# International School of Liquid Crystals
# 6th Workshop

# New Challenges in Computational Modeling: Techniques for Processes, Molecular Systems and Anisotropic Materials

**Directors of the Workshop: A. Laganà, P. Pasini**
***E. Majorana* Centre for Scientific Culture, Erice**
**25-28 October 2001**

## October 25

Afternoon: Arrival
21.15: Welcome Reception at the Marsala Lecture Hall (S. Rocco)

## October 26

| | | |
|---|---|---|
| **8.45-9.00** | A. Lagana`<br>P. Pasini<br>G.F. Tantardini<br>C. Zannoni | Opening and Welcome |

1st Session**:**
**Metachem: Metacomputing for complex computational chemical applications**

| | | |
|---|---|---|
| **9.00 – 9.50** | **M. Livny** | Distributed computing:tools and perspectives. |
| **9.50 – 10.20** | F. Semeria | Monte Carlo simulations of a biaxial liquid crystal model using the Condor processing system. |
| **10.20 –10.50** | S. Boschi | Computational Chemistry at CINECA. |
| **10.50 – 11.20** | | **Coffee Break** |
| **11.20 – 12.10** | **D. Laforenza** | Le “Griglie computazionali”: verso un nuovo modo di fare Scienza. |
| **12.10 – 12.40** | O. Gervasi | A GRID based computational approach to the simulation of crossed beam experiments. |
| **12.40 – 13.10** | L. Pacifici | Parallel restructuring of reactive scattering codes using a skeleton based environment. |

**Lunch Break**

2nd Session: **Computational techniques for molecular systems**

| | | |
|---|---|---|
| **15.30 – 16.00** | **P. Lazzeretti:** | Fast coupled Hartree-Fock algorithm for the calculation of parity-violating contributions to electronic energies of enantiomeric molecules. |

| | | |
|---|---|---|
| **16.00 –16.30** | G. Giorgi | Theoretical study on selective grafting mechanisms to systems containing silicon |
| **16.30 –17.00** | L. Muccioli | Molecular Dynamics simulation of the Odd-Even effect in liquid crystals |
| **17.00 – 17.30** | D. De Fazio | Hyperquantization Algorithm for chemical reaction dynamics. |

**17.30** Assemblea del Gruppo Interdivisionale di Chimica Computazionale

**October 27**

2nd Session**: : (cont'ed)**

| | | |
|---|---|---|
| **9.00 - 9.50** | **F. Gianturco** | Modelling structures and dynamics in highly quantum molecular processes. |
| **9.50 – 10.20** | A. Polimeno | Computational approaches to mesoscopic dynamics of isotropic and anisotropic fluids |
| **10.20 – 10.50** | G.F. Tantardini | Adsorption of atomic Oxygen on Al (100), Al (110) and Al (111). |
| **10.50 – 11.20** | | **Coffee Break** |
| **11.20 – 11.50** | M. Persico | Molecular rotation and alignment in multiphoton processes. |
| **11.50 – 12.20** | C. Angeli | Study of homonuclear diatomic molecules containing multiple bonds using the NEV-PT perturbation theory. |
| **12.20 – 12.50** | L. Gagliardi | Quantum Chemistry Methods for Heavy Elements. |

**Lunch Break**

3rd Session: **Process Computational Technologies**

| | | |
|---|---|---|
| **15.30 –16.20** | **M. Morbidelli** | Multi-objective Optimization of Continuous Chromatographic Separation Processes through Genetic Algorithms. |
| **16.20 – 16.50** | G. Continillo | Numerical and experimental investigation of extinction mechanisms of gas flames in packed beds. |
| **16.50 – 17.20** | L. Russo | Approximate Inertial Manifold in the study of constitutive equation for mesophases under flow: a comparative analysis. |
| **17.20 – 17.50** | M. Di Stefano | Theoretical Investigations of the atmospheric system Thionyl fluoride. |
| **17.50 –18.30** | **A. Lagana`** | Concluding remarks. |
| **18.30 – 19.30** | | **Poster Session** |
| **20.30** | **Social Dinner** | |

**October 28:** Departure