## Seminars 2006

November 17, 3:30 pm, Aula Touschek, Department of Physics

Prof Antonio Scala - SMC Roma1

Simulating hard rigid bodies

Hard rigid bodies are a reference system to understand the properties of molecular fluids, especially regarding the steric effects. Nevertheless, apart the case of hard spheres systems, there are no general recipes for Monte Carlo or Event Driven Molecular Dynamics simulations. We introduce a new algorithm to calculate the distance between two convex surfaces. Building up on such result, we introduce a new event-driven (ED) molecular dynamics algorithm for simulating systems of hard convex bodies. In order to optimize collision detection between elongated objects, we introduce a new nearest-neighbour list based on oriented bounding parallelepipeds. We show in detail algorithm's efficiency simulating a system of hard ellipsoids of revolution (HE) and discuss the possible applications of our new techniques in various scientific and technological fields.

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October 25, 3:30 pm, Aula Touschek, Department of Physics

Prof Marek Cieplak - Polish Academy of Science

Nanoscale fluid flows in the vicinity of patterned surfaces

October 12, 3pm, Aula Conversi, Department of Physics

Prof Stefano Ruffo - Universita` di Firenze

Dinamica lenta in sistemi con interazioni a lungo raggio

October 9, 12 am, Aula Touschek, Department of Physics

Prof Giuseppe Suffritti - Universita` di Sassari

Modelling the diffusion in microporous materials: examples and challenges

May 8

Prof Giancarlo Jug - Università dell'Insubria

Why are window-glasses sensitive to weak magnetic fields at low temperatures?

April 12

Dr Emanuele Paci - Leeds University

From peptide conformation to protein translocation in vivo: What can we learn from simulating simple models?

January

Dott Andrea Ricci - Johannes Gutenberg Universitaet, Mainz

Elastic properties and Structures for 2-d model collisions in confined geometry