



## Global to Regional Oceanographic Modelling (GROM) supported by the DEISA research infrastructure

Using DEISA computing resources, **Pierre Bahurel** and his team from Mercator Ocean in France have, together with ESEOO in Spain, developed new oceanographic models that will help us to understand the evolution of the climate over the last decades and to provide an ocean analysis and forecasting service on a daily basis. A supercomputing infrastructure is essential for oceanographic modelling in order to generate ever more realistic simulations of the ocean's behavior.

Mercator Ocean was founded, as a consortium company, in 2002, with the aim of establishing an operational system for describing the state of the ocean at any given time and place on the planet.

"The ocean is an integral part of our environment, upon which many depend for survival, and it is a basic element of the Earth's climate. It is also an important site of transit for both goods and people", points out Pierre Bahurel, head of Mercator Ocean.

"Therefore, understanding both the state of the ocean and the ways in which it might change is crucial. Operational oceanography is essential for many scientific activities in the fields of oceanic physics, marine biology, and meteorology, and it has also practical benefits for the security and the improvement of maritime transportation", continues the French researcher.

### Global and regional oceanographic modelling

In collaboration with ESEOO in Spain, Mercator Ocean launched the GROM project in 2006, with the general aim of developing global and regional operational oceanographic models.

"The project we are currently working on is to build and validate new ocean model configurations on a global to regional scale, with

which we can simulate mesoscale or sub-mesoscale physical processes such as eddies, meanders, fronts or currents", explains **Yann Drillet**, ocean modeller at Mercator Ocean.

Mercator Ocean's team uses two types of models to conduct its research. The first one is called an "eddy-permitting" model, which allows a realistic representation of the main ocean currents. The second model is called "eddy-resolving", and offers finer representations of a number of mesoscale features of the ocean, essential for operational forecasting and for many activities (such as pollution detection and forecasting, ship routing, offshore fishing and halieutic resource management) for which the impact of these mesoscale processes is crucial.

"Our final goal is to develop a global eddy-resolving model (1/12°)", says Bahurel. Such a model is essential for understanding the evolution of the climate over the last decades and for providing an ocean analysis and forecasting service on a daily basis. We are also working on a better resolution for regional eddy-resolving models (1/36°) in specific areas, capable of representing sub-mesoscale and high frequency physical processes such as tides and storm waves, and providing useful large ocean forcings to scientists or operators involved in coastal oceanography", he explains.

### Modelling the ocean requires high computation capacities

Modelling the ocean requires, however, very high computation capacities. In order to vali-

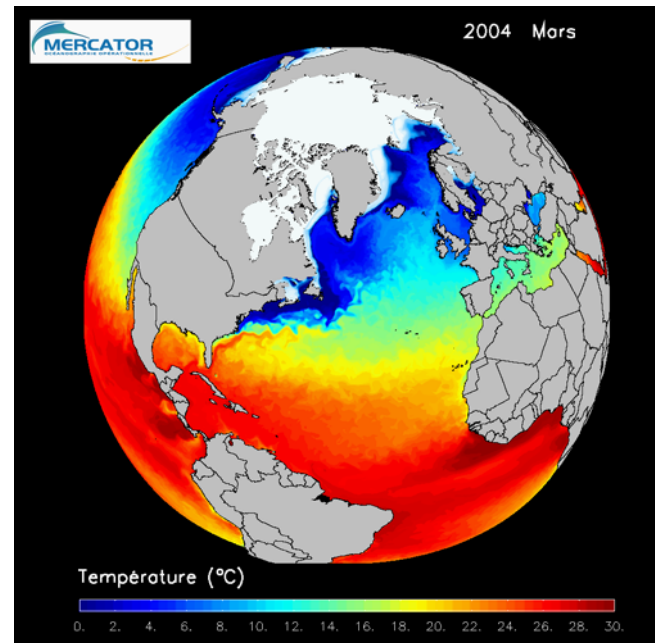


Figure 1: Temperature of the sea surface (coloured regions) and sea ice extension (white regions) in March 2004, as simulated by the global high resolution model developed by Mercator-Ocean. Note the trajectory of the gulf stream, one of the globe's larger western boundary currents, which draws warm water from the Caribbean Sea and the Gulf of Mexico and flows into the North East Atlantic.

date the simulations both physically and statistically, Mercator Ocean's team needs to know the model's behavior over relatively long periods – and each year simulated requires tens of thousands of computing hours. Physical processes in the ocean, such as mesoscale phenomena or "mixing" are often very complicated to model, and others such as tides and storm waves, considerably increase the computation needs.

