

# Introductory to the HPC National Competence Center

CaSToRC, Cyprus



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EURO

# Computation-based Science and Technology Research Center - CaSToRC

CaSToRC is one of four research centers of The Cyprus Institute designated by the Government as the National HPC Competence Center under the EuroCC project, with the mission to:

*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*

## **Objectives:**

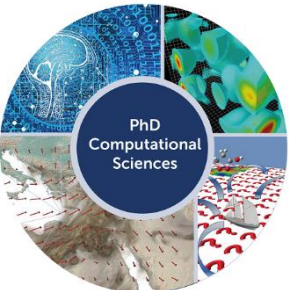
- To carry out research in computational sciences and engineering of international caliber
- To deliver graduate education programs in Simulation and Data Science, and Computational Sciences
- To provide training, advanced user support to academia and industry and access to a computational resources

# CaSToRC – Educational Programmes



- Master of Science (MSc) degree in Simulation and Data Sciences (SDS)

- Provide a unique interdisciplinary approach to solve critically important problems, using applied mathematics, physics, chemistry, biology, statistics and computing. Through modelling, simulation, data mining, and study of specific phenomena via computer analysis, students will learn to apply computation and data analytics to gain new insights.



- Doctor of Philosophy in Computational Sciences

- Educate students and carry out significant research in Computational Science with specialization in important fields that require High Performance Computing such as Climate Modelling, Computational Physics, Machine Learning, Scientific Computing, Computational Chemistry, 3D Visualization and Computational Biology.

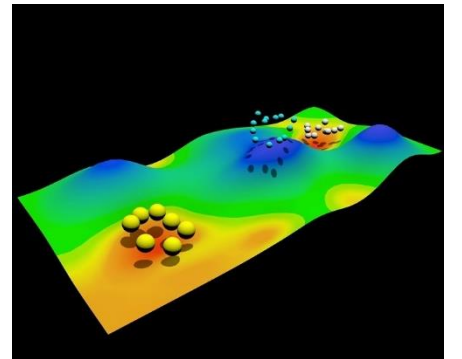
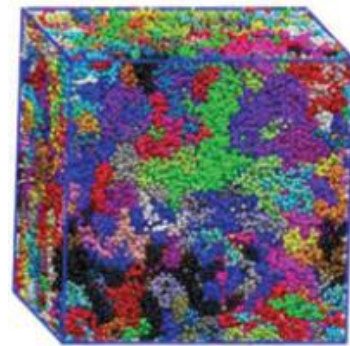
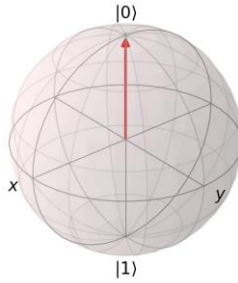


- European Joint Doctorates: Simulation in MULTISCALE physical and biological systems (STIMULATE)

- Delivers an interdisciplinary European Joint Doctorate (EJD) program in computational science, which educates students to best address the challenges posed by exascale computing and data-intensive science

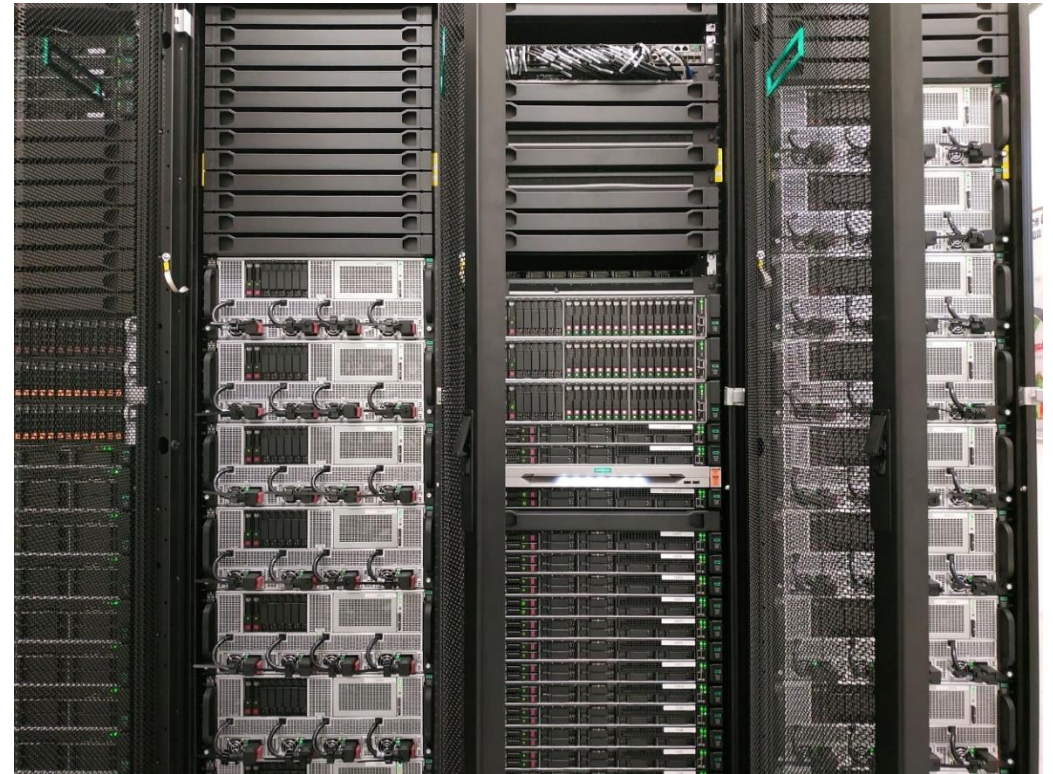
# CaSToRC - Research

- Research in Computational Sciences is carried out in the following fields:
  - Modelling and algorithms
  - Data Science
  - Climate Modelling
  - Computational Physics
  - Computational Engineering
  - Computational Biology
  - Quantum Computing
- CaSToRC is open to collaboration opportunities with other academic research groups, industry and government organisations



