

# Davide Micheletti

I introduce myself: I am Davide Micheletti and I am a PhD student in the group of Professor Zannoni at the University of Bologna (Italy). I benefited of the HPC Transnational Access to visit the SARA Computing Centre and the Computational Physics group of Professor Daan Frenkel at AMOLF Institute in Amsterdam. I spent ten weeks in the Netherlands and I had a very good time. The organization was perfect; I lived in one of the AMOLF apartments which was ten minutes walk from SARA and fifteen minutes by bike from the centre of Amsterdam, in other words the best possible accommodation! The motivations for applying to HPC-Europa were the need to use High Performance Computing facilities and to search for scientific support and collaboration. My research project dealt with coarse-grained simulations of polymeric materials. I run Monte Carlo simulations on a large number of processors to measure the stress-strain isotherms of liquid crystalline elastomers at different temperature conditions.

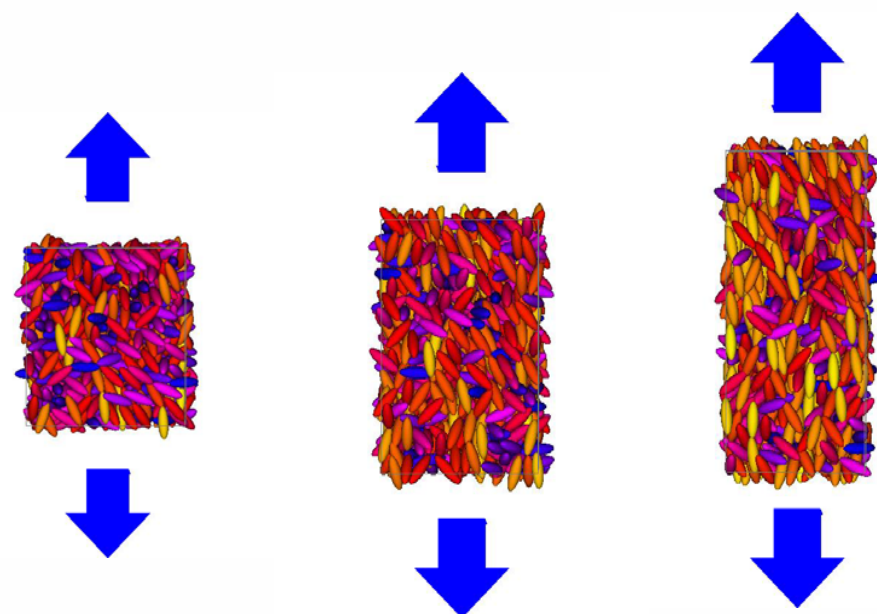
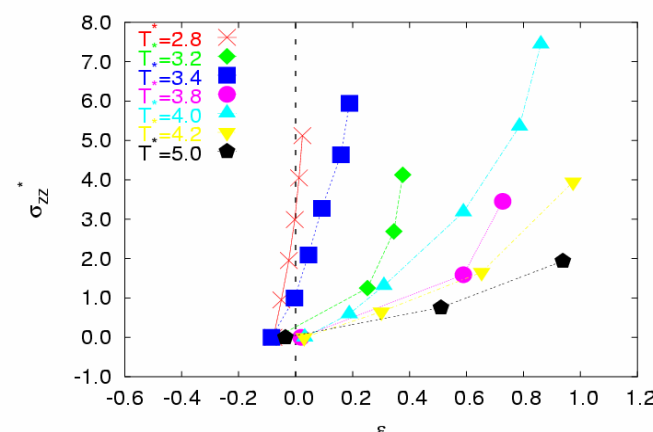


Figure 1: Snapshots taken from Monte Carlo stress-strain simulations. From the left to the right, we show elastomers samples in the isotropic phase equilibrated at different value of the adimensional engineering stress  $\sigma_{eng}^* = 0, 1, \text{ and } 2$ . In addition, we apply a colour code as a function of monomer orientation with respect to the stretching direction: if a monomer is parallel to that, it will be yellow coloured, otherwise if it is perpendicular, it will be blue coloured. For orientations between 0 and 90°, the colour gradually fades from yellow to blue.

Figure 2: Adimensional engineering stress  $\sigma_{eng}^*$  as function of strain  $\epsilon$ .



## Curriculum



**Dr Davide Micheletti** has received in October 2002 a degree in Industrial Chemistry, at the University of Bologna.

He is now attending a **PhD** in Physical Chemistry of Materials at the University of Bologna on modelling and simulation of elastomers.

His PhD supervisor is Professor Claudio Zannoni.



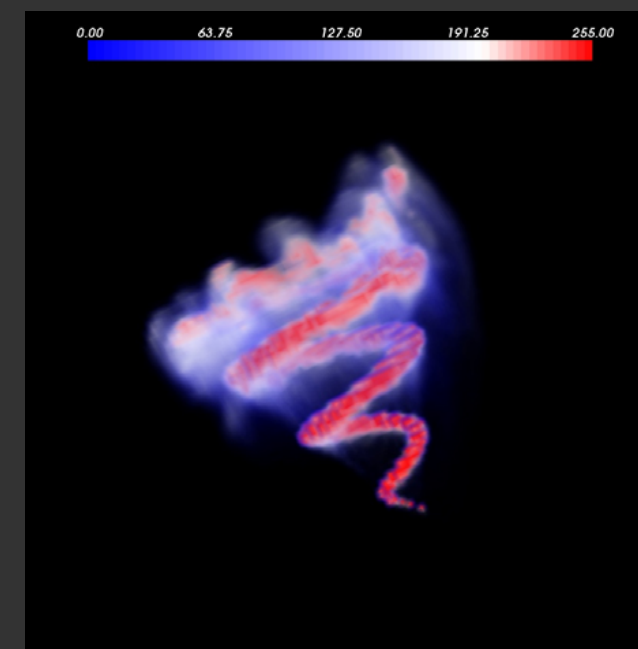
# HPC-Europa

Pan-European Research Infrastructure on High Performance Computing

## HPC-Europa is at its first birthday and the success is great !

In the first year of activity a total of 270 applications were made to the Transnational Access programme, from 28 different Countries. The selection panel offered places to 188 user-projects, 97 of which started - and in most cases completed - before the end of 2004, with an acceptance rate of 70%, spreading in a reasonably well-balanced breadth of scientific disciplines. These users spent some 155 visitor-months at the six different infrastructures, and used about 750 000 Allocation Units (AUs). The AU is defined as "the computational power delivered by a computer executing for one hour at the sustained rate of one GFlop/s". A number of very successful projects have so far been carried out and a lot of scientific papers are in preparation or have already been submitted to refereed scientific publications. Even though the first year of activity must be considered as a start-up and integration period, the different NAs and JRAs are already co-operating to create a set of tools and methodologies to support the TA and the computational sciences community in general.

HPC-Europa will strongly continue in this mission to enable users to make effective use of HPC facilities, thus enabling them to tackle new scientific challenges which would not otherwise be tractable.



Networking Activities



Research Activities

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Transnational Access



www.hpc-europa.org

# Transnational Access' series of Surgeries

by Rainer Keller - HLRS and Irina Nazarova - EPCC

The HPC-Europa Consortium is offering our guest scientists the possibility to get in touch with leading experts of different fields of Computer Science in Europa. Using the AccessGrid (<http://www.accessgrid.org>), this allows to organize live meetings of interested audience at all sites of the HPC-Europa consortium. AccessGrid offers a very good audio and video-stream quality with very little hardware requirements for small installations. In order to participate, a medium-range personal computer with only the software needs to be installed. For active participation with several people at one site, however, the installation of large-screen displays and active noise-cancellation is necessary.

With additional tools, the use of AccessGrid offers the possibility not only to share the Powerpoint presentation, i.e. have the current slide available at each site, but also use a Whiteboard-application to draw and interactively get in touch with the audience and with the presenter as we experienced at our first pilot surgery.

## The first pilot surgery

In the first of a series of the so-called "HPC-Europa Surgeries", one of Europe's leading experts on OpenMP, Dr. Mark Bull from EPCC was giving an "Introduction to OpenMP" on the 25th of February. The presentation was given to an audience of nine at EPCC and eleven guests and staff members at HLRS over the AccessGrid, with scientists gathering in the multimedia labs of both partners.

As participants were asked to submit questions or topics of interest, the presentation was covering not only beginners aspects of this Shared Memory parallel programming technique, but also going into the detail of user's questions. This proved to be a good concept, as everyone in the audience was addressed. Specifically very detailed questions regarding implementation details of OpenMP were interesting to our guests, as they are likely to port their software onto other platforms and would like to know the caveats in advance. Also Professor Barbara Chapman, also a member in the OpenMP steering committee, shared some insight on the future development of the OpenMP-standard to be released.



## The second surgery

For the second surgery, again the topic of parallel programming was chosen, this time with regard to distributed memory programming with the Message Passing Interface (MPI, <http://www.mpi-forum.org>). Over 23 guest scientists and staff members of EPCC, CINECA, SARA and IDRIS participated as Dr. Rolf Rabenseifner from HLRS, held the talk entitled "Introduction to MPI". This time, quite a lot of questions were submitted, therefore Dr. Rabenseifner chose to answer them in detail to get to know the audience, beforehand.

In such a tutorial, it's not possible to cover every single one of the over 200 functions of the MPI-standard within two hours, so we provided the presentation material and the questions submitted as PDFs to all the sites before the meeting for printout. With the increased number of participating sites, the increased possibility for technical problems, such as drop-outs or broken microphones became more apparent.



## The future surgeries

The concept of a surgery with the partner's sites participating over the AccessGrid has proven to be a good concept to give a thorough tutorial on topics relevant to Transnational Access guests. Especially the possibility to give input relevant to the guests' programming problem was proved to be very good.

With two hours, the length of such a tutorial is too short to go too much into detail with such broad topics as OpenMP or MPI, but in discussions afterwards we came to the conclusion, that an even longer tutorial with a break in the middle could ease this. Nevertheless with multimedia-labs using AccessGrid, the talk may be presented in a very lively and interactive way.

In the future, we plan to have these surgeries for our HPC-Europa guests on a regular basis every two months. The topics will be chosen to reflect the need of our sites' guests. One may think of a tutorial on how to make use of compiler optimisation techniques or performance analysis using the tools developed in JRA1.

In order to increase the value of such tutorials, we are planning to record the surgery to be offered as movie and the presentation with additional tools to record the input of the presenter using Lecturnity and distributing via VNC.



# Duncan Sanders

Granular Dynamics Group, University of Nottingham



In late July 2004 I presented some work on vibrated granular media at the Max Planck Institute for the Physics of Complex Systems in Dresden, Germany. At the workshop I met Prof. Hans Herrmann. We discussed our respective work and decided it might be useful to carry out some joint research. Prof. Herrmann, an HPC-Europa host, encouraged me to apply to the programme to visit the HLRS in Stuttgart.

From this point the process was very quick. I submitted a project proposal online in August, received confirmation of my successful application in September and flew to Southern Germany in October. In arriving at The University of Stuttgart, I was met by Ms Doerthe Pesek from the HLRS who showed me to the apartment which was to be my home for the next five weeks. The Stuttgart campus is large and the office where I worked was very cosmopolitan and well-equipped. I speak little German but everyone in the office spoke English and on the occasions when I tried to speak German to strangers they would almost always reply in English.

I was given a UNIX machine to use and for the first few days I refined a code I had written in Nottingham.

After a little difficulty in setting up my accounts, I had full access to the machines of the HLRS. One of the slightly older machines was almost continually empty. This was perfect for my research as I ran through a huge parameter space, every day launching new jobs that would have taken weeks back home.

I had hoped to create a parallel version of my simulation but it quickly became clear that this wasn't a sensible approach. I was investigating attractive forces in heated granular media and needed to simulate a wide range of conditions. I found the best way was to farm out the same simulation with different parameter files to as many nodes as possible.

I received lots of support while in Germany and would thoroughly recommend the HPC-Europa programme to anyone interested in serious computational work. When it was time to come home I realised I had produced a huge amount of work in just five weeks.

Away from work I had a great time with the HPC-Europa programme. Stuttgart is an international city and I made friends from the US, Switzerland, Austria and, of course, Germany.