

EURO²

EuroCC Belgium

Empowering the Belgian supercomputing community

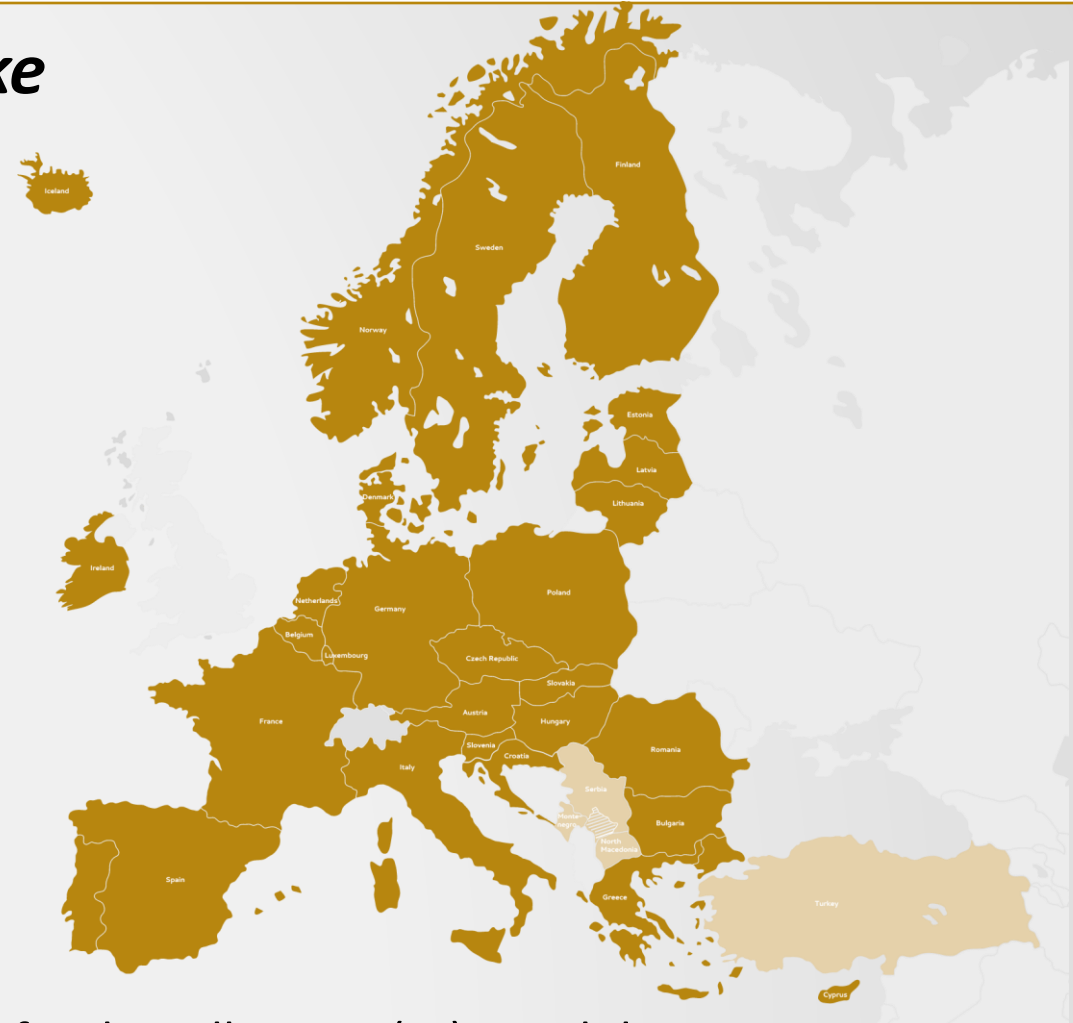
A network of NCCs

National Competence Centers



Mission: promote and facilitate HPC uptake

- EuroHPC JU actions already presented
 - Pre-exascale and exascale infrastructures
 - “Chip act”
- Focus on “competences”
 - 2020: EuroCC + Castiel projects first phase
 - “CC” for “Competence Centers”
 - 2023: EuroCC + Castiel phase 2
 - Focus on SMEs and international collaboration
 - Also address indus., acad. and public admin.
 - Castiel 2 also coordinates Centers of Excellence
 - Increase national HPC competences, High-Performance Data Analytics (HPDA) and Artificial Intelligence (AI) capabilities



