EuroTeQ Engineering University

Course

Part of the EuroTeQ course catalogue spring/summer 2023

Multiscale Modelling for Polymer Mechanics

Subject area: Mechanical Engineering

University:	TU/e
Level:	MA all years
Teaching mode:	hybrid: some students participate online, other students attend real-life
Instructor(s):	Dr. sc.nat. M. Hütter; Dr.ir. L.C.A. van Breemen

Short description

The focus of this course is on modeling the mechanical behavior of polymers in the solid state. Of particular interest is the combination different length scales to arrive at mechanical models that build on the underlying structure. To that end, several numerical techniques are discussed, namely Molecular Dynamics, Metropolis Monte Carlo, and Finite Element Modeling. Both sequential and concurrent level-coupling will be examined, based on concepts from non-equilibrium thermodynamics

Full description

The course will give an introduction to/repetition of the most common and important simulation techniques, namely to

- Molecular Dynamics (MD) simulations (particle-based),
- Metropolis Monte Carlo (MC) simulations (particle-based),
- Finite Element Method (FEM) (continuum),

that are used nowadays to model and predict the thermo-mechanical properties of polymers.
To that end, the course will include the following subtopics:

- Controlling the temperature and pressure with thermo- and barostats (MD, MC);
- Imposing external deformation and temperature gradients (MD, FEM);
- Calculation of the mechanical and thermal response (stress tensor and heat flux) (MD);
- Implementation of constitutive material models for hyper-elastic, visco-elastic, and visco-plastic behavior (FEM);
- Coupling of particle-based and continuum scales (MD, MC, FEM), using nonequilibrium thermodynamics.

In order to increase the accuracy and efficiency of the simulations, the course covers also

- Time-integration schemes (Euler, Verlet) (MD);
- Efficient energy and force calculations for large systems (neighbour lists and cell lists) (MD, MC);
- Averages and the usefulness of fluctuations (MC);
- Boundary conditions, periodic or free (MD, MC, FEM);
- Calculation of stresses and tangential stiffness (FEM);
- Mesh-convergence (FEM).

Implementation of material models is done in Matlab (MD, MC, FEM), and Marc Mentat (FEM). The above simulation techniques will be applied to study and predict the behavior of polymers

Learning outcomes

After passing the course, the student is able to

- Understand how Molecular Dynamics (MD), Metropolis Monte Carlo (MC), and Finite Element Modeling (FEM) can be employed for the analysis of solid polymers on different length scales; in particular: understand how these techniques can be used in combination (sequential vs. concurrent coupling);
- Apply (conceptually) a combination of MD, MC, and FEM to specific cases, and correspondingly analyze points in the modeling strategy that need special attention;
- Understand how temperature and pressure are controlled with thermo- and barostats (MD, MC), and how external deformation is imposed (MD, MC, FEM);
- Understand how macroscopic mechanical and thermal properties can be extracted from MD and MC, by way of statistical averages or fluctuation formulae;
- Understand the procedures behind the implementation of constitutive material models for hyper-elastic, visco-elastic, and visco-plastic behavior (FEM);
- Understand, analyze, and apply improvements for the accuracy and efficiency of the simulations, particularly in terms of: time-integration schemes (Euler, Verlet) (MD), efficient energy and force calculations for large systems (neighbor lists and cell lists) (MD, MC), periodic/free boundary conditions (MD, MC, FEM), calculation of stresses and tangential stiffness (FEM), and mesh convergence (FEM).

Recommended in particular for students of the following study programmes

Applied Physics, Material Science

General information

Contact hours per week:	8
Total workload:	140 (in student hours for the whole course)
ECTS credits:	5
Language:	English
Course start date:	06 February 2023
Course end date:	23 April 2023
Add. info about start date:	
Weekly teaching day/time:	
Time zone:	CET (Denmark, Germany, France, Netherlands, Switzerland, Czech Republic)

Further information:

Prerequisites:	Recommended: Solid Mechanics; Statistical Mechanics.
Activities and methods:	Lectures, Self study: preferably on campus, with support if needed.
Presence on campus:	

Final examination

Form:	oral
Date:	
Location/format:	Oral exam for EuroTeQ students
Re-sit possibility:	yes
Transcript available:	on request
Add. info/requirements:	

Registration

To register for this course, follow the registration requirements of your **home university** as specified here: www.euroteq.eu/courses-registration.

Administration

Number of places:	50
Minimum participants:	
Internal course code:	4LM30
Contact:	M.Huetter@tue.nl

This course is part of the EuroTeQ Engineering University joint course catalogue 2023. This is a collaborative activity of the partner universities DTU, L'X, TU/e, TalTech, CTU, TUM as well as Technion. Students from these universities can participate in the offered courses. It is the responsibility of the student to check if you fulfil the requirements to participate in a specific course. Students are also advised to check with their home institution how to get recognition of the ECTS credits gained in courses of the EuroTeQ course catalogue. For further information about EuroTeQ Engineering University, visit www.euroteq.eu or get in touch with the above-mentioned point of contact.