



# EURO

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“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



**EuroHPC**  
Joint Undertaking

- **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



ΑΡΙΣΤΟΤΕΛΕΙΟ  
ΠΑΝΕΠΙΣΤΗΜΙΟ  
ΘΕΣΣΑΛΟΝΙΚΗΣ

# 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

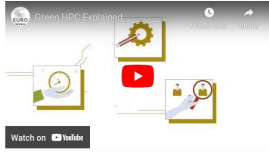
- Introduction to HPC


**Understanding HPC**

In this section you may find useful videos (created by EuroCC) that will help you familiarize yourself with High Performance Computing and EuroCC project:



Watch on  YouTube



Watch on  YouTube

## WHAT IS A SUPERCOMPUTER?

"Supercomputers" are computer systems used in scientific applications that require the execution of several millions of mathematical operations to limited resources (eg cache, storage space) they could not be performed at all. Supercomputers overcome these limitations by using thousands of computers (commonly referred to as "nodes") that communicate with each other using a very fast network and which in turn, 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 modern science.

## IS THERE A NATIONAL HPC INFRASTRUCTURE IN GREECE?

In 2013, the ARIS HPC system, the Greek supercomputer, was deployed and operated by GRNET S.A. ARIS consists of 332 computational nodes of Greek users in multiple scientific fields. GRNET additionally offers application support and training services. Computational nodes are available to all Greek users in order to allow full and equal access to the ARIS national high performance computing system. GRNET launches calls, addressed to SMEs, to use the ARIS supercomputer.

## 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 ways to access the ARIS supercomputer. You can contact the ARIS supercomputer support team or the 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 being PRACE operational services, as well as to the prototyping of new services. Regular training courses take place in the fields of efficient HPC applications. For more information, visit the PRACE training portal.

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

## 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 free of charge. The best place to discover all upcoming training events in Europe is the PRACE training portal.

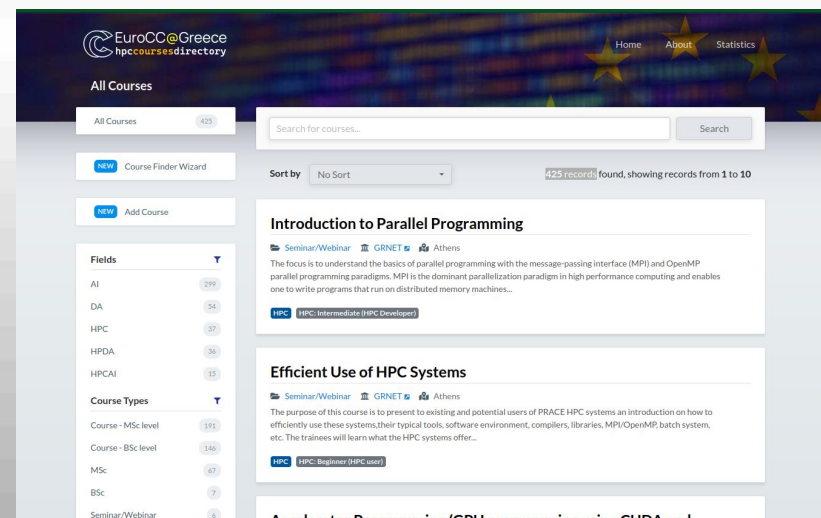
## HOW CAN I HAVE ACCESS TO EUROPEAN-WIDE HPC-RELATED TRAINING COURSES?

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 free of charge. 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 interesting information.

## 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:

- 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.)



The screenshot shows the EuroCC@Greece hpcoursesdirectory website. The header includes the logo and navigation links for Home, About, and Statistics. The main content area is titled 'All Courses' and features a search bar, a 'Course Finder Wizard', and an 'Add Course' button. A sidebar on the left lists various fields and course types with their respective counts:

Fields	Count
AI	299
DA	54
HPC	37
HPDA	36
HPCAI	15

Course Types	Count
Course - MSc level	191
Course - BSc level	146
MSc	87
BSc	7
Seminar/Webinar	6

The main content area displays a search bar with the text 'Search for courses...', a 'Search' button, and a 'Sort by' dropdown menu. Below the search bar, it indicates '425 records found, showing records from 1 to 10'. The first course listed is 'Introduction to Parallel Programming', which is a seminar/webinar in Athens, focusing on parallel programming with MPI and OpenMP. The second course is 'Efficient Use of HPC Systems', also a seminar/webinar in Athens, focusing on the efficient use of HPC systems and their tools.


- Repository of video lectures (YouTube)
  - Topics: HPC, AI, Biomolecular, CFD, Computational chemistry, Energy, Material sciences, Seismology
  
- Links to external repositories of training resources


**Video Lectures**

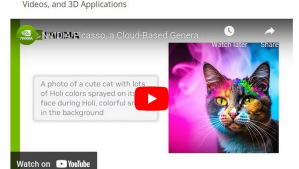
In this section you can find valid video lectures on HPC, coming from entities related to the EuroCC Competence Centers


**ARTIFICIAL INTELLIGENCE**

- GTC 2023 Keynote with NVIDIA CEO Jensen Huang
- NVIDIA Picasso, a Cloud-Based Generative AI Service for Creating Images, Videos, and 3D Applications



March 2023  
**Keynote  
Premiere**  
Watch on  YouTube



A photo of a cute cat with lots of Holi colors sprayed on its face during Holi, colorful in the background.  
Watch on  YouTube



# 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	<b>Introduction: EuroCC@Greece</b>	⌚ 15m
Presentation language: Greek			
<b>Speaker:</b> Pavlos Sermpetzis (Senior Researcher, EuroCC@Greece / Aristotle University of Thessaloniki)			
10:15	→ 10:30	<b>Molecular sensor design using HPC</b>	⌚ 15m
Presentation language: English			
<b>Speaker:</b> Stepas Toliautas (Associate Professor, Vilnius University / NCC Lithuania)			
10:30	→ 11:00	<b>Development of a high-performance quantum Monte Carlo library (QMCKI)</b>	⌚ 30m
Presentation language: English			
<b>Speaker:</b> Viitay Gopal Chilkuri (Associate Professor, Aix Marseille Univ / CNRS / Centrale Méditerranée / iSm2, Marseille, France & TREX CoE)			
11:00	→ 11:30	<b>Introduction to AUTH's HPC infrastructure "Aristotelis"</b>	⌚ 30m
Presentation language: Greek			
<b>Speaker:</b> Paschalis Korosoglou (HPC engineer, IT AUTH)			
11:30	→ 11:45	<b>Break</b>	⌚ 15m
11:45	→ 12:45	<b>Charge Transfer Unveiled: An Exciting Journey Through TD-DFT</b>	⌚ 1h
Presentation language: Greek			
<b>Speaker:</b> Emmanuel Koukaras (Assistant Professor, Aristotle University of Thessaloniki)			
12:45	→ 13:45	<b>Machine Learning in chemistry for everyone: A practical guide for quick development of predictive models</b>	⌚ 1h
Presentation language: Greek			
<b>Speaker:</b> Georgios Fanourgakis (Assistant Professor, Aristotle University of Thessaloniki)			
13:45	→ 14:00	<b>Questions / Open discussion</b>	⌚ 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/1FAIpQLSdHpJyAbLuWwpelBy812mEirEOGzYnV5JFMnSQkCu4altMnJA/viewform>



# Thanks!

**Web:** <https://eurocc-greece.gr/>

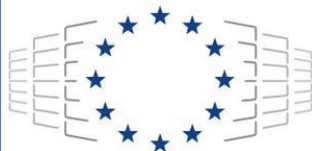
**Twitter:** @EuroCC\_Greece

**LinkedIn:** eurocc-greece

**YouTube:** @euroccgreece9501

**Newsletter:**

<https://eurocc-greece.gr/newsletter/>



**EuroHPC**  
Joint Undertaking

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