

---

**Modulbezeichnung:** Multiscale Materials Simulation (CE\_MuSim) 15 ECTS  
 (Multiscale Materials Simulation)

Modulverantwortliche/r: Paolo Moretti

Lehrende: Erik Bitzek, Paolo Moretti, Michael Zaiser

---

Startsemester: WS 2017/2018

Dauer: 2 Semester

Turnus: jährlich (WS)

Präsenzzeit: 150 Std.

Eigenstudium: 300 Std.

Sprache: Englisch

---

**Lehrveranstaltungen:**

Introduction to Advanced Maths and Calculus (WS 2017/2018, Seminar, 1 SWS, Paolo Moretti)

Scientific Programming with PYTHON (WS 2017/2018, Sonstige Lehrveranstaltung, 1 SWS, Paolo Moretti)

Multi-scale Simulation Methods I (Lecture) (WS 2017/2018, Vorlesung, 1 SWS, Paolo Moretti)

Multi-scale Simulation Methods I (Tutorial) (WS 2017/2018, Übung, 1 SWS, Paolo Moretti)

Computer Lab for CE 1(3 practicals WW8) (WS 2017/2018, Praktikum, 2 SWS, Michael Zaiser et al.)

Foundations of Finite Element Simulation (Lecture) (WS 2017/2018, optional, Vorlesung, 1 SWS, Michael Zaiser)

Foundations of Finite Element Simulation (Tutorial) (WS 2017/2018, optional, Übung, 1 SWS, Michael Zaiser)

Seminar Computational Materials Science I (WS 2017/2018, optional, Seminar, 2 SWS, Michael Zaiser et al.)

Dislocation Theory and Dislocation Simulation (Lecture) (WS 2017/2018, optional, Vorlesung, 1 SWS, Michael Zaiser)

Dislocation Theory and Dislocation Simulation (Tutorial) (WS 2017/2018, optional, Übung, 1 SWS, Michael Zaiser)

Multi-scale Simulation Methods II (Lecture) (SS 2018, Vorlesung, 1 SWS, Paolo Moretti)

Multi-scale Simulation Methods II (Tutorial) (SS 2018, Tutorium, 1 SWS, Paolo Moretti et al.)

Modelling Materials with Finite Element Simulations (Lecture) (SS 2018, optional, Vorlesung, 1 SWS, Michael Zaiser)

Modelling Materials with Finite Element Simulations (Tutorial) (SS 2018, optional, Übung, 1 SWS, Stefan Liebenstein)

Seminar Computational Materials Science II (SS 2018, optional, Seminar, 2 SWS, Michael Zaiser et al.)

Generalized Continuum Models of Materials Mechanics (SS 2018, optional, Vorlesung, 1 SWS, Michael Zaiser)

Computational models of biomaterial failure (SS 2018, optional, Vorlesung mit Übung, 2 SWS, Paolo Moretti)

Numerische Methoden in den Werkstoffwissenschaften - Atomistische Methoden (SS 2018, optional, Vorlesung mit Übung, 2 SWS, Erik Bitzek)

---

**Inhalt:**

These lectures provide a broad overview of simulation methods operating on length scales from the atomistic to the continuum scale. Simulation methods introduced include Molecular Dynamics, equilibrium and kinetic Monte Carlo simulation, mesoscopic methods such as e.g. Dislocation Dynamics and the Phase Field method, and continuum-level modeling of materials behavior in Finite Element simulations. The introduction of methods operating on different scales is complemented by a discussion of multiscale approaches, i.e. the linking of models operating on different scales. For most of the tutorials 'Python' will be used as programming language, which will be introduced in a separate short course. This course is accompanied by practicals where the students will have the opportunity to numerically implement 'one-scale' models in a hands-on manner. This will be complemented by examples of information passing between different scales and the construction of simple multiscale models.

**Lernziele und Kompetenzen:**

Students will develop a fundamental understanding for the role of computer-based simulation methods in modern materials science. They obtain a detailed overview over most commonly used simulation methods and of their application. They learn the practical realization of simulation tasks based on analysis of materials science problems. Through fundamental understanding of theory they will understand the theory behind simulation methods. They will be able to develop models and to work on novel problems.

---

**Studien-/Prüfungsleistungen:**

CE TAF Module 2 Multiscale Materials Simulation (Prüfungsnummer: 463131)  
mündliche Prüfung, Dauer (in Minuten): 30 Prüfungssprache: Englisch

Erstablingung: SS 2018, 1. Wdh.: keine Angabe

1. Prüfer: Paolo Moretti, 2. Prüfer: Michael Zaiser

---