



THE CYPRUS  
INSTITUTE

RESEARCH • TECHNOLOGY • INNOVATION



EURO

**EuroCC support Opportunities Academia**

**CaSToRC - Dr. Jacob Finkenrath**

### Outline:

- Overview on the activities of the NCC in HPC for Academia
  - Results on Survey on HPC
- Training and Events
  - Beginner to Advance events
- HPC Resources on National and European Level
  - PRACE and upcoming EuroHPC system
  - Software efforts in HPC
- Expression of Interest for Support

## EuroCC will strengthen the HPC competences on the national level by

- Establishing a National Competence Centre (NCC) of high-performance computing (HPC) in participating countries.
  - NCCs will coordinate activities in all HPC-related fields at the national level
  - serve as a contact point for customers from industry, science, and the general public alike
- Elevate participating countries to a common high level in the fields of **HPC, HPDA and AI** through National Competence Centres (NCCs),
  - NCC will be responsible for surveying and documenting the core HPC, HPDA, and AI activities and competencies in their respective countries.

**CaSToRC is acting as the National Competence Center in HPC for Cyprus**

### Strengthen the HPC Competences in the Cypriot community by inter-connecting, supporting and training

- **Connecting:** *HPC to academic and industrial partners by*
  - Call for expression of interest for projects
  - Events like industrial week/user forum and hackathons
- **Training:** *On High Performance Computing*
  - Courses on HPC for all level: from beginners to advance
  - Support of interns and personnel to strengthen HPC competences
- **Supporting:** *Application to HPC machines and resources*
  - Training and support for technical aspects for computing time applications
  - Consulting by High Level Support Team at NCC for your HPC project



by using our Cyclone for scientific research in Cyprus

## Initialization

### Initialization Phase of project (Sep. 20 - Feb. 21)

#### Outreach and raising interest in NCC and HPC:

- Dissemination of our activities via our CaSToRC email list
- Direct outreach to more than 25 academic groups at 9 academic institutions (so far) to understand HPC needs and interest
  - positive feedback and raised interest for our trainings, services and resources
- Virtual Seminar series started Nov. 2020 on “How HPC can enable innovation and research”

#### Support effort:

- Activities of High Level Support Team
  - support of HPC projects
    - for upcoming phase we target to extend this via our call for “Expression of Interest for Support”
  - Internship: hosting one at our side and we are recruiting and looking for projects
  - HLST participates in training events (like Machine learning in HPC), (note we are recruiting)

#### Evaluation of Needs:

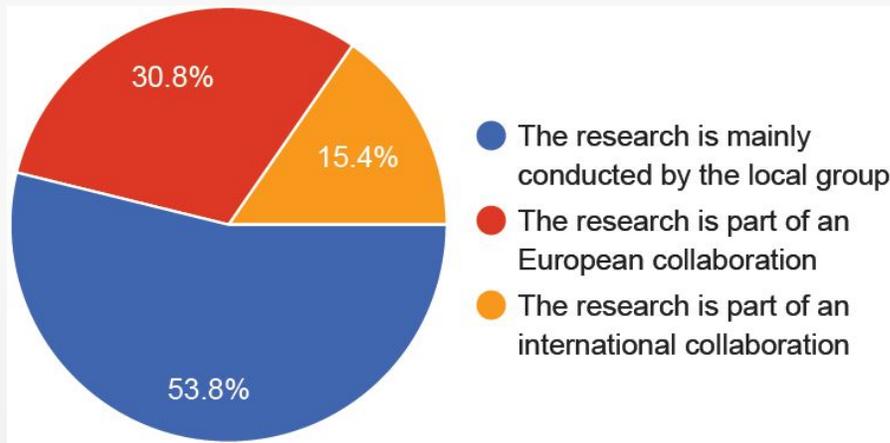
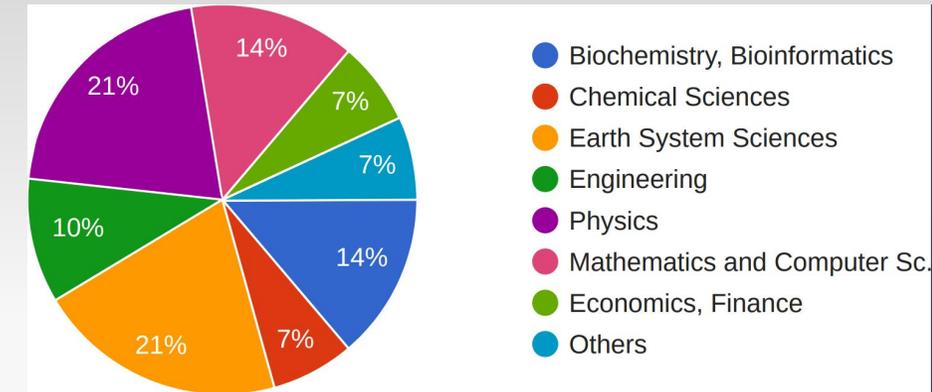
- First Survey on HPC needs and competences (Oct. 20):

