 1) scientific community 2) EuroHPC infrastructures & NCCs 3) public & private industry parties benefiting from the products & downstream services on geohazards 11 open-source flagships codes 15 simulation cases For the 3rd pillar (public & private parties): codesign with mini-apps with EPI, EUPEX and EuPilot initiative. Some TRL 8 or 9, that went into operations.
CEEC	Centre of Excellence in Exascale CFD	Adress the extreme-scale computing challenge to enable the use of CFD simulations at exascale.	7 WPs: 3 technical WPs (2,3,4) supporting the execution of lighthouse cases WP1, future technologies WP5, dissemination WP6 and PM WP7.
HiDALGO2	Centre of Excellence in Urban-migration simulation topics	bring together advanced solutions (HPC HPDA AI) to provide stakeholders & decision makers tools that would mitigate tragic consequences of climate & civilization phenomenon by delivering necessary knowledge	The objectives are distributed in Conceptual services: 4 areas: technological, multidisciplinary, socio-scientific, team working objectives. 4 current use cases: urban air project (TRL6), urban buildings (), renewable energy sources, wildfires. Project components (see the slides). Main topics of interest for phase 2: Exascale support for Global Challenges, DATA Exploration and visualisation
MaX3	MAX designs new materials at the exascale	Turn MaX lighthouse codes into exascale-enabled applications Enabling materials for grand challenges	7 WPs: -1 MGT -4 technical WPs -WP5 training & community engagement, WP6 communication, exploitation & dissemination

CoEs - Industry topics October 2023 © 2023 Members of the CASTIEL 2 Consortium

	1	I	T
<u>SPACE</u>	Scalable Parallel Astrophysical Code for Exascale Center of Excellence (CoE) for HPC astrophysical applications	outstanding quality & volume of data => exceptional challenges to their theoretical interpretation. 8 codes in 3 main themes 5 objectives: to evolve the 8 codes, evolve data analysis & visualization ecosystem, dvp ML techniques, address the energy efficiency issue, federate the A&C community	3 private companies in the consortium WP1: Management WP2/3: science (interaction in WP2 with HW providers) WP4: tools (transversal for the others) WP5: dissemination, outreach, training for the A& C community
<u>MultiXScale</u>	Performance, portability, productivity	Application co-design for exascale, accelerate development, deployement of scientific workflows interest in co-design Objective: increase performance, productivity and portability for scientists & pilot multiscale usecases of societal and industrial significance.	2 private companies in the consortium Scientific WPs (2,3,4): WP4 includes 3 showcases – one of them is helicopter design with industry partner Leonardo; Technical WPs (1,5); Collaboration with EESSI as a deployment mechanism for software. Large interest from cloud providers. WP7: – Two tasks with specific focus on industry, "Task 7.1 – Scientific applications provisioned on demand" and "Task 7.4 - Industry-oriented training activities"
Plasma-PEPSC	Plasma exascale performance simulations CoE	Fusion energy research and modern industries depends on plasma science and technology, plasma simulations for societal challenges, HPC, supercomputers and virtual prototyping have an important role in predicting observations and in design => pushing flagship plasma simulation codes to tackle exascale enabled grand challenges.	3 technical WPs (2.3.4.5) with use cases; WP6: dissemination, community building, training and exploitation . WP1 drives the project (on tech viewpoint) WP7 on admin management Methods: performance optimization and co-design
BioExcel-3	Center of excellence for Computational Biomolecular Research	Supports computational molecular life sciences (neurosciences, drug discovery etc.) and developing exascale for life science. Provide researchers with high-quality user-friendly software, to increase their expertise and skills. Codes world leading open-source software like GROMACS, HADDOCK	2 technical work-packages (core software and workflows), WP on user-driven development, WP on training and dissemination, WP on management. Industry interactions are part of the user-driven development as well as outreach and dissemination. One SME is a member of the consortium.
ESiWACE-3	Excellence in simulation of Weather and Climate in Europe	Focus on supporting the modelling community to reach a higher TRL for exascale supercomputing and foster knowledge transfer in EU. Objective: evolution: enable leading EU weather and climate models to leverage performance of pre-exascale systems, revolution: make use of exascale.	3 pillars: scalability of codes and of software development, usability of workflows in HPC environment and exploitability of data. Pillar 2 includes community building wrt earth system modelling Pillar 1: WP1,2,3,about tech development. Pillar 2: WP4,5,6 about services and networking with community. WP5-> training & capacity building Partners, includes industry company Atos! Core services -> infrastructures -> R&I -> Community engagement

3 Objectives regarding Industry outreach and provision of services

There are two types of CoEs: Type 1 (preparing applications in the Exascale era) and Type 2 (for supporting supercomputing applications for Science and Innovation).

- Four CoEs are Type 1: MaX, SPACE, Plasma-PEPSC and CEEC
- Six CoEs are Type 2: ChEESE-2P, BioExcel-3, EXCELLERAT P2, ESiWACE3, HiDALGO2 and MultiXscale

The CoEs-Type 2 generally have interest or clear goals to interact with industry, whereas the CoEs-Type 1 are more academic-oriented, with a smaller interest to interact with industry. The following Table 2 summarizes the information regarding provision of services by the CoEs:

Table 2: Provision of services & Services portal

СоЕ	COE- TYPE	Provision of services	Existing services Portal
EXCELLERAT-2	Type 2	Yes	https://services.excellerat.eu/
CEEC	Type 1	No	-
HiDALGO2	Type 2	Yes, provision of solution access to SMEs. 4 families of applications and 2 are directly targeting industry, there are also potential for industry with regard to their applications, or the general used techniques	-
ChEESE2	Type 2	Yes, mainly focused on the public sector.	-
MaX3	Type 1	Max3 did offer a set of services for expert users from industry in the past, it is not their current highest priority	http://www.max-centre.eu/services
SPACE	Type 1	No	-
MultiXScale	Type 2	In some way: Training yes, otherwise not directly. Cloud providers are providing apps sw as services to their users (customers)	-
Plasma-PEPSC	Type 1	No	-
BioExcel-3	Type 2	Yes but any details to be discussed case- by-case	https://bioexcel.eu/services/
ESiWACE-3	Type 2	Maybe very indirectly by Meteo Centres / DestinE)	https://www.esiwace.eu/services