Amtliche Bekanntmachungen der TU Bergakademie Freiberg

Nr. 30, Heft 2 vom 27. September 2024

Modulhandbuch

für den

Masterstudiengang

Computational Materials Science

Inhaltsverzeichnis

Abkürzungen

KA: schriftliche Klausur / written exam
MP: mündliche Prüfung / oral examination
AP: alternative Prüfungsleistung / alternative examination
PVL: Prüfungsvorleistung / prerequisite
MP/KA: mündliche oder schriftliche Prüfungsleistung (abhängig von Teilnehmerzahl) / written or oral examination (dependent on number of students)

SS, SoSe: Sommersemester / sommer semester
WS, WiSe: Wintersemester / winter semester

SX: Lehrveranstaltung in Semester X des Moduls / lecture in module semester x

SWS: Semesterwochenstunden

<table>
<tr><td>Data:</td><td>AlassCod. MA. / Examination number: -</td><td>Version: 16.07.2024</td><td>Start Year: SoSe</td></tr>
<tr><td>Module Name:</td><td colspan="3">AI-assisted Programming in Computational Materials and Mechanics</td></tr>
<tr><td>(English):</td><td colspan="3"></td></tr>
<tr><td>Responsible:</td><td colspan="3">Eidel, Bernhard / Prof. Dr.-Ing. habil.</td></tr>
<tr><td>Lecturer(s):</td><td colspan="3">Eidel, Bernhard / Prof. Dr.-Ing. habil.</td></tr>
<tr><td>Institute(s):</td><td colspan="3">Institute of Mechanics and Fluid Dynamics</td></tr>
<tr><td>Duration:</td><td colspan="3">1 Semester(s)</td></tr>
<tr><td>Competencies:</td><td colspan="3">Students are able to identify, evaluate and use resources for a programming project in the WWW. They learn to use latest AI-assistants to generate, test and improve computer codes in Python. Students learn to apply these competencies in a coding project individually assigned by the Lecturer.
Students learn to write a report about their coding project following scientific standards in structure, content and style. They learn to present and defend their results.</td></tr>
<tr><td>Contents:</td><td colspan="3">Most important ingredients are:
Learning effective search strategies for resources in the WWW (literature, computer codes, datasets, AI-tools, etc.)
Analysis of the model equations and a solution method for problems of mechanics/materials science/physics
Prompt Engineering for Code generation in Python by a Chatbot or alternative coding assistants
Code assessment – tests for verification of the generated code. Bug detection/fixing. Analysis of strengths and weaknesses of the AI-based coding assistants
Writing a scientific report in LaTeX about the coding project
Presentation and defense of the project</td></tr>
<tr><td>Literature:</td><td colspan="3"></td></tr>
<tr><td>Types of Teaching:</td><td colspan="3">S1 (SS): Lectures (2 SWS)
S1 (SS): Exercises (2 SWS)</td></tr>
<tr><td>Pre-requisites:</td><td colspan="3">Mandatory:
Introduction to Scientific Programming, 2017-05-18
Software Tools for Computational Materials Scientists, 2024-07-16
Numerical Analysis of Differential Equations, 2024-01-29</td></tr>
<tr><td>Frequency:</td><td colspan="3">yearly in the summer semester</td></tr>
<tr><td>Requirements for Credit Points:</td><td colspan="3">For the award of credit points it is necessary to pass the module exam. The module exam contains:
AP: Individual AI-assisted coding project with report<hr>Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst:
AP: Individuelles KI-assistiertes Programmier-Projekt mit Bericht</td></tr>
<tr><td>Credit Points:</td><td colspan="3">5</td></tr>
<tr><td>Grade:</td><td colspan="3">The Grade is generated from the examination result(s) with the following weights (w):
AP: Individual AI-assisted coding project with report [w: 1]</td></tr>
<tr><td>Workload:</td><td colspan="3">The workload is 150h. It is the result of 60h attendance and 90h self-studies.</td></tr>
</table>