# CaSToRC - Infrastructure

- The main HPC System available via CaSToRC is Cyclone
  - Hybrid System
  - Peak/Sustained Performance
    - ~600 TFlop/s
  - Number of Nodes
    - 17 forty-core compute nodes
    - 16 forty-core compute nodes each with 4 NVidia V100 GPUs
- Other prototype systems
- Cyclone is the production platform for academia
  - 2 production calls per year, preparatory access call is always open



# CaSToRC - Projects

- CaSToRC is participating in the following ongoing EU projects



Coordination of the European Joint Doctorate programme STIMULATE



WP2 and WP3 Co-Leader  
Leader of WP8 LyNcs project  
"Linear Algebra, Krylov-subspace methods, and multigrain solvers for the discovery of New Physics"



National Competence Center



Build up a science community, especially R&D and technology needs of the SESAME Members and beyond



**ERA-Chair:** Computation-Based Engineering for "computer design of materials and processes" via novel algorithmic approaches and computational tools.

Support the development and inclusion of the national Open Science Cloud initiatives in 15 Member States and Associated Countries in the EOSC governance



# CaSToRC – NCC Activities and Opportunities

- Training and Skills Development
  - A number of training events have been identified and will take place
- Technology Transfer/Business Development and Collaboration with Industry
  - Industry week is in first week of March and registration is open
    - Will include on the first day a user forum
  - For academia and industry to network and collaborate in projects
- Facilitation of access to scientific and technical expertise and knowledge pools
  - Access to resources, High Level Support, more specific training and internships
- Awareness Creation and Collaboration
  - Seminar series, collaborations with other academic groups, industry, government

# HPC Beginner Training Event

- This is our first event and a “pre-requisite” to our “HPC Intermediate Training Event” taking place Monday 19 - Wednesday 21 April 2021
- We would have loved to host you at The Cyprus Institute, but we all know we can’t at the moment.
- Online training is different, we will all do our best given the situation
- Please raise your hands for any questions
  - Speaker will be able to respond to you when possible
- Please try to not get distracted with other aspects online/at the office
- Recordings of sessions will be made and uploaded where you can refer to them later



# HPC Beginner Training Event

- **Day 1 (Monday 15<sup>th</sup> February 2021)**
- 09:30 - 10:00: Welcome and Participant Introductions
- 10:00 - 10:15: Introduction to NCC
- 10:15 - 11:15: Introduction to High-Performance computing
- 11:15 - 11:30: Break
- 11:30 - 12:30: Introduction to Data Analysis with Artificial Intelligence Algorithms
- 12:30 - 13:30: Lunch Break
- 13:30 - 14:30: How to access HPC infrastructure and Training Opportunities
- 14:30 - 14:45: Break
- 14:45 - 17:00: Basics of Parallel programming and performance optimization

# HPC Beginner Training Event

- **Day 2 (Tuesday 16<sup>th</sup> February 2021)**
- 10:00 - 12:00: Connecting to a system, Linux Introduction, Scripting
- 12:00 - 13:30: Lunch Break
- 13:30 - 15:00: Introduction to Slurm, Submitting jobs on systems, Queues, Modules

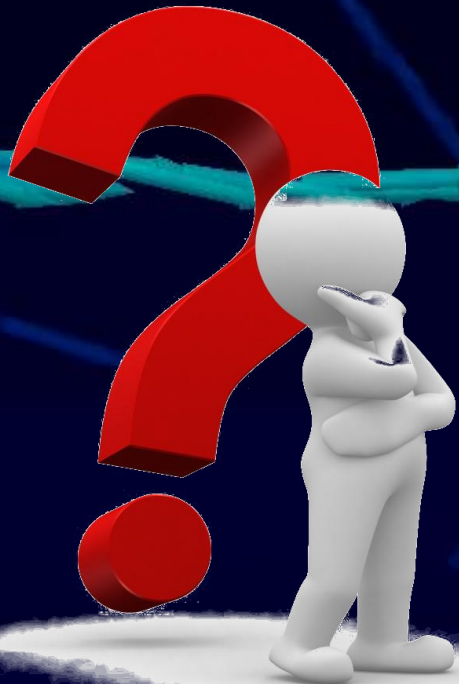
Between 16:00 - 17:00, there will be a Joint EuroCC/SimEA seminar titled "**Special Displacement Method for the Calculation of Materials' Properties at Finite Temperatures**" with speaker Dr. Marios Zacharias of Cyprus University of Technology, which participants can follow if they wish.

- Zoom connection for this is different – find on CaSToRC website

# HPC Beginner Training Event

- **Day 3 (Wednesday 17<sup>th</sup> February 2021)**
- 10:00 - 11:30: Brief introduction to Parallel Computing with OpenMP - Session 1
- 11:30 - 11:45: Break
- 11:45 - 12:30: Brief introduction to Parallel Computing with OpenMP - Session 2
- 12:30 - 13:30: Lunch Break
- 13:30 - 15:00: Brief introduction to Parallel Computing with OpenMP - Session 3

Thank You!



Questions?



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