D3.1
Connection to other CoEs

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Abstract	The report details the activities of the dealii-X project towards other CoEs in Europe. We are active in several directions. A major activity is the involvement in the CASTIEL 2 project, where we collaborate in terms of joint codes and the important activities on CI/CD, which enables the use of our software on European supercomputers. Furthermore, dealii-X engages in a seminar series that also invites partners from other CoEs to participate for in-depth exchange. Finally, dealii-X contributes to training and workshops, organized through the infrastructure of the partner LRZ.
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Distribution List

- Project Coordinators (PCs)

- Work Package Leaders (WPLs)

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1 dealii-X within CASTIEL 2

The dealii-X project is a Centre of Excellence (CoE) funded in as a project in the European High-Performance Computing Joint Undertaking under the powers delegated by the European Commission.

The use of supercomputers is at the heart of the dealii-X project. In the European Union, 10 CoEs were started in 2023, and 4 additional CoEs started in the two subsequent years. These projects share the goal to create codes that efficiently utilize modern high-end supercomputers up to emerging exascale systems (including EuroHPC systems) and to make these codes available to the relevant user groups. The dealii-X project share these goals, and shares the challenges of many other projects in terms of porting effort for our codes to ensure scalability on each target system. Given the similar tasks faced by several projects, the EuroHPC centres of excellence are coordinated through the project CASTIEL 2, the Coordination & Support for National Competence Centres on a European Level Phase 2, project number 101102047, who state their mission as[1][2]

> The project encourages collaboration, exchange of knowledge between HPC practitioners, expertise and best practices between Participating States and the mapping of skills and competences across Europe to support cohesion and a more consistent level of expertise across Europe. In this next phase of the project, the CASTIEL 2 project also takes on an additional role of providing similar coordination support to the EuroHPC Centres of Excellence (CoEs).
> The CoEs gather HPC expertise in the development of HPC applications by scientific domain at a European level, CASTIEL 2 will build a stronger HPC community which will foster strategic collaboration in HPC research and deployment of skills and in expertise in HPC technologies and applications between CoEs and NCCs.

[1] https://eurohpc-ju.europa.eu/research-innovation/our-projects/castiel-2_en
[2] https://www.eurocc-access.eu

> The objective of CASTIEL 2 and EuroCC 2 is to strengthen the European Union (EU)'s technological autonomy and competitiveness by ensuring a coordinated and consistent high level of knowledge sharing across Europe in HPC and related disciplines such as high-performance data analytics (HPDA) and HPC-based artificial intelligence.

CASTIEL 2 has the role of coordinating the work of the various CoEs. Among the CoEs, around 50 codes for scientific computations are developed and maintained, which differ vastly in size, maturity, scalability and age. As a CoE, dealii-X has picked up on various levels of integration with the CASTIEL 2 project as a coordinating agency, as well as with other CoEs in terms of similar scientific strategies. The actions of these steps are described on the following pages.

2 Online presentation of CASTIEL 2

In exchange with the partners at CASTIEL 2, the dealii-X project has delivered their input to various web pages. On `https://www.hpccoe.eu/`, we are now listed as a project[3] with the main project description

> dealii-X aims at developing a scalable, high-performance computational platform to create accurate digital twins of human organs using the deal.II finite element library. The framework will combine sophisticated numerical methods with exascale computing capabilities to create cutting-edge multiphysics and multidisciplinary simulation models. Lighthouse applications representing crucial processes in the human brain, the cardiovascular and respiratory systems as well as the liver will be tackled to gain new insights into biological processes of the human body and aiding in personalized medicine. A primary focus is on a new generation of solvers, including novel methods for large linear, nonlinear and coupled systems, matrix-free finite element algorithms for GPUs and discretization schemes.

We have integrated the dealii-X web page at `https://www.dealii-X.eu`, where

[3] `https://www.hpccoe.eu/eu-hpc-centres-of-excellence2/dealii-x/`

we report on the recent developments of the dealii-X project in terms of codes, scientific achievements, and prizes, to just name a few. We have clarified this involvement with CASTIEL 2 and are committed to provide future updates as requested by our partners. One point of contact is the interaction of dealii-X with partners from Ginkgo, who are active in the MICROCARD-2 project.

As part of these effort, we have contributed to Work Package 2 of CASTIEL 2 concerning the summary of the consortium, objectives, area of activity, codes and use cases.

3 Integration of dealii-X codes into WP2 of CASTIEL 2

In December 2024 to February 2025, we have intensively collaborated with Work Package 2 of CASTIEL 2 concerning the codes and use cases. We have presented our three main mathematical codes, `deal.II`, `PSCToolkit` and `MUMPS` for the CoE codes whitebook version 1.3, using the following descriptions:

Code	Category	Description	Main uses
deal.II	Multi-physics	Wide range of finite element algorithms, multigrid methods, matrix-free and matrix-based algorithms	Discretization of partial differential equations
PSCToolkit	Linear solver	Framework for solving large and sparse linear systems	Linear algebra applications
MUMPS	Linear solver	A numerical software package for solving sparse systems of linear equations	Linear algebra applications

The provided information also contains URLs to the code repositories, owners of the code, the open-source status of the software packages, the size of user communities and related information. Similar descriptions have been provided for the application codes involved in the dealii-X CoE, including the lifex, 4C, ExaDG, polyDEAL, LiverX and ExaBrain projects.

