



## Turbulence in fusion plasm

**T**imo Kiviniemi's research group is studying plasma cohesion in a tokamak-type fusion reactor. The group's researchers were the first in the world to show that it is possible to simulate both the formation of an electric field and its impact on turbulence by using the same software.

– Nuclear fusion is a very challenging research field. At the moment, it involves three main problems: heating, cohesion and materials' durability. Our research deals with the cohesion of fusion plasma, says Timo Kiviniemi who works at the Laboratory of Advanced Energy Systems at Helsinki University of Technology.

The electronically charged particles in plasma, electrons and ions (nuclei), usually adhere to the magnetic flow surfaces of plasma, moving along the magnetic field lines on the flow surfaces. However, heat and particle transport occurs in plasma as they move outwards, perpendicular to the flow surfaces, and finally the particles disappear into the wall structures.

– Most of the particle and heat transport in fusion plasma is due to turbulence. When this process is better understood, we hope to be able to reduce it, says Timo Kiviniemi.

A stepwise improvement in cohesion was observed under laboratory conditions as early as in the 1980s, but even today it still cannot be fully explained. One of the essential theories is that the rotational speed of plasma on different flow surfaces, i.e. at different distances from the plasma core, changes so fast that the non-simultaneous timing of the rotation movement tears eddies apart. The assumption is that plasma rotation is due to an electric field formed within plasma.

Kiviniemi's research group is now investigating how the intensively fluctuating electric field is generated and why it makes turbulence disappear – this knowledge will help in finding a way to suppress the impeding turbulence.

The simulation was performed using Elmfire software with the "full-f" approach instead of the "delta-f" method. The full-f code calculates the whole particle distribution, which makes it well suited for calculating plasma dynamics in the presence of strong perturbations. Other gyrokinetic simulations are normally based on the delta-f method, in which the simulation reveals only the standard deviation from an expected distribution. Even though simplified geometry is applied in gyrokinetics, the full-f method requires a considerable amount of computing resources, both memory and CPU.

Timo Kiviniemi's research group is one of the biggest users of CSC's computing resources. Elmfire runs have also been distributed to the supercomputing environment at Rechenzentrum Garching (RZG) in Germany, a member organization of DEISA. The resources provided by DEISA have been of great help for the research. More information is available at <http://www.deisa.org/applications/projects2006-2007/fullfgk.php>.

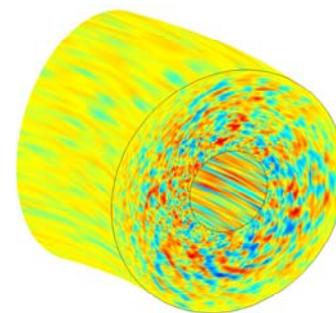


Fig 1. The poloidal cross section of saturated turbulence from an ELMFIRE simulation.

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## DEISA Extreme Computing Initiative awards 2008

**F**rom the DECI call 2007, 45 projects have now been accepted for operation in DEISA in 2008, with a total award of around 30 million processor-core hours. An allocation of 1 million processor-core hours could in principal be spent by using 16 processor-cores for about 62,000 hours (or 7 years), or by using 1024 processor-cores for about 1000 hours (or 40 days). Since DECI is dedicated to capability computing, using large fractions of a big supercomputer (or several supercomputers) simultaneously was mandatory, and only such capability computing projects were considered for execution in DEISA.

The DEISA Applications Task Force, a European team of HPC experts led by Hermann Lederer from RZG, supports the enabling of the applications in the projects to be used within the heterogeneous DEISA infrastructure and also helps to select the most suitable architecture for each project, depending on its specific requirements. In this way, DEISA is also opening up the respective most powerful HPC architectures avail-

able in Europe for the most challenging projects, mitigating the rapid performance decay of a single national supercomputer within its short life-time cycle of typically about 5 years.

The 45 projects retained for operation in 2008 cover major areas of science including Materials Science (12 projects), Astro Sciences (8 projects), Engineering (8 projects), Life Sciences (8 projects), Earth Sciences (4 projects), Plasma Physics (3 projects), and Informatics (2 projects). The projects to be supported involve scientists from 14 different European countries and collaborators from three more continents.

This huge continental demand for capability computing resources in Europe also clearly documents the need for a persistent European HPC ecosystem.

