1st Workshop on Molecular Theories and Simulations

Gaeta, 10−12 May 2002

Organizing committee:

A. Amadei (Roma, TOV)
M. Aschi (L'Aquila)
A. Di Nola (Roma, La Sapienza)
D. Roccatano (L'Aquila)

Final Program

Friday 10 May

afternoon: welcome and rooming in.

Saturday 11 May

10:00 **Bert de Groot** (Göttingen, D)
Water permation across biological membranes: Structur e, dynamics and mechanism of aquaporin−1 and GlpF

10:40 **Isabella Daidone** (Roma, I)
Folding/unfolding simulations using Biased Molecular Dynamics

11:20 Coffee break

11:50 **Giorgio Colombo** (Milano, I)
Simulation MscL gating under pressure

12:30 **Steve Hayward** (Norwich, UK)
Understanding Protein Domain Motions by Construction of a Database

13:10 Lunch

15:40 **Roberto Improta** (Napoli, I)
Quantum mechanical methods for the study of biological systems

16:20 Coffee break

16:50 **Emil Apol** (Groningen, NL)
Equations of state for temperature and electric field bas ed on the quasi−Gaussian entropy theory

17:30 **Maira D'Alessandro** (Roma, I)
Statistical mechanics and thermodynamics of simulated ionic solutions

18:10 Discussion

Sunday 12 May

10:00 **Riccardo Spezia** (Roma, I)
The Perturbed Matrix Method: applications from gas ph ase to biological macromolecules

10:40 **Emma Langella** (Napoli, I)
A comprehensive computational strategy for the study of organic radicals in biochemical processes

11:20 Coffee break

11:50 **Cecilia Bossa** (Roma, I)
Long time scale Molecular Dynamics simulations of My oglobin

12:30 Departure

Hotel Summit − Gaeta (LT)