



CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Other HP2C projects and their chief initiators

Materials science

Electrons in molecules and solids

Density functional theory (DFT) is one of the most important modelling methods in materials science, solid-state physics and chemistry. The BigDFT code solves quantum mechanical equations within the framework of density functional theory, thereby facilitating the determination of almost all the physical and chemical properties of new materials. BigDFT uses novel mathematical functions, so-called wavelets, to illustrate electronic wave functions and charge distribution. One of BigDFT's key fields of application is the prediction of the existence of new nanomaterials.

BigDFT – Large Scale Density Functional Electronic Structure Calculations in a Systematic Wavelet Basis Set; Stefan Goedecker, Professor at the University of Basel

Accurate simulation of quantum mechanical effects

MAQUIS is another important project from solid-state physics, in which unusual and technologically interesting properties of materials are modelled with the exact simulation of all the quantum mechanical effects.

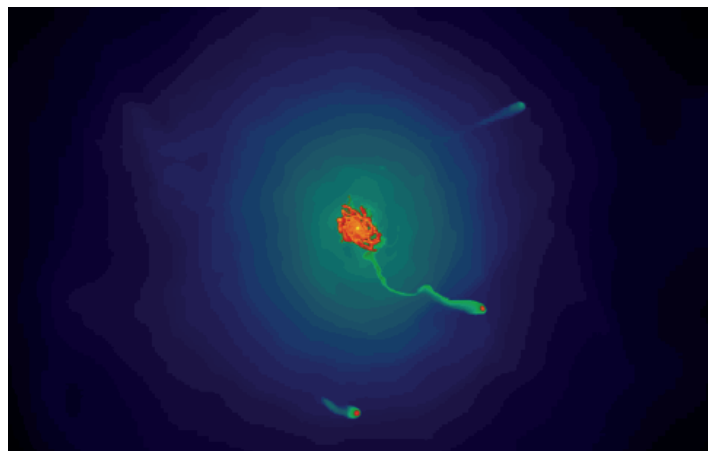
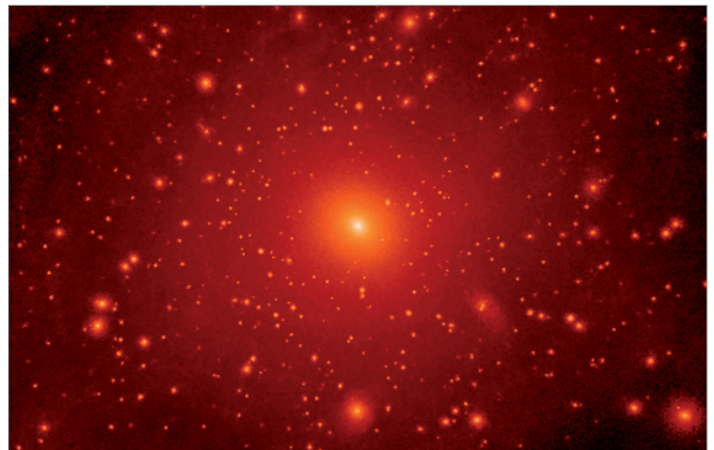
MAQUIS – Modern Algorithms for Quantum Interacting Systems; Thierry Giamarchi, Professor at the University of Geneva

Astrophysics

Stellar explosions

Supernovae – stellar explosions – are key events and studying them can help explain the origin of heavy elements and their distribution in the universe more precisely. However, the explosion mechanisms are poorly understood and it is not easy to reproduce a stellar explosion in a computer model realistically. This is complicated by the very close interaction of many individual physical processes under extreme temperatures and matter density, which can only be achieved and explored in astrophysical explosions. With the team now focusing on the processes that are considered “essential” in the development of its algorithms, it should be possible to perform reliable three-dimensional simulations.

SUPERNOVA – Productive 3D Models of Stellar Explosions; Matthias Liebendörfer, Professor at the University of Basel



“Thanks to HP2C, we have been able to upgrade our galaxy formation models” says Romain Teyssier. The cosmology team of the University of Zurich is now able to model the dynamics of the yet-to-be-discovered “dark matter” (image above), but also the evolution of the ordinary matter, settling into a realistic rotating disk like our own Milky Way (see the central region of the image below). (Image: Cosmology group George Lake, University of Zurich)

**Origin of the cosmos**

The project is aimed at modelling the formation and development of large-scale structures and galaxies in the universe. Beginning from the initial conditions, which can be observed through the cosmic microwave background radiation, the scientists can develop their virtual universe over thirteen billion years under the influence of the laws of gravity and fluid mechanics. Simulating the origin and development of the cosmos is extremely important for science as it constitutes a test of the basic model of physics. Only with simulations can we verify whether astronomic observations coincide with results of the underlying physical laws.

COSMOLOGY – Computational Cosmology on the Petascale; George Lake, Professor at the University of Zurich

Medicine**The cardiovascular system**

Scientists are pursuing the goal of simulating the electrophysiology and mechanics of the heart in combination with the circulatory system. The simulations are physiologically and pathologically useful for practice and should facilitate improvements in diagnostics for vascular disease, make surgical interventions more plannable and lead to the more effective treatment and cure of inflammatory vascular diseases.

CARDIOVASCULAR/LIVE5 – HPC for Cardiovascular System Simulations; Alfio Quarteroni, Professor at EPF Lausanne

Simulating the ear

The goal is to simulate the human ear based on realistic biophysical principles with a view to developing hearing aids more effectively.

EAR MODELLING - Numerical Modelling of the Ear: Towards the Building of new Hearing Devices; Bastien Chopard, Professor at the University of Geneva

Biology**Natural selection**

Darwinian selection explains the adaptation of living organisms to their environment. In order to detect the traces of selection in genomes, the scientists need to find traces of rare small events, typically adaptive changes in a few percent of a protein, tens to hundreds of millions of years ago. The Selectome project is optimizing software to allow efficient scanning on supercomputers for Darwinian selection in tens of thousands of genes, from hundreds of genomes.

SELECTOME – Selectome, looking for Darwinian Evolution in the Tree of Life; Marc Robinson-Rechavi, Professor at the University of Lausanne

Climate**How does climate change affect the Alps?**

As our knowledge grows, climate models are becoming increasingly complex. At the same time, however, high-resolution models are important locally to improve our understanding of the effects of climate change on the alpine regions. By revising or replacing the existing codes and algorithms, the aim of the project is to make the regional weather and climate model COSMO-CCLM used by ETH Zurich and MeteoSchweiz more efficient and adapt it to new computer architectures.

COSMO-CCLM – Regional Climate and Weather Modelling on the Next Generation's High-Performance Computers: Towards Cloud-Resolving Simulations; Isabelle Bey, Executive Director of C2SM (Centre for Climate Systems Modelling) at ETH Zurich.

More accurate weather forecasts

The OPCODE Project is closely related to COSMO and primarily intended to promote local weather simulations. Under the project, for instance, essential developments that are still outstanding for COSMO are to be carried out for the implementation of the models on state-of-the-art computer architectures with graphics processors.

OPCODE - Operational COSMO Demonstrator; Oliver Fuhrer, MeteoSchweiz