By making available to Mercator Ocean some 450000 CPU hours on the ECMWF IBM, the DEISA Extreme Computing Initiative (DECI) made possible some major achievements within the GROM project:

"These computation capacities have enabled us to carry out interannual simulations, which

are crucial for testing the validity of our models, for setting up systems of operational oceanic forecasting, and for deepening our understanding of the ocean more generally. Thanks to DEISA, we have been able to develop new models starting from the global eddy-permitting model to the regional eddy-resolving models”, explains Drillet.

The results obtained by Mercator Ocean with the help of DEISA have proved extremely innovative and promising:

“We have been able to develop a global eddy-permitting model ( $1/4^\circ$ ) that allows us to represent an excellent degree of variability and eddy kinetic energy in all the oceans of the globe”, begins Drillet.

“We have also been able to study for the first time the coupling between sea ice and a global eddy-permitting ocean”, he adds. “Understanding this coupling is essential to efforts to realistically simulate circulation in the high latitude ocean, which has consequences for large-scale ocean circulation and deep water formation. An important aspect of the ocean forecasting is to provide information on sea ice-free transport pathways particularly in the Arctic Ocean and in the Canadian straits”.

Considerable achievements have also been made at a more regional level, especially in the North Atlantic area: “We have managed to represent correctly the Gulf Stream pathway and in particular the separation of the current from the coast at Cap Haterras to become a zonal jet in the Atlantic”, says Drillet. According to the researcher, “the eddy-resolving simulation obtained ( $1/12^\circ$ ) is the most realistic simulation ever produced”.

“The accuracy of these simulation results in the key area of the North Atlantic region is new for to the entire physical oceanographic modelling community”, points out Drillet.

“It allows us to represent the position and the intensity of the Gulf Stream and its North Atlantic current extension, which has a strong influence on oceanic and atmospheric properties”, says Bahurel.

“It also enables us to represent the cold and warm eddies that are formed in this current and which transport temperature and salinity properties in the Sargasso Sea in the south and along the North American coast”, adds Drillet.



Figure 2: Photo of Pierre Bahurel, head of Mercator Ocean (on the right) and Yann Drillet, Ocean Modeller at Mercator Ocean.

“We have also developed a regional model within the North East Atlantic and the Western Mediterranean Sea areas, which allows us to refine locally the modelling process. It makes it now possible to introduce new physical phenomena, such as tides, into these models, and to get a better representation of the level of fresh water penetration from rivers into the ocean. This vastly improved the quality of our simulations, and created many new potential applications, especially on the continental shelf where human and biological activities are more important”, says Bahurel.

### First steps towards finer resolutions

The final goal for Bahurel’s team remains the development of a global eddy-resolving model with a resolution comparable to that realised in regional models ( $1/12^\circ$ ). This model is now under development but it is still too large for the computation facilities currently available.

“The process of improving the horizontal resolution in the ocean modelling is not complete. One of our objectives is to be able to simulate sub-mesoscale processes or coastal phenomena with a resolution of 1km. This will be soon possible with regional models thanks to progress in the level of computational power”, says Bahurel.

“At the global scale, ocean observations have to be improved in terms of resolution, global coverage and real time distribution. Given that the atmosphere is the ocean’s engine, we will also have to improve our knowledge of this component. It is crucial for the future development of our environment monitoring and forecasting capabilities”, concludes Bahurel.

