Digital Transformation in the Healthcare Sector: How High-Performance Computing can transform your Business.

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FORTH
INSTITUTE OF COMPUTER SCIENCE

Interactive workshop at Health IT Conference

18/10/2023

Eleni Kanellou

EURO Greece

- *Who are we? Introducing EuroCC*
- *What is HPC?*
- *HPC in Europe: a bit of history*
- *Why is HPC important?*
- *Why use HPC in Business?*
- *HPC impact on life sciences*
- *Adapting HPC for SMEs*
- *HPC services for SMEs*

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Where are you from?

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What is your area of expertise?

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Have you ever though any of the following?

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EuroCC: Who are we?

EuroCC@Greece, the Greek Competence Center

- Competence mapping
- Knowledge transfer
- Awareness/ dissemination
- Collaboration with industry
- Assistance for access to infrastructure
- Training needs identification / training provision / skills development

EuroCC@Greece Consortium partners

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grnet

coordinator

FORTH
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DEMOKRITOS

ARISTOTLE UNIVERSITY OF THESSALONIKI

National Technical University of Athens

SUPPORTED BY

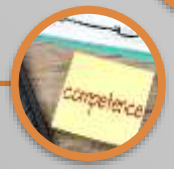
GENERAL SECRETARIAT FOR RESEARCH AND INNOVATION

EuroHPC Joint Undertaking

The project has received funding from the European High-Performance computing Joint Undertaking (JU) under grant agreement No 951732 and the Greek Secretariat for Research and Technology.

The EuroCC Network

National Competence Centres (NCCs) are the **central points of contact** for HPC and related technologies in their country.



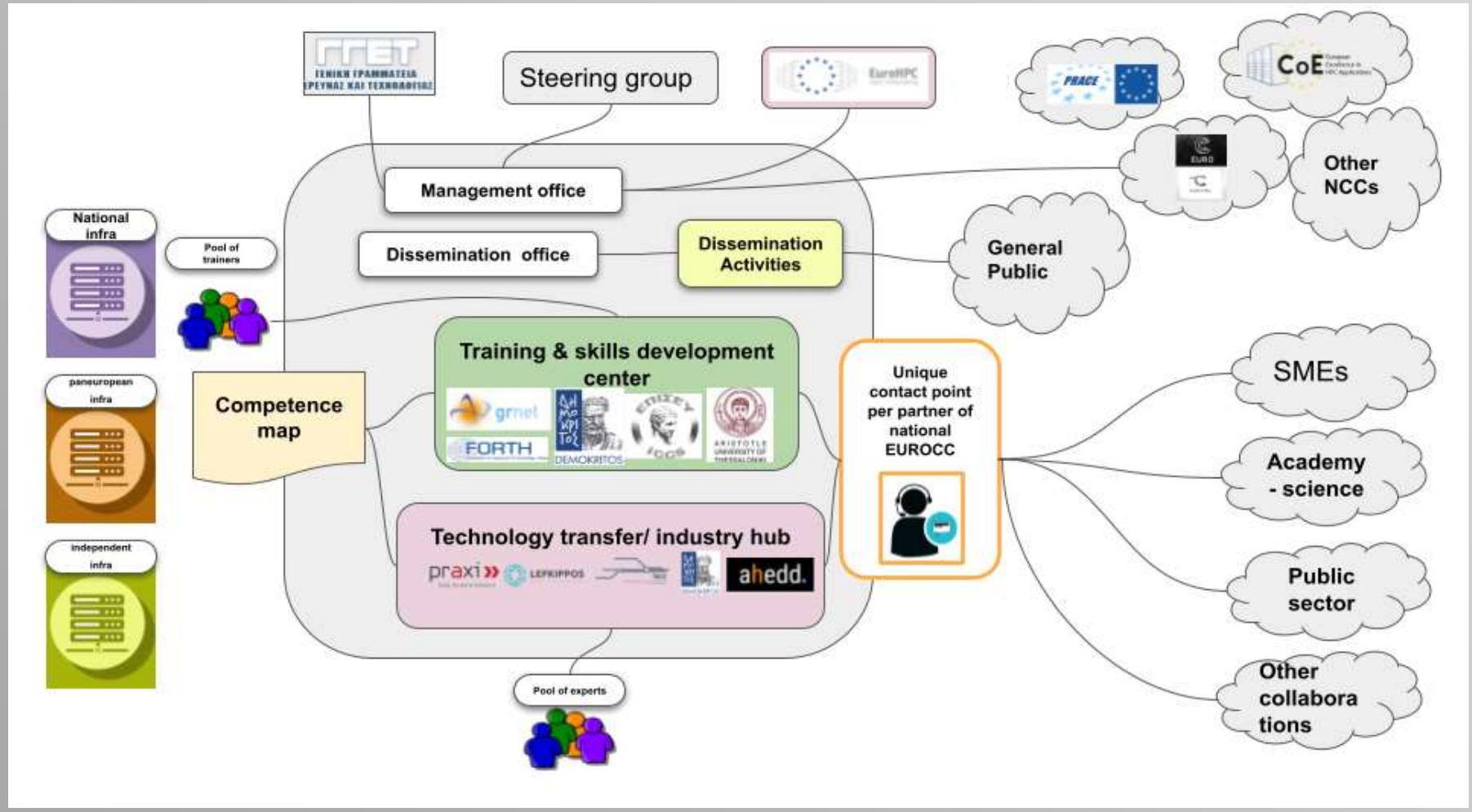
They develop and display a comprehensive and transparent map of **HPC competences and institutions** in their country

They act as a **gateway for industry and academia** to providers with suitable expertise or relevant projects, may that be **national** or **international**

They collect **HPC training offers** in their country and display them on a central place together with international training offers collected by other NCCs

They foster the **industrial uptake** of HPC

EuroCC@Greece within an Ecosystem



EuroCC2

The EuroHPC JU continues to fund a second phase of the project, dubbed *EuroCC2*.