**Results are used to design our training and support program**

## Academic Survey - Results

Survey for the academic community received 28 replies:

- completed by research groups from 10 different institutions
- more than 50% of the groups conduct their research locally



### Main topics of interest for training :

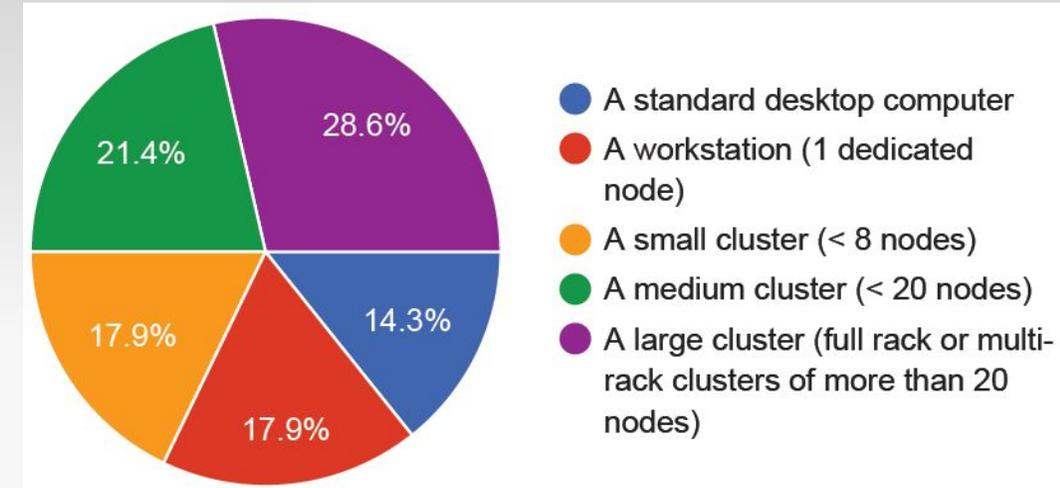
- Python for HPC
- Scientific software packages
- New computational methods for simulations
- Machine learning

## Academic Survey - HPC Competences

### Competence uniformly distributed in:

- Parallel computing, software development and proposal writing
- Usage and interaction of HPC software - ranging between high-level to low level.
- Usage of computational resources from standard computers to large HPC clusters

- Most used programming languages are in the following order:
  - Python, Fortran, C and C++, R
- Most of the HPC applications implement multi-threading and Message Passing Interface (MPI) parallelization
- Only half have GPU support
  - While all the others have expressed interest in supporting it in the near future.



**major interest in training and support for accessing computational resources**

## Training Events at NCC

- **Medium Level** (19 - 21 April 2021)
  - advanced aspects of HPC including MPI, OpenMP and Hybrid Programming and Python for HPC
  - Software profiling, improving scalability and performance of codes
  - Post processing of data and automating execution of workflow
- **Beginner Level** (15 - 17 Feb. 2021), Next one scheduled Q3 - 21  
we had 40+ participants and addressed a broad level
  - Hands-on training on how to remotely access, use the NCC infrastructure and basic OpenMP
  - How to run applications on the infrastructure
  - Basics of parallel programming, machine learning using HPC, Python using HPC
- For news and upcoming events: Check our webpage and meetup  
<https://www.meetup.com/high-performance-computing-cyprus/events/>

- **HPC NCC Seminar series, every 2 week**
  - addresses how HPC enables research
    - 2.03 Mr Brendan McGinty, Dr Seid Koric (National Center for Supercomputing Applications) CSA Industry Overview with Computational Breakthroughs and Synergies with AI
    - 16.03 Prof. Martha Constantinou (Temple University) Synergy of HPC and Nuclear Physics to Resolve Long-standing Puzzles
- **Hackathons (17 - 21 May 2021)**
  - we are looking for groups and projects from academia
    - Users can apply and will get specific support for their projects within the event
- **Internship program (open)**
  - Looking for projects from academia and industry
    - paid and with rolling application via Graduate School with a duration of up to ~ 6 month
    - connecting interns to HPC related projects from academia and industry
  - Looking for interns
    - work on HPC projects by support by our HLST