## DEISA events



### DEISA Training

March 5 – 7, Stuttgart, Germany  
HLRS – High Performance Computing Center Stuttgart

The first part of the training gives a global description and introduction to the usage of the DEISA infrastructure. The second part of training introduces new ways to access to the DEISA infrastructure. On the third day of the training Use Cases will be presented.

The speakers and their subjects at the sixth DEISA Training Session are:

- *DEISA Overview*, **Thomas Bönisch**, HLRS
- *DEISA Access, filesystems and job submission*, **Denis Girou**, IDRIS
- *DEISA Common Production Environment*, **Denis Girou**, IDRIS
- *UNICORE*, **Michael Rambadt**, FZJ
- *The DESHL Client*, **Malcolm Illingworth**, EPCC
- *The DEISA Life Sciences Portal*, **Isabelle Dupays**, IDRIS
- *The Globus Toolkit*, **Helmut Heller**, LRZ
- *Direct Numerical Simulation of a separated turbulent channel flow with a smooth profile*, **Matthieu Marquillie**, University of Lille 1
- *ESSENCE - DEISA and the creation of a large ensemble of climate model runs*, **Dr. Sterl**, The Royal Netherlands Meteorological Institute, De Bilt
- *Coupled Computations on the Heterogeneous DEISA Network*, **Harald Klimach**, High Performance Computing Center Stuttgart, University of Stuttgart
- *GeoSys/RockFlow: A parallelized FEM code for thermo-hydro-mechanical (THM) coupled problems in porous media*, **Prof. Kolditz**, Helmholtz Centre for Environmental Research, Leipzig

The registration at [www.deisa.org/training](http://www.deisa.org/training) for the DEISA Training Session will close on February 21, 2008. Welcome!

### DEISA Symposium 2008

Advancing Extreme Computing in Europe  
April 28 – 29, Edinburgh, UK  
[www.deisa.org/symposium](http://www.deisa.org/symposium)

# Ab initio simulations of Protein-Surface Interactions mediated by Water

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The interaction of a hydrophilic protein  $\beta$ -sheet with a gold surface in water at room temperature has been simulated via ab initio molecular dynamics for the first time. Mechanisms of protein-surface interactions that were not known before have been evidenced. The outcome of the project will help us elucidating how proteins can selectively recognize inorganic surfaces such as metals.

## Lots of questions to answer

Recent combinatorial biotechnologies have shown that the molecular recognition capability of proteins can be specifically oriented toward inorganic surfaces. However, at present the principles regulating protein-surface interactions are poorly understood. What features of the surface and of the proteins determine which protein is able to bind to a given surface and how? In addition, the exact role of water in the process of protein-surface interaction is unknown.

The comprehension of such mechanisms would foster several technological applications based on the rational design of protein/surface interactions, ranging from biomaterials to nanobioelectronics. The aim of PSI-Wat is to elucidate the mechanisms of interaction between a surface and a protein, including the role played by water.

In particular, we have chosen to focus on the interaction of a polypeptide with one of the experimentally most studied surfaces, namely Au(111), for which from the theoretical view-point very little is understood and even the wetting behavior without the protein has not been studied yet via ab initio molecular dynamics (AIMD). As for the protein specimen, an anti-parallel  $\beta$ -sheet structure has been used, a system that joins realism with computational convenience and that is the proposed structure for an experimentally identified gold binding protein.

## Car-Parrinello method was exploited

We have performed fully AIMD simulations at finite temperature, using plane-wave Density Functional Theory, on a system that is composed of an Au(111) slab and an anti-parallel  $\beta$ -sheet of poly-Serine (a natural amino acid occurring in experimental gold-binding peptides), immersed in explicit water molecules

and replicated by 3D periodic boundary conditions. In particular, the Car-Parrinello approach has been exploited to calculate the time evolution of the system. The initial set up has been performed by preliminary classical molecular dynamics simulations.

The AIMD of the protein/gold/water system was carried out on Mare Nostrum at the Barcelona Supercomputing Center with the ab initio molecular dynamics code included in the Quantum-ESPRESSO suite (<http://www.quantum-espresso.org>). Fine-tuning and optimization of the code on Mare Nostrum has been performed with the support of the DEISA staff. The simulated system is composed of 4 layers of Au (112 atoms), 130 protein atoms and 115 water molecules, giving a total of 587 atoms and approximately 2500 electrons. We have simulated the time evolution of the system via Car-Parrinello method for 15 ps (plus 2 ps of initial thermalization), a duration long enough to obtain meaningful averaged quantities (also considering the large number of atoms in the system). Each ps of dynamics required approximately 100h on 200 processors of Mare Nostrum.

## New mechanisms were found

The results of our simulations show the mechanisms of interaction between the three components of the system, i.e., between water and gold, poly-Serine and gold, and poly-Serine and water. In particular, analogies and differences in the behavior with respect to gold of water and the related side-chain of the Serine (hydroxyl group, OH) could be identified. Remarkably, some of the found mechanisms were not known before, and requires AIMD for a correct description.

In particular, the dynamics of gold atoms is important to explain the interaction with the protein and with water. In addition, our calculations demonstrate for the first time that such large systems, including metals, can be simulated by Car-Parrinello AIMD for a meaningful duration and yielding scientifically sound results, when the extreme computational power provided by initiative like DEISA is available. The full analysis of the trajectories and of the electronic structure will eventually allow us to give the quantitative description of the phenomena.

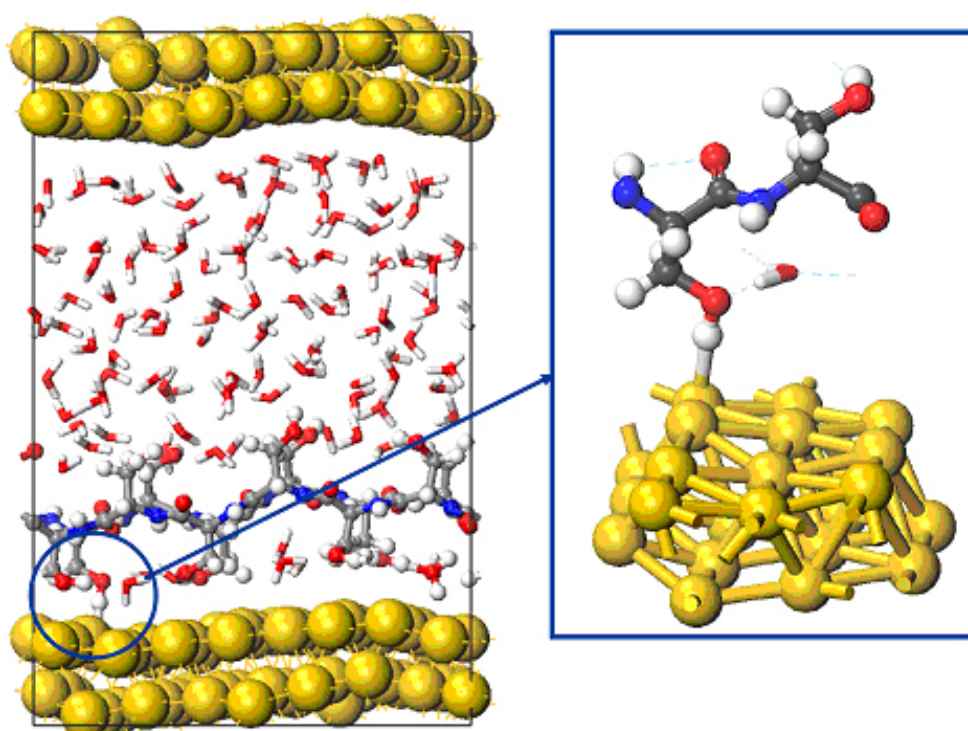


Figure 1. Snapshot from the ab initio molecular dynamics of the protein/gold/water system. The atoms represented in the left panel of the figure are repeated by 3D periodic boundary conditions, creating an infinite gold slab and an infinite poly-Serine  $\beta$ -sheet. The right panel highlights the instantaneous interaction between the Serine side-chain and the gold surface, that takes place (in this example) via the hydrogen atom of the hydroxyl group.