Data:	ADVTCMS. MA. Nr. 3587 / Examination number: 44511	Version: 12.08.2024	Start Year: WiSe 2018
Module Name:	**Atomistic Simulation Methods**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with the current state-of-the-art simulation methods for atomistic problems and most recent developments in computational methods for the nanoscale. They will be introduced to the fundamentals of statistical mechanics and interatomic potentials. Participants will also be introduced to the usage of machine learning methods in atomistic simulations, particularly for interatomic potentials. They will also be taught novel methods for visualization and analysis of their simulation results. Students will use widely-available open-source simulation software in hands-on exercises. They will learn the theoretical underpinnings of these advanced methods and will be able to apply those to new problems.		
Contents:	Key topics include: Statistical mechanics; Molecular dynamics; Monte Carlo methods; Kinetic Monte Carlo; Interatomic potentials; Machine learning potentials; Visualization and analysis methods including machine learning motivated methods.		
Literature:	D. Frenkel, B. Smit. Understanding Molecular Simulation: From algorithms to applications, Wiley VCH R. Lesar. Introduction to Computational Materials Science, Cambridge University Press E. Tadmor, R. Miller. Modeling Materials: Continuum, atomistic and multiscale techniques, Cambridge University Press J.M. Haille. Molecular Dynamics: Elementary Methods, Wiley VCH		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Software Tools for Computational Materials Scientists, 2024-07-16 Theory, Modelling and Simulation of Microstructures, 2024-07-01 basic experience with a Linux environment (bash/shell); knowledge of crystallography		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 8 students or more) [MP minimum 15 min / KA 90 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 8 und mehr Teilnehmern) [MP mindestens 15 min / KA 90 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	CerEng. MA. Nr. / Examination number: -	Version: 20.06.2024	Start Year: WiSe 2024
Module Name:	**Ceramic Engineering**		
(English):			
Responsible:	Aneziris, Christos G. / Prof. Dr.-Ing. habil.		
Lecturer(s):	Aneziris, Christos G. / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Ceramics, Refractories and Composite Materials		
Duration:	1 Semester(s)		
Competencies:	Students will understand, apply, improve and generate ceramic materials: • in micro structural design, • ceramic processing, • testing and • application		
Contents:	Most important ingredients are: • definition, bonding, • micro structure, density, porosity • mechanical properties, • thermal and thermo mechanical properties • chemical properties • sintering • basics in ceramic technology, theoretical • ceramic technology pressing/extruding/casting, experimental • engineering ceramics, alumina/zirconia • engineering ceramics, silicon carbide • functional ceramics, non linear dielectric/piezoelectric properties - barium titanate • refractories, carbon bonded materials • silicate ceramics • Exercise: theoretical density / Enthalpy • Visiting of ceramic plant or research institute		
Literature:	Introduction to Ceramics, David Kingery Introduction to the Principles of Ceramic Processing, James Reed Physical Ceramics, Yet-Ming Chiang, Dunbar Birnie III, W. David Kingery		
Types of Teaching:	S1 (WS): incl. exercises and and practical course / Lectures (2 SWS)		
Pre-requisites:	**Recommendations:** Basic fundamentals of materials science		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 6 students or more) [MP minimum 30 min / KA 90 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 6 und mehr Teilnehmern) [MP mindestens 30 min / KA 90 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 30h attendance and 90h self-studies.		

Data:	KOTM. MA. Nr. 3120 / Examination number: 41907	Version: 18.05.2017	Start Year: SoSe 2018
Module Name:	**Continuum Mechanics**		
(English):			
Responsible:	Kiefer, Björn / Prof. PhD.		
Lecturer(s):	Kiefer, Björn / Prof. PhD.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will elevate their understanding of the mathematical foundations of continuum solid mechanics. Moreover, they will be familiar with classical theoretical approaches that describe the kinematics, kinetics and constitutive behavior of three-dimensional continua at small and large deformations, including the governing balance laws. The successful participant will be able to apply this knowlegde to the modeling of specific problems in geometrically and physically nonlinear solid mechanics.		
Contents:	Most important ingredients are: • tensor algebra and analysis • balance laws (mass, momentum, energy, entropy) • thermodynamic consistency • spatial and material descriptions • kinematics of continua at finite deformations • definition of various stress measures • constitutive theory		
Literature:	P. Chadwick: Continuum Mechanics: Concise Theory and Problems, Dover Publications, 1999 Gurtin, Fried, Anand: The Mechanics and Thermodynamics of Continua, Cambridge University Press, 2009 Holzapfel: Nonlinear Solid Mechanics: A Continuum Approach For Engineering. John Wiley & Sons, 2000 Lai, Rubin, Krempl: Introduction to Continuum Mechanics. Butterworth-Heinemann, 1993 Malvern: Introduction to the Mechanics of a Continuous Medium, Prentice Hall, 1969		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Taught in English and German. / Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Basic knowledge in engineering mechanics		
Frequency:	yearly in the summer semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 10 students or more) [MP minimum 30 min / KA 120 min] Possible in German. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 10 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] In Deutsch möglich.		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		

Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies. To help deepen the understanding of the subject matter, (voluntary) homework problems are given out along with the exercise sheets.

