



## Simulating automotive noise generation

### Testing and taking advantage of the DEISA research infrastructure in an industrial context

Using the DEISA research infrastructure within the Joint Research Activity (JRA5) framework, the Fiat Research Center (CRF), in Italy, carried out a number of different computational fluid dynamics and aeroacoustic simulations in the important area of automotive noise generation.

"Noise reduction is an important concern in terms of human well-being and health, and is a significant issue for a wide range of applications, including for the automotive industry", says **Roberto Tregnago**, researcher at CRF. "The research that we are doing at CRF focuses on different types of noise generation, and, in particular, on aerodynamic noise, which results from the interaction between the airflow and the moving vehicle. Aerodynamic noise increases with the speed of the vehicle, and becomes dominant above 100 km/h", he explains.

#### Computational simulation: an essential tool for studying noise generation and optimizing industrial production

Computer simulations have become increasingly useful for the study of noise generation. Computational fluid dynamics (CFD) and computational aeroacoustics (CAA) are the two main numerical applications used by researchers to simulate noise generation.

"These two applications enable us to study the features of fluid dynamics that contribute to noise generation, and to develop new ways of reducing noise pollution. By using CAA, the aeroacoustic properties of a new car design can be adequately simulated. Several layout alternatives can be numerically tested, a practice that is at the moment unfeasible in physical testing", says Tregnago.

"However", Tregnago continues, "these applications are highly demanding in terms of computing power. That is why a partnership with a research infrastructure, such as DEISA, can be of genuine interest to automotive industries."

#### Raising industrial simulation capabilities through the partnership with DEISA

The Joint Research Activity JRA5, which focused on computational fluid dynamics (CFD) and computational aeroacoustics (CAA), provided the framework for such a partnership.

"CRF joined the DEISA project in order to explore – and take advantage of – the possibilities offered by a distributed computational grid in resolving engineering problems in the area of noise generation. Our main objective was, in particular, to test the DEISA infrastructure in an industrial context, and to push back the boundaries of numerical simulation for industrial applications", says Tregnago.

"Practically, we defined four relevant test cases related to simulations that are very important for the automotive design process: The first test was a shape-noise aeroacoustic simulation on a detailed car body; the second focused on open sunroof buffeting; the third on noise generation and propagation inside ventilation ducts; and the final test dealt with shape optimisation of car bodies. Each test case was scheduled with four degrees of increasing complexity, both in terms of model dimension and time/frequency resolution."

"The simulation was realised on a Fiat Grande Punto. It was performed with a time step of  $5.0 \times 10^{-5}$  s in order to increase the quality of the pressure wave resolution. This corresponds to a Nyquist frequency of 10 000 Hz. Computed time history was accumulated up to 0.6 seconds, with a global resource consumption of roughly 30 000 CPU hours (in DEISA normalized

units). The numerical signal has been recorded at every time step, in 138 different positions on the underbody of the car, in order to obtain accurate noise maps that show the noise power spectra over the whole vehicle for a given frequency."

"In order to validate these numerical results, a number of experiments were also carried out in FIAT Auto's aeroacoustic wind tunnel. Twenty flat microphones were placed in the same positions as a subset of the numerical probes, in order to enable us to compare the experimental power spectra of the pressure signal at each location with that derived from the numerical simulation."

The simulation, according to Tregnago, was genuinely promising: "Globally, the comparison of the results of the simulation with those of the experiment shows them to be largely in accord. In particular, the simulation was able to predict – within acceptable limits – the suppression of the peak in the spectrum due to fluid-acoustic resonance that increases noise within the passenger compartment, and the level of accuracy reached has allowed us to propose some design solutions to the problem of noise emission."

"The high quality results obtained with these simulations enable us to move away from sim-

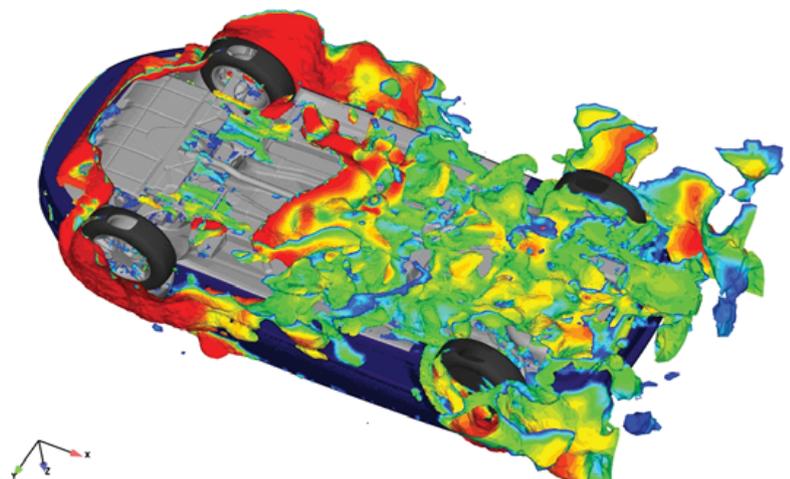


Fig. 1. Iso-surface of density coloured by velocity magnitude

ple trend prediction towards providing detailed measurements within a short period of time. The competitiveness of the company has been increased through the achievement of a streamlined design process and the improved performance of the final product", he notes.

"CRF's experience with the DEISA infrastructure has, however, demonstrated that appropriate numerical techniques, together with suitably high performance multiprocessor systems, do represent powerful tools for industry. They enable us to tackle problems that would be impossible to face with standard resources within the time constraints of a product development process. Thanks to the increasing power of supercomputers, it is likely that we will see, in the near future, comprehensive simulations of these designs that also encompass elements of multi-disciplinary optimisation."



Fig. 2. Instantaneous acoustic pressure distribution on the underbody of the vehicle. The image depicts the computed acoustic pressure at a certain point in time on the surface of the vehicle underbody. In the red regions, the instantaneous fluctuating pressure is higher, while in the blue regions it is lower. This pressure distribution stimulates the underbody panels that generate noise within the cabin.

## New DEISA publications

### DEISA Advancing Science in Europe

A publication on the scientific results and success stories of DEISA.

### DEISA Digest

A selection of articles on the key results of some of the research projects carried out within the DEISA.

Publications are online at:

<http://www.deisa.eu/press/publications.php>

## Advancing Extreme Computing in Europe

### 4th DEISA Symposium in Edinburgh



The DEISA Symposium 2008 was held in Edinburgh, UK, starting with lunch on the 28th of April and ending with lunch on the following day. Overall, the Symposium was enjoyed and indeed warmly received by all that attended.

There were 132 people from 16 countries in attendance. The venue was a Geology Museum named Our Dynamic Earth, which is set at the foot of an extinct volcano in the edge of Edinburgh's Old Town.

An exhibition area on the first floor contained 11 posters from the DEISA Extreme Computing Initiative 2007 and some further exhibits describing EPCC and the UK HPC services available within DEISA. The two lunches and the evening reception were enjoyed within this exhibition space, which also permitted delegates to stroll out onto the battlements to admire the views.

The talks were split into two groups, where the first day saw talks of a general nature about the current status of HPC Grids both in Europe and in America, whilst the 2nd day saw talks from actual users of the DEISA infrastructure.

#### First day: talks from key players in the field of HPC e-Infrastructures

The first day was introduced by Arthur Trew, the Director of EPCC, where he welcomed Jane Nicholson, from the UK's EPSRC funding council. This was immediately followed by a description of the DEISA infrastructure itself, by Paolo Malfetti, and then a talk on some of the ground breaking science achieved thanks to DEISA, presented by Hermann Lederer.

Thomas Eickermann then presented the current state of PRACE, whilst Marian Garcia Vidondo described the service provided

by GEANT2, which provides the network between the DEISA sites.

After the break, Victor Alessandrini invited Alistair Dunlop to present the findings of the OMII-Europe project. Thereafter both Ed Seidel and Al Kellie gave their impressions on the requirements for the future of HPC from an American perspective.

#### Second day: talks from DEISA users

The following day saw presentations from Xavier Daura on simulating protein dynamics for vaccine research; Karsten Reuter on molecular switches at metal surfaces; and Jukka Heikkinen on plasma turbulence.

The final session saw talks from Lucas Visscher, Sascha Husa and Stefano Corni, who presented their work on simulating photodissociation, black hole coalescence and interactions of protein with surfaces mediated by water, respectively.

Overall, the Symposium was found to be very interesting with a wide variety of interesting talks. We all look forward to an equally successful DEISA Symposium 2009, which will be held in Amsterdam.

Presentations of the Symposium are available at: <http://www.deisa.eu/symposium/Edinburgh2008/>



# Simulating the Local Universe

Gustavo Yepes, *Universidad Autónoma de Madrid, Spain*; Stefan Gottlöber, *Astrophysikalisches Institut Potsdam, Germany*; Anatoly Klypin, *New Mexico State University, USA*; Yehuda Hoffman, *Racah Institute of Physics, Israel*

The SIMU-LU project has been able to simulate the formation and evolution of a system pretty similar to our own galaxy and its closest neighbour: the Andromeda Galaxy.

We have carried out the most accurate representation of the formation of the Local Universe performed to date, starting from cosmological initial conditions compatible with the most recent astronomical observations. To this end, we have been running a set of high-resolution N-body cosmological simulations from initial conditions which include observational constraints on the mass distribution and velocity fields derived from nearby galaxies and clusters around us. We were able to run these simulations with up to 1 billion dark matter particles in different computational volumes. The simulations reproduce the main features of the mass distributions we observe in our local neighbourhood such as the Coma and Vir-

go clusters, and the Great Attractor and Local Superclusters.

By zooming in to the region where we are supposed to live, the Local Group, we have been able to simulate the formation and evolution of a system pretty similar to our own galaxy and its closest neighbour: the Andromeda Galaxy. The outcome of these numerical experiments will provide us with a deep insight into the dynamics of our local environment and will constitute the starting point to do more realistic simulations, in which ordinary matter (i.e. gas and stars) will be included together with the more exotic, yet dominant, components of the universe: Dark Matter and Dark Energy.

## Advanced simulation methods

To simulate the evolution of a self-gravitating fluid in an expanding universe, we need to solve a coupled system of the 3D Poisson and Vlasov equations. These are the standard equations of motion for particles interacting via gravity, simultaneously solving Poisson's PDE for the gravitational potential and Newton's ODE for the acceleration of each particle with the particularity that the phase space variables are implicit functions of time due to the expansion of the universe.

We have used two of the most advanced cosmological simulation N-body codes developed till now. The Adaptive Refinement Tree (ART) code employs standard particle-mesh techniques to compute particle accelerations and advance their coordinates and velocities in time. A regular cubic grid covers the entire computational volume and defines the minimum resolution of the simulation. This grid is then refined to form additional higher resolution meshes in the regions of interest

The GADGET code, on the other hand, uses a combination of Particle Mesh algorithms to compute the long range gravitational forces and a Tree algorithm with monopole expansion of the potential to account for the short scale force. Both codes use domain decomposition techniques to split the particle and mesh information among the different processors and use MPI communication among different nodes. They have been extensively tested in large distributed memory, SMP and NUMA architectures such as the MareNostrum (BSC) and HLRB2 (LRZ) supercomputers where these simulations have been done.

## Studies of the dynamics of the Local Supercluster

The purpose of our DECI project was to perform very large cosmological simulations of 1 billion particles in a computational cubic volumes ranging from 64 to 160 Mpc (i.e. 200 to ~500 million light years) on a side. We need to resolve objects that are expected to be formed if dark matter is in the form of cold, weakly interacting massive particles (WIMPs) with differences in mass over many orders of magnitude: from the largest superclusters of galaxies with masses of up to  $10^{16}$  solar masses or more, to the tiniest dwarf galaxies orbiting around the normal ones (with masses less than  $10^{10}$  solar mass).

The novelty of our approach resides in the generation of the initial conditions. We impose observational constraints onto the random realizations of the initial density fluctuation field. Thus, we force the formation of structures similar to those we see today. We have the advantage of dealing with known, well-studied astronomical objects. This significantly simplifies the comparison of the model with the observational data. For instance, we are able to study many details of the dynamics of the Local Supercluster to which our Local Group of galaxies belongs. The results of these simulations will constitute an excellent database to study in detail many aspects of the distribution of matter in our backyard. Now, the next step is to include the ordinary matter into the simulation so that we can witness the birth of stars inside the dark matter halos and make realistic comparison with the most recent astronomical observations of the real objects in our universe.

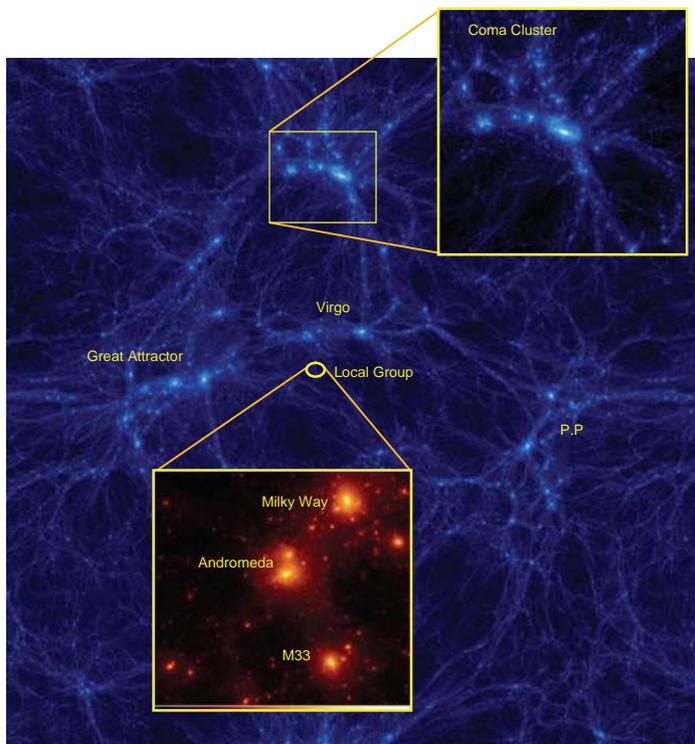


Fig. 1. Dark matter density distribution of the Local Universe simulation. The boxsize is 160 Mpc across. Several objects of the real universe are identified. The circle shows the position of our Local Group. A blown up panel shows the detailed structure of the simulated Local Group. The resolution of this small region of 2 Mpc radius is equivalent of having a total of  $4096^3$  (70 billion) particles in the whole box, which translates in a dynamical mass range of more than  $10^6$ .

# JRA6: Coupled applications

Gilles Grasseau, IDRIS-CNRS, Orsay, France

The Joint Research Activity JRA6 offers the opportunity to research projects using coupled simulations to take advantage of HPC facilities, such as the DEISA infrastructure. As a result of this work, research teams have the possibility to tackle new classes of numerical investigations.

Many complex systems can be seen as made of components that obey their own physical laws, and these components interact weakly with one another through boundary conditions, for example. Code-coupling which deals with multi-physics, multi-models and multi-scale numerical simulations, is especially well-suited for inter-disciplinary research projects in which different legacy codes cooperate within the whole coupled application.

Generally, due to the complexity of these applications, coupled codes run with a moderate efficiency on parallel machines as available in the DEISA infrastructure. The major contribution of the JRA6 team has been to enhance the coupled applications in HPC context, such as DEISA infrastructure, and, as a result, provide research teams with the possibility to tackle new classes of numerical investigations.

The main scientific and technical results of the nine coupling projects driven by this JRA are presented in the following.

## Combustion in 3D

Radiative heat transfer plays an important role in the turbulent combustion, but is often neglected in simulations because of its complexity and the related heavy numerical cost. DEISA Extreme Computing Initiative (DECI) allowed French researchers at the Energetique Moléculaire et Macroscopique Combustion laboratory to validate the 2D results with a more realistic description, such as an LES, 3D radiative code, etc., and validate the coupling approach for large configurations.

The results obtained in the DECI context demonstrate the importance of radiation heat transfer in turbulent combustion (see Figure 1).

### Deploying of a coupled architecture for aeroacoustic simulations

The research from the Institut für Aerodynamik und Gasdynamik in Stuttgart proposes a smart

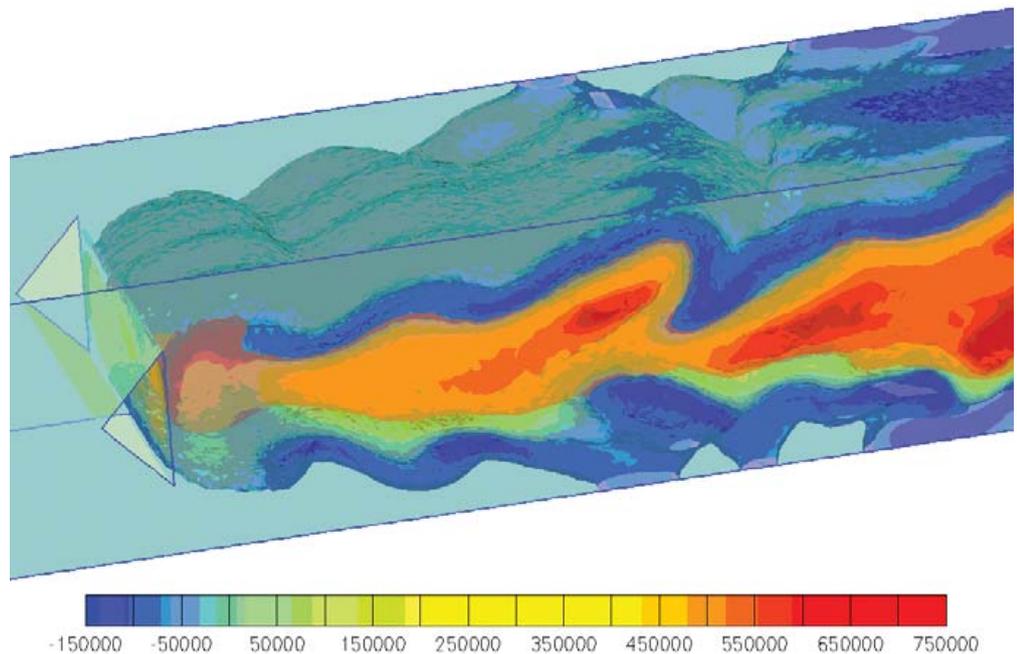


Fig. 1. A 3D flame numerical simulation in a diedra flame-holder case (EM2C laboratory). Instantaneous field of the radiative power (in  $\text{KW.m}^{-3}$ ) is here shown. Positive (respectively negative) radiative powers are lost (absorbed) by gases. Up to 256 processors for the Radiative Heat Transfer and 120 processors for the Combustion part have been deployed on one site of the DEISA Infrastructure.

way to treat aeroacoustic problems by applying different Navier-Stokes numerical models with different refinement according to the domain complexity topology and the obstacle proximity (see Figure 2).

The JRA6 contribution has mainly consisted of greatly enhancing the parallelism level and thus opening access to totally new problem classes. Furthermore, the benefit of deploying the application on heterogeneous configurations (vector and scalar architecture) has been demonstrated.

### High added value to the design of inhibitors

In order to design better inhibitors involved in many diseases, such as Alzheimer or AIDS, the Chemistry Department at Ecole Normale Supérieure in Lyon is studying the whole enzymatic process using a coupling approach: The reactive centre is described using a quantum method (CPMD), whereas the rest of the solvated protein is described by a classical molecular dynamics method (GROMACS). The JRA6 team has brought high added value to this research by enhancing the initial coupled application (CPMD/

GROMACS) to explore much bigger molecular configurations.

### Driving molecular dynamics simulations

Large-scale computer simulations of biological systems provide valuable insight into molecular processes as diverse as enzymatic catalysis and membrane fusion. By adding external forces (with the graphic interface), the simulation systems can be driven towards states of particular interest (see Figure 3), which are unlikely to be observed spontaneously. Furthermore, the mechanical properties of (macro) molecules and their assemblies can be examined in this way by researchers of the Theoretical biochemistry laboratory at Institut de Biologie Physico-Chimique in Paris.

Driving GROMACS MD simulations with the well-known sophisticated visualization tool VMD has been the first step of our work in the HPC context.

### Fluid-structure coupling for medical applications

Some of the modern medical numerical investigations deal with simulating blood flow in

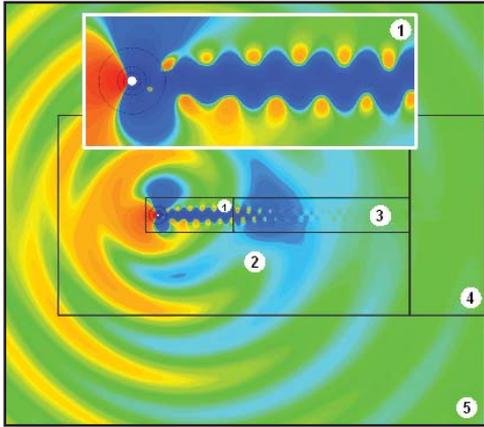


Fig. 2. Visualization of the pressure field generated by a von Karman Vortex Street decomposed into (1) unstructured Navier-Stokes (overlapped circles represent different mesh resolutions), (2) structured nonlinear Euler, (3) structured Navier-Stokes, (4) structured nonlinear Euler and (5) structured linearized Euler.

veins, including the interactions on the lung assisted by artificial ventilation. Due to the complexity of the considered biological models, such simulations lead by Lehrstuhl für Numerische Mathematik in Munich, require taking into consideration of a wide range of different physical properties and more and more details.

In order to exploit efficiently all these components, the JRA6 activity tackled global optimization problems and, in particular, the component mapping onto the heterogeneous DEISA infrastructure.

### Coupled application between 3D natural convection and radiation

The JRA6 contribution, in collaboration with Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur in Orsay, enabled deploying the numerical coupled application between 3D natural convection and radiation for the thermal efficiency of buildings. The numerical tools have been optimised by providing two parallelism levels which offers the possibility to simulate cavities with high Rayleigh numbers. The middleware capability for heterogeneous configuration (vector architecture and scalar architecture) over the DEISA infrastructure has been validated.

### Combustion in 2D

Combustion, radiation heat transfers and pollutant formation are the three main phys-