The latest phase of this initiative will build on the achievements of EuroCC, in particular supporting and further developing the HPC Competence Centres and building the overall European HPC ecosystem.

Started on 1st January 2023, the project EuroCC2 will run for a 3-year period with a total budget of up to €62 million, provided by the Digital Europe Programme.

What is HPC?

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What is High-Performance Computing?

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High-Performance Computing

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What is HPC?
Technology that takes advantage of the power of **supercomputers** or **computer clusters** to solve computational problems that are advanced or massive, be it in terms of data volume or complexity.

Why is it useful?
HPC can lead to major advancements in fields like scientific research or technological product development, because it make it possible to analyse *huge volumes of data,* or perform complex simulations, that would otherwise be impossible to do with standard computers.

How does it work?
A small HPC cluster can have 16 nodes with 64 cores, or four cores per processor, which, combined with networking capabilities, enables the high-performance computer to compute things **much faster** than a normal computer.

Where is it used?
The adoption of HPC has been particularly robust in industries that need to *quickly analyze large data sets*, including genome sequencing, molecular dynamics, computational chemistry, etc. In the future, almost all industries will likely turn to HPC to tackle large volumes of data.

HPC in the broader sense

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HPC:
computing systems having extremely high computational capabilities. Today these systems are able to perform more than 10^{15} operations per second (petascale) and are expected in a few years to reach 10^{18} operations per second (exascale)

HPDA
= HPC + Big Data:
Analyze extremely large datasets quickly and/or efficiently

AI:
Systems capable of learning and making decisions

Cloud:
On-demand access to computing resources such as servers, storage, databases, networking, software, analytics, and intelligence

Quantum Computing

HPC in Europe: A bit of history

Once upon a time, in Europe…

Around 2017…

The EU was a heavy consumer of HPC but owned no supercomputer out of the global top 10 ones.

While EU industry only provided about 5% of HPC resources worldwide, it consumed about 1/3 of them!

Biggest issues:

- Lack of high-reaching and sufficient computing capacity in line with its human and economic power;
- Not competitive enough European supply industry;
- Risk of getting technologically deprived or delayed of strategic know-how for innovation and competitiveness
- Risk of having the data produced by EU research and industry processed elsewhere for lack of corresponding capabilities in Europe;
- Risk of getting technologically deprived or delayed of strategic know-how for innovation and competitiveness
- Lack of coordination and synchronised innovation procurement policies between the Member States;
- No Member State can develop the necessary HPC ecosystem on its own in a competitive timeframe with respect to the USA, China or Japan

EU HPC strategy

Converge HPC, Big Data and Cloud Computing technologies;

Build a competitive European HPC ecosystem

Realize and procure extreme scale supercomputers in 2020/2021 and in 2022/2023 based on EU technology.

Sources: https://digital-strategy.ec.europa.eu/en/library/high-performance-computing-factsheet
https://ec.europa.eu/newsroom/document.cfm?doc_id=47053

The EuroHPC JU

The European High Performance Computing Joint Undertaking

- EuroHPC JU: Legal and funding entity, created in 2018
- Public Members:
  - the European Union (represented by the EC)
  - Assorted member states
- Private members:
  - European Technology Platform for HPC (ETP4HPC)
  - European Quantum Industry Consortium (QuIC)
  - Big Data Value Association (BDVA)
- Provides financial support through procurement or R&I grants
  - Budget of ~ EUR 7 billion for the period 2021-2027

Mission: make Europe a world leader in High-Performance Computing

Develop a world-class supercomputing infrastructure, available to Europe's private and public users, scientific and industrial users everywhere in Europe

Stimulate a technology supply industry (from low-power processors to software and middleware, and their integration into supercomputing systems)

Support research and innovation activities: developing and maintaining an innovative European supercomputing ecosystem, with emphasis to SMEs

Ease access to European HPC opportunities in different industrial sectors, delivering tailored solutions for a wide variety of users

Strengthen the European knowledge base in HPC technologies and bridging the digital skills gap

Source: https://eurohpc-ju.europa.eu/about/discover-eurohpc-ju_en

EuroHPC JU Supercomputers

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Access to JU Machines

https://eurocc-greece.gr/how-to-apply-for-access-to-eurohpc-ju-supercomputers/

Why is HPC important?

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Why is HPC important?

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Reduced physical testing	By relying on HPC-powered simulations, physical tests can be eschewed. This can be very beneficial for industries where physical testing is costly and cumbersome, such as the automotive industry where crash tests can be replaced by simulations.
Fault tolerance	HPC clusters have more than one processing nodes, meaning that even if some of the nodes fail, the rest of the HPC system can continue its operation. Thus, even if overall processing is slowed down by the reduced computing power, there will be no problem of processing availability.
Higher Processing Speed	HPC clusters do not only exploit the availability of multiple nodes. They also contain highly performant processing and communication devices, such as the latest CPUs, graphics processing units (GPUs), and low-latency networking fabrics such as remote direct memory access (RDMA), coupled with all-flash local and block storage devices, HPC can perform massive calculations in minutes instead of weeks or months.
Lower Cost	The use of HPC shortens the time to complete production, given that it speeds up production processes. This translates to less wasted time and money. Furthermore, as remote HPC services become available, even small businesses and startups can afford to run HPC workloads, paying only for what they use and scaling up and down as needed (e.g. by relying on cloud-based HPC).
Improvement of existing processes	Faster processing time and quicker data analysis facilitates the automation and streamlining of workflows.
Innovation	Discoveries that are made possible for the first time through the use of HPC, make it a power that drives innovation across nearly every industry around the world.

Supercomputer vs. conventional computer

Genetic Diagnostics: HPC speedup?	Early detection and treatment of diseases: HPC speedup?	3D Brain Mapping: HPC simulation?
From few months down to weeks	From months down to month	Can handle tenths of histological brain slice images
From month down to few days	Weeks down to days	Can handle hundreds of histological brain slice images
From year down to few months	From day down to hours	Can handle many thousands of histological brain slice images

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Gnetic Diagnostics: HPC speedup?