Data:	CPTA MA Nr. 3658 / Examination number: 44509	Version: 01.07.2024	Start Year: SoSe 2025
Module Name:	**Crystal Plasticity, Texture and Anisotropy**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will be exposed to the materials science fundamentals of plasticity in single and polycrystals. They will learn mathematical and physical concepts concerning orientation distributions, texture and anisotropy and will be able to apply this knowledge for understanding material properties. They will learn about experimental methods for determining and characterizing crystallographic texture of a material. Participants will be introduced to the fundamentals of plasticity in single crystals in terms of both single as well as multiple slip. Furthermore, various approaches to modeling polycrystal plasticity, i.e., via mean-field and full-field approaches will be dealt with. Participants will be able to understand the advantages and limitations of the models and can transfer this knowledge to simulations. A further emphasis is on fundamental concepts of grain boundaries together with approaches towards modeling them. The students will get acquainted with various tools for data analysis and simulations, and will learn to apply them to new problems.		
Contents:	Key topics are: Mathematical foundations of orientations, orientation distributions, texture; Graphical representation of orientations; Experimental methods of texture determination; Anisotropic elasticity; Plasticity of single and polycrystals; Homogenization models for polycrystal plasticity.		
Literature:	• U.F. Kocks, C. Tomé, H.-R. Wenk. Texture and Anisotropy, Cambridge University Press • O. Engler, V. Randle. Introduction to Texture Analysis: Macrotexture, Microtexture and Orientation Mapping, CRC Press • F. Roters, P. Eisenlohr, T. Bieler and D. Raabe. Crystal Plasticity Finite Element Methods: In Materials Science and Engineering, Wiley VCH • L. Priester. Grain Boundary and Crystalline Plasticity, Wiley VCH		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Programming experience in Python (which will be used in the exercises). This is satisfied by participating in the module „Software Tools for Computational Materials Scientists“.		
Frequency:	yearly in the summer semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: PVL: Homework assignment MP/KA (KA if 8 students or more) [MP minimum 30 min / KA 120 min] PVL have to be satisfied before the examination.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: PVL: Hausarbeit MP/KA (KA bei 8 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min]		

	PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.
Credit Points:	4
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.

Daten:	DEU A1/ 1.Sem. BA. Nr. 948 / Prüfungs-Nr.: 71101	Stand: 04.08.2017	Start: WiSe 2016
Modulname:	**Deutsch A1/ 1. Semester**		
(englisch):	German A 1/ 1st Semester		
Verantwortlich(e):	Polanski, Katja		
Dozent(en):			
Institut(e):	Internationales Universitätszentrum/ Sprachen		
Dauer:	1 Semester		
Qualifikationsziele / Kompetenzen:	Im Kurs werden Grundlagen in Phonetik, Orthographie, Grammatik und Lexik vermittelt. Die Teilnehmer erwerben Grundkenntnisse und Grundfertigkeiten im Hören, Sprechen, Lesen und Schreiben auf der Basis der Allgemeinsprache sowie landeskundliche Kenntnisse.		
Inhalte:	Kommunikation im Alltag (Menschen kennen lernen, Einkaufen, Restaurantbesuch, Tagesabläufe, Uhrzeit); Grammatik: zum Beispiel Fragestellungen, Zahlen, Konjugation der Verben, Präsenz und Präteritum, Mengenangaben, Plural der Nomen, Komposita		
Typische Fachliteratur:	Begegnungen A1+, Schubert Verlag		
Lehrformen:	S1 (WS): Übung (4 SWS)		
Voraussetzungen für die Teilnahme:	**Empfohlen:** Keine Vorkenntnisse der deutschen Sprache notwendig		
Turnus:	jährlich im Wintersemester		
Voraussetzungen für die Vergabe von Leistungspunkten:	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [90 min] PVL: Aktive Teilnahme an mindestens 80% des Unterrichts PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Leistungspunkte:	4		
Note:	Die Note ergibt sich entsprechend der Gewichtung (w) aus folgenden(r) Prüfungsleistung(en): KA [w: 1]		
Arbeitsaufwand:	Der Zeitaufwand beträgt 120h und setzt sich zusammen aus 60h Präsenzzeit und 60h Selbststudium.		