NCC Belgium - Goals

Mission: promote and facilitate HPC uptake

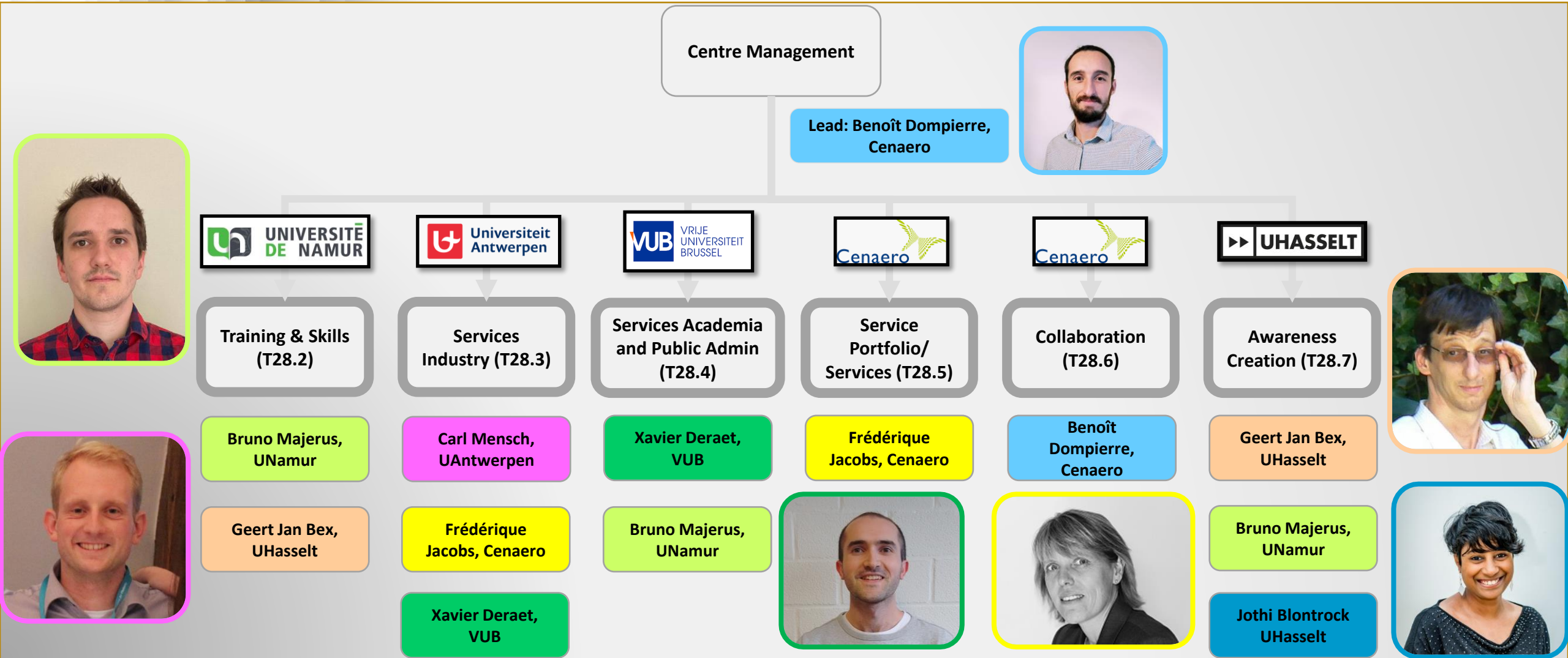


NCCs act as central contact point at the national level

- Communicate
 - Raise awareness about HPC (focus on SMEs and industry)
 - Grow/Maintain the Belgian HPC Network by regular communication
- Support
 - Provide a clear overview of existing tools, training & services (+ easy access)
 - Provide a way to send requests (+ transfer to relevant parties)
 - Identify gaps in services and training, and find a way to fill them
 - Direct support to stakeholders
- Collaborate
 - Promote national and international collaboration

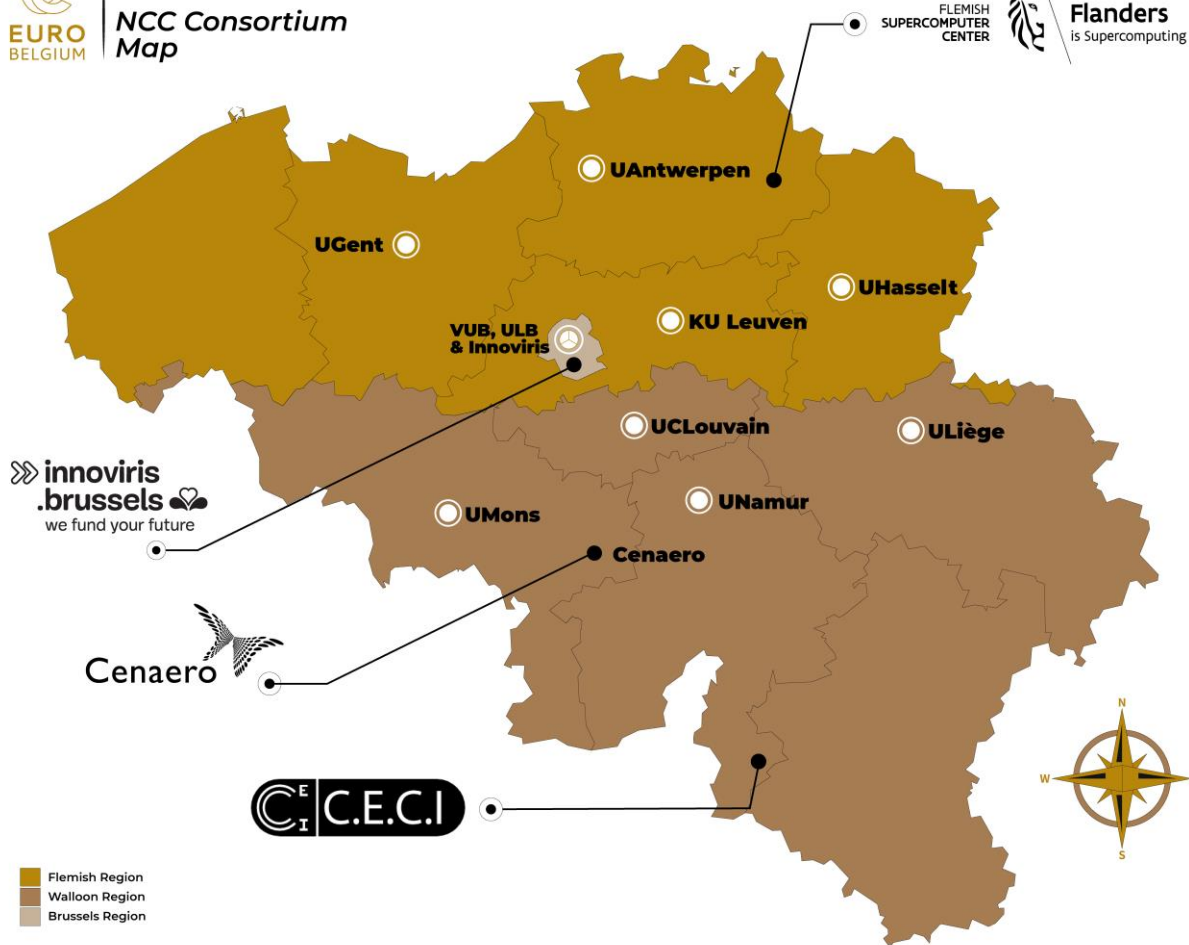
NCC Belgium – Who are we?