Furthermore, we have delivered details on the technical aspects of the codes (size of project, dependencies, workflows, parallelization, supported hardware, scal-

ability, development plans), the porting status to various JU systems in the European union, highlighting the focus of dealii-X on the systems Lumi (porting to general GPU architecture), Leonardo (high priority), and JUPITER (high priority). We also engage in exchange of ideas concerning these systems. Furthermore, we have been open in checking for synergies in various developments, and will actively interact with partners at various scientific conferences. As a concrete step, the activities in WP2.6, with the details listed in deliverable D2.6, the dealii-X project aims to work towards a metascheduler for the simpler use of software across supercomputers. We will seek active collaboration with other CoEs concerning the use of distributed infrastructure and include available scheduling protocols developed within the EU in the past as much as possible.

To foster this exchange, the dealii-X project will be represented in the NCC-CoE-all-hands meeting in Tallinn, Estonia, in September 23–25, 2025.

The dealii-X consortium has been joining the **PMT-CoE leader meetings** of CASTIEL 2, organized by the partners at HLRS (Stuttgart, Germany) since November 2024, as collaborated on a joint Kokkos workshop on February 27, and various other meetings.

Finally, we have provided **champions** and **deputy champions** for the main areas of CASTIEL 2, namely the competences (WP2), the training (WP3), the industry contacts (WP4) and communication (WP5).

4 Collaboration on CI/CD

An additional area of tight interaction is on continuous integration and continuous deployment, where we have started interaction with the CI/CD team of CASTIEL 2. We have been introduced into the existing infrastructure established at EuroHPC. We are eager to use the upcoming months to interact with the European Environment for Scientific Software Installations (EESSI)[4], where we want to get our main codes, starting from the core code `deal.II`, to be deployed at various HPC systems. This collaboration with enable us to get continuous feedback on the state of our software, which will add a crucial facet to the testing infrastructure of deal.II. In addition, this is also of great benefit to our users, as EESSI is subscribed to build a common

[4] https://www.eessi.io/

stack of scientific software installations for HPC systems as well as a variety of other systems.

The goal at this point is to interact with EESSI, to join the monthly meetings as well as bi-weekly status updates, in order to get our main codes deployed until October 2025. Initial, the coordination with CI/CD is done by dealii-X's PI Martin Kronbichler. From April 2025, Ivan Pribec from the BADW-LRZ partner will join the activities and coordinate with other CoEs. Overall, the consortium is committed to increase the redundancies of duties on this topic work to several partners, with primary focus on the partners from WP1 and WP2, to ensure a high responsiveness and good progress.

5 dealii-X Seminar Series

To enhance collaboration and knowledge exchange among project partners, we have initiated the development of an online seminar series showcasing cutting-edge research by dealii-X collaborators and guest speakers. Launching in June 2025, the seminars will follow a standard format of a 45-minute lecture followed by a 15-minute Q&A session. Recordings of the sessions will be made available on the project webpage and shared via social media channels. This initiative will be carried out in close collaboration with the VPH Institute, which will assist in editing and publishing the multimedia content (WP4).

Through the seminar initiative, we will also establish contacts to other EuroHPC CoEs. It is planned that several talks will be given by researchers in adjacent projects, giving the dealii-X members insights cutting-edge progress of related topics. This setup will foster the collaboration between the projects. As a platform to learn from other researchers and other projects, the activities in the seminar series will boost the qualifications of our team members and create opportunities for research results beyond the present state of the art.

6 Training and Workshops

One of the consortium's key goals is to enhance the training of clinical researchers and practitioners through specialized workshops and interactive, hands-on sessions. LRZ has a well-established mission to provide education on programming and HPC-related topics. In response to growing demand, its course offerings have expanded significantly in recent years to include GPU programming, deep learning, and AI. These training sessions are promoted through LRZ's existing HPC network as well as EuroCC dissemination channels.

LRZ has actively contributed to several European projects, including CompBioMed and LEXIS, where it played a key role in organizing meetings, application-focused workshops, and hackathons (e.g., the preCICE workshop and the CompBioMed-SEAVEA hackathon).

As part of the dealii-X consortium, the first workshop is scheduled for December 2025, in Trieste, Italy, hosted by the partner SISSA. The event will feature an open users and developers workshop, followed by project-specific sessions addressing critical topics such as co-design, exascale computing, and machine learning/deep learning. These sessions aim to strengthen partner collaboration and foster multi-disciplinary research.