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Early detection and treatment of diseases: HPC speedup?

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3D Brain Mapping: HPC simulation can handle how many histological brain slice images?

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Supercomputer vs. conventional computer

- Genetic Diagnostics: HPC speedup?
  - From few months down to weeks
  - From month down to few days
  - From year down to few months
- Early detection and treatment of diseases: HPC speedup?
  - From day down to hours
  - From months down to month
  - Weeks down to days
- 3D Brain Mapping: HPC simulation?
  - Can handle tenths of histological brain slice images
  - Can handle hundreds of histological brain slice images
  - Can handle many thousands of histological brain slice images

HPC Best Use Examples

Source: https://digital-strategy.ec.europa.eu/en/library/high-performance-computing-best-use-examples

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Why use HPC in Business?

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What would you say are roadblocks to product development cycles?

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Can you classify the aforementioned roadblocks to some of the following categories?

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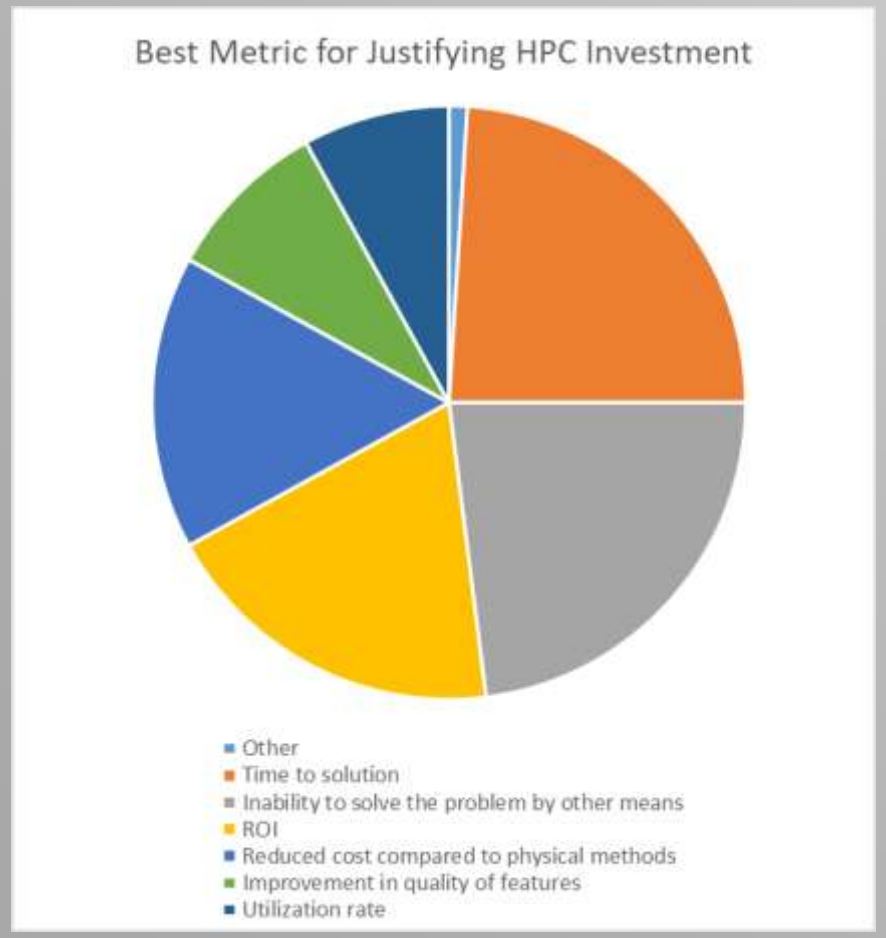
Why use HPC in business



- HPC significantly reduce R&D costs and development cycles, producing higher quality products and services, reducing the time of product development cycles.
- **Example**: HPC has enabled automakers to reduce the time for developing new vehicle platforms from an average of 60 to 24 months, saving EUR 40 billion while improving crashworthiness, environmental friendliness, and passenger comfort
- High return on investment in HPC: each Euro invested in HPC on average returned EUR 867 in increased revenue and EUR 69 in profits.

Sources: https://digital-strategy.ec.europa.eu/en/library/high-performance-computing-factsheet
U.S. Council on Competitiveness report, "Solve. The Exascale Effect: The Benefits of Supercomputing Investment for U.S. Industry," Intersect360 Research, 2014

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How HPC can benefit the life sciences sector

Life Sciences meet Digital Technologies

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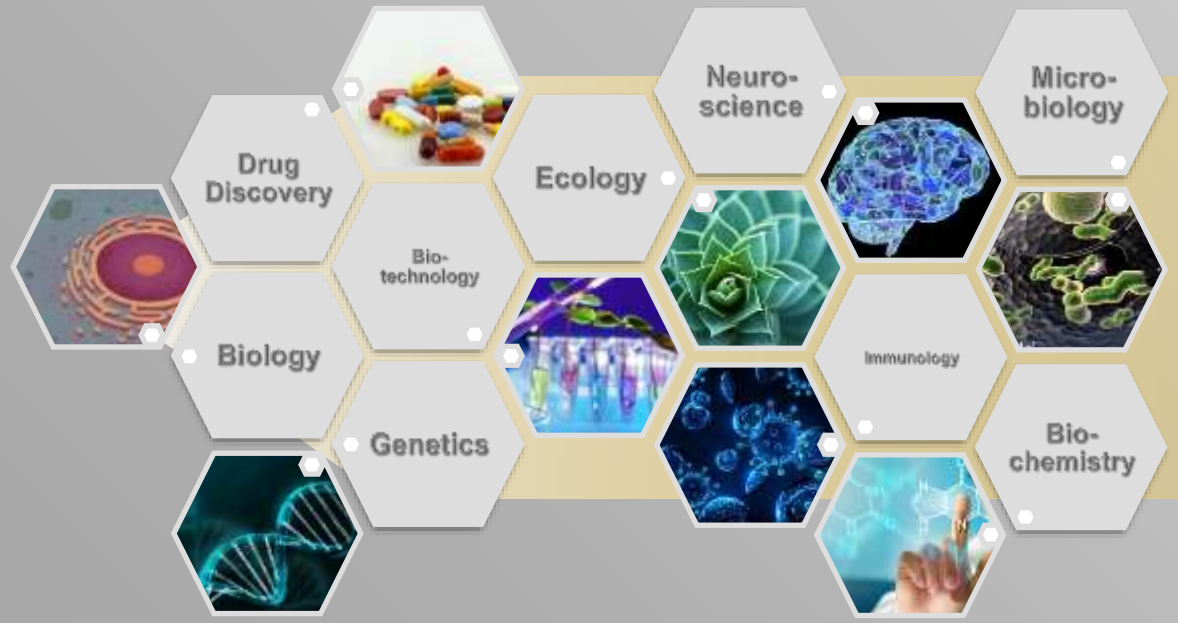

