

Fostering Innovation with HPC, advanced simulations and AI

12 January 2021

**Christos Christodoulou
Innovation Scout, SimEA, CaSToRC**



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No [810660](#)

Outline

- Overview of CaSToRC
- Innovation with HPC, advanced simulations and AI
- Management and Innovation Office (MIO)
- Innovation actions
- Upcoming projects

Why HPC?



Fighting COVID-19

COVID-19

Data, Artificial Intelligence & Supercomputers



A major asset in detecting
of the virus, developing
and devising strategi

A supercomputer analysed data on COVID-19 and helped come up with the "bradykinin hypothesis" [COMMENTS](#)

By [Rafael Cereceda](#) & [Emma Beswick](#) • last updated: 07/09/2020



Racing the Clock, COVID Killer Sought Among a Billion Molecules

Oak Ridge researchers use Summit supercomputer to reduce search time from years to hours.

May 26, 2020 by [GEETIKA GUPTA](#)



ences. Copyright Carlos Jones/ORNL and Carlos Jones

Coronavirus: Using European supercomputing, EU-funded research project announces promising results for potential treatment*

HPC enables tackling large-scale and complex problems

The massive computing power offered by HPC, in combination with modelling and simulations and AI help scientists **rapidly** advance their understanding of COVID-19 leading to accelerated development of **new treatments** and **preventative measures**

Overview of CaSToRC

- Computational-based Science and technology research center
- Created in **2009** (Cyl created in 2005)
- More than **30 researchers**
- Secured more than **€16 million** in external funding
€12 million from the EU
- **Dual mission**
 1. Computational-based research and education
 2. Provision of comp. resources and know-how to user communities

Overview of CaSToRC

CaSToRC has been designated as the National Competence Center (NCC) for HPC in Cyprus

The European HPC Joint Undertaking (EuroHPC JU) is a pan-European HPC action involving 33 countries aiming to advance scientific discovery and innovation

- **Upcoming budget:** (2021-2030): 8 billion Euro (co-funded between EU and member countries)

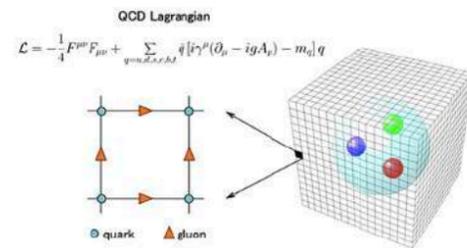
EuroCC aims to enhance the EU uptake of HPC by academia and industry by creating NCCs for HPC in each member country

Overview of CaSToRC

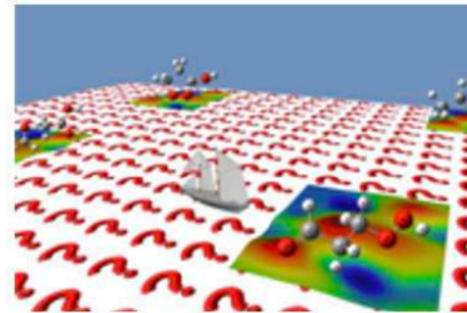
CaSToRC hosts prestigious ERA Chair project SimEA

- ERA Chair projects aim to bring excellence by bringing outstanding academics under the direction of the ERA chair holder to research institutions and universities
- At the same time one of the main goals of ERA Chair projects is to implement structural changes necessary to achieve excellence on a sustainable basis