Data:	DisTheo. MA. Nr. 3206 / Examination number: 45102	Version: 08.06.2017	Start Year: WiSe 2017
Module Name:	**Discrete Element Method**		
(English):			
Responsible:	Schwarze, Rüdiger / Prof. Dr.-Ing.		
Lecturer(s):	Schwarze, Rüdiger / Prof. Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students should remember the fundamentals of the discrete element method. They should be able to distinguish the different numerical techniques and algorithms applied in the discrete element method. They should be able to apply the discrete element method to simple problems in the field of granular materials.		
Contents:	Most important ingredients are: • modeling strategy (conceptual and numerical model); classification of DEM • contact detection; interaction force-displacement laws, contact and friction laws • algorithms for solving the equations of motion • modelling of granular material • introduction to simulation tools and software (Yade, LIGGHTS,etc.) • practical hints; applications; practical exercises in 2d and 3d.		
Literature:	Pöschel, T. & Schwager, T.: Computational Granular Dynamics, Springer Jing, L & Stephansson, O.: Fundamentals of Discrete Element Methods for Rock Engineering, Elsevier Matuttis, H.G. & Chen, J.: Understanding the Discrete Element Method, Wiley		
Types of Teaching:	S1 (WS): Discrete Element Method / Lectures (2 SWS) S1 (WS): Discrete Element Method / Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Fundamental of Microstructures, 2010-12-02 Continuum Mechanics, 2016-07-11 Introduction to Scientific Programming, Fundamentals in mechanics		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 5 students or more) [MP minimum 30 min / KA 60 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 5 und mehr Teilnehmern) [MP mindestens 30 min / KA 60 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	MechTest. MA. Nr. 3207 / Examination number: 50409	Version: 05.04.2018	Start Year: WiSe 2018
Module Name:	**Experimental Methods of Structure Characterization of Matters**		
(English):			
Responsible:	Rafaja, David / Prof. Dr. rer. nat. habil.		
Lecturer(s):	Wüstefeld, Christina / Dr.-Ing.		
Institute(s):	Institute of Materials Science		
Duration:	1 Semester(s)		
Competencies:	Students get familiar with basic principles and applications of selected methods for microstructure analysis of matters (mainly optical, scanning and transmission electron microscopy, diffraction methods) and learn how these methods can be used for analysis of the real structure of materials.		
Contents:	- Crystal symmetry operations, point and space groups in crystallography - Interaction of electrons, X-rays and neutrons with matter - Applications of optical, scanning and transmission electron microscopy, and X-ray, electron and neutron diffraction in the analysis of real structure and microstructure of matters: - Phase identification and quantification, use of crystallographic databases - Determination of the grain and crystallite size, - Global and local preferred orientation of crystallites - Residual stress analysis		
Literature:	- L. Reimer: Scanning Electron Microscopy, Springer, Berlin 2010 - V. Randle, O. Engler: Introduction to texture analysis, macrotexture, microtexture and orientation mapping, Gordon & Breach, Amsterdam, 2000. - H.P. Klug, L.E. Alexander: X-ray diffraction procedures for polycrystalline and amorphous materials, New York, Wiley, 2nd edition 1974. - C. Giacovazzo, H.L. Monaco, G. Artioli et al.: Fundamentals of Crystallography, IUCr Texts on Crystallography 15, 3rd edition, 2011 - D.B. Williams, C.B. Carter: Transmission Electron Microscopy: A Textbook for Materials Science, Springer, New York 2016		
Types of Teaching:	S1 (WS): Lectures (3 SWS)		
Pre-requisites:	**Recommendations:** Profound knowledge of English, basics in materials science, mechanics, advanced mathematics, physics for scientists.		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 5 students or more) [MP minimum 30 min / KA 120 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 5 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	FMC. MA. Nr. 3208 / Examination number: 41908	Version: 01.11.2019	Start Year: WiSe 2017
Module Name:	**Fracture Mechanics Computations**		
(English):			
Responsible:	Kiefer, Björn / Prof. PhD.		
Lecturer(s):	Kiefer, Björn / Prof. PhD.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Development of an understanding of the fracture of materials and structures from the point of view of a design engineer; students acquire knowledge about theoretical (numerical) stress analysis of cracked structures as well as fracture mechanics concepts of brittle, ductile and fatigue failure. Development of the ability to design fail-safe structures with defects, qualitatively assess the safety and durability as well as estimate the duration of life for subcritical crack growth under (random) in-service loads.		
Contents:	Most important ingredients are: fundamentals of fracture mechanics, including fracture mechanics concepts and relevant load parameters for elastic and plastic materials under static as well as cyclic loading. Suitable Finite-Element techniques for the calculation of load parameters are introduced. The application of fracture mechanics concepts to the assessment of safety and durability of structures is demonstrated with the help of real-world examples.		
Literature:	M. Kuna: Finite Elements in Fracture Mechanics: Theory - Numerics - Applications, Springer, 2013 D. Gross, T. Seelig: Bruchmechanik – Mit einer Einführung in die Mikromechanik, Springer, 2011 M. Kuna: Numerische Beanspruchungsanalyse von Rissen, FEM in der Bruchmechanik, Vieweg-Teubner 2010 T. L. Anderson: Fracture Mechanics: Fundamentals and Applications, CRC Press 2004		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Taught in English and German. / Exercises (2 SWS)		
Pre-requisites:	**Recommendations:** Basic knowledge in theoretical mechanics		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 12 students or more) [MP minimum 30 min / KA 120 min] Possible in German.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 12 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] In Deutsch möglich.		
Credit Points:	5		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 150h. It is the result of 60h attendance and 90h self-studies.		

