



## Passage of a droplet

**T**urbulence is a chaotic state of fluid motion. Not only is the fluid motion complicated, but also the flow. You may change slightly the starting configuration of your flow and after a while the flow configuration is completely different", says Federico Toschi whose research group at the National Research Council (CNR), Italy, received their by-far largest supercomputing resources from DEISA to study statistical properties of small droplets transported by an incompressible homogeneous and isotropic turbulent flow.

Toschi explains that it is impossible to know the exact starting configuration for the velocity field with infinite accuracy in any experimental or natural situation. It is a property of turbulence that even a tiny error in the knowledge of the starting configuration gets amplified exponentially. "This means that in practice you are not able to describe in a deterministic way the configuration of your system. Therefore a turbulent flow necessarily needs to be described statistically." Many natural systems are turbulent: they behave in a very complicated, chaotic way with a lot of vortices.

Fluids are everywhere and they can transport particles. "There are many possible examples such as the formation of rain droplets in clouds: At the beginning droplets are very small, and then they keep growing on top of condensa-



Fig. 1. Trajectories of particles with different inertia, released from the same spatial position. The red curve is a particle with no inertia (fluid element, hence following the fluid material line); the yellow curve is a particle with the largest inertia in our simulation. As mass grows, particles are less and less sensitive to small scale vorticity and to rapid velocity variations; particles with high inertia are expelled from high vorticity regions.

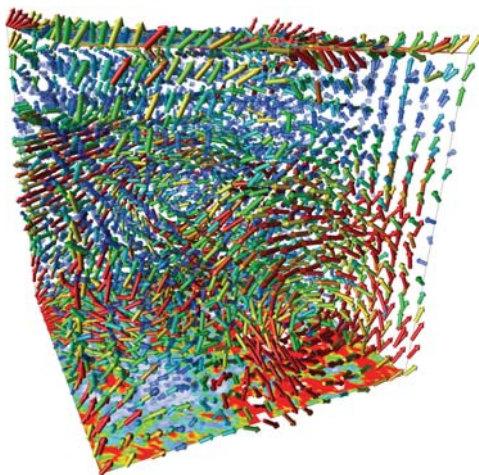


Fig. 2. A snapshot of an Eulerian turbulent velocity field from the Direct Numerical Simulation of Navier-Stokes equation. As it can be seen the turbulent field is characterized by the presence of vortex and vorticity at all scales. In the figure we can see a large vortical structure. Particles are evolved in such velocity fields.

tion nuclei. When they are large enough, they can even collide with other droplets to form larger droplets until they are too heavy. Then they fall and hence the rain begins."

Toschi's HEAVY project run on the DEISA infrastructure addresses this important question to determine the properties of particles transported by a flow, when the flow is turbulent. "I wanted to study very accurately the statistical properties of particles transported in a turbulent field, in its simplest realization – homogeneous and isotropic turbulence".

Toschi explains that the results of the numerical simulation have already been compared with some state-of-the-art experiments. Also in these experiments the aim is to have a flow field that is the simplest possible – i.e. homogeneous and isotropic. "Inside this turbulent flow experimentalists are tracking the evolution of particles, and a part of our work is to see and validate to which extent we are able to compare our results with experiments", says Toschi.

"These experiments are very challenging, because you have to follow the individual trajectory of particles and that is very complicated. By comparing the results of the experiments

with the dynamics of neutral tracers, one is also able to validate the accuracy of the experiment. Vice-versa experiments can be used to validate the model used for the transport of particles."

### Possible fields of application

Understanding the evolution of impurities and micro-droplets in a turbulent environment is of great interest in a variety of applications ranging from health preservation to engineering and atmospheric sciences. "Dispersion of pollutants in a city is one of the possible fields of application", continues Toschi. "Pollutants get transported by wind and its turbulent fluctuations. Of course there is a great deal of factors you will have to take into account, such as the geometry of a city: streets, buildings and boundary layers."

Toschi's study is an idealised situation, where only the basic physical properties of particles transported by turbulence are observed. "However this is already a piece of information and may allow predicting which area of a city can be affected and to which extend."

Another possible field of application is combustion. "The fuel is spread as very small droplets into the combustion chambers. Again there are many complications due to on-going physical and chemical phenomena", says Toschi. "But one of the phenomena is the dynamics of droplets in a turbulent environment. By having a better knowledge of the dynamics of these particles one could for example enhance the efficiency of combustion and diminish the produced pollution."

### Reynold numbers and need for more powerful supercomputers

Although supercomputers are getting more and more effective, the lack of computing power still limits scientific discoveries. "The present capacity of the fastest supercomputers in the world is not enough in our field of study. The very large simulation now performed deals with the evolution of a particle in a turbulent

field. In the turbulent field there are fluctuations from a very large scale to a smaller and smaller scale. There are strong fluctuations, for example, in vorticity”, explains Toschi.

The ratio between the largest scale and the smallest scale in a system is connected to a di-



Fig. 3. The numerical simulation of the HEAVY project was concluded in April 2007. Now Federico Toschi and his research group are analysing the results. All the data will be made available for the entire science community in order to enable new research with different perspectives and interests.

dimensionless number, called the Reynolds number. “At the moment it is impossible to numerically integrate a turbulent flow with realistically large Reynolds numbers”, adds Toschi. “For example the Reynolds number of the wind behind of an airplane can easily be in the order of 108. Today with the largest supercomputers it is possible to integrate a Reynolds number, which is at least three orders of magnitude smaller than that. Laboratory experiments can reach Reynolds numbers higher than in the numerical simulations”.

This is important when studying a turbulent flow, because in a turbulent flow there are fluctuations all the way from the largest to the smallest scale, and these are coupled in a very complicated way.

Toschi concludes: “If you want to know the statistical properties of particles or of a pair of particles that get separated, or if you want to know how a concentration of pollutants gets dispersed by turbulence, a realistic Reynolds number is a must”.

#### Sharing data

The run was concluded in April 2007. Since then the data has been re-organised for future analysis. Toschi’s group has started com-

paring data of numerical simulations with the data from previous experiments. The idea is to gather together findings of different numerical simulations and experiments on this same physical phenomenon. Toschi tells that as soon as they have finished this step of analysis all the data will be made available for the entire science community in order to enable new research with different perspectives and interests. The data will be stored at the International Computational Fluid Dynamics Database, iCFDdatabase (<http://cfd.cineca.it>) hosted by CINECA, Supercomputing Centre in Bologna. This is very important since the simulations are very demanding from the computational point of view, of the order of half million computing hours. Opportunity to run this kind of simulations is rare. Therefore Toschi’s group allow other researcher to exploit all the data.

In the future Toschi plans to study particles that are lighter than the flow, such as air bubbles in a flow. The goal is to consider more and more realistic situations, for example taking into account the fact that a particle may have finite sizes. The fluid dynamics of this kind of particles can be different than that of very small particles. Toschi sees the collision of particles as a very important and interesting research topic, too.

## 4th DEISA Symposium: Advancing Extreme Computing in Europe

This year’s annual DEISA Symposium will take place April 28 – 29 at Our Dynamic Earth in Edinburgh. Its purpose is to provide a forum where scientists from around the world can discuss HPC e-Infrastructures in general and for DEISA users to share their experiences and results.

The DEISA Symposium will take part over two days. The first day will feature talks from key players in the field of HPC e-Infrastructures including DEISA, and also from PRACE. The second day will see talks from prominent DEISA users, reporting on both their experience of the DEISA infrastructure and on their groundbreaking results.

Speakers for the second day have been confirmed:

- **Xavier Dura**, U. Barcelona, Spain, *Simulation of protein dynamics in vaccine research (Life Science)*



Fig.1. Our Dynamic Earth is a charitable trust committed to the education and life long learning of Earth Sciences.

- **Karsten Reuter**, FHI-MPG, Germany, *Molecular Switches at Metal Surfaces (Materials Science)*

- **Jukka Heikkinen**, U. Helsinki, Finland, *Plasma turbulence and flows at conditions of transport transients (Plasma Physics)*

- **Lucas Visscher**, U. Amsterdam, The Netherlands, *Simulating the Photodissociation of Triiodide (Materials Science)*

- **Joerg Schuhmacher**, TU Ilmenau, Germany, *How fast can vorticity grow in turbulence? (Fluid Mechanics)*

- **Stefano Corni**, INFN-CNR, Italy, *Protein-Surface-Interactions mediated by Water (Nanobioscience)*

Registration is now open at  
<http://www.deisa.org/symposium/>

# First-principles statistical mechanics for molecular switches at surfaces

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The large-scale density-functional theory calculations enabled by this DEISA project have provided unprecedented atomic-scale insight into the structural and electronic properties of the prototypical molecular switch azobenzene adsorbed at coinage metal surfaces. The computations reveal an interaction that is far more complex than the anticipated weak physisorption, particularly for copper, with the final bonding resulting from quite different interactions of different molecular moieties with the solid surface. The understanding emerging from the trend study of Cu, Ag and Au surfaces clearly identifies Ag as a preferred system where a controlled reversible switching should be possible.

## Azobenzene on copper, silver, and gold surfaces

In view of the rapidly advancing miniaturization in microelectronics and sensing, molecules are envisioned as fundamental building blocks in a future “molecular nanotechnology”. Since controlled switching between defined states is a crucial basis component for storage and logic, molecules offering this functionality (e.g. through externally stimulat-

ed changes between conformational isomers) attain a central importance. Considering contacting and defined integration into a larger framework, it is more precisely the molecular function when the molecule is stabilized at a solid surface that is of key interest.

A necessary prerequisite for an atomic-scale understanding of this function of the adsorbed switch is a detailed structural and electronic characterization of the stable (or meta-stable) molecular states. The project thus concentrated on achieving this crucial microscopic information for the molecular switch azobenzene, when adsorbed at the technologically relevant close-packed surfaces of the coinage metals Cu, Ag, and Au. Azobenzene is a prototypical molecular switch known to undergo conformational changes between a cis- and a more stable trans- isomer in solution. The main objective was therefore to identify and characterize (meta) stable cis- and trans- adsorption geometries at the three metal surfaces.

## Many DEISA sites employed in parallel

The CASTEP code was executed on many DEISA sites in parallel to minimize the project turnaround time, benefitting greatly from DEISA's

united computing power, unparalleled in Europe. Groups of tasks were distributed over different sites, each employing 128 processors at the IBM Power4/5 sites RZG (Garching, Germany), IDRIS (Orsay, France), FZJ (Jülich, Germany), and CINECA (Bologna, Italy), and using up to 510 processors on the SGI Altix system HLRB-II at LRZ (Garching, Germany). The multitude of total energy and force evaluations required for the project involved computing the explicit electronic structure of up to one thousand electrons, expanded in a basis approaching a million plane waves. With each such evaluation taking of the order of several hours, parallel and efficient usage of all available DEISA sites was crucial to the success of the project.

## Best molecular switch: azobenzene on silver

Our study reveals an essentially zero net binding of both conformational isomers (cis- and trans-) at Ag(111) and Au(111). This is significantly different at Cu(111), where the bonding, particularly of the cis- isomer, is even strong enough to reverse the gas phase energetic order of the two isomers. We are able to rationalize these findings as a competition between covalent bonding of the central azo (-N=N-) bridge to the substrate on the one side, and the surface interaction of the two closed-shell phenyl (-C<sub>6</sub>H<sub>5</sub>) rings on the other side, with steric effects due to the specific molecular geometry as an additional important factor. Deficiencies in the description of either of these interactions at the employed generalized gradient approximation level will therefore crucially affect the deduced energetic order of the (meta)stable adsorption modes. This concerns, notably, van der Waals contributions to the interaction of the -C<sub>6</sub>H<sub>5</sub> moiety with the coinage metal surface. Currently, the identified correlation of the cis- isomer stability with the N-substrate bond strength already permits a first prediction of suitable candidate materials for a controlled reversible switching, namely those that offer an intermediate N-substrate bonding leading to roughly energetically degenerate cis- and trans- bound states. Corresponding experimental work was already initiated with silver as one material that fulfils this property within the local collaborative research centre (Sonderforschungsbereich) SFB-658 of the German Research Council.

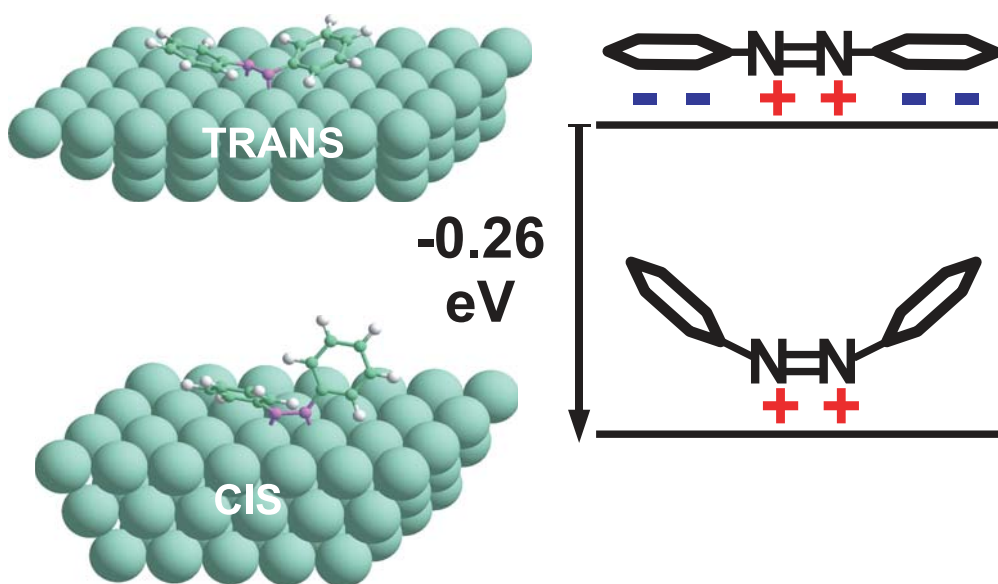


Fig. 1. Left panels: Perspective views of adsorbed trans- (top) and cis- (bottom) azobenzene at Cu(111). Cu = green spheres, N = small violet spheres, C = small green spheres, H = small white spheres. Right panels: Corresponding schematic views of adsorbed trans- (top) and cis- (bottom) azobenzene, depicting the different interaction of the molecular moieties with the surface. In the two-dimensional trans- configuration the short covalent N-Cu bond lengths conflict with the strong Pauli repulsion of the closed-shell phenyl rings at these molecule-surface distances, eventually rendering the three-dimensional cis- configuration energetically more favourable.

# DEISA Life Sciences portal in a pre-production phase

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In its attempt to stimulate and ease the exploitation of the sheer supercomputing power by the Life Sciences community, DEISA has reached a significant new level. An application team within the Joint Research Activity JRA4 has guided DEISA's middleware group into the conception of a web based portal for new HPC users. These users would not spontaneously try to benefit from the supercomputer solutions even if their challenges were well beyond the capacities of their laboratory's facilities.

The DEISA Life Sciences portal conceals the complexity of the supercomputing Grid allowing a user to submit stereotypical jobs through a simple web form. This web site is currently in a pre-production phase. It will be available to all the community after a screening by the Scientific Evaluation Committee. At present, eight DEISA sites are integrated into the portal.

## Three bioinformatics' applications available

In the first version of the portal there are three main bioinformatics' applications: BLAST, NAMD and RaxML. They are derived into a variety of services, one for each DEISA site, where they were installed. A regular user is only allowed to see and use a limited number of those services.

