What is E-CAM?

E-CAM is an e-infrastructure centre of excellence funded by the European Union for the five years commencing 1st October 2015 with a total budget of 4.8M€. It supports software, training and consultancy in simulation and modelling, and in particular the use of complex simulations of materials, including biological systems, for both fundamental scientific studies and for industrial applications. It focuses on three key issues.

First is the need for an expert consultancy service to industry. European industry, including *inter alia* such important sectors as pharmaceuticals, food, advanced materials and semiconductor devices, could benefit greatly from increased use of computational simulations in its R&D activity, but needs expert advice and assistance from the scientific community in identifying such opportunities.

Secondly, there is a pressing need for algorithmic and methodological innovation. Improvements in computational power increasingly rely on the use of massively parallel computation and specialist hardware accelerators both of which require new codes and libraries as well as novel methods.

Thirdly, and crucially, we need to train and mentor the next generation of scientific programmers and computational scientists, both in industry and in academia. They need to be recognised as valuable professionals with a vital role to play in delivering the full potential of computational simulation.

Who is involved?

E-CAM is based around CECAM's distributed European network of simulation science nodes and the physical computational e-infrastructure of PRACE. The 18 institutional partners in E-CAM bring together 15 CECAM nodes, 2 PRACE Centres, and one centre for industrial computing.

- 1. UCD, Dublin, Ireland, E-CAM coordinator.
- 2. EPFL, Lausanne, Switzerland (CECAM HQ)
- 3. FU Berlin, Germany
- 4. Università La Sapienza, Rome, Italy
- 5. Maison de la Simulation IDRIS, Paris, France
- 6. TU Wien, Austria
- 7. U Cambridge, United Kingdom
- 8. MPI for Polymer Research, Mainz, Germany
- 9. Ecole Normale Supérieure de Lyon, France
- 10. FZ Juelich, Germany
- 11. U Barcelona, Spain
- 12. Daresbury Laboratory, United Kingdom
- 13. SISSA Trieste, Italy
- 14. U Amsterdam, the Netherlands
- 15. CSC, Espoo. Finland
- 16. Scuola Normale Superiore Pisa, Italy
- 17. NUIG, Galway, Ireland (ICHEC)
- 18. U Aalto, Finland

E-CAM will involve a broad spectrum of industrial associates (12 are already identified), affiliated research groups and individual scientists in its activities. It will cooperate closely with other centres of excellence and EU initiatives to help grow the European computational science ecosystem.

What will be delivered?

E-CAM will develop at least 150 robust software modules directed at industrial and academic users in the areas of:

- electronic structure calculations;
- · classical molecular dynamics;
- quantum dynamics;
- meso-scale and multi-scale modelling.

These modules will be freely available under an open-source licence from a central repository.

It will provide advanced training in the production, documentation and use of this software through a system of extended software development workshops. It will directly hire and train 20 postdoctoral researchers and indirectly benefit many more, including scientists and programmers working in industry, through participation in its workshops.

It will hold a series of scoping workshops with its industrial partners to identify problems of mutual interest and areas where industry could benefit from E-CAM's consultancy services. These will be developed over the five years from an initially exploratory phase to the point where they provide a significant income stream and a sustainable business model for E-CAM.

More generally, E-CAM aims to raise awareness of the importance and value of computational scientists and programmers, and to challenge stereotypes of gender and status in this regard.



Geographical distribution of E-CAM partners



The official E-CAM web-site is <u>http://e-cam2020.eu</u>.

For more information on CECAM go to <u>http://www.cecam.org</u> and for PRACE go to <u>http://www.prace-ri.eu</u>.

E-CAM is one of the eight centres of excellence for computing applications implemented as part of the Digital Agenda Europe

http://ec.europa.eu/digital-agenda/en/digitalinfrastructures





Relationship of CECAM to E-CAM



Funded by the European Union

A European Centre of Excellence for Software, Training and Consultancy in Simulation and Modelling