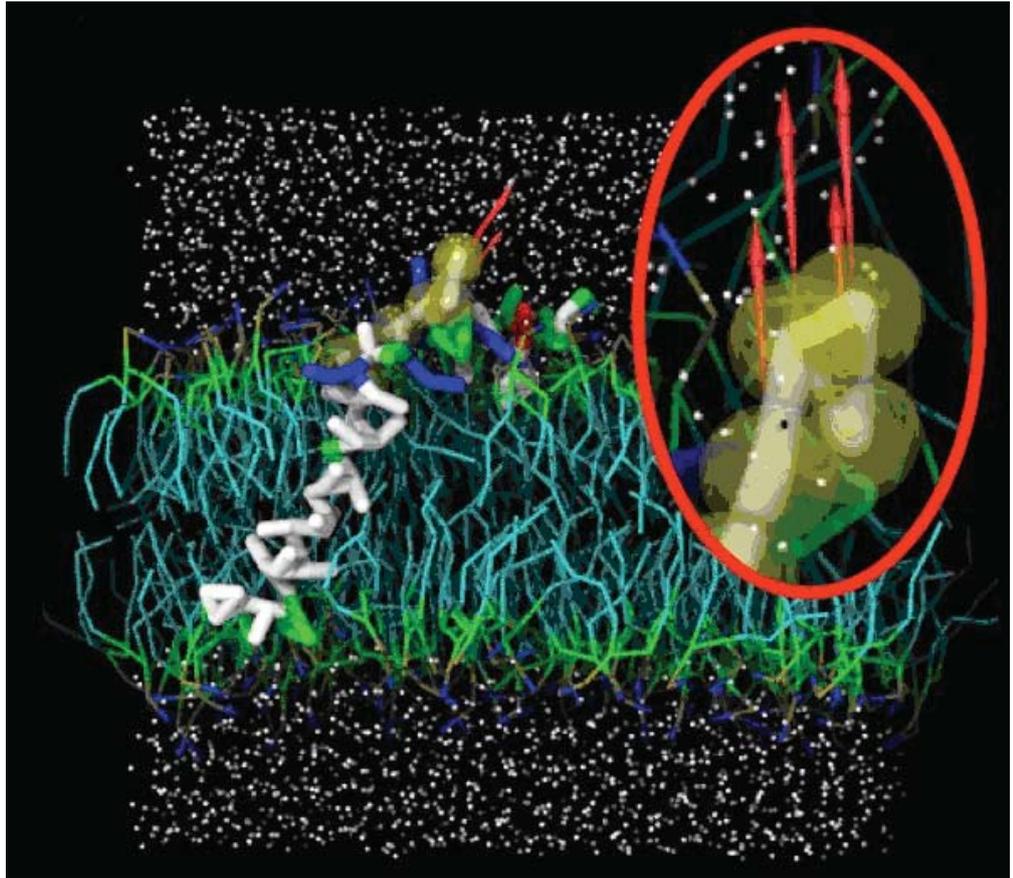


Figure 3: A single snapshot of a coarse grained molecular dynamics simulation of a protein (*Synaptobrevin transmembrane domain*) in a lipid bilayer. The protein is shown as licorice, lipids as lines and water as points. The red arrows (see figure zoom) show the user external forces applied interactively in the simulation. Here, the membrane anchoring of protein is probed by pulling on one particular side (on tryptophane residues).

ical phenomena involved in this coupling project. Numerical investigations driven by Energetique Moléculaire et Macroscopique Combustion laboratory and made possible by the technical work achieved in JRA6, demonstrate that taking into account the radiative heat transfers not only modify the instantaneous and mean temperature fields as expected, but also the flame structure itself and its dynamics, which was little expected.

### Investigations of water cycles over dry and wet regions

Exploiting a multi-models architecture that couples three components: atmosphere, vegetation and hydrologic processes, permits very innovative and relevant investigations lead researchers at Laboratoire d'Etudes des Transferts en Hydrologie et Environnement in Grenoble about the water cycle over dry regions as well wet ones. Switching from dry to wet hydrological components offered the

possibility to collaborate with researchers of AMMA – the African Multidisciplinary Monsoon Analysis international project. These results are now part of the international AMMA project.

### Observational predictions on the very first objects in the universe

Dark matter evolution, baryonic gas dynamics and chemical reactions inside the baryonic gas are the different physical phenomena involved and coupled together in this project propose by Laboratoire de l'Univers et de ses Théories in Meudon, France.

In order to exploit large physical configurations, substantial enhancements of the coupled application (parallelism level, load balancing and general optimizations), have been achieved to run efficiently on the DEISA infrastructure. This numeric tool, which considers the dark energy effects, provides precious observational predictions about the very first objects in the universe.