

Course title:

Soft Matter Modelling: Molecular Simulations and Soft Matter in Flow

Duration [number of hours]: **24**

PhD Program [MERC/MPHS/SPACE]: **MPHS**

Name and Contact details of unit organizer(s):

Dr. Antonio Baldanza, Dr. Maurizio De Micco, Prof. Giuseppe Milano, Prof. Pier Luca Maffettone,

Affiliation(s): SSM, UNINA

Email: a.baldanza@ssmeridionale.it, m.demicco@ssmeridionale.it

Website: www.docenti.unina.it/giuseppe.milano ,

Email: giuseppe.milano@unina.it

Website: www.docenti.unina.it/pierluca.maffettone,

Email: p.maffettone@unina.it

Course Description [max 150 words]:

“Soft Matter” (or complex fluids) is ubiquitous in many technological and industrial processes. This course has two parts, the first introduces the basics of molecular simulations and will give example applications of this class of techniques to typical soft matter materials including atomistic and coarse-grained modelling approaches. The second part is focused on Soft Matter under flows. Soft matter can flow like liquids, it possesses a measurable viscosity, can bear stresses, and typically shows viscoelastic behaviour under flow conditions. A common characteristic is its large and nonlinear response to weak forces. This course introduces the fluid-dynamics of viscoelastic liquids. Rheological models for macromolecular systems will be presented. Introduction to Brownian Dynamics computations with Matlab will be given.

Syllabus [itemized list of course topics]:

- A first introduction to Molecular Simulations (1 h)
- Basics of Statistical Mechanics for Molecular Simulations (3 h)
- Molecular Dynamics: integration, force calculations (1 h)
- Monte Carlo: from Monte Carlo integration to Metropolis (2 h)
- Force Fields (1)
- How to increase simulation speed: main algorithms, coarse-graining (3h)
- Molecular Simulations: some example applications (1h)
- Introduction to Soft Matter and Continuum Mechanics (2h)
- Introduction to Brownian Dynamic simulations (2h)
- Rheology (2h)
- Modelling flexible and rigid macromolecules dynamics (3h)
- Brownian Dynamic simulation of flexible and rigid macromolecules (3h)

Assessment [form of assessment, e.g., final written/oral exam, solutions of problems during the course, final project to be handed-in, etc.]:

Team’s work on a project

Final discussion on all the reports

Suggested reading and online resources:

Suggested books:

1. Frenkel and Smit, *Understanding Molecular Simulations: From Algorithms to Applications*, Academic Press, 2023
2. Larson RG, *The structure and rheology of complex fluids*, Oxford University Press, 1999
3. Doi M, *Soft Matter Physics*, Oxford University Press, 2013