The interface is based on a classic web form through which a user selects all the available options of a software package, along with some basic job characteristics. Once the job form is filled out, a user may submit his job through a single click. The interface then provides a very simple page allowing the monitoring of the job and its results, where the process is seamless and hides the actual complexity. An efficient way for retrieving the output data has also been set up. The output data and the logs of the job are available for a determined amount of time.

## Initial users very satisfied

The portal is at the moment in a final test phase and seven pilot projects were selected to test it. The first version of the portal received a very warm welcome from its test users from the Life

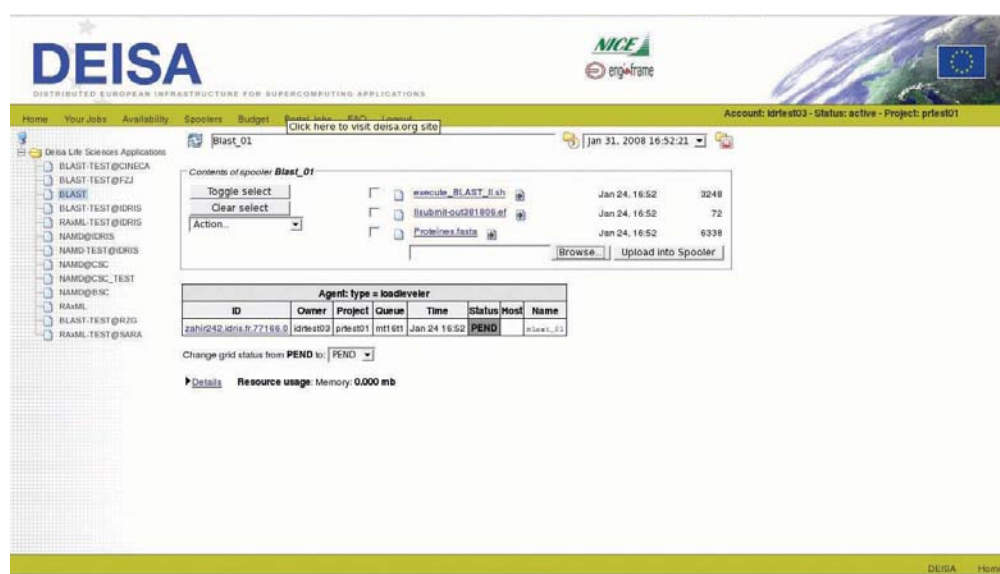


Fig. 1. Screenshot from DEISA Life Sciences portal.

Sciences community. Since the testing phase has been going well, the portal will soon enter the production phase. Then, in the next phase, the portal will be extended by deploying new software and features for the interface, taking into account the needs and suggestions of the community. Some reviews of the portal now follow:

"This access allows us to have a calculation capacity which we could not have had internally. To date, we are very satisfied with using the server –, their availability and their speed. They are very appropriate for our analyses. We are eager to see some evolution on the way calculations are submitted and the results downloaded on our computers. One point of paramount importance for us was the security and confidentiality of all data submitted to the Biportal. As a private company and as an end-user of Biportal, we are particularly confident and optimistic about the interest that such a tool brings to in-silico studies of new therapeutic molecules."

Xavier GALLET *Bioinformatician, Research Scientist Nautilus Biotech, Evry.*

"The portal granted me access to a run power that allowed me to carry out more than 25 ns of simulation of my protein in a few days whereas it would have taken months with the computer

system at my laboratory. [...] The NAMD job submission through downloading the configuration file is simple. [...] Once, the jobs through retrieving the results were conducted without any difficulties even for files over 250 Mb. [...] I am very satisfied with the service offered and I hope to benefit from the portal again."

Dr Lorraine Brillet, *CEA, Grenoble.*

"The portal's conception seems to be effective and it is easy to use. Finally, the downloading of compressed file results as an option is a good asset and the transfer is rapid"

Dr Bruno Maignet, *CNRS Research Director, LORIA, Nancy.*