Data Analysis and Data Management

Bioinformatics

Modeling and Simulation

Machine Learning and AI

Collaborative Research and Data Sharing

Data Privacy and Security

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What are the challenges for life sciences?

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Example: Drug Discovery and Pharmaceuticals

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CHALLENGES…	…AND HOW TO FACE THEM
• Surfacing of new diseases • Aging population means new patient profiles • Medical data records growing exponentially • Having to solve for enormous number of biological factors	• Make new discoveries faster than ever • Work with larger data sets • Collaborate more efficiently • Scale up parallel simulations • Exploit HPC-powered advances in genomics

Several years to decades to develop products 

Personalized treatments in shorter time

HPC Success Stories in Life Sciences

Showcasing Success Stories from the FF4EuroHPC Project

PediDose: A Pediatric Simulated Dosimetry Platform for Clinical Use

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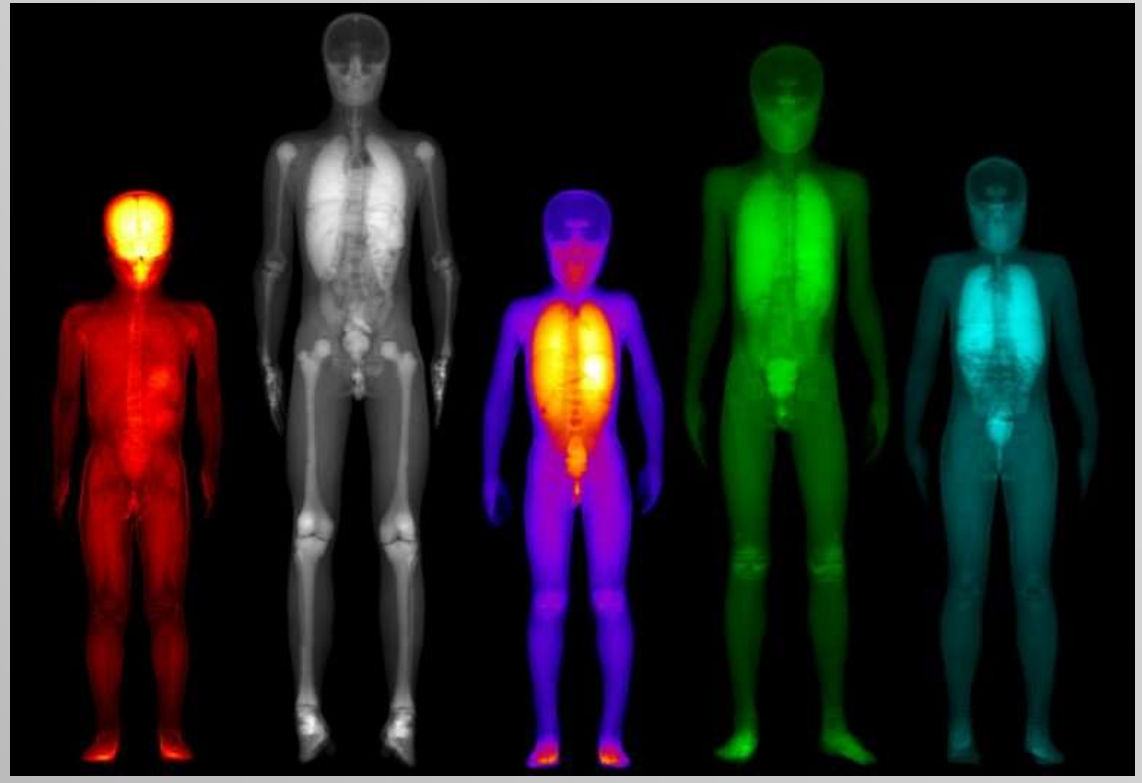
Who?	The Problem	The Challenge
Greece End User: iKnowHow Domain Expert: BioEmTech HPC Expert: GRNET	• Radiation dose calculations from radiopharmaceuticals in nuclear imaging like PET have been a challenge • No commercial solutions for personalised dosimetry existed so far • Developing and optimising dosimetry protocols in pediatric applications is a particular problem as children are more sensitive to ionizing radiation • Current clinical practice relies on rough estimations	• Experimental dosimetry and validation in order to improve dosimetry protocols is difficult • Stochastic nature of radiation is best approached with statistical computing approaches such as Monte Carlo simulations • However, those have a high computational cost

PediDose: A Pediatric Simulated Dosimetry Platform for Clinical Use

The HPC Solution	The Business Benefit
• IKH and BIOEMTECH created a precise dosimetry software (“PediDose”) • Monte Carlo simulation was applied to about 30 advanced anthropomorphic phantoms covering 31 organs • By employing HPC resources (129 parallel jobs), a speedup by a factor of 80 was achieved • A ML predictive dosimetry model was developed and trained with these computed results, thus permitting an individual dose calculation	• PediDose has been technically integrated into the evorad® suite, a competitive healthcare software for medical imaging (PACS) from IKH • This add-on is expected to generate additional net income for IKH of about €1.25 Mio within the next five years • PediDose will be offered on a license basis to other vendors of medical software • Medical market entry for BIOEMTECH facilitated through partnership with IKH



Advanced HPC Based Drug Discovery with Converged Deep Physics and AI

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Who?	The Problem	The Challenge
France End User: **Iktos** Domain Expert: **Qubit Pharmaceuticals** HPC Expert: **Qubit Pharmaceuticals**	• The development of new drugs consists of two phases: Discovery and development • The discovery phase can be split into 5 steps: target identification, hit discovery, hit-to-lead, lead optimisation, and pre-clinical • Conventional drug discovery strategies (based on in vitro and in vivo techniques) are costly and time-consuming	• Discovery costs around €800m and lasts around 5 year, often outsourced to SMEs • Computer-aided drug design has emerged as a new in silico method • Many SMEs are competing in this field! • Thus, qualitative and quantitative improvement of the method is needed to have competitive advantage!

Advanced HPC Based Drug Discovery with Converged Deep Physics and AI

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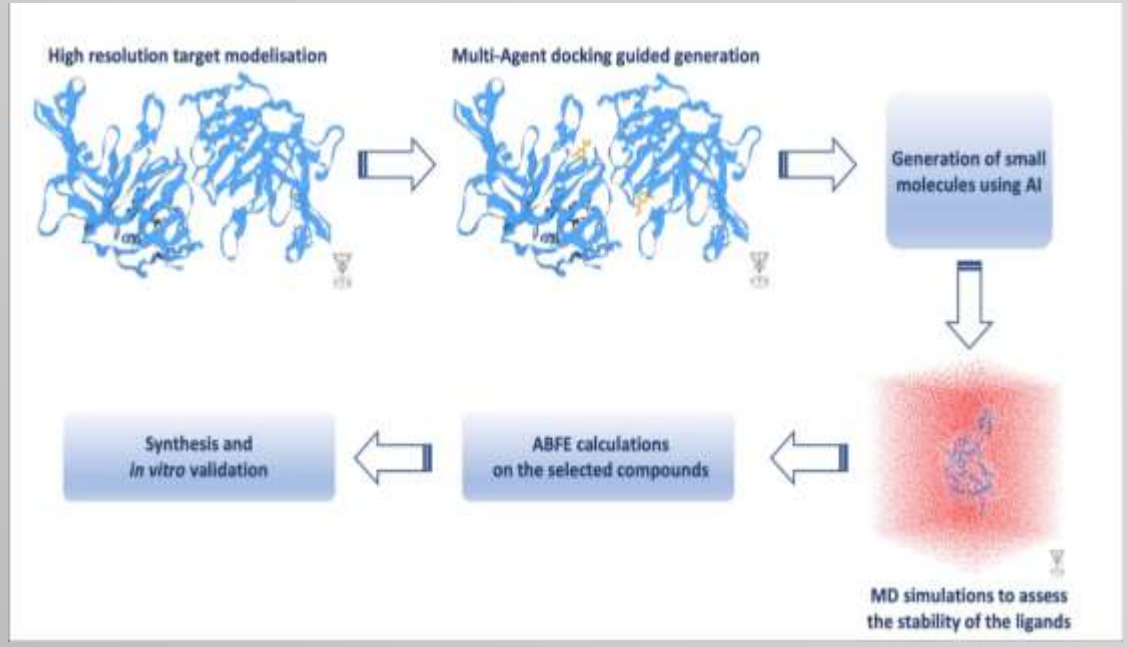
The HPC Solution	The Business Benefit
• Drug discovery strategy and toolchain aiming at the early stages of the drug discovery process, with a focus on small molecules targeting novel proteins • Physics-based/AI-assisted workflow run on HPC • ML algorithms can be trained using high-quality data from molecular simulations to understand protein target engagement that is not yet well described in the literature • Entire drug discovery process improved and sped up shortened by 25%	• Potential to cut drug discovery time by 25% and reduce overall drug development costs by 20% • This add-on is expected to generate additional net income for IKH of about €1.25 Mio within the next five years • Potential savings of several million euros or potentially much more (depending on the actual steps covered). • Comptetitive advantage in a challenging market • Technology developed is expected to increase success rates from 10% to 40% in other further drug discovery problems

