Recent publications

Chemical physics
The supercooled state of dipolar liquids
Supercooled liquids have a strikingly slow dynamics without a clear structural cause. The ensuing glass transition is considered to result from an increase of cooperativity between the dynamics of molecules. Ricardo Palomar and Gemma Sesé have studied the case of dipolar liquids via molecular dynamics, and found that the dynamics in the supercooled state does not significantly depend on the dipolar nature of the fluid. The studied appeared in the Journal of Chemical Physics on Aug. 12, 2008.

Biomedicine
Culturing malaria
The fight against malaria requires growing its parasite in vitro, a process that is not well understood yet. A group of FEN researchers from the SIMBIO group has studied, in collaboration with researchers from GlaxoSmithKline, how the geometry of the culture affects the parasite’s development. The work has been published in the Malaria Journal on Oct. 8, 2008.

Biological modeling
Web-based microbial simulation
Individual-based models of microbial systems are more difficult to analyze and communicate than traditional analytical models. Joan Carles Cañadas and a researcher from the SIMBIO group have developed a web-based simulation of yeast populations in liquid media that allows the user to explore the way in which the population reacts to changes in parameter values, initial conditions or assumptions. The model is described in the Nov. 2008 issue of the Journal of Industrial Microbiology and Technology.

Complex systems
The emergence of language conventions
Linguistic categories (colors, animals...) are culture-dependent conventions accepted by communities without central coordination. Individuals may conceptualize the world differently, but they must reach an agreement to understand each other. FEN researcher Andrea Baronchelli and co-workers have developed a game model to show that categories may emerge simply through cultural exchange. The results were published in the Proceedings of the National Academy of Sciences of the U.S.A. on June 10, 2008.

Systems biology
The quantized dynamics of cells
Certain cell types exhibit quantized behavior, e.g. in the distribution of cell cycles; only a discrete set of cycle times are possible. Jordi Garcia Ojalvo and collaborators from the Southwestern Medical Center in Dallas have proposed a simple mechanism for this phenomenon, in which noise plays a vital role. The work has been published in the Proceedings of the National Academy of Sciences of the U.S.A. on Oct. 14, 2008.

Physical chemistry
Encapsulating dyes
Cyclodextrins are useful molecules that stabilize sparingly soluble organic molecules in aqueous phases. Elvira Güردia and Jordi Martí, with collaborators from Argentina, have used extensive molecular dynamics simulations to study the solvation dynamics of the dye Coumarin 153 after encapsulation by β-cyclodextrins. The work was published in the Journal of Physical Chemistry B on July 2, 2008.
Our postdocs

Núria Domedel Puig, biologist

“Since I was primarily trained as a biologist, working in a physics department is a very challenging and exciting task. Prof. Jordi Garcia Ojalvo and I are working on a project funded by the Red Española de Esclerosis Múltiple. We study the cellular response to interferon beta (IFNβ), a widely used drug against this disease. Our collaborators from the Universidad de Navarra, headed by Dr. Pablo Villoslada, generate time series data from human blood samples that we then analyse. The goal is to build a mathematical model that reproduces IFNβ signalling. We wish to gain insight into how IFNβ treatment alters cellular behaviours, and why some patients fail to respond to this treatment.”

Núria Domedel Puig obtained her PhD in Bioinformatics from Birkbeck College (University of London, UK) in June 2008. She has joined the Department financed by the Red Española de Esclerosis Múltiple (REEM).

Ioannis Skarmoutsos, phys. chemist

“I joined the Department on April 2008, and since then I have started my research in collaboration with Prof. Elvira Guardia. In general, my impressions about the hospitality and the labor environment in DFEN are excellent. My research focuses mainly on the determination of the local structural effects and related dynamics in supercritical fluids (SCFs), by employing molecular dynamics simulation. It is well-known that SCFs exhibit solvent properties which may be varied from gaslike to liquidlike values with small changes in pressure or temperature. The origin of this peculiar behavior of SCFs has been attributed to density inhomogeneities in such systems. Our main goal is to reveal the microscopic mechanisms responsible for the static and dynamic behavior of these inhomogeneities, and their interconnection with dynamic properties of SCFs.

Ioannis Skarmoutsos obtained his PhD in chemistry from the National and Kapodistrian University of Athens (Greece) in 2007 and is in Barcelona since April 2008. He is currently a postdoctoral fellow, financed partly by our Department.

Side Note
Instant replay of a supernova explosion

X-ray spectra from the Chandra and XMM-Newton Observatories have allowed to characterize for the first time the energetics and the explosion mechanism of a supernova (SNR 0509-67.5), some 400 years after the event. Eduard Bravo participated in the study, which has been published in The Astrophysical Journal on June 20, 2008. The results have been confirmed by the optical detection of the light echo of the supernova explosion. For more information, see http://chandra.harvard.edu/press/08_releases/press_032008.html