Governance structure & tasks



NCC Belgium – Who are we?

Main partners and Infrastructure



• Tier 1 + Tier 2

VLAAMS
SUPERCOMPUTER
CENTRUM



Vlaanderen
is supercomputing



• Tier 1

Cenaero



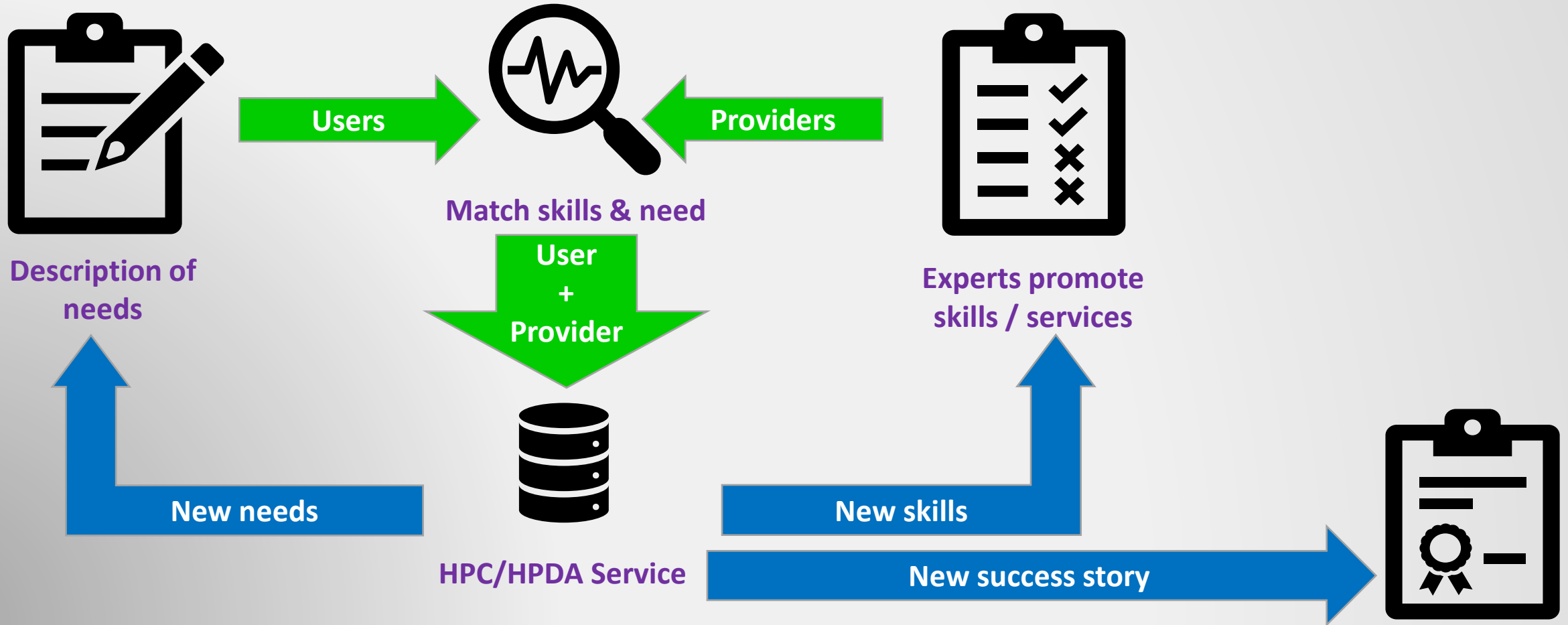
• Tier 2

CÉCI

NCC Belgium – Services

A simple concept

Meeting point between needs and HPC/HPDA expertise



NCC Belgium – Services

What kind of benefits for the users?

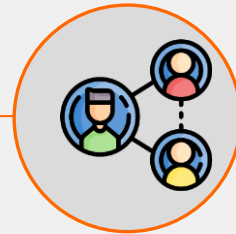
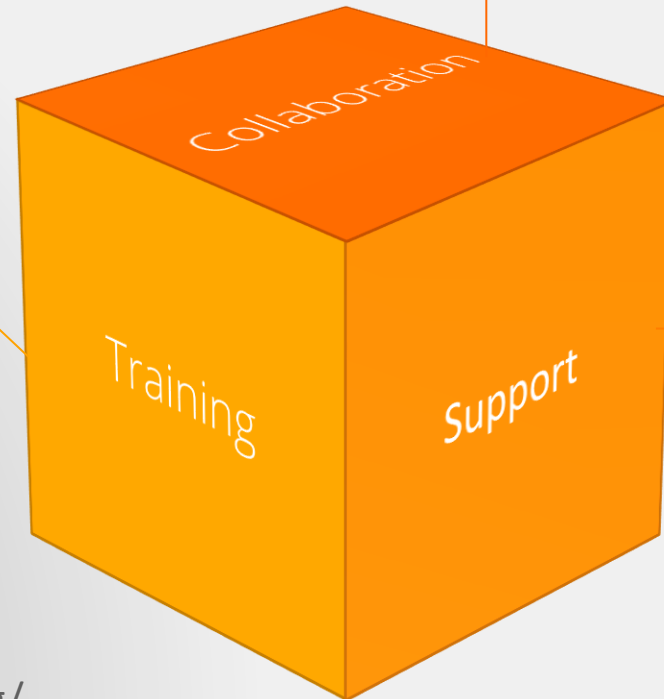


Develop new skills

- With or without diploma
- On purpose training
- Workshops (+ hands-on)
- Online resources
- Belgium + Europe

<https://www.enccb.be/training>

<https://www.eurocc-access.eu/training/>



Facilitate collaboration

- Network of experts and services providers
- Set-up of communities
- Organisation of events
- Publication of user stories

<https://www.enccb.be/marketplace>



Support to increase HPC adoption

- Audit / Definition of needs
- Access to infrastructure
- Technology transfer (soft & hard)
- Proofs of concepts
- Support to find resources and funding

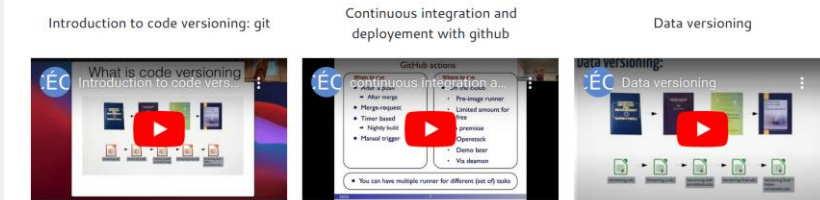
NCC Belgium – Highlights

Main achievements 2023 and perspectives

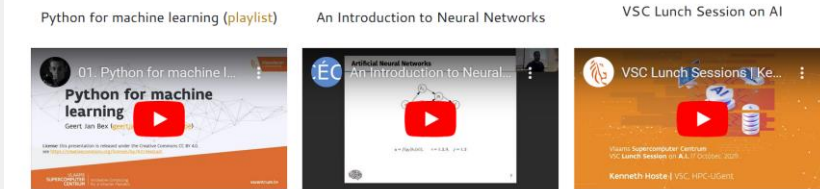
Training

- Online trainings (open to all)
 - Quantum Computing Demystified
 - Performance-aware C++ programming
- Creation of a training video portal
- Development of new trainings
 - New training by CÉCI and VSC
 - Data
 - LM/ChatGPT for HPC
 - → LUMI for sysadmin; FPGA; code Licensing; C++ software engineering in preparation
 - Development of teaching kit / starting kit (Including video EN and FR)
 - Personas: data science profile nearly done

Git and GitHub



Machine learning and AI



Data



NCC Belgium – Highlights

Main achievements 2023 and perspectives



Training

- Collaboration at the European scale on various topics
 - Training baseline
 - Certification
 - Sharing training material
 - European-wide shared training and assimilated events
 - List of trainings: <https://www.enccb.be/training>
 - “CASTIEL” and “NCCs” organised events
 - On-site / Online / Hybrid

NCC Belgium – Highlights

Main achievements 2023 and perspectives



Training: “CASTIEL” and “NCCs” organised events

- Next events (known by today)
 - 6 November 2023: MATLAB for HPC (NCC Germany) hybrid
 - 7- 8 November 2023: National Meeting of the National Network for Advanced Computing 2023, Vila Real, Portugal (NCC Portugal) on-site
 - 8 November 2023: Parallel Computing with MATLAB and Scaling MATLAB Code to the HPC Cluster. (NCC Czech Republic) hybrid
 - 9 November 2023: Training Event “High-Performance Computing, High-Performance Data Analysis and Large-Scale Machine Learning” (MCC Cyprus) hybrid
 - November 8–10, 2023: GUIX HPC: Reproducible software deployment for high-performance computing, (NCC France) In English, on-site
 - 13-15 November 2023: Workshop High Performance Programming (NCC Sweden) online
 - 27 November- 1 December 2023: Hackathon Optimizing for AMD GPUs (NCC Poland) in Kraków, Poland on-site
 - November 28 2023: OpenFoam, the open source CFD alternative? (NCC France) In English, online
 - 28-29 November 2023 : Parallel programming tools MPI, OpenMP (NCC France) on-site
 - 4-8 December 2023: Artificial Intelligence for computational physics (NCC France) on-site
 - 4-5 December 2023: DataSummit Luxembourg & Schengen-X (NCC Luxembourg) on-site
 - 6 December 2023: EuroCC2 Central Europe Regional Workshop, Kraków/Poland (NCC Poland) on-site
 - 12 December 2023: Flow simulation for the drone and the light aircraft industries (NCC France) In English, online
 - 11-13 December 2023: Multi-architecture parallelism using Kokkos/C++ training (NCC France) on-site
 - 13 December 2023 : The EBRAINS Project: A Gateway to Collaborative Neuroscience Webinar
 - 30 January 2024: Explore and visualize large-scale data with ParaView (Open Source software) (NCC France) In English, online
 - 14-16 Feb, 2024: High-Level GPU Programming course, in Espoo, Finland (NCC Finland) on-site
 - 21-24- February 2024: 28th International Information Technology Conference IT (co-organizer NCC Montenegro) hybrid

NCC Belgium – Highlights

Main achievements 2023 and perspectives



Collaboration (National and European)

- Continuous development of our network
 - Contacts with companies, hubs, clusters, universities, TTOs/KTOs
 - General outreach
 - Identification of the needs, opportunities, challenges and blockers
 - Identification of the services and skills
 - → Continuous improvement of our services
 - Identification of synergies with
 - Belgian EDIHs (Eu Digital Innov Hubs): Digitalisation of SMEs
 - CoE (Centers of Excellence): Towards exascale
 - Other NCCs (Netherlands, France, Spain, Portugal, Austria, ...): How to make more with less
 - International initiatives such as Inno4scale / FF4EuroHPC / HPC4SME / PRACE / ...

NCC Belgium – Highlights

Main achievements 2023 and perspectives



Collaboration (National and European)

- Direct support to LUMI's actions
 - Belgian LUMI page on our website
 - Contact to the LUMI-BE team at lumi-be-support@enccb.be

A screenshot of the LUMI website. At the top right is the 'EURO BELGIUM' logo. Below it is a navigation menu with links: Home, News, Stories, Training, Industry, LUMI, Marketplace, About us, Testimonials, Contact. A search bar is on the right. The main heading is 'What is LUMI?' with a 'Featured' tag. Below is the 'LUMI' logo and a paragraph: 'LUMI is one of the pan-European pre-exascale supercomputers. It is also the fastest supercomputer in Europe (the Top500 list published in May 2023) and the third fastest globally. LUMI is also the seventh greenest supercomputer on the planet. The LUMI data center as also recognized in the 2023 Data Centre World Awards for the Green Data Centre of the Year in March 2023.' Below the text is a video player showing a wolf in a server room. The video title is 'LUMI – world-class supercomputer' and it includes 'Watch later' and 'Share' buttons. At the bottom of the video player, it says 'Watch on YouTube' and 'EuroHPC world-class supercomputer'.

LUMI, an HPE Cray EX system, has a sustained computing power of 375 petaflops (HPL, High-Performance Linpack) in its final configuration. LUMI is also one of the world's leading platforms for artificial intelligence. [Read more technical facts about LUMI.](#)

NCC Belgium – Highlights

Main achievements 2023 and perspectives



Collaboration (National and European)

- Development of a service portfolio
 - Implementation of a marketplace like platform
 - Thanks to the collaboration with NCC France
 - Currently only in French, English version in testing phase within a task force (5 to 10 NCCs)

The screenshot displays the EURO BELGIUM website interface. At the top right, there are navigation links for 'Offres', 'Membres', 'Communautés', and 'Mon compte'. The main content area is divided into several sections:

- PROFIL:** Profile of M. Benoit Dompierre, Chef de produit / Chef de projet at CENAERO. Description: 'Strong technical and scientific background in HPC, I progressively turned to new challenges with project & team leading'. Skills: HPC, HPDA, IA, Responsable du NCC Belgique.
- ORGANISME:** Information about CENAERO, Charleroi, BELGIQUE. Description: 'Your trustworthy R&T partner in modeling and numerical simulation'. Text: 'Cenaero fournit des méthodes et des outils de simulation numérique. Reconnu au niveau international, Cenaero est principalement actif dans...'. Skills: HPC, HPDA, IA / Machine learning / Deep learning, Simulation numérique.
- MES COLLABORATEURS-TRICES:** Section for collaborators, listing 3 registered users: Thibaut Van Hoof, Frédérique Jacobs, and Olivier Pierard. Status: 'Aucun-e invité-e'.
- Mes offres:** A section with a 'Nouvelle offre' button and three service cards:
 - LOGICIEL - Minamo:** 'Minamo is a surrogate-based optimisation (SBO) & data mining platform'. Skills: IA / Machine Learning / Deep Learning, Data Analytics.
 - LOGICIEL - Morfeo process:** 'Morfeo process is a thermo-mechanical kernel to perform process simulation such as additive manufacturing, welding or machining'. Skills: Jumeau numérique, Fabrication additive.
 - LOGICIEL - Morfeo Life:** 'Morfeo Life is a thermo-mechanical kernel to perform crack propagation simulation under LEFM hypothesis'.
- Référencer une offre:** A central section with six buttons for referencing offers:
 - Référencer une offre de matériel
 - Référencer une offre de logiciel
 - Référencer une offre de prestation de service, conseil ou expertise
 - Référencer une offre d'accès à des infrastructures de calcul
 - Référencer une formation
 - Référencer une architecture HPC
 - Référencer une offre d'emploi
 - Référencer un événement

NCC Belgium – Highlights

Main achievements 2023 and perspectives

Communication

- Publish content (user stories, news, ...)
 - Website (<https://www.enccb.be/>)
 - Social networks (LinkedIn, Twitter)
- Collaboration
 - Participation to / co-creation of events
 - Sharing external communication
 - National and international
- Preparation of EuroCC newsletter
 - Please contact us if your are interested in

News Stories Training Industry LUMI Marketplace About us Testimonials Contact

Search

Faster processor communications to better understand fluid turbulences

Featured User story



Pierre Balty is a PhD. student with Prof. P. Chatelain at the Institute of Mechanics, Materials, and Civil Engineering at the UCLouvain. The main focus of their research group is the theoretical investigation of turbulence in fluids, also known as computational fluid dynamics (CFD). This field of study is of great interest to develop wind turbines with better yield, planes with low consumption, or aerodynamic cars. In such devices, small perturbations can dramatically influence the fluid's behavior at large scales. Therefore, it is important to have efficient numerical tools that accurately perform CFD computations of large domains that resolve the most minor details in a reasonable amount of time.