Data:	IHPC. MA. Nr. 3210 / Examination number: 11110	Version: 05.03.2015	Start Year: WiSe 2012

Module Name:	**Introduction to High Performance Computing and Optimization**
(English):	
Responsible:	Rheinbach, Oliver / Prof. Dr.
Lecturer(s):	Rheinbach, Oliver / Prof. Dr.
Institute(s):	Institute of Numerical Mathematics and Optimization
Duration:	1 Semester(s)
Competencies:	The students shall have an understanding of and ability to apply: • parallel computing on shared and distributed memory multiprocessor systems • parallel algorithms The students know relevant terms in English.
Contents:	Ingredients can be: • Portable parallel programming with OpenMP and MPI (Message Passing Interface); hybrid parallelization; accelerators • Code profiling, tracing and optimization methods using tools (profiler, VAMPIRE, etc.); • Relevant software libraries (e.g., BLAS, LAPACK, SCALAPACK, etc.) • Design and analysis of algorithms • Parallel solution of linear systems (dense/sparse systems) • International literature and relevant terms in English
Literature:	Georg Hager, Gerhard Wellein, Introduction to High Performance Computing for Scientists and Engineers, Chapman & Hall, 2010 OpenMP Standard, www.openmp.org Barbara Chapman, Gabriele Jost, Ruud van der Pas, Using OpenMP: portable shared memory parallel programming, MIT Press, 2008 William Gropp, Ewing Lusk, Anthony Skjellum, Using MPI: Portable Parallel Programming with the Message-Passing Interface, MIT press, 2000 Michael Quinn, Parallel Programming in C with MPI and OpenMP, McGraw-Hill, 2003 Anne Greenbaum, Iterative Methods for Solving Linear Systems, SIAM, 1997
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)
Pre-requisites:	**Recommendations:** Basics knowledge in scientific programming and algorithms.
Frequency:	yearly in the winter semester
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA: MP = individual examination (KA if 30 students or more) [MP minimum 30 min / KA 120 min] PVL: Programming Project PVL have to be satisfied before the examination.
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA: MP = individuelle Prüfung (KA bei 30 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: Programmierprojekt

	PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.
Credit Points:	4
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA: MP = individual examination [w: 1]
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.

Data:	ISP. MA. Nr. 3211 / Examination number: 11609	Version: 18.05.2017	Start Year: WiSe 2017
Module Name:	**Introduction to Scientific Programming**		
(English):			
Responsible:	Rheinbach, Oliver / Prof. Dr.		
Lecturer(s):	Prüfert, Uwe / Dr. rer. nat. Rheinbach, Oliver / Prof. Dr.		
Institute(s):	Institute of Numerical Mathematics and Optimization		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with the syntