EURO

Pavlos Sermpezis

“Computational chemistry & HPC” seminar

Aristotle University of Thessaloniki - December 09, 2024

EuroCC@Greece - at a glance

- **EuroCC**
  - European project to establish **National Competence Centres (NCCs)** …
  - … on **High Performance Computing (HPC)** …
  - … in **33 European countries**
  - Started in **2020**
  - Funded by EuroHPC JU & GSRI

- **EuroCC@Greece** is the **NCC** for **HPC** in **Greece**

EuroCC@Greece - at a glance

- **Members**
  - GRNET – National Infrastructures for Research and Technology *(coordinator)*
  - National Center for Scientific Research “Demokritos”
  - Foundation for Research and Technology – Hellas (FORTH)
  - Institute of Communication and Computer Systems of NTUA
  - Aristotle University of Thessaloniki

The role of EuroCC@Greece

- Mission & Role of the National Competence Centre (NCC)
  - **Point of contact** and coordination on a national level for HPC
  - **Cover needs of HPC users**
    - access to resources, technological consultancy, training courses, networking, etc.
  - Set up a cross-European network of NCCs

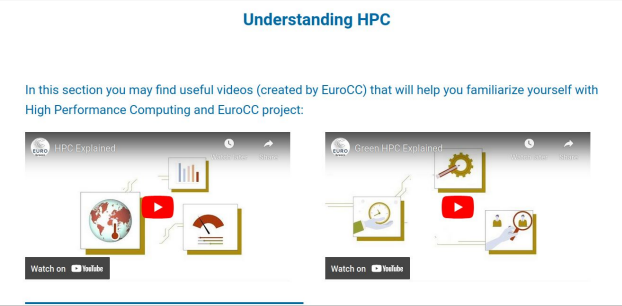
- Users
  - **Research & academic institutions**
    - e.g., to advance competitiveness
  - **Public administration**
    - e.g., to improve effectiveness
  - **Industry**
    - e.g., to promote innovation

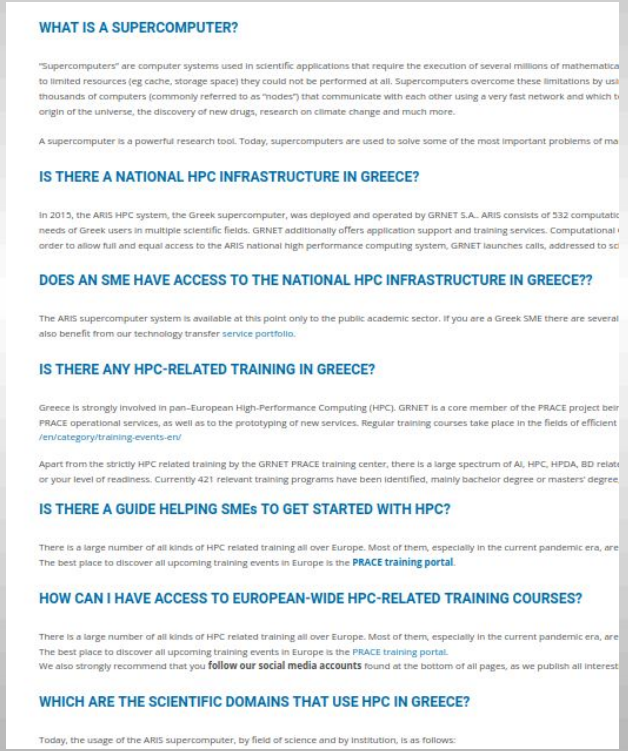
“Services” of EuroCC@Greece

- Learn about HPC
- Access to training resources (courses, videos, tools, code, etc.)
- Access to infrastructure
- Industrial innovation (tech transfer, funding opportunities, internships)
- Mapping of competences
- HPC “marketplace”
- Information (news, newsletter, etc.)
- Event organization

Training

- Introduction to HPC





WHAT IS A SUPERCOMPUTER?

"Supercomputers" are computer systems used in scientific applications that require the execution of several millions of mathematica
to limited resources (eg cache, storage space) they could not be performed at all. Supercomputers overcome these limitations by usi
thousands of computers (commonly referred to as "nodes") that communicate with each other using a very fast network and which t
origin of the universe, the discovery of new drugs, research on climate change and much more.

A supercomputer is a powerful research tool. Today, supercomputers are used to solve some of the most important problems of ma

IS THERE A NATIONAL HPC INFRASTRUCTURE IN GREECE?

In 2015, the ARIS HPC system, the Greek supercomputer, was deployed and operated by GRNET S.A.. ARIS consists of 532 computatic
needs of Greek users in multiple scientific fields. GRNET additionally offers application support and training services. Computational
order to allow full and equal access to the ARIS national high performance computing system, GRNET launches calls, addressed to sc

DOES AN SME HAVE ACCESS TO THE NATIONAL HPC INFRASTRUCTURE IN GREECE??

The ARIS supercomputer system is available at this point only to the public academic sector. If you are a Greek SME there are several
also benefit from our technology transfer service portfolio.

IS THERE ANY HPC-RELATED TRAINING IN GREECE?

Greece is strongly involved in pan-European High-Performance Computing (HPC). GRNET is a core member of the PRACE project beir
PRACE operational services, as well as to the prototyping of new services. Regular training courses take place in the fields of efficient
/en/category/training-events-en/

Apart from the strictly HPC related training by the GRNET PRACE training center, there is a large spectrum of AI, HPC, HPDA, BD relate
or your level of readiness. Currently 421 relevant training programs have been identified, mainly bachelor degree or masters' degree

IS THERE A GUIDE HELPING SMEs TO GET STARTED WITH HPC?

There is a large number of all kinds of HPC related training all over Europe. Most of them, especially in the current pandemic era, are
The best place to discover all upcoming training events in Europe is the **PRACE training portal**.

HOW CAN I HAVE ACCESS TO EUROPEAN-WIDE HPC-RELATED TRAINING COURSES?

There is a large number of all kinds of HPC related training all over Europe. Most of them, especially in the current pandemic era, are
The best place to discover all upcoming training events in Europe is the PRACE training portal.
We also strongly recommend that you **follow our social media accounts** found at the bottom of all pages, as we publish all interest

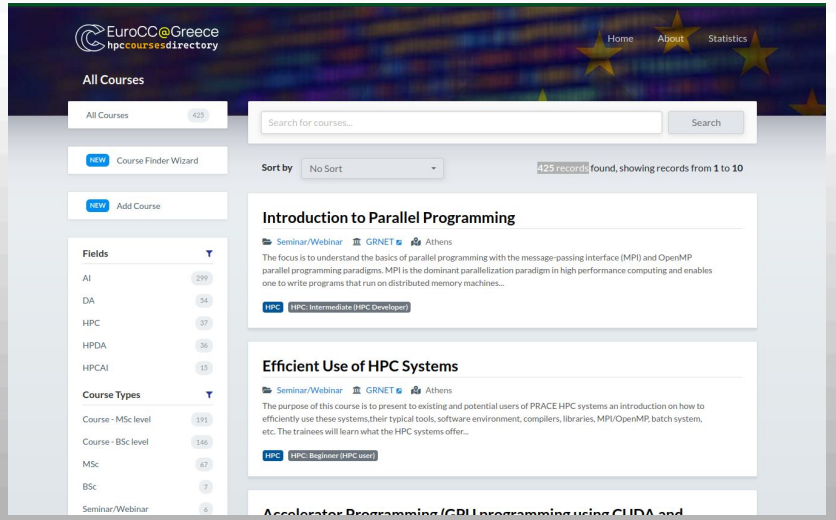
WHICH ARE THE SCIENTIFIC DOMAINS THAT USE HPC IN GREECE?

Today, the usage of the ARIS supercomputer, by field of science and by institution, is as follows:

Training

- HPC PRACE training center
  - seminars: Parallel Programming, GPU programming, CUDA, biomolecular modeling in HPC, ML/AI in HPC, Meteorological and climate modeling, etc.

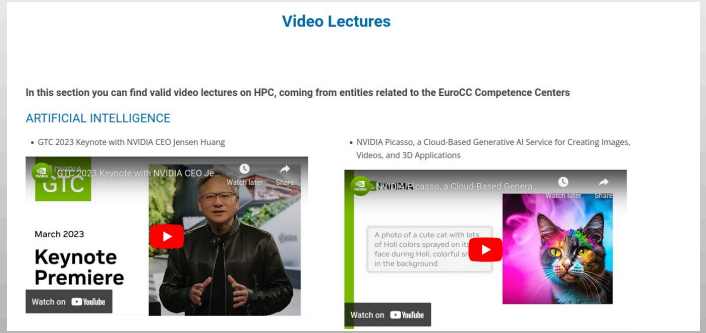
- Repository of HPC training courses
  - http://hpc-courses.chemeng.ntua.gr/
  - 425 courses (BSc, MSc, seminars, summer schools, etc.)



Training

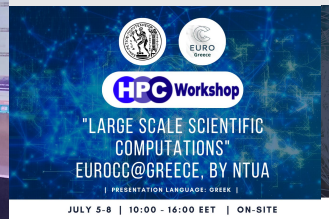
- Repository of video lectures (YouTube)
  - Topics: HPC, AI, Biomolecular, CFD, Computational chemistry, Energy, Material sciences, Seismology

- Links to external repositories of training resources



Training

- Several training events every year



Access to HPC resources

- HPC infrastructures in Greece
  - GRNET - “ARIS”
  - AUTH - “Aristotelis”
  - ICS-FORTH
  - Demokritos

- External infrastructure
  - MELUXINA
  - Leonardo

contact us!!

HPC marketplace

- **HPC marketplace**: database (or “yellow pages”) of HPC providers in Greece

- **“HPC providers”**
  - HPC service providers (industry & academia)
  - HPC infrastructure providers
  - HPC experts (independent professionals)
  - … that provide any type of HPC and/or Big Data and/or AI services

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

Tech transfer & Industry hub

- **Services to industry**
  - Access to HPC infrastructure
  - Access to funding
  - Tech transfer services
  - Consultation in HPC, AI and HPDA technologies
  - Mentoring on business aspects
  - Networking
  - Facilitation of industrial internships

Computational chemistry & HPC agenda

10:00 → 10:15	**Introduction: EuroCC@Greece** Presentation language: Greek **Speaker**: Pavlos Sermpezis (Senior Researcher, EuroCC@Greece / Aristotle University of Thessaloniki)	15m
10:15 → 10:30	**Molecular sensor design using HPC** Presentation language: English **Speaker**: Stepas Toliautas (Associate Professor, Vilnius University / NCC Lithuania)	15m
10:30 → 11:00	**Development of a high-performance quantum Monte Carlo library (QMCkl)** Presentation language: English **Speaker**: Viiay Gopal Chilkuri (Associate Professor, Aix Marseille Univ / CNRS / Centrale Méditerranée / iSm2, Marseille, France & TREX CoE)	30m
11:00 → 11:30	**Introduction to AUTH's HPC infrastructure "Aristotelis"** Presentation language: Greek **Speaker**: Paschalis Korosoglou (HPC engineer, IT AUTH)	30m
11:30 → 11:45	**Break**	15m
11:45 → 12:45	**Charge Transfer Unveiled: An Exciting Journey Through TD-DFT** Presentation language: Greek **Speaker**: Emmanuel Koukaras (Assistant Professor, Aristotle University of Thessaloniki)	1h
12:45 → 13:45	**Machine Learning in chemistry for everyone: A practical guide for quick development of predictive models** Presentation language: Greek **Speaker**: Georgios Fanourgakis (Assistant Professor, Aristotle University of Thessaloniki)	1h
13:45 → 14:00	**Questions / Open discussion**	15m

Live interactive Q&A tool:
https://hackmd.io/@pkoro/SygDY4e41x

Find the links also at the **zoom chat**

EuroCC@Greece training questionnaire:
https://docs.google.com/forms/d/e/1FAIpQLSdHpJyAbIuWwpelBy812mEirEOGzYnV5JFMnSQkCu4aItMnJA/viewform

Thanks!

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

Twitter: @EuroCC_Greece

LinkedIn: eurocc-greece

YouTube: @euroccgreece9501

Newsletter: https://eurocc-greece.gr/newsletter/

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