**All the retained projects are listed at <http://www.deisa.org/applications/projects2007-2008/index.php>.**

### Next DEISA events

6th DEISA training session  
5 - 7 March '08, Stuttgart, Germany.  
<http://www.deisa.org/training>

4th DEISA Symposium  
28 - 29 April '08, Edinburgh, UK.

# On the molecular working of a twisted nematic cell

Claudio Zannoni, Università di Bologna, Dipartimento di Chimica, Fisica e Inorganica

One of the most successful stories in advanced materials is that of liquid crystal (LC) displays. The basic concept underlying the most classic among these devices, the twisted nematic (TN) display, is that a pixel is activated by a change of molecular organization in a few micron thick cell. According to this concept, an initial configuration of the local preferred direction (the director) is established between two orienting surfaces (rubbed glass or polyimide), rotated 90 degrees from one another, that confine the LC. An experimental fact is that polarized light is going through the pixel in this "rest" state and this is compatible with a microscopic helical configuration. If the chosen LC has a positive dielectric anisotropy and a suitable voltage is applied across the cell in correspondence of the pixel, then polarized light is not rotated and light does not go through the device, compatibly with a monodomain organization. When the field is switched off the original organization is re-established.

The classic textbook picture explaining the working of a TN-LCD, is that of uniformly twisted layers, but to the best of our knowledge there is little evidence that the molecular organization at rest is a uniform helix at molecular level. Moreover, the way the organization is established is not obvious, for instance as the organization at rest is re-established after an aligning cycle does the reorganization take place from the centre of the cell or from the surface? Uniformly or not? Is a uniform helix really formed? Or how helical is the structure?

Trying to work out the microscopic working of the TN display is a particularly challenging problem, as it implies considering a huge number of degrees of freedom, which are to follow for very long times from a microscopic point of view, as the average TN-LCD response varies in the range 8-15 milliseconds, while the typical time scales we are to date able to access through conventional computer simulations is of the order of nanoseconds.

Within the DEISA project, we have tackled this problem setting up a molecular resolution model of a TN cell containing  $O(10^6)$  model particles, simulated using the Monte Carlo (MC) method. To this purpose, we developed an MPI parallel MC code using a replicated data scheme, by modifying the canonical Markov chain of the Metropolis algorithm to allow for multiple simultaneous moves to be performed at the same time by different proc-

essors. This kind of moves are not possible in conventional MC algorithms due to the intrinsic non deterministic nature of MC, but in our case the big sample size allows every processor to pick an energetically independent particle in suitably chosen cells in which the whole sample is subdivided.

We modeled the LC rod-like molecules contained in the LCD cell as Gay-Berne single ellipsoidal interaction sites, discarding all the intramolecular degrees of freedom. Our TN cell is arranged as to model a 0.1 micron x 0.1 micron x 0.05 micron display cell. Although a fully realistic model would have to consider an order of magnitude bigger sample, this is currently unfeasible with the available resources. The initial configuration (see fig. 1 a), is characterized by the LC molecules uniformly aligned perpendicular to the display surfaces to give the dark pixel state, while the display boundaries are modeled with layers of fixed particles oriented along the incoming and outgoing polarizers directions (rotated 90 degrees from one another). The system is then allowed to relax through MC simulation to the "rest" equilibrium state, which is reached only after 150000 hours of computing time (See fig. 1 b).

Following the time evolution of this equilibration process we can notice that the mechanism of clearing of the pixel proceeds by the local induction of order by the two confining surfaces which induce an almost parallel alignment to their orientation on the LC molecules filling the

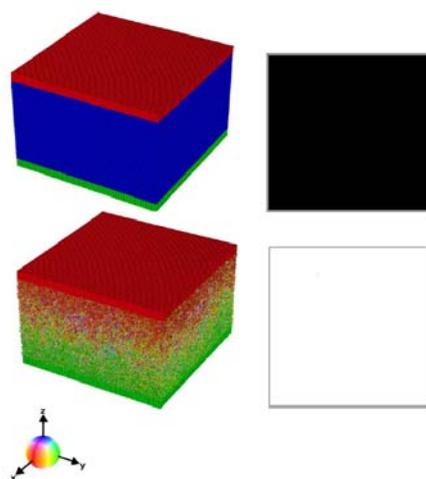


Fig 1. Snapshots of the molecular configurations (left) and corresponding computed pixel images (right) for: a) the initial dark state (top) and b) the final states (bottom), after 150000 hours of Monte Carlo simulation. Molecules are color coded according to their orientations.