Pierre Balty received the master's degree from UCLouvain, in 2019 and is currently working toward the PhD degree under the supervision of Prof. Philippe Chatelain within the Institute for Mechanics, Material, and Civil engineering, UCLouvain. His research focuses on hybrid Eulerian-Lagrangian numerical methods, their deployment on distributed systems, and their applications to wind energy. To pursue his research, Pierre collaborate with international research group from the Massachusetts

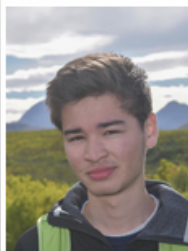
Faster MPI= GPU-to-GPU Communication
on LUMI by Thomas Gillis @16:35

NCC Belgium – Highlights

Main achievements 2023 and perspectives

We talk about LUMI!

Tim Lebailly (KU Leuven, Department of Electrical Engineering) is currently testing the GPU partition of LUMI for his project "Spatial-Aware Self-Supervised Learning". His experience with LUMI:



“LUMI is great for Belgium as it allows users to get very large amounts of compute. Currently, I am finishing my allocation on Hortense (Tier-1) in Ghent. To give an example, during the pilot phase on LUMI, I was able to run an experiment over 4 days which is equal to a bit more than my full allocation on Hortense for 8 months! This gives me the opportunity to scale up my research to state-of-the-art neural networks.

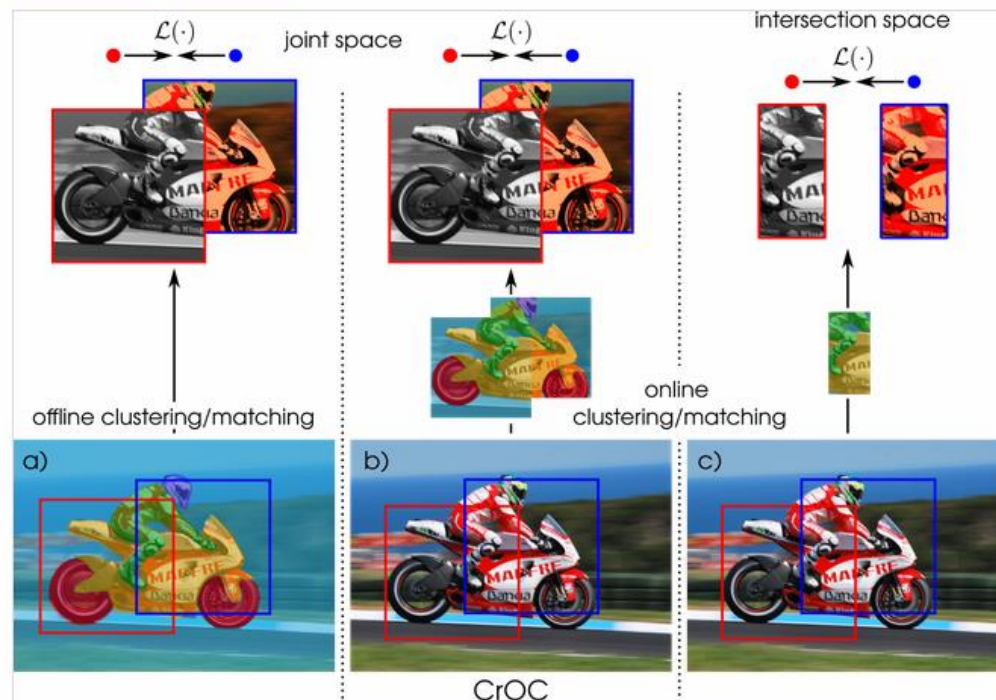
Also, given that LUMI is so big, the queue time is significantly smaller as the jobs you run don't have system-wide impact as opposed to smaller supercomputers like Hortense. In that regard, the user experience is really nice.

Though it's not for the faint-hearted. It uses AMD GPUs, and the documentation resources online are very limited (as opposed to NVIDIA hardware), so it's not as trivial to get your code running (as opposed to Hortense, for instance). As time goes on, the support for users will improve, and the LUMI support team will make the experience easier for a new user by providing native installs/containers for different types of common software.”

From Good to Great: The Advantages of Upscaling from Tier-2 to Tier-0 for Research

User story

Featured



Costly and not scalable labelling in machine learning

Machine learning [1] covers a wide range of methods for computers to learn how to do things without being explicitly programmed: it teaches a computer to learn and improve from experience, just like humans do. Supervised learning is a type of machine learning where the computer is trained using labelled data. For example, the data might consist of pictures of animals with labels indicating which animal is in the image. The computer uses this labelled data to learn how to identify each animal on its own. Once the computer has been trained using the labelled data, it can make predictions on new, unlabelled data. For example, if you give the computer a picture of an animal it hasn't seen before, it can use what it learned from the labelled data to predict what animal it might be.

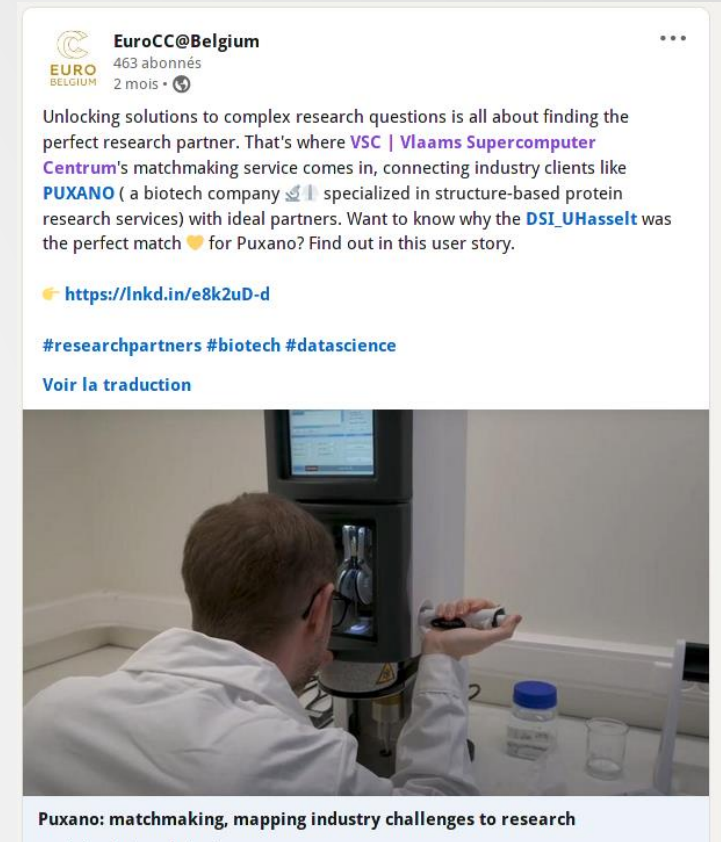
This type of machine learning gives excellent results in many applications, but the labelling is costly and not scalable.

