Modulbezeichnung:	**Basics in Computational Materials Science and Process Simulation 1+2: Particle-based Methods, Continuum Methods (Basics Compu 1+2)** (Basics in Computational Materials Science and Process Simulation 1+2: Particle-based Methods, Continuum Methods)	**5 ECTS**
Modulverantwortliche/r:	Michael Engel	
Lehrende:	Michael Engel, Manuel Münsch, Andreas Bück, Frank Wendler	

Startsemester: WS 2020/2021	Dauer: 2 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 60 Std.	Eigenstudium: 90 Std.	Sprache: Englisch

Lehrveranstaltungen:

Basics in Computational Materials Science and Process Simulation 2 (SS 2021, Vorlesung, 2 SWS, Manuel Münsch et al.)

Basics in Computational Materials Science and Process Simulation 1 (WS 2020/2021, Vorlesung, 2 SWS, Michael Engel et al.)

Inhalt:

This module provides the students with an overview on the simulation methods and computational techniques used in materials science and engineering as well as chemical and bioengineering. Basics in Computational Materials Science and Process Simulation 1: The lecture Basics in Computational Materials Science and Process Simulation 1 introduces the Hard- and Software environment for scientific computing as well as the basic concepts of particle based modelling and simulation in materials science and process technology. The lectures provide an overview of different techniques, methods, and applications thereof from the atomic scale via the mesoscale to the microscale:

- electronic structure calculations
- atomistic simulations
- molecular modelling
- discrete element method
- population balance in particle technology

Basics in Computational Materials Science and Process Simulation 2: The lecture Basics in Computational Materials Science and Process Simulation 2 provides an introduction to numerical methods to solve typical engineering problems. Emphasis is placed on practical application of these methods to processes involving thermodynamics, fluid mechanics and materials deformation. In particular, it addresses:

- programming with MATLAB
- solution of nonlinear equations
- numerical differentiation and integration
- numerical solution of differential equations
- numerical solution of transport problems: the Finite-Difference Method
- introduction to the Finite Element Method
- simulation of transport phenomena using FEM packages (ABAQUS)
- modelling of deformation processes: Elasticity and Plasticity
- numerical simulation of deformation phenomena with FEM

Lernziele und Kompetenzen:

Students who successfully participate in this module can

- demonstrate knowledge of scientific computing environments and can apply shell commands
- explain basic techniques and methods of numerical modelling of particulate systems on various scales from atoms to molecules to granular matter as well as continuum simulation methods
- describe limitations and strengths of common simulation algorithms and data structures
- describe interatomic and intermolecular interactions and their computational implementation
- apply numerical methods to solve nonlinear differential equations
- apply finite elements to represent continuous fields and set up finite element models for deformation and transport processes

- apply standard programs to solve engineering problems in fluid dynamics and mechanics of materials

Literatur:

- Scientific Computing with MATLAB and Octave (4th Edition, Springer), A. Quarteroni, F. Saleri and P. Gervasio
- The Finite Element Method (World Scientific), Z. Chen

Further recommended reading will be announced in the lectures.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Advanced Materials and Processes (Master of Science)**

(Po-Vers. 2019w | TechFak | Advanced Materials and Processes (Master of Science) | Gesamtkonto | Pflichtmodule | Computational Materials Science and Process Simulation (CMSPS))

Studien-/Prüfungsleistungen:

Computational Materials Science and Process Simulation 1+2: Particle-Based Methods, Continuum Methods (Prüfungsnummer: 1761)

(englische Bezeichnung: Basics in Computational Materials Science and Process Simulation 1+2: Particle-Based Methods, Continuum Methods)

Prüfungsleistung, Klausur, Dauer (in Minuten): 120
Anteil an der Berechnung der Modulnote: 100% Prüfungssprache: Englisch

Erstablegung: SS 2021, 1. Wdh.: WS 2021/2022
1. Prüfer: Michael Engel

Computational Materials Science and Process Simulation 1: Particle-Based Methods (Prüfungsnummer: 1762)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60
Anteil an der Berechnung der Modulnote: 50%
weitere Erläuterungen:
Gemäß Corona-Satzung wird als alternative Prüfungsform festgelegt: mündliche Prüfung mit 30 Minuten Dauer
Prüfungssprache: Englisch

Erstablegung: WS 2020/2021, 1. Wdh.: SS 2021
1. Prüfer: Michael Engel

Computational Materials Science and Process Simulation 2: Continuum Methods (Prüfungsnummer: 1763)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60
Anteil an der Berechnung der Modulnote: 50% Prüfungssprache: Englisch

Erstablegung: SS 2021, 1. Wdh.: WS 2021/2022
1. Prüfer: Manuel Münsch