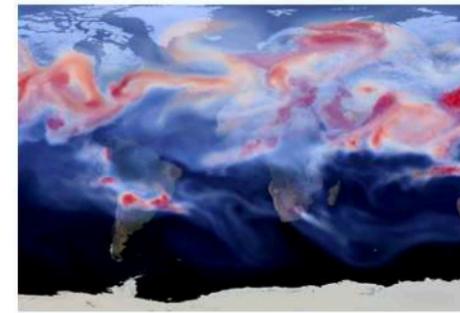
CaSToRC Research Areas



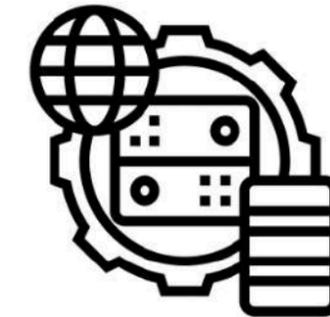
Nuclear and Particle Physics



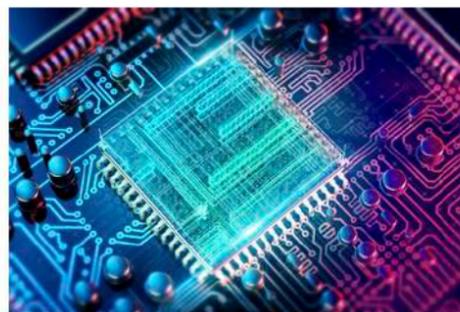
Fluid Dynamics
Heat Transfer



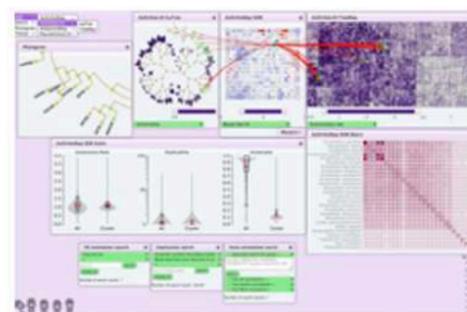
Climate and Environmental Modelling



Big Data
Machine learning



Scientific Computing
Novel Architectures

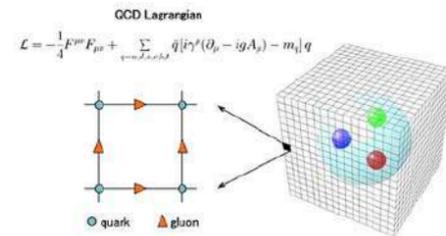


Computational Biology
3D Visualization

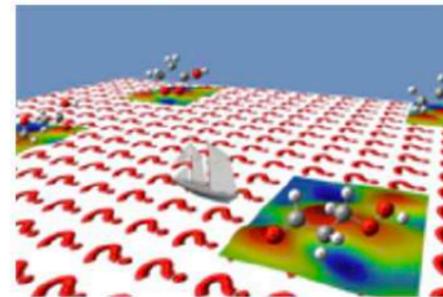


Digital Cultural Heritage

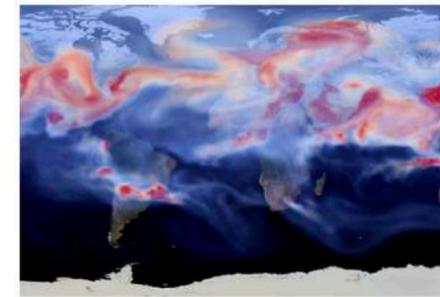
CaSToRC Research Areas - SiMEA



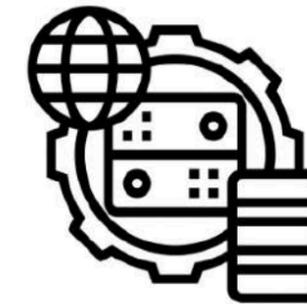
Nuclear and Particle Physics



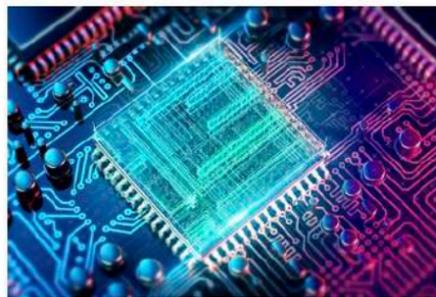
Fluid Dynamics
Heat Transfer



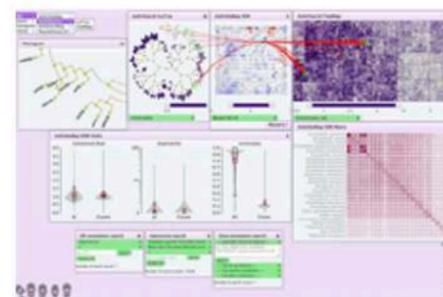
Climate and Environmental Modelling



Big Data
Machine learning



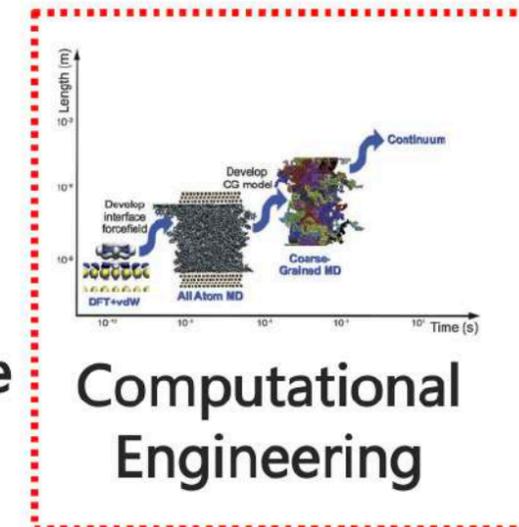
Scientific Computing
Novel Architectures



Computational Biology
3D Visualization

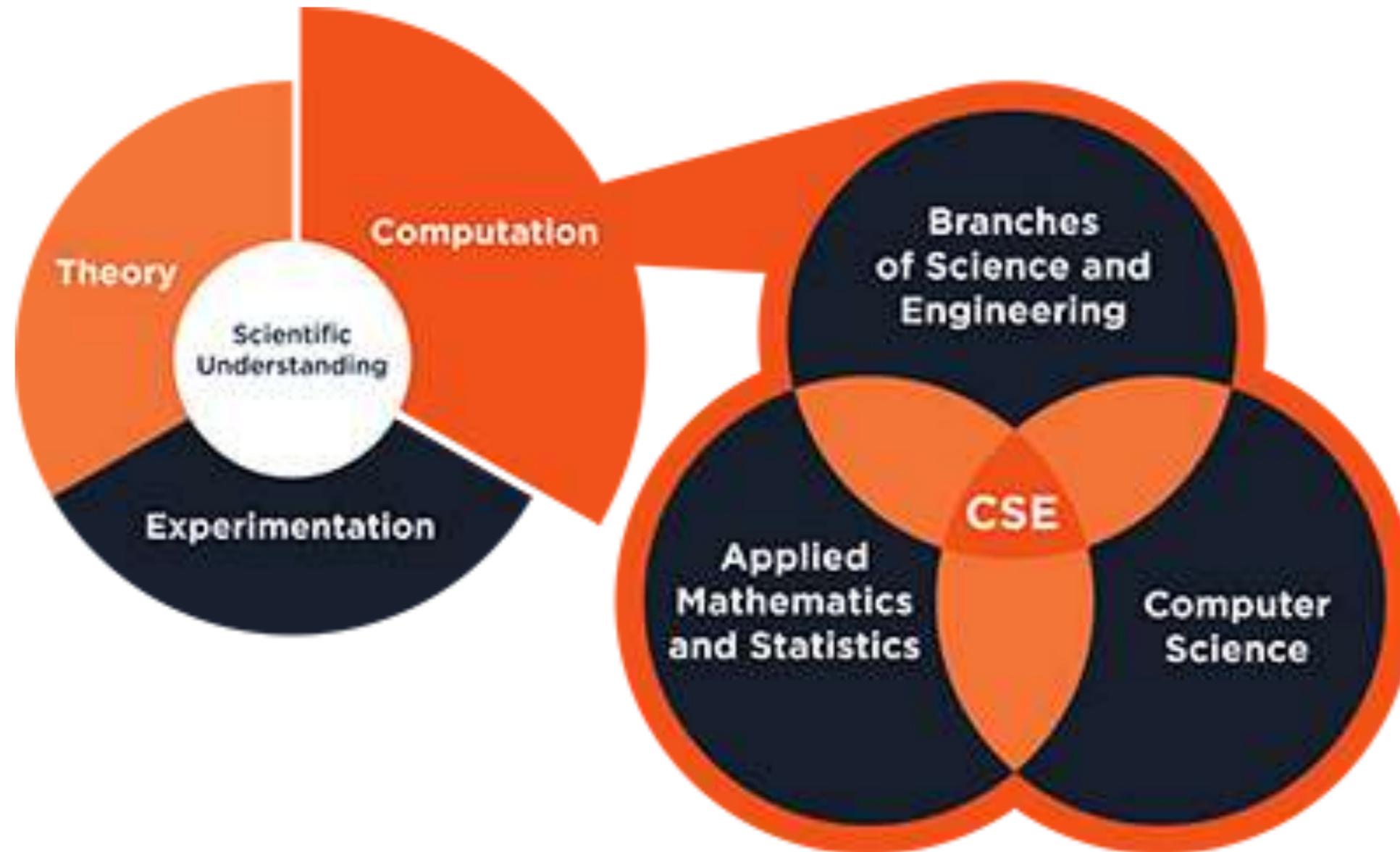


Digital Cultural Heritage



Computational Engineering

Why is computation important?



Why is HPC important?

Necessary to model and simulate **complex problems** and physical phenomena such as weather, fluid dynamics, molecular interactions

Industry leverages HPC to improve products, reduce production costs and **decrease the time** it takes to develop new **products**

Results come in minutes/hours instead of days or weeks

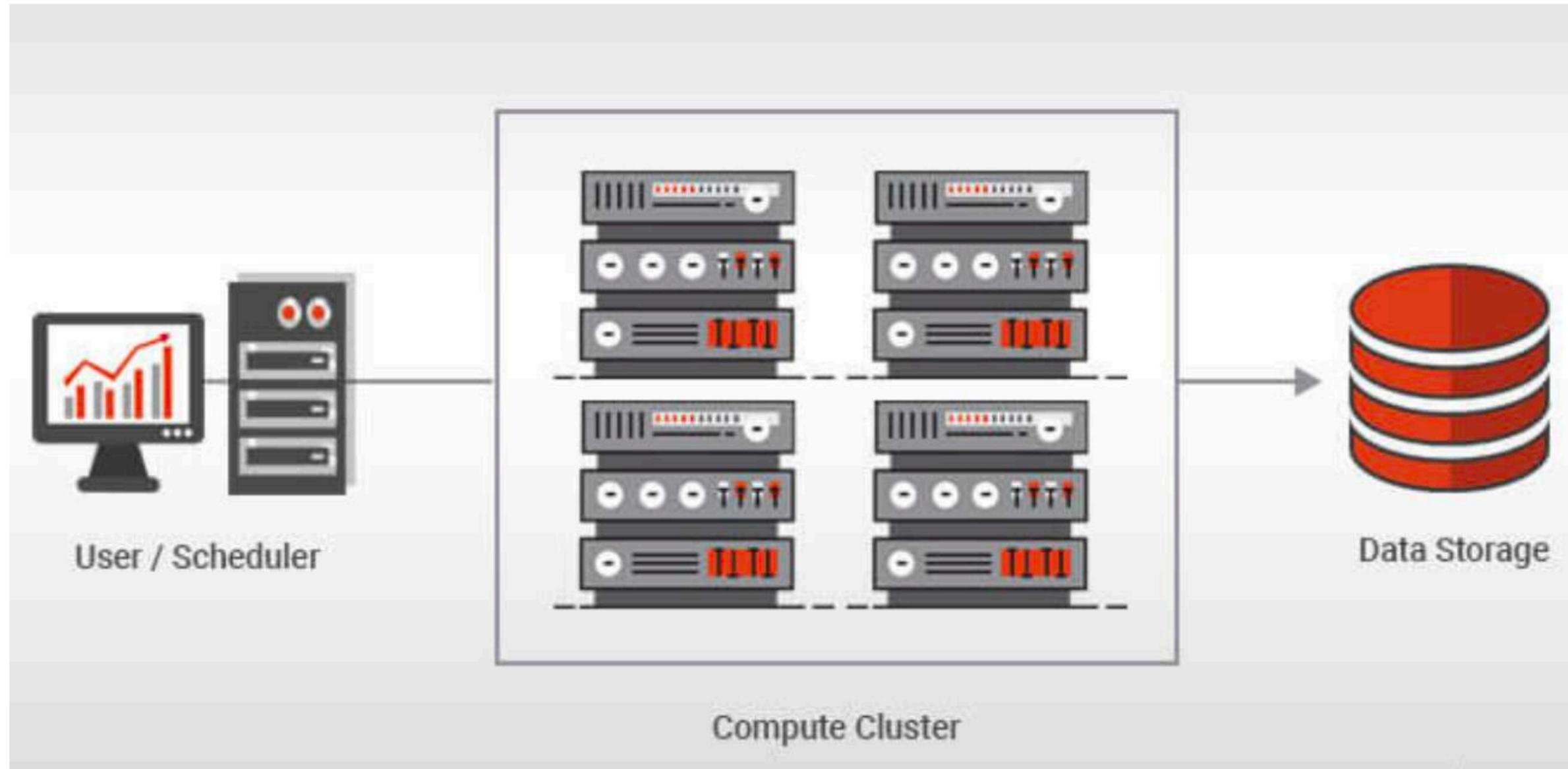
Why is HPC important?

Flood of data¹

- Average internet user: ~ 1.5 GB / day
- A smart hospital: 3 TB / day
- A self driving car: 4 TB / day
- A connected plane: 40 TB / day
- A connected factory: 1 PB / day

¹Approximated numbers by Cisco

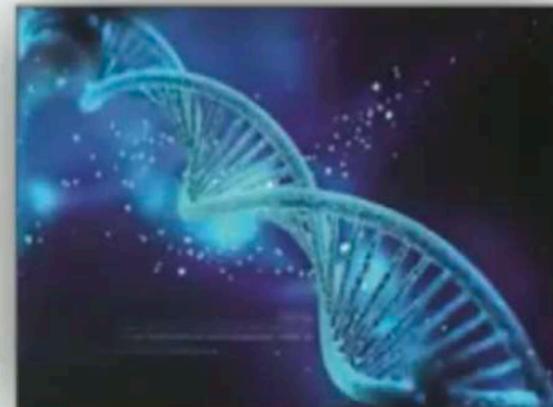
How does HPC work?



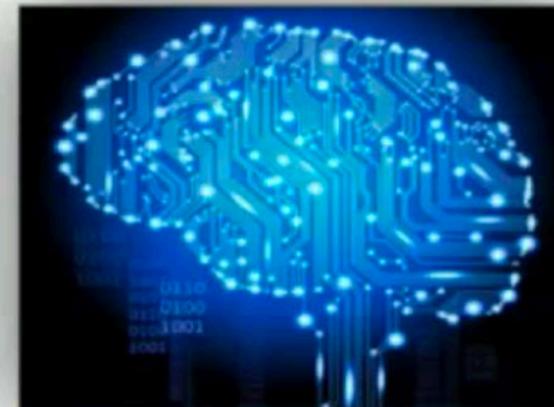
Innovation with HPC, advanced simulations and AI



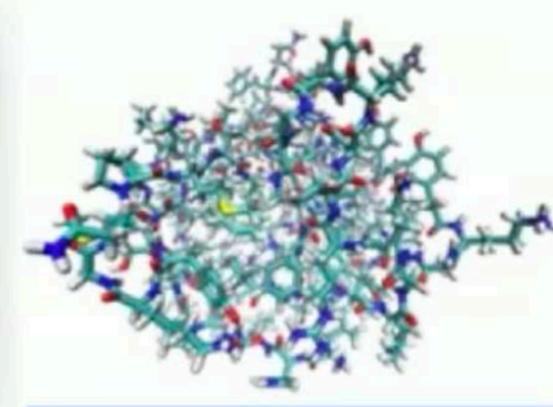
ASTROPHYSICS



GENOMICS / BIO-INFORMATICS



ARTIFICIAL INTELLIGENCE



MOLECULAR DYNAMICS*



BIG DATA ANALYTICS



FINANCIAL



WEATHER & CLIMATE

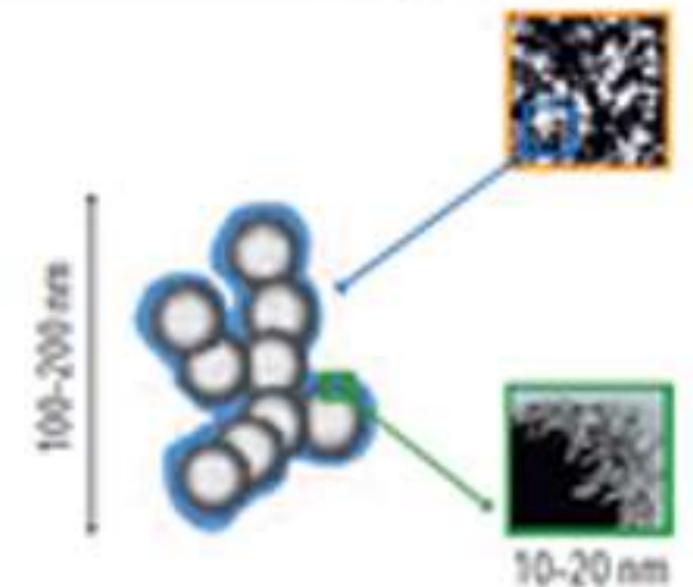


CYBER SECURITY

Innovation in materials design

Polymer nanocomposites

- (Nano-)particles dispersed in polymer matrix
- Lead to better properties of the nanocomposite material
- Applications in a variety of fields: biomedical, food-packaging, etc



Innovation in materials design

Graphene-based nanostructured materials

- Super-strong two-dimensional material that can be easily functionalized to tailor its properties
- Applications in organic electronics, gene therapy, bioimaging, biosensors, tissue engineering, antibacterial agents, 3D bioprinting, photothermal therapy, drug delivery
- Face masks against COVID-19 and other viruses contain some form of graphene²

²<https://medicevo.com/products/medicevo-graphene-face-mask-5-pc>



Innovation in materials design

Polymer thin-films

- Every day applications: food packaging, adhesive, electronics
- Smart materials that change properties at different environments
- Example: chromoactive glasses change colour when subjected to a certain variation in temperature, light, pressure

Anti-blue light glasses

Photochromic sunglasses



Innovation in Medicine

Fighting Covid-19

- Virtual high-throughput screening to rapidly identify compounds that can fight COVID-19^{3,4}
- Advanced simulations used to test interaction between molecules and the virus active sites
- The massive computational power of HPC helps accelerate the discovery of these compounds
- Machine-learning brings accurate, physics-based, computationally tractable models
- E.g., exscalate4cov: **5 million molecules simulated per second** on Eni's HPC5 (81 petaflops), most powerful industrial supercomputers in the world

^{3,4} https://ec.europa.eu/commission/presscorner/detail/en/ip_20_890, <https://pubs.acs.org/doi/10.1021/acs.jcim.0c01010>

Innovation in Banking

- The banking and finance sectors are nowadays full of complex problems, coming together with a massive amount of data
- An example is risk assessment, where new regulations require more detailed models
- This has led to the creation of many computationally-intensive tasks that require the use of HPC to be solved

Innovation in Energy sector - Oil and gas

- Finding oil (seismic processing), producing oil (reservoir simulation), or optimizing production (pipeline and facilities simulation) is a computationally intensive problem
- HPC and AI reduce hours of calculations to minutes, helps enterprises rapidly adapt to market changes
- Energy exploration generates **exabytes** of seismic data used for the discovery and extraction of oil that are not easy to process
- With ML algorithms and HPC, the efficiency and speed of exploration, drilling and production is immensely increased

Innovation with HPC, advanced simulations and AI

Digital transformation

- Natural language processing and computer vision can help automate various problems to help industry and government to digitally transform
- Translate languages, voice \leftrightarrow text conversion, create human-like conversational agents, classify or detect objects in images
- Applications: Reduce administrative work, optimise internal operations, etc

Scope of the NCC together with SimEA

The main scope of the NCC/SimEA is:

- Advance competitiveness in research
- Improve the effectiveness of government services
- Promote innovation by engaging with industry

The above will be pursued through **SimEA** and **EuroHPC** with the help of the newly established Management and Innovation Office (MIO) at CaSToRC

Management and Innovation Office (MIO)

Scope

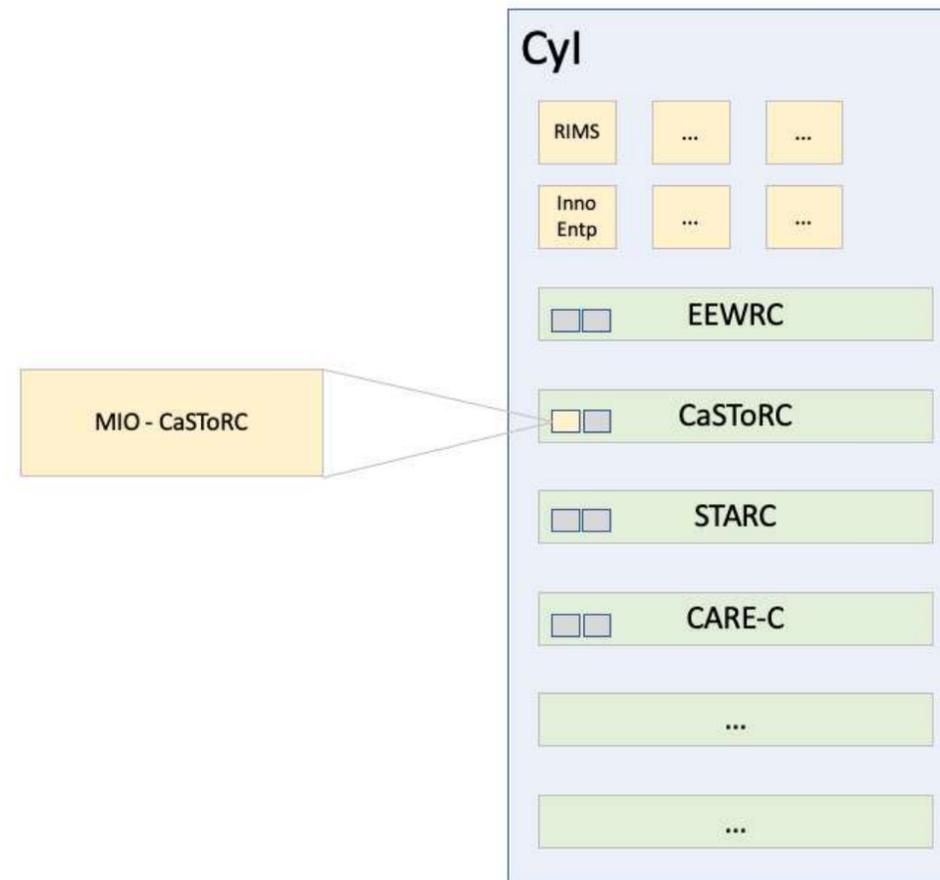
Forge links between academia, government, industry and the overall innovation ecosystem using CaSToRC's expertise in HPC, Artificial Intelligence (AI) and data science

Enhance the research management structure of the centre by optimizing the mobilization of resources and personnel to be engaged in the centre's innovation programs

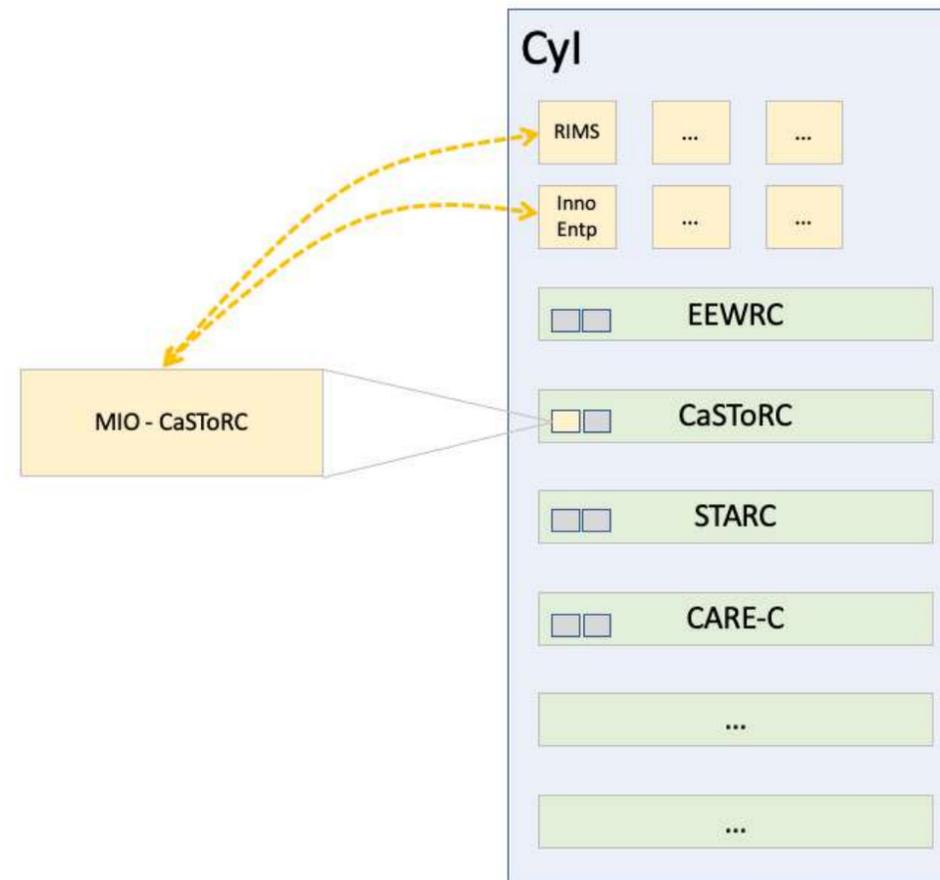
Vision

Establish CaSToRC as a one-stop shop for local academic, industrial and government stakeholders to integrate HPC and data science approaches in their workflows

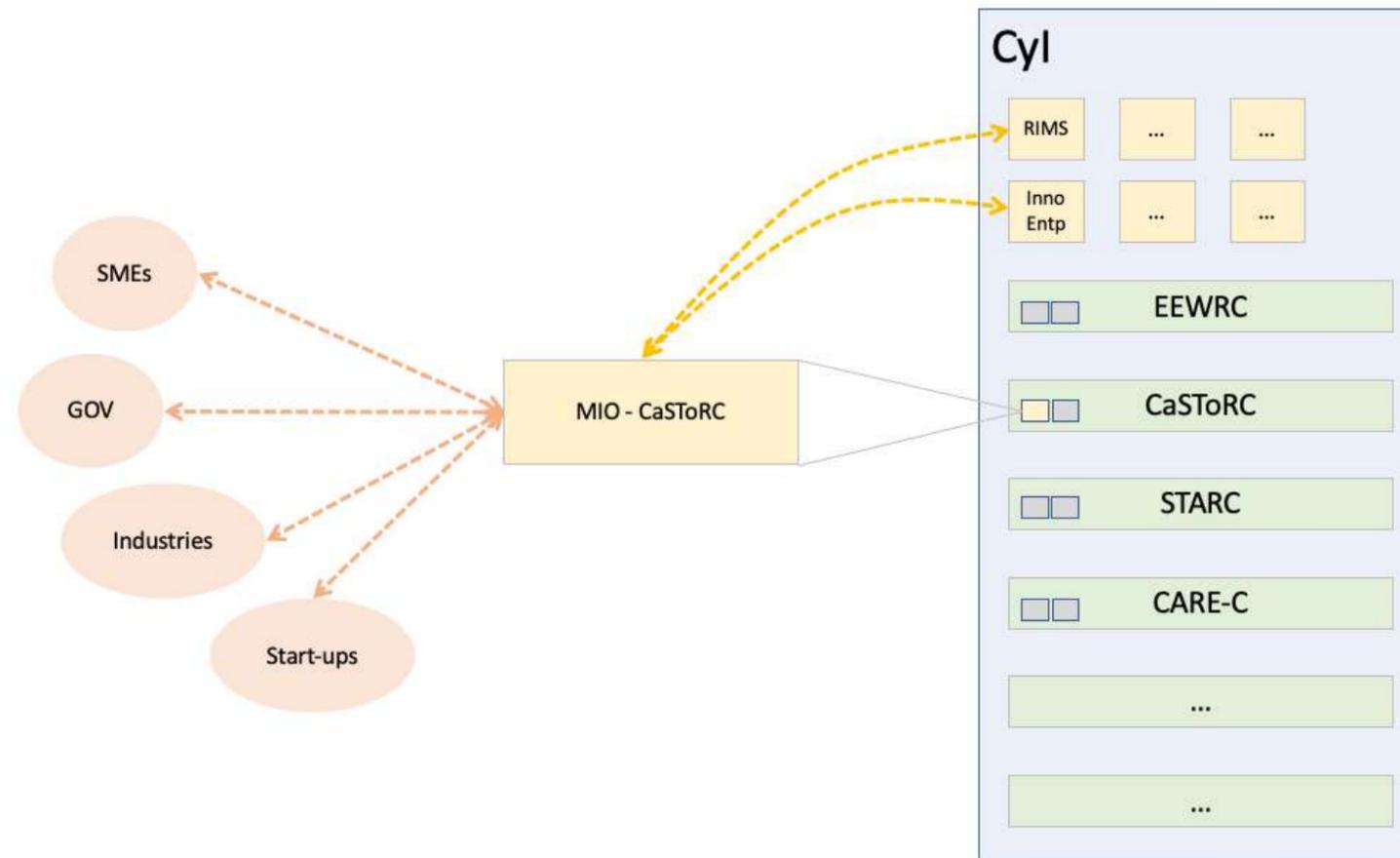
Management and Innovation Office (MIO)



Management and Innovation Office (MIO)



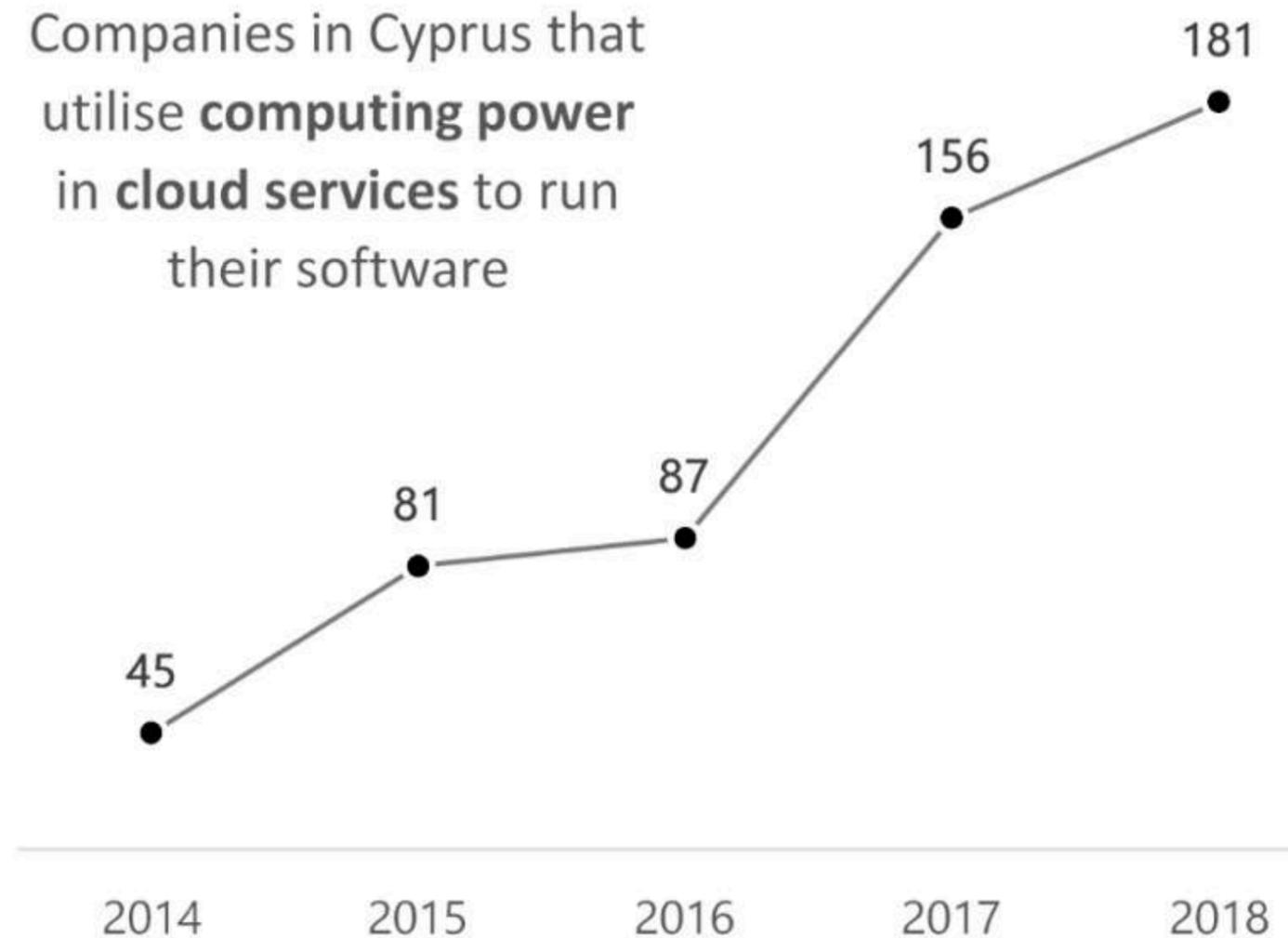
Management and Innovation Office (MIO)



Market analysis - MIO

Companies in Cyprus utilising computing power in cloud services to run software increased more than double in 2 years (2016 to 2018)⁵

These companies are target to the center's innovation actions

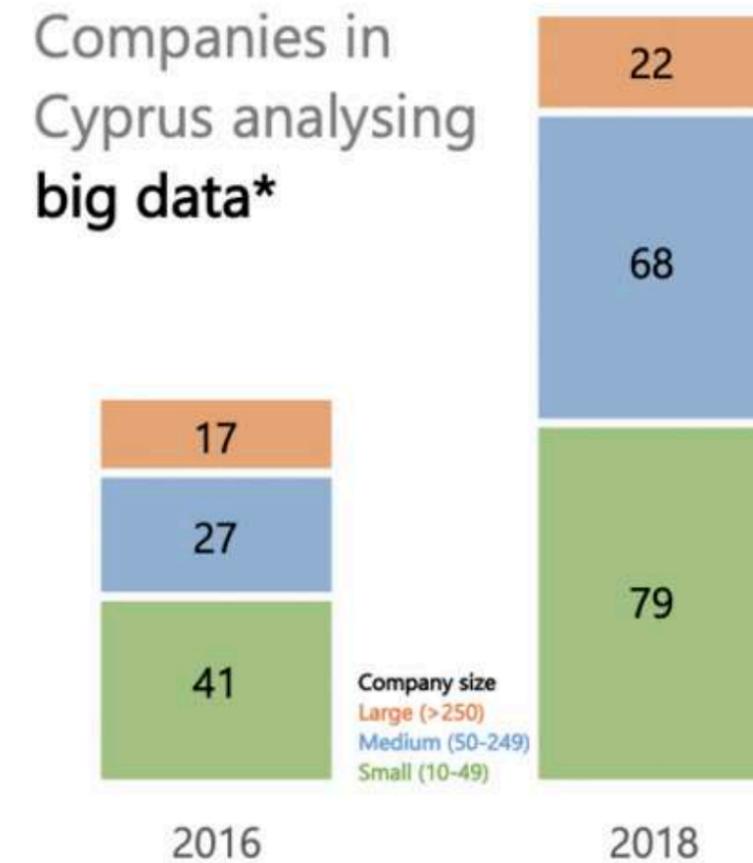


⁵Source: Cyprus Statistical Service (CyStat)

Market analysis - MIO

An increasing amount of companies analyse big data⁵

As with the companies utilising computing power in the cloud, these companies will potentially benefit from the use of HPC



*Datasets too large/complex to be dealt with by traditional data-processing application software

⁵Source: Cyprus Statistical Service (CyStat)

MIO + industry support team



Kathy Christoforou
Scientific Coordinator



Andreas Gavrielides
Scientific Coordinator



Christos Christodoulou
Innovation Scout



Kyriakos Hadjiyiannakou
Industry Support



Stelios Erotokritou
Scientific Coordinator

<https://castorc.cyi.ac.cy/training-user-support/user-support>

<https://simea.eu/management-and-innovation-office>

<https://castorc.cyi.ac.cy/about/people>

Innovation actions

1. Raise awareness of the potential of HPC through seminars and interaction with CaSToRC personel
2. Training program: courses on HPC, hackathons, hands-on software development
3. Access to local HPC resources and services
4. Consultancy for technology transfer and business development
5. Internship program, Co-development projects with academic groups and industry
6. Advances user support to scale software for EU machines and access to exascale resources

Upcoming/Existing projects

- Real estate value prediction
- Leaf disease classification
- Design and developing of plastic bags from bioplastic
- Developing next generation car tires

Upcoming events

- Industry weeks: First one in March 2021
- Trainings (industry + academia): First one in February 2021
- Seminar series: Weekly webinars (bit.ly/castorc-seminar-series)

More info

- castorc.cyi.ac.cy/news-and-events
- simea.eu/activities/seminar-series
- Open positions: jobboard.cyi.ac.cy

CaSToRC: HPC National Competence Center Spring 2021 Online Seminar Series

12 Jan	Dr. Christos Christodoulou (The Cyprus Institute)	Fostering innovation with HPC, Advanced Simulations, AI and Big Data (Joint EuroCC/SimEA seminar series)
19 Jan	Asst. Prof. Vangelis Daskalakis (Cyprus University of Technology)	High-Performance Computing in Structural Biology (EuroCC seminar series)
26 Jan	Prof. Panagiotis Grammatikopoulos (Okinawa Institute of Science and Technology)	Computer Simulation Aspects of Nanoparticle and Nanodevice Design (SimEA seminar series)
2 Feb	Prof. Zoe Cournia (Academy of Athens)	Multiscale Modeling of Biomolecules and Materials (Joint EuroCC/SimEA seminar series)
16 Feb	Dr. Marios Zacharias (Cyprus University of Technology)	Special Displacement Method for the Calculation of Materials' Properties at Finite Temperatures (Joint EuroCC/SimEA seminar series)
2 Mar	Mr Brendan McGinty, Dr Seid Koric (National Center for Supercomputing Applications)	NCSA Industry Overview with Computational Breakthroughs and Synergies with Artificial Intelligence (Joint EuroCC/SimEA seminar series)
9 Mar	Dr. Thomas Montenegro-Johnson (Birmingham University)	Active (non-) Particles: Donuts, Curved Rods, and Flexibility (SimEA seminar series)
16 Mar	Prof. Martha Constantinou (Temple University)	Synergy of High-Performance Computing and Nuclear Physics to Resolve Long-standing Puzzles: The Proton Spin and Mass (EuroCC seminar series)
23 Mar	Dr. Igor Chernyavsky (The University of Manchester)	TBC (SimEA seminar series)
6 Apr	Prof. George Froudakis (University of Crete)	Designing Novel Nanoporous Materials for Applications in Energy and Environment. From Multi-Scale Modeling to Materials Informatics (Joint EuroCC/SimEA seminar series)
20 Apr	Prof. Andreas Efstathiou (European University Cyprus)	The CYGNUS Models for the Spectral Energy Distributions of Galaxies and their Supermassive Black Holes (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=Um8wdTdHeStFMtM3LzNRL3I3Um55QT09>; Passcode: Vs5Cz1
To receive updates on these events, register at: <https://www.meetup.com/high-performance-computing-cyprus/>

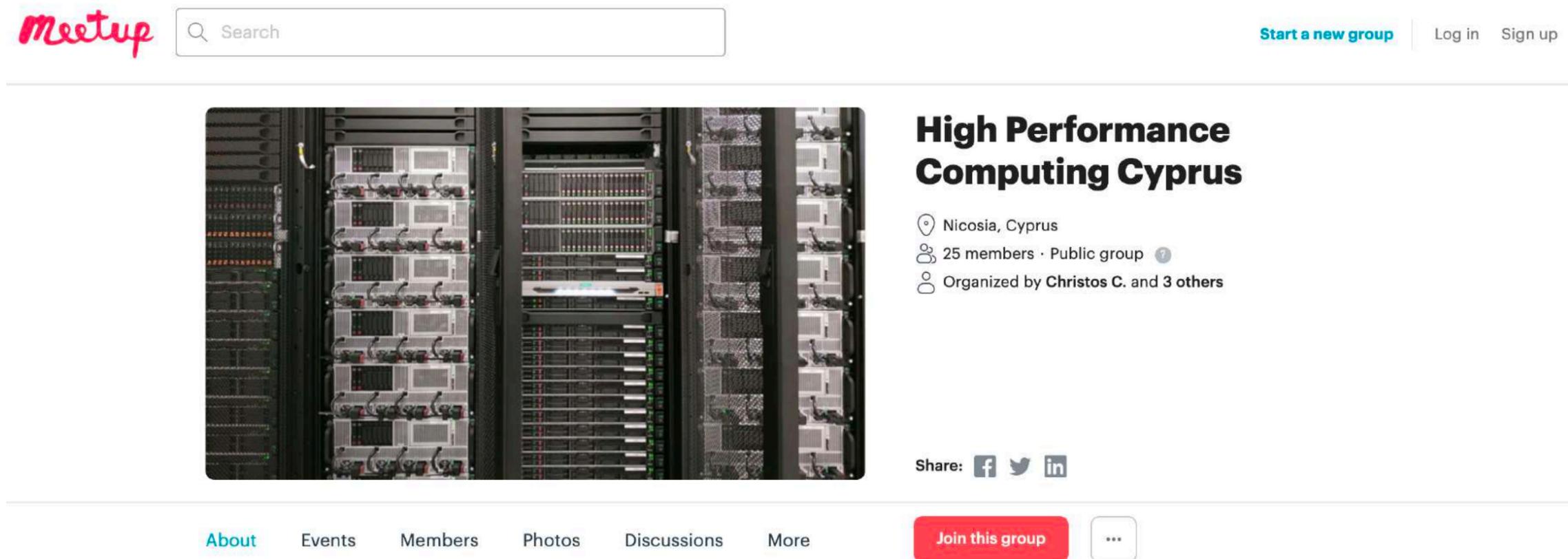


The SimEA and EuroCC projects have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 810660 and No. 951740, respectively.

🚀 **Don't miss an event** 🚀

Become a member of our meetup

bit.ly/hpc-meetup



The screenshot shows the Meetup website interface. At the top left is the Meetup logo in red script. To its right is a search bar with a magnifying glass icon and the text 'Search'. Further right are links for 'Start a new group', 'Log in', and 'Sign up'. The main content area features a large image of server racks on the left. To the right of the image is the group title 'High Performance Computing Cyprus' in bold black text. Below the title, there is a location pin icon followed by 'Nicosia, Cyprus', a group icon followed by '25 members · Public group', and a person icon followed by 'Organized by Christos C. and 3 others'. Below this information are social media share icons for Facebook, Twitter, and LinkedIn. At the bottom of the group page, there is a navigation menu with links for 'About', 'Events', 'Members', 'Photos', 'Discussions', and 'More'. To the right of the navigation menu is a red button that says 'Join this group' and a white button with three dots.

Credits

- Slide 3: COVID-19 virus pattern in rows on pink background by Zamurovic Brothers from Noun Project
- Slide 16: `comp-physics-lincoln.org`
- Slide 21: Boston Children's hospital

Thank you

Does your company have a computationally intensive project?

Get in touch!

 c.christodoulou@cyi.ac.cy

 castorc.support@cyi.ac.cy



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No [810660](#)