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How to increase awareness through use cases?



- Use cases on our website and on social media



- Use cases on presentation (examples just after)
 - Industry contacts want to see how HPC can help them through examples
 - Work between Belgium and CASTIEL to develop a one-page template for use cases
 - Use cases from all countries → better sectorial coverage



Matchmaking, mapping industry challenges to research

Company

PUXANO is a biotech company offering structure-based protein research services to pharma and biotech companies. The company differentiates from others by developing its own technologies to accelerate the process of obtaining protein structures.

Challenges & Solution

The procondor platform helps to optimize the protein sequence in a semi-automated manner. Puxano initially used the platform internally, but wanted to automate it further and make it available for others to use.

To meet this computational demand, Puxano has employed the HPC services of VSC. Furthermore, VSC introduced Puxano to the Data Science Institute of UHasselt (DSI). DSI helped Puxano design a suitable database structure. The developed database is being incorporated into the Puxano analysis pipelines and serves as the core source of information for the Puxano (web-based) service platform.



Benefits

- ✓ VSC as match-maker between Puxano and DSI
- ✓ DSI gave new insights to design a suitable database structure
- 👉 « The developed database serves as the core source of information for the Puxano (web-based) service platform. »

“Our key objective was to rethink our script for protein construct design into a software platform. The idea was to find out which type of database structure served best to integrate protein information in different formats, have efficient data storage, easily updatable and searchable. Our collaboration with academia was very valuable for the success of the project” **Wouter Van Putte, Director & co-Founder @Puxano**

Full story:





Unraveling the behavior of the hIDO1 protein

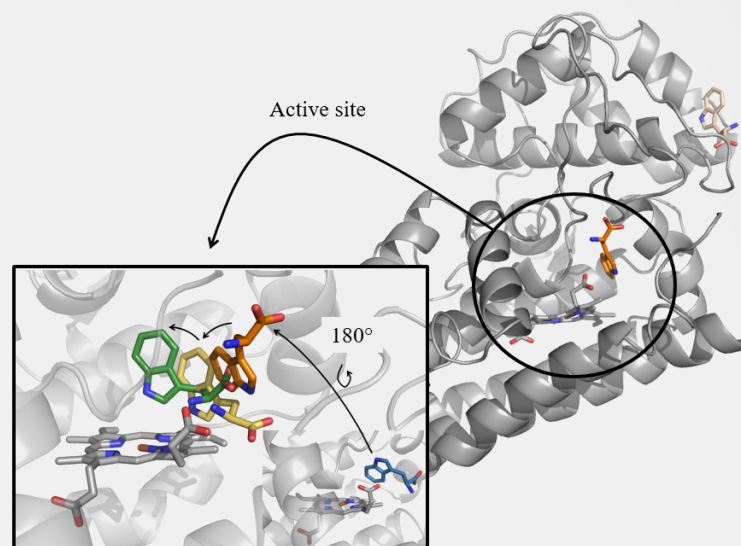
Research group

CBS (Structural Biological Chemistry) Laboratory is part of University of Namur and develops actively research projects in medicinal chemistry.

Challenges & Solution

In cancer, it may be that one kind of enzyme is suractivated, which affects the pathway where it is involved, and thus, the overall behaviour of the cell. Therefore, inhibition of such proteins (therapeutic targets) is an important part of cancer research. The suractivation of the human Indoleamine 2,3-dioxygenase 1 (hIDO1) protein is linked to induce immune escape and resistance to immunotherapy.

For the design of new inhibitors, it is essential to understand the full structure of the protein including the interaction with its substrate (dynamic loop) to understand the response to drugs. In order to capture the motion of this loop during substrate entrance, Molecular Dynamics (MD) numerical simulations are essential.



Benefits

- ✓ Synergy between Molecular and the crystallographic observations, with the protein's behaviour in vivo
- ☞ « Crucial advances in the understanding of this enzyme for the design of new drugs for, e.g., the treatment of cancer..»

“In molecular dynamics, the movement of each atom over a given period of time, sufficient to capture the phenomenon, is computed and then analysed. One simulation occurs in 1 month whereas it would have taken more than a year on a personal computer. The assistance of CECI's team was crucial to the successful completion of the simulations and the provision of sound advice.” **Manon Mirgaux, PhD Scientist UNamur**

Full story:





The Role of HPC in Ensuring Nuclear Reactor Safety

Company

Founded in Belgium 150 years ago, Tractebel is today one of the world's leading engineering companies for energy, water and infrastructure projects.

Challenges & Solution

In 2012, the federal agency of nuclear control of Belgium reported defects in the vessels of the nuclear reactor Doel 3 and Tihange 2. Among a lot of analyses, numerical simulation has been chosen to assess the risk level.

