

## Provisional Program

May 30 -June 1 2018

**May 30,**

**15:00-19:00**

Giovanni Ciccotti      Molecular Simulation (MS) vs Theoretical Physics

Gianni Battimelli      A project for an Archive for the history of MS

Oliveri Darrigol      Discrete mathematics and discrete physics in the works of Ludwig Boltzmann.

**May 31**

**09:00-13:00**

Arianna Borrelli      The Monte Carlo method in early particle physics

Marie Farge      The role of supercomputers to study turbulence

Giovanni Paoloni      Research Institutions and Science Policy: Why and how should one study them

Vittorio Marchis      Mechanical fantasies, epistemology of the machine in the immaterial knowledge

**15:00-19:00**

Luigi Cerruti                      Folding, Unfolding, Misfolding, Non-folding  
Molecular Simulation and the Proteins Folding  
Problem

Ignacio Pagonabarraga

Sara Bonella                      CECAM Historical Archives: First steps and a Few  
Questions

Gianni Battimelli                A case study on the history of MS: B.Alder and the  
inception of Molecular Dynamics

**June 1**

**09:00-13:00**

Michel Mareschal                The early years of Computational Statistical  
Mechanics

Martyn Guest                      The Story of two Community Codes, DL\_POLY and  
GAMESS-UK, with an Overview of their  
Performance Evolution: Analysing, Understanding  
and Exploiting HPC Technology

Paul Durham                      Origins and Development of the Collaborative  
Computational Projects at Daresbury Laboratory

General Discussion                Is it timely and desirable to create an archive\_for  
and the history\_of molecular simulation? If so,  
which is a good strategy and what are the steps in  
order of complexity/difficulty?