display. This is a very slow process, characterized by the progressive alignment of the molecular layers, starting from those closer to the two surfaces. The resulting distribution of local directors at this point is far from being that of a perfect linear helix. On the contrary, the molecular layers align almost parallel to the closest display surface, and are not affected by the farthest surface. Some sort of helicoidal ordering starts to form only when the two fronts of perpendicular oriented particles, come into contact in the middle of the sample. However, the temperature dependent fluctuations of molecular orientations in the middle of the sample make the conventional picture of a uniformly helicoidal configuration too simplistic, and evidences how this requirement is not necessary to achieve a good optical behavior.

Having reached an equilibrated configuration corresponding to a light pixel, we switched on an electric field in the central region of the display. Our aim was to investigate on the mechanics underlying the disruption of helicoidal order to give a black pixel. The interesting result is that the dark region of the pixel starts to grow from the centre of the square area affected by the field, expanding in concentric spherical shells, instead of uniformly all over that area (see fig 2).

The calculations were carried out at the CSC in Finland, employing 128 processors and at CINECA in Italy, using 64 processors, for a global amount of 200000 CPU hours.

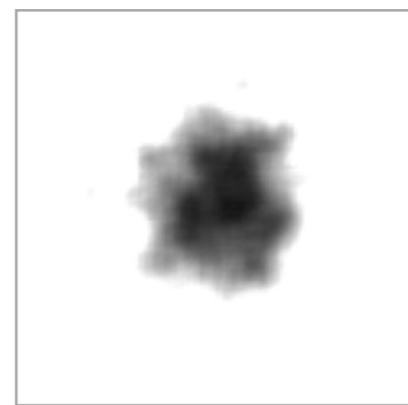


Fig 2. Pixel image computed after 50000 cycles of  $\text{\AA}$  MC simulation with an electric field switched on in the middle of the display.

## HIV simulation as a GIN demo between Australia and Europe



Fig 1. Six supercomputing machines were involved in the simulation

A range of simulations of known mutants against one particular HIV drug were run in the DEISA and Australian Partnership of Advanced Computing (APAC) grid infrastructures for the Grid Interoperability NOW (GIN) demonstration. This demonstration was presented at SC07, in Reno, Nevada.

HIV is a disease that affects some 40 million people worldwide. Certain drugs can improve patient health by binding to and inhibiting critical viral enzymes. Virus can mutate and become resistant to these drugs.

According to Michael Kuiper from VPAC, the simulation run in APAC and DEISA grids is designed to gather drug binding interaction energies of anti-HIV drugs bound to the active site of HIV protease, including drug-resistant versions of the protein. Though still a developing methodology, it is hoped that this technique can give an accurate assessment of the likely effectiveness of each antiviral drug with respect to any given mutant strain of HIV. With this information, patients who develop drug resistance will be given the next best effective drug for their HIV strain while reducing the chance of further resistance.

In order to assess the drug binding interactions, each drug and respective HIV mutant enzyme is run as a short molecular dynamics simulation to try and get an averaged energy of interaction between the drug and the HIV protease strain. A number of simulations were run with the drug Amprenavir (Apv) with various HIV strains. The runs were for 200000 steps, collecting data every 500 steps. The trajectory

data is post-processed to measure the energy of interaction between the drug and each hiv strain. Since these methods are developing, various weights were given to each type of interaction, (such as van der Waal and electrostatic interactions) to help parameterize the measurements.

The simulation involved six supercomputing machines: CINECA and IDRIS of the DEISA sites, SAPAC, VPAC, Monash and iVEC from the APAC grid. Input data were stored on the VPAC storage server and they were moved via GridFTP. The jobs were submitted on DEISA by using

DESHL; a UNICORE command line interface and on APAC by using Globus WS-Gram client. The simulation outcomes were again uploaded on the VPAC storage server for post-processing and visualization. The resources requested were 16 processors per site for about five hours.

This demo was one of the DEISA talks given at the FZJ's booth at the SC07 exhibition.

**All the presentation slides are at [http://www.deisa.org/news\\_events/deisa\\_events/deisa\\_sc07.php](http://www.deisa.org/news_events/deisa_events/deisa_sc07.php)**



Fig 2. Four DEISA talks were given at SC07.