These simulations were highly computationally demanding. A single computation required a high quantity of memory (up to 128Gb for the first computations). Due to the high number of configurations to compute (some hundreds), combined with the memory needs, the use of HPC infrastructure was a requirement.



Benefits

- ✓ HPC helped in the assessment of structural integrity
- ✓ Safe restart of the reactors (combined with inspections)
- ☞ « Tractebel acquired unique expertise and now conducts its own analyses on various parts of nuclear power plants internally but also for its partners. »

“Multiple crack configurations required much caution to perform the computation within the available hardware resources while satisfying high-quality standards in the results. Cenaero developed methodologies to face the challenges (number of configurations, memory and restitution time limitations, post-processing).” **Valéry Lacroix, Technical manager of seism & structural integrity group @Tractebel**

Full story:



NCC Belgium

What's next?



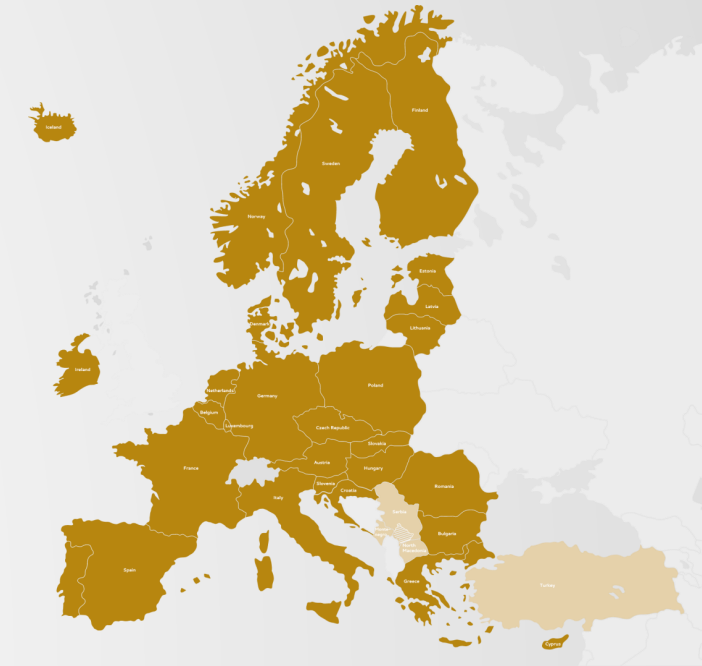
From our side

- Continuous development of
 - Our offer
 - Training
 - Service to industry, academia and public administration
 - Service portfolio platform
 - Our network
 - Our communication



EuroCC Belgium

Empowering the Belgian supercomputing community



NCC Belgium

What's next?



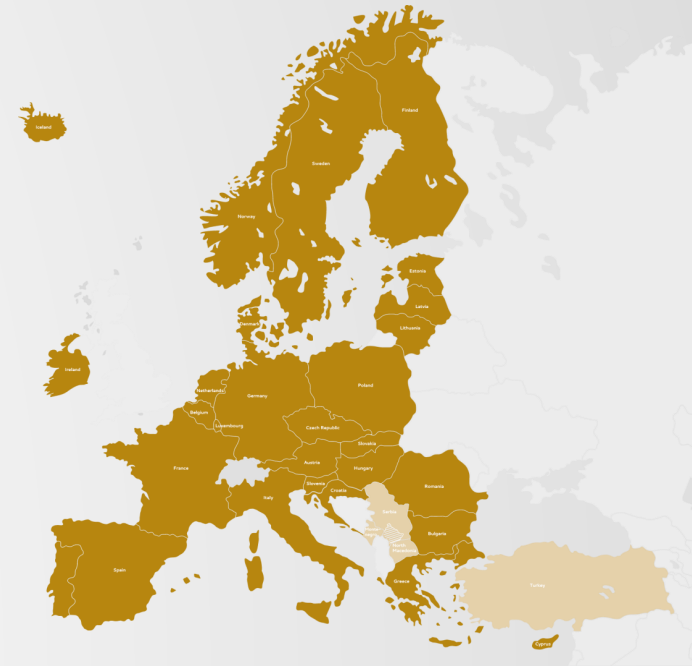
From your side

- Please contact us if
 - You need support (information, networking, access to infrastructure, advices, ...)
 - You want to share your experience/feedback with us and/or with the community
 - You want to develop your network
 - You want to promote your services / skills / trainings / ...



EuroCC Belgium

Empowering the Belgian supercomputing community



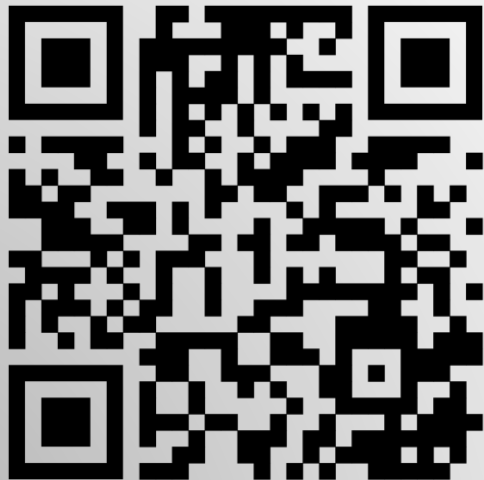
NCC Belgium

What's next?



Keep in touch with us

- If you are here today, you should benefit from us
 - <https://www.enccb.be/>
 - contact@enccb.be



<https://www.linkedin.com/company/76535472/>



https://twitter.com/EuroCC_Belgium



Thanks!



VLAAMS
SUPERCOMPUTER
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Vlaanderen
is supercomputing



Cenaero



EuroHPC
Joint Undertaking

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.