### CaSToRC: HPC National Competence Center Spring 2021 Online Seminar Series

|        |  |  |
|--------|--|--|
| 12 Jan | Dr. Christos Christodoulou<br>(The Cyprus Institute)                                   | Fostering innovation with HPC, Advanced Simulations, AI and Big Data<br>(Joint EuroCC/SimEA seminar series)  |
| 19 Jan | Asst. Prof. Vangelis Daskalakis<br>(Cyprus University of Technology)                   | High-Performance Computing in Structural Biology<br>(EuroCC seminar series)  |
| 26 Jan | Prof. Panagiotis Grammatikopoulos<br>(Okinawa Institute of Science and Technology)     | Computer Simulation Aspects of Nanoparticle and Nanodevice Design<br>(SimEA seminar series)  |
| 2 Feb  | Prof. Zoe Cournia<br>(Academy of Athens)   | Multiscale Modeling of Biomolecules and Materials<br>(Joint EuroCC/SimEA seminar series)   |
| 16 Feb | Dr. Marios Zacharias<br>(Cyprus University of Technology)                              | Special Displacement Method for the Calculation of Materials' Properties at Finite Temperatures<br>(Joint EuroCC/SimEA seminar series)                                     |
| 2 Mar  | Mr Brendan McGinty, Dr Seid Koric<br>(National Center for Supercomputing Applications) | NCSA Industry Overview with Computational Breakthroughs and Synergies with Artificial Intelligence<br>(Joint EuroCC/SimEA seminar series)                                  |
| 9 Mar  | Dr. Thomas Montenegro-Johnson<br>(Birmingham University)                               | Active (non-) Particles: Donuts, Curved Rods, and Flexibility<br>(SimEA seminar series)  |
| 16 Mar | Prof. Martha Constantinou<br>(Temple University)                                       | Synergy of High-Performance Computing and Nuclear Physics to Resolve Long-standing Puzzles: The Proton Spin and Mass   |
| 23 Mar | Dr. Igor Chernyavsky<br>(The University of Manchester)                                 | TBC<br>(SimEA seminar series)  |
| 6 Apr  | Prof. George Froudakis<br>(University of Crete)  | Designing Novel Nanoporous Materials for Applications in Energy and Environment. From Multi-Scale Modeling to Materials Informatics<br>(Joint EuroCC/SimEA seminar series) |
| 20 Apr | Prof. Andreas Efstathiou<br>(European University Cyprus)                               | The CYGNUS Models for the Spectral Energy Distributions of Galaxies and their Supermassive Black Holes<br>(Joint EuroCC/SimEA seminar series)                              |

You can watch the webinars live on the allocated dates at 16:00 (Cyprus time) via  
Zoom: <https://zoom.us/j/9947402955?pwd=Um8wdTdHeStfMTM3LzNRL3l3Um45QT09> Password: Vs5Cr1  
To receive updates on these events, register at: <https://www.meetup.com/high-performance-computing-cyprus/>



The SimEA and EuroCC projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 810660 and No. 951740, respectively.

## HPC Facility - Cyclone

- Technical specification of out production machine **Cyclone**
  - various calls to access: production, preparatory and etc.

### Cyclone Specifications

|                                   |  |
|-----------------------------------|--|
| <b>Peak/Sustained Performance</b> | ~600 TFlop/s   |
| <b>Number of Nodes</b>            | 17 forty-core compute nodes                                  |
| <b>Processors/node</b>            | 16 forty-core compute nodes, each with 4 NVidia V100 GPUs    |
| <b>Memory/node</b>                | 2 twenty-core sockets per node, each is Intel Xeon Gold 6248 |
| <b>Scratch disk storage</b>       | 96 GB memory per cpu node 192 GB memory per compute node     |
| <b>Disk storage</b>               | Approximately 5 TBytes                                       |
| <b>Node-node interconnect</b>     | 135 TB NVMe Storage  |
| <b>accelerators</b>               | 3.2 PB Storage   |
| <b>OS info</b>                    | HDR 100  |
|                                   | GPUs available   |
|                                   | OS, Compute Node: CentOS                                     |
|                                   | OS, Front End & Service Nodes: CentOS                        |



