Modulbezeichnung:	**Schwerpunktfach Computational Material Science and Process Simulation (Compu focal)** (Focal Subject Computational Material Science and Process Simulation)	**15.0 ECTS**
Modulverantwortliche/r:	Michael Engel	
Lehrende:	Paolo Moretti, Wolfgang Peukert, Manuel Münsch, Erik Bitzek	

Startsemester: SS 2022	Dauer: 2 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 150 Std.	Eigenstudium: 300 Std.	Sprache: Englisch

Lehrveranstaltungen:

Modellbildung in der Partikeltechnik / Numerical Methods in Particle Technology (SS 2022, Vorlesung, 2 SWS, Wolfgang Peukert)
Numerische Methoden in den Werkstoffwissenschaften - Atomistische Methoden (SS 2022, Vorlesung mit Übung, 4 SWS, Erik Bitzek)
Multi-scale Simulation Methods I (Lecture) (WS 2022/2023, Vorlesung, 1 SWS, Paolo Moretti)
Multi-scale Simulation Methods I (Tutorial) (WS 2022/2023, Übung, 1 SWS, Paolo Moretti)
Numerische Methoden der Thermofluiddynamik (WS 2022/2023, Vorlesung, 2 SWS, Manuel Münsch)
Numerische Methoden der Thermofluiddynamik - Übung (WS 2022/2023, Übung, 1 SWS, Manuel Münsch et al.)
Pre-course on Linux and Matlab (Block Lecture) (WS 2022/2023, Übung, 1 SWS, Michael Engel)

Empfohlene Voraussetzungen:

Recommendation: Basic knowledge of the PYTHON programming language (according to the course Scientific Programming with PYTHON). The student's knowledge will be assessed with short (voluntary) tests at the beginning of the lectures. In case the test is not passed, choosing the focal subject "Computational Materials Science and Process Simulation" is discouraged.
Attending the pre-course on Linux and Matlab (Block Lecture) offerend prior to lectures of the winter term is mandatory. (first offered WS 2018).
Operational IDM account required

Inhalt:

The elective focal subject module "Computational Materials Science and Process Simulation: Discrete Methods" provides the students with an in-depth understanding of state-of-the-art discrete simulation methods in the fields of materials science and engineering as well as chemical and bioengineering and their synergies.
Pre-course on Linux and Matlab:
Introduction to fundamental computational material science tools. Overview of the topics will be covered:

- Linux
- Linux Bash shell, scripting
- Gnuplot
- MATLAB

Numerical Methods in Materials Science - Atomistic Methods:
The lecture Numerical Methods in Materials Science - Atomistic Methods covers all aspects of atomistic simulations, including

- advanced methods for the generation of atomistic samples
- atomic interaction potentials
- molecular dynamic integration algorithms for different Thermodynamic ensembles (NVE,NVT,NPT)
- energy minimization algorithms and structure optimization
- introduction to Density Functional Theory
- determination of defect properties
- advanced analysis and visualization methods

- modelling thermally activated events: transition state theory, nudged elastic band calculations, Monte Carlo and (adaptive) kinetic Monte Carlo methods

The theoretical concepts are put into practice in a series of hands-on exercises and simulation projects.
Numerical Methods in Particle Technology:
The lecture Numerical Methods in Particle Technology provides an overview on modern numerical simulation methods in the field of particle technology. After a repetition of the principle basics of particle technology the following methods and topics are addressed:

- single particles in fluids
- hybrid models for adhesion and sintering

The elective focal subject module "Computational Materials Science and Process Simulation: Continuum and Multiscale Methods" provides the students with an in-depth understanding of state-of-the-art continuum-scale simulation methods in the fields of materials science and engineering as well as chemical and bioengineering and their synergies.
Numerical Fluid Dynamics:
The lecture Numerical Fluid Dynamics covers

- governing equations and models in fluid mechanics
- steady problems: the Finite-Difference Method
- steady problems: the Finite-Volume Method
- unsteady problems: methods of time integration
- advection-diffusion problems
- solution of the incompressible Navier-Stokes equations
- grids and their properties
- boundary conditions

The theory taught in the lectures is extended and applied to several transport problems in the corresponding exercise class:

- discretization of the Blasius similarity equations
- parabolization and discretization of the boundary layer equations
- finite-Difference discretization of heat-transfer problems
- approximation of boundary conditions
- finite-Volume discretization of heat-transfer problems
- discretization and time-stepping of the Navier-Stokes equations
- projections methods: the SIMPLE and PISO Methods

Multiscale Simulation Method I:
The "Multiscale Simulation Method I" lecture provides 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. This course is accompanied by exercises 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 who successfully participate in this module can

- describe and critically assess the most frequently used simulation algorithms in fluid dynamics and mechanics of materials
- create samples and simulation setups for various continuum simulation methods
- apply state-of-the-art programs for numerical simulations at the continuum scale
- analyze and evaluate the simulation results of aforementioned methods
- plan multiscale modeling approaches for specific engineering problems

At the end of the pre-course on Linux and Matlab, the students should be able to 1. Use the computer pools at FAU and work with Linux Operation system 2. Use the bash and shell scripts for fundamental data processing 3. Plot and analyse data by using Gnuplot 4. Use Matlab to solve simple problem such

as matrix operation, writing scripts and functions.

- work in a team to solve engineering problems using computers

Literatur:

- J.H. Ferziger, M. Peric, Computational Methods for Fluid Dynamics, Spinger, 2008
- R.J. Leveque, Finite Difference Methods for Ordinary and Partial Differential Equations, SIAM, 2007
- R. LeSar, Introduction to Computational Materials Science: Fundamentals to Applications

Further literature will be announced in the lectures.

Studien-/Prüfungsleistungen:

Computational Materials Science and Process Simulation 1: Modelling Electrons, Atoms and Particles (Prüfungsnummer: 1811)
(englische Bezeichnung: Computational Materials Science and Process Simulation 1: Modelling Electrons, Atoms and Particles)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 45
Anteil an der Berechnung der Modulnote: 50% Prüfungssprache: Englisch

Erstablegung: SS 2022, 1. Wdh.: WS 2022/2023
1. Prüfer: Wolfgang Peukert

Computational Materials Science and Process Simulation 2: Numerical Fluid Dynamics and Multiscale Simulations (Prüfungsnummer: 1812)
(englische Bezeichnung: Computational Materials Science and Process Simulation 2: Numerical Fluid Dynamics and Multiscale Simulations)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 45
Anteil an der Berechnung der Modulnote: 50% Prüfungssprache: Englisch

Erstablegung: WS 2022/2023, 1. Wdh.: SS 2023
1. Prüfer: Manuel Münsch
