



**POLITECNICO
DI TORINO**



Excellence course – Corso di eccellenza

"The Theory of Coarse-Graining and its applications towards the modelling of complex fluids"

Prof. Pep Espanol

Sala DIDATTICA - DISAT

20 Lectures – 20 hours

Summary: In this course we present in detail the fundamentals of the theory of coarse-graining, explore different applications that range from thermodynamics of small systems to fluctuating hydrodynamics and complex fluids (colloidal suspensions and other viscoelastic fluids), and describe particle-based simulation methodologies like DPD and SDPD for the simulation of complex fluids.

| Day | Time | Topic | |
|--------------------------------|---------------|---|--|
| Mon May 6 th | 10:00 – 11:00 | The microscopic level | Introduction to the course |
| | 11:00 – 12:00 | | The microscopic level |
| | 14:30 – 15:30 | | Flow in phase space: Ergodicity, Irreversibility, Equilibrium |
| | 15:30 – 16:30 | | Probabilities in Phase space. Levels of description. The Maximum Entropy Principle |
| Tue May 7 th | 10:00 – 11:00 | The coarse- grained dynamics | Green's view of coarse-graining |
| | 11:00 – 12:00 | | The Zwanzig projection operator technique |
| | 14:30 – 15:30 | | The GENERIC framework |
| | 15:30 – 16:30 | | Near equilibrium and Mori theory of projection operators |
| Wed May 8 th | 09:00 – 10:00 | The theory of coarse- graining at work | External Forcing: summary and overview of applications |
| | 10:00 – 11:00 | | Thermodynamics of small systems |
| | 14:30 – 15:30 | | Colloids, Smoluchowski and Langevin descriptions |
| | 15:30 – 16:30 | | Blob Models of complex molecules |
| Thu May 9 th | 09:00 – 10:00 | Hydrodyna mics | Discrete diffusion |
| | 10:00 – 11:00 | | Discrete fluctuating hydrodynamics |
| | 11:00 – 12:00 | | Boundary conditions |
| | 13:00 – 14:00 | | Nanoparticles embedded in a fluid |
| Fri May 10 th | 10:00 – 11:00 | Fluid particle models | Lagrangian fluid particles: the continuum limit and the Lagrangian description |
| | 11:00 – 12:00 | | The DPD model and the SDPD model |
| | 14:30 – 15:30 | | The SDPD model for viscoelastic fluids |
| | 15:30 – 16:30 | | Summary of the course |

The course is organized by the Scudo (Doctoral School of Politecnico di Torino) for its graduate students. However, the course can also be attended by a limited number of external students (free of charge). Students potentially interested are invited to contact Daniele Marchisio (daniele.marchisio@polito.it).