- Cyclone Suitable to get started and scale up your applications
  - Environment similar to European systems, first step towards European Tier 0 systems

# Support Opportunities Academia - CaSToRC

## Access to Supercomputers in Europe



### PRACE: Partnership for Advance Computing in Europe

- Access to PRACE systems via regular Call for Proposals
  - Production Access, DECI, Shape, Preparatory A-D, etc.
- Top HPC systems in Europe
  - CPU (x86): Juwels, Joliot Curie, Hawk, SuperMUC-NG, Marenstrum, etc.
  - GPU (Nvidia) : Juwels-Booster, PizDaint, Marconi 100,.. etc.

with the current Top 7 system Juwels-Booster with 70 PetaFlops at JSC

- use Preparatory access for the first step

**Get in contact with us !**  
**Our HLST can help with their experience**



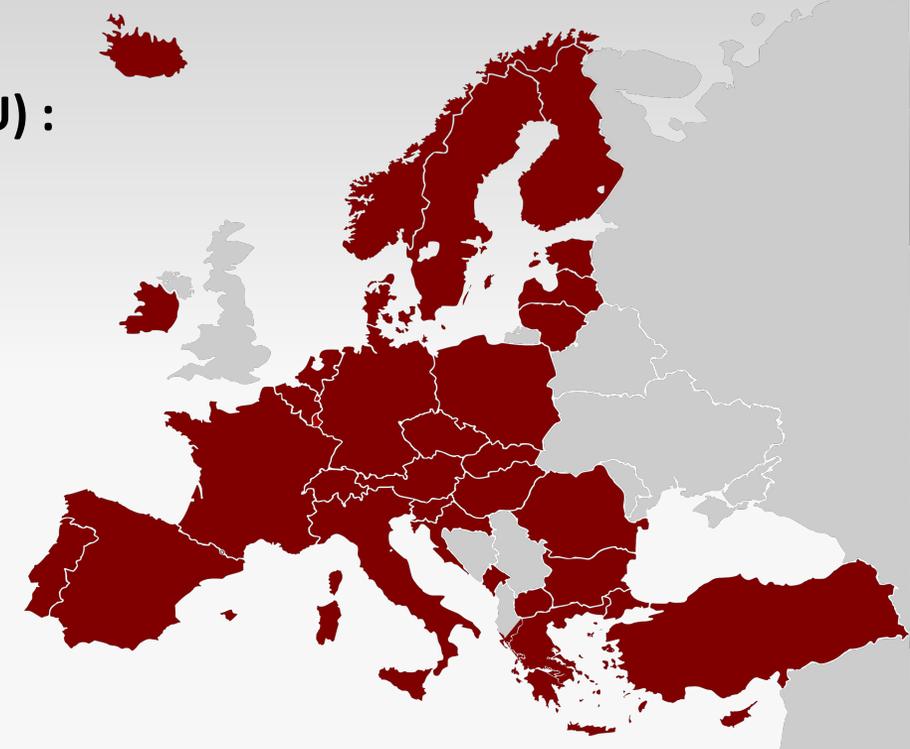
## Towards Exa-Scale Computing in Europe

### European High Performance Computing Joint Undertaking (EuroHPC JU) :

- buy and deploy top-of-the-range supercomputers
- develop innovative exascale HPC technologies and applications.

The JU is currently supporting two main activities:

- Supporting research and innovation activities:  
Developing a European supercomputing ecosystem, stimulating a technology supply industry
  - Within this effort is **EuroCC**
- Developing a pan-European supercomputing infrastructure:
  - **3 Pre-Exascale machines and 5 PetaFlop machines**



**Pushing Europe into the ExaScale Era**

Upcoming Budget (2021 - 2033): 8 billion Euro

## Overview : EuroHPC Joint Undertaking

### European High Performance Computing Joint Undertaking (EuroHPC JU) :

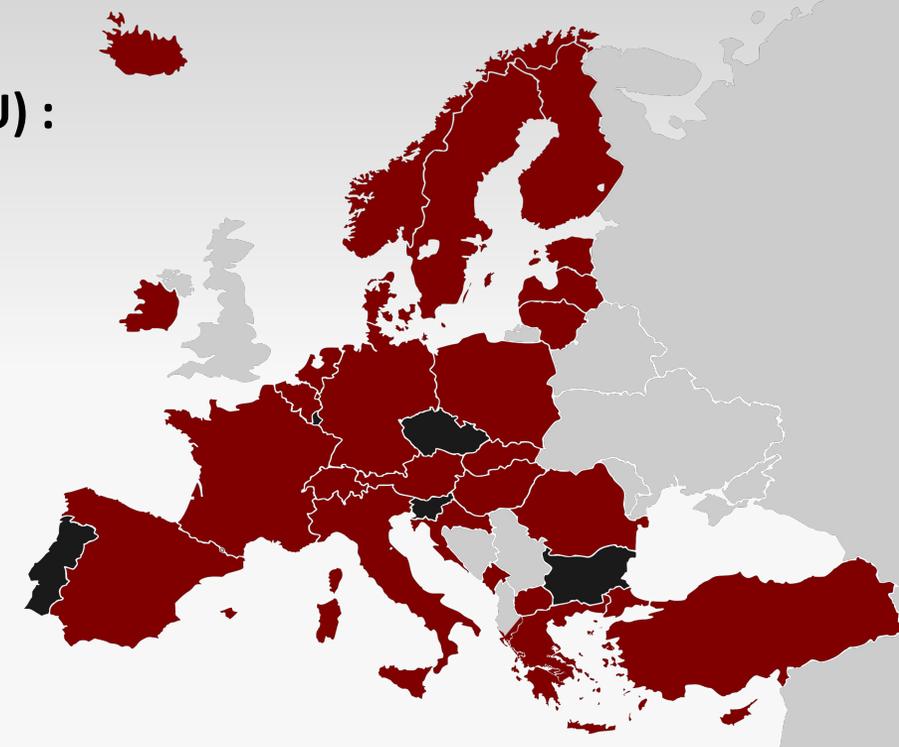
- buy and deploy top-of-the-range supercomputers
- develop innovative exascale HPC technologies and applications.

### 5 PetaFlop machines in Bulgaria, Czech, Luxembourg, Slovenia, Portugal

- ~ 4 - 15 new PetaFlops HPC machines
  - Bulgaria: *PetaSC* with 4.4 PetaFlops using AMD Epyc
  - Czech: with 15 PetaFlops using Nvidia A100
  - Luxembourg: *Meluxina* with 15 PetaFlops using Nvidia A100
  - Slovenia: *Vega* with 6.8 PetaFlops using Nvidia A100
  - Portugal: *Deucalion* with 10 PetaFlops using Fujitsu A64FX CPUs
- planned for coming online 2021 - 2022

with Cyclone Nvidia V100 partition you can prepare your applications

- most of the systems are based Nvidia GPUs



**Pushing Europe into the ExaScale Era**

## Overview : EuroHPC Joint Undertaking

### European High Performance Computing Joint Undertaking (EuroHPC JU) :

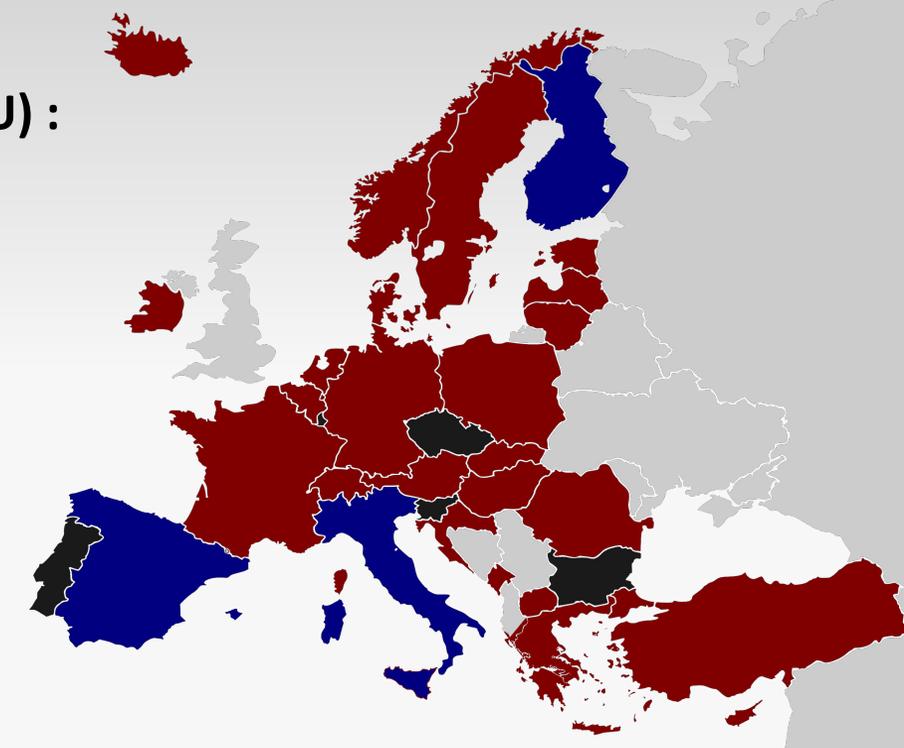
- buy and deploy top-of-the-range supercomputers
- develop innovative exascale HPC technologies and applications.

### 3 Pre ExaFlop machines in Finland, Italy and Spain

- ~ 200 - 500 new PetaFlops HPC machines
  - Finland: **Lumi** with 500 PetaFlops using AMD Instinct M100
  - Italy: **Leonardo** with 300 PetaFlops using Nvidia A100
  - Spain: **Marenostrum 5** with more than 200 PetaFlops (arch. tbd)
- expected to come online Q4 2021 - 2022

EuroHPC Pre Exa-Scale machines are coming with different architectures

- similar to current worldwide HPC trends



Pushing Europe into the ExaScale Era

At NCC we are following the new trends  
Get in touch !

## Specific Software and New computational Methods

### Various Center of Excellences in HPC

- *addressing Exa-scale computing in various scientific fields*
- *maybe possible synergy with your research*

see <https://www.hpccoe.eu/>

A short list:

- BioExcel (Comp. Biomolecular)
- ChEESE (Solid earth)
- CoEC (Combustion)
- CompBioMed (Comp. Biomedicine)
- E-CAM (Material and Comp. Science)
- EoCoE (Green Energy oriented)
- ESiWACE (Weather and Climate)
- EXCELLERAT (Engineering)
- HiDALGO (Global Systems Science )
- MaX (Material design)
- NOMAD (Comp. Material Science)
- RAISE (AI and Sim. based Engineering)
- PerMedCoE (Personalised Med.)
- POP (Perf. Optimization)
- TREX (Chemistry)



**Develop Exascale solutions in various (your) fields !  
(Best practice how to scale up)**

## Expression of interest for Academia (NOW OPEN)

### Targeted Research/Academic programme

Call for **academic and research community** to **express their interest** in HPC Support

#### Aims to:

- Helping HPC beginners from research and academic institutions to leverage access and usage of HPC
- Help experienced research groups to scale up or optimise HPC applications
- Increase the efficiency, expertise and competitiveness of Cyprus-based research groups.
- Enable the uptake of the key future technologies of HPC, Big Data Analytics and AI in Cyprus
- Projects will **will be assisted** by members of the NCC High Level Support Team of CaSToRC
- Funding from the NCC are available to support the technical personnel involved in the development

See: <https://docs.google.com/forms/d/e/1FAIpQLSfVidSNmJPTTo2A7nLS9bD38sIOj-an4NRKXKibER7wCI8lCNQ/viewform>

**Please contact me if you have any question !**

*Cultivate the use of HPC, Simulation and Data Science and to serve the needs for compute- and data-intensive applications for academia, government and industry.*

### We are recruiting and seeking for

- Expression of interests for HPC support from academia and industry
- Team members for HLST from all areas
- Internship students and post graduates for HPC related projects

News and Events will be announced via:

- Our Email list: <https://castorc.cyi.ac.cy/subscribe-to-castorc>
- Our social media channels, webpage, etc.

## Useful Links and References

- Regular updated webpage: <https://castorc.cyi.ac.cy/national-hpc-competence-centre>
- Open positions for NCC via <https://jobboard.cyi.ac.cy>  
or see <https://jobboard.cyi.ac.cy/?q=1042297719> and <https://jobboard.cyi.ac.cy/?q=774774257>
- Call for Expression of Interest  
see <https://docs.google.com/forms/d/e/1FAIpQLSfVidSNmJPTTo2A7nLS9bD38sIOj-an4NRKXKibER7wCl8lCNQ/viewform>
- Inauguration of the Cypriot NCC at the 10th September 2020  
<https://castorc.cyi.ac.cy/inauguration-of-the-national-hpc-competence-centre>  
<https://www.youtube.com/watch?v=s1bKebGFIWQ&feature=youtu.be&t=10s>
- User support: <https://castorc.cyi.ac.cy/training-user-support/user-support>  
Contact: [castorc.support@cyi.ac.cy](mailto:castorc.support@cyi.ac.cy) or contact person for users from academia [j.finkenrath@cyi.ac.cy](mailto:j.finkenrath@cyi.ac.cy)



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