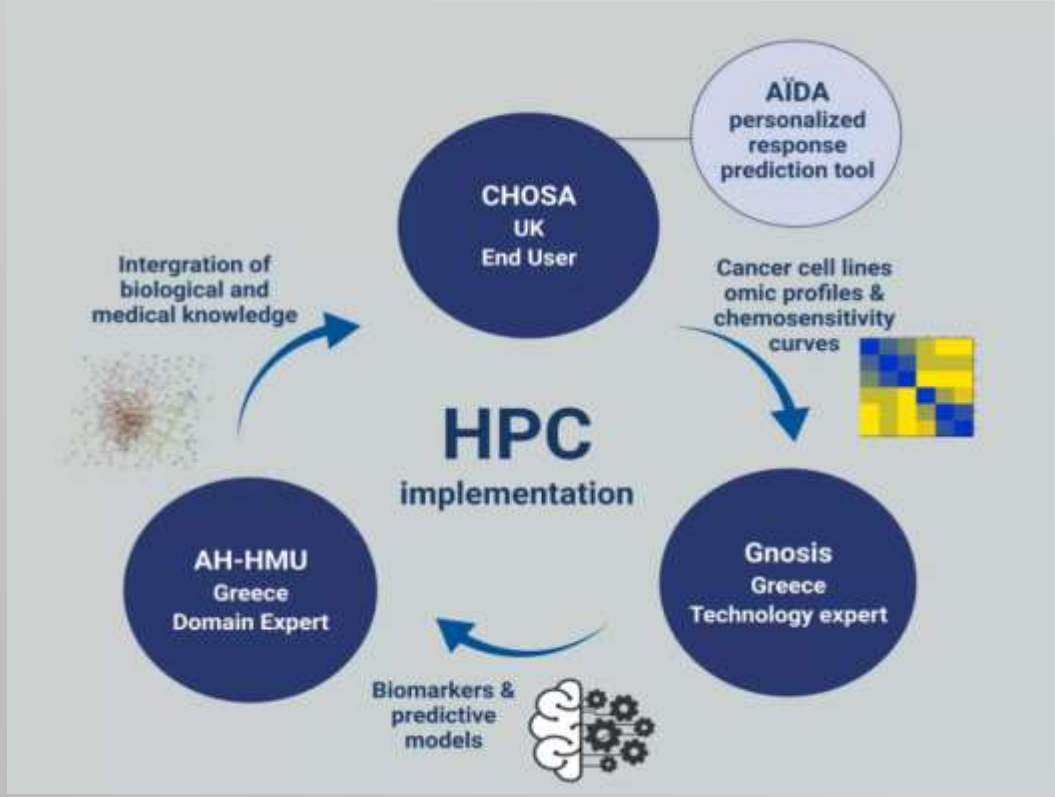


High-Performance Computing Enhances Treatment Precision in Breast Cancer

Who?	The Problem	The Challenge
United Kingdom End User: **CHOSA Oncology Ltd** Domain Expert: **Hellenic Mediterranean University** Technology Expert: **JADBio**	• Many cancer patients fail to respond to their drug treatment, resulting in heavy human and economic loss • Lack of efficacy is mainly attributed to host/tumour variations at the genetic and molecular level, which clinical practice still struggles to integrate • New digital genomic technology delivers treatment regimens that assess and use the DNA, RNA, protein, and metabolites in the individual patient's tumour	• Current technologies focusing on just one or a few genetic biomarkers or using complex ex vivo laboratory tumour models are predictive of treatment outcomes only in highly selected cases and difficult to implement effectively • Building an easy-to-use and intelligent platform to identify effective drugs in each individual requires the analysis of huge data sets.

High-Performance Computing Enhances Treatment Precision in Breast Cancer

The HPC Solution	The Business Benefit
• Extensive analyses of a huge volume of publicly available data (called NCI-60), which link different types of cancer to the anticancer activity of over 50,000 compounds • Using the JADBio autoML platform and HPC resources, ML models for these selected compounds were built to estimate the models' performance in predicting treatment outcomes • Analyses ve required a prohibitive amount of time without the employment of HPC	• After further validation, the models will be used to set up a complete platform called 'Allied Intelligence for Drug Accuracy' (AÏDA) which predicts the efficacy of different cancer drugs for each individual patient • No similar solutions exist at the moment • With a focus on breast cancer, a business potential of up to €69m, based on an anticipated price of €3,000 per service.



More HPC Success Stories

For more inspiration:

EuroCC2
Success Story Booklet
now available!

EuroCC2 Success Stories

https://eurohpc-ju.europa.eu/system/files/2023-06/EuroCC_booklet_2023%20(1).pdf

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Adapting HPC for SMEs

HPC Needs by Stakeholder Type

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Big Industry

- May have in-house HPC capabilities
- May have more liberal spending limits
- May have easier access to technology experts
- May be more time constraint-bound, in order to ensure competitiveness
- May have strict data or code confidentiality constraints.
- May have the capability of investing in research

Academia

- May not have continuous flow of funding
- May have more freedom in accessing public HPC infrastructures
- May have HPC capabilities in-house
- May have to create novel/custom procedures or workflows
- May be allowed limited access to proprietary solutions, due to copyright issues etc

Public Sector

- May rely on limited funding
- May face more regulations or restrictions on where and how to spend funding
- May be less deadline-bound
- May need robust HPC solutions, as decision-making may be slower

No “one size fits all”!

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What would you say is the biggest challenge in adopting HPC for your SME?

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The challenges in the case of the SME

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COST

Prohibitive cost of in-house infrastructure

Limited budget for infrastructure hire

Limited budget for solution acquisition

FLEXIBILITY

Computational requirements and needs may fluctuate during development

Workflows may need to be adapted to available infrastructure

DATA

Data transfer time may be an issue

Data confidentiality may affect choice of infrastructure

Data storage needs may affect the cost

EXPERTISE

Adapting workflows to HPC may require experts outside of the SME's field

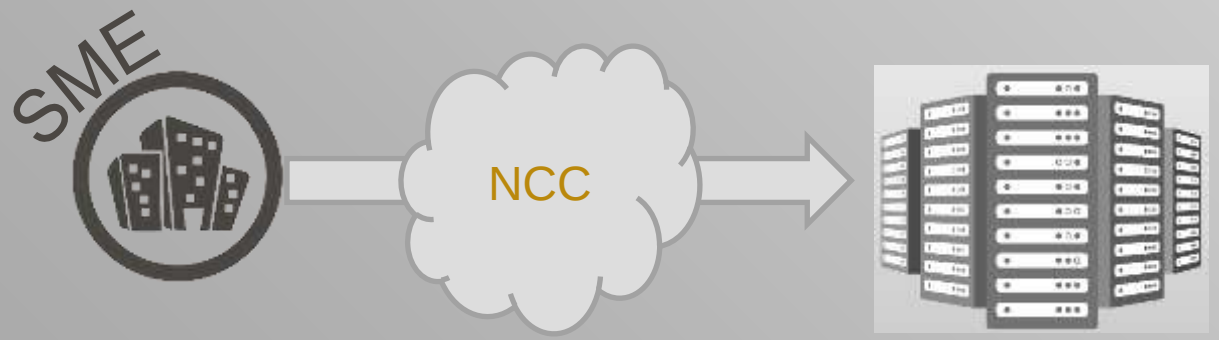
Experts should have a combination of backgrounds to better serve the SME's HPC need

INVESTMENT

Competitive markets

Must carefully choose where to invest time and budget

Exploratory research may be prohibitive



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Which of these challenges would you rank as more demanding?

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Access to infrastructure

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HPC for hire

+ Flexibility, more freedom of choice

- Extra cost that may be prohibitive

Cloud Solutions

+ Versatile

- Still incur cost, versatile under conditions

National Infrastructures

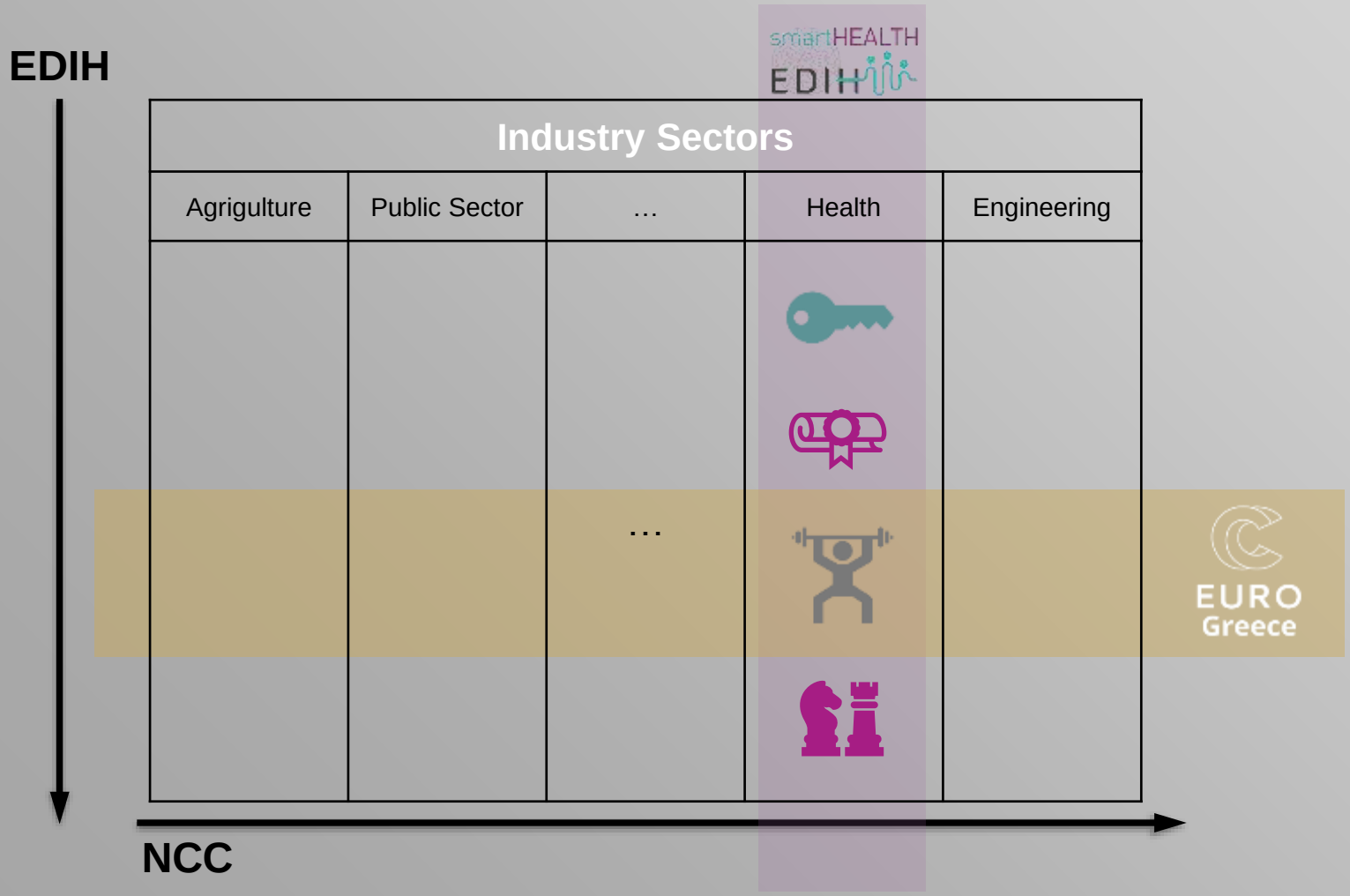
+ Lower cost

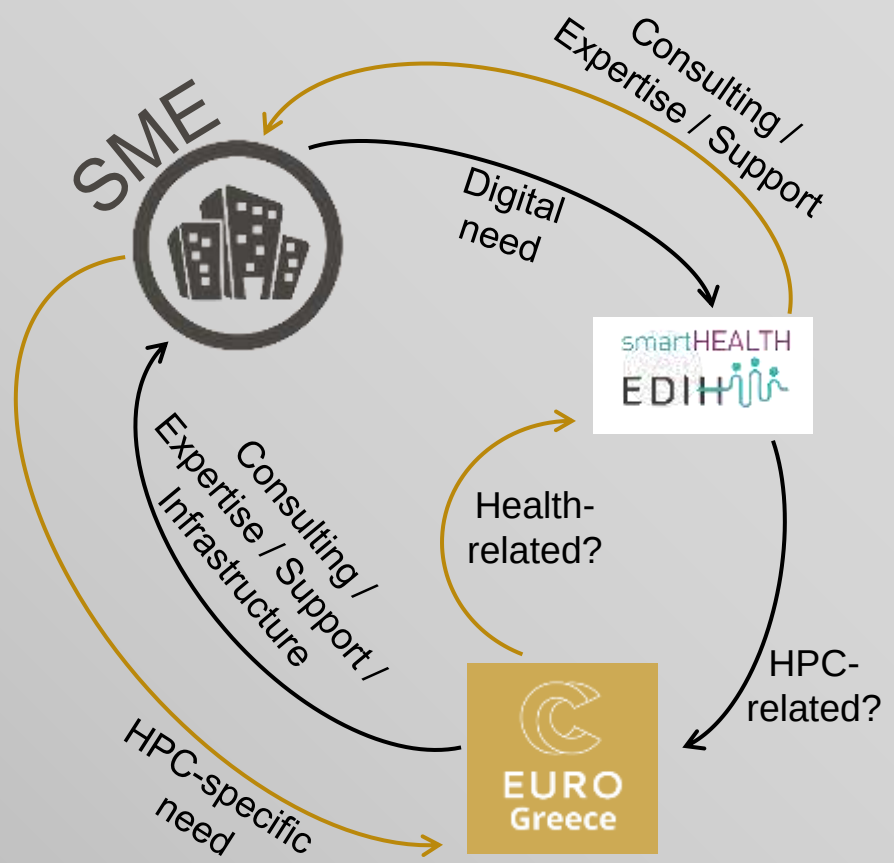
- Eligibility may be restricted

Access to infrastructure

Available resources and how to use them

Contact your NCCs and EDIHs





EuroCC@Greece Website

EuroCC@Greece Website

https://eurocc-greece.gr /

EuroCC@Greece Website

Industrial Training Course

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Industrial Training Course

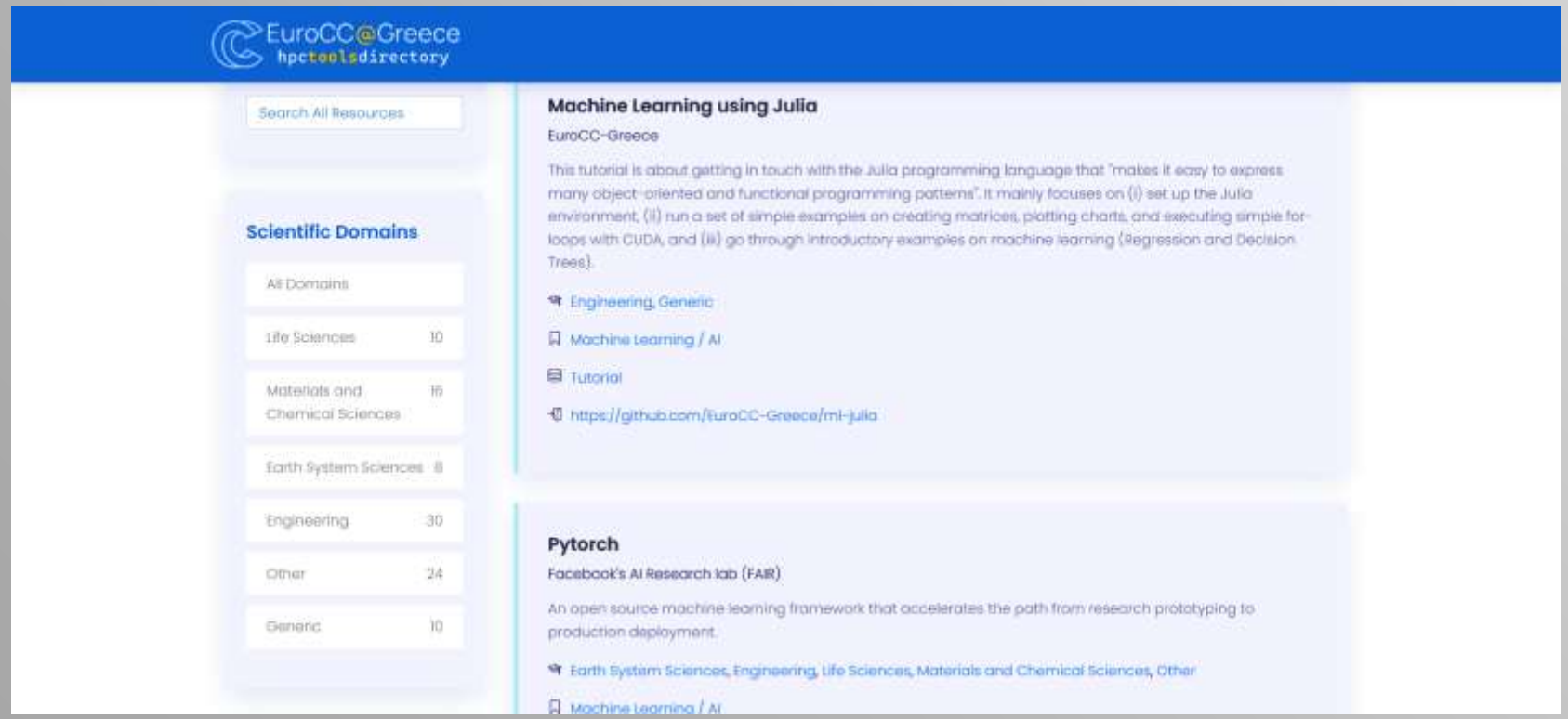
https://mssg.ipta.demokritos.gr/tng4hpc4ind/

HPC Marketplace

HPC Marketplace

https://hub.eurocc-greece.gr/

HPC Tools Directory



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HPC Tools Directory

https://hpctools.chemeng.ntua.gr/

Call for expression of interest

Are you an industry or government stakeholder looking for access to HPC resources?

- Apply to our program and secure assistance in your project projects by members of the High-Level Support Team of EuroCC@Greece.

Fill out the form or e-mail
contact@eurocc-greece.gr

Express Your Interest in HPC!

Get in touch and stay connected!

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contact@eurocc-greece.gr

Newsletter

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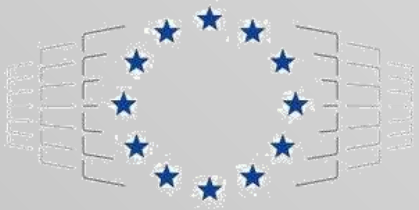
Contact Us!

Thanks!



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Joint Undertaking

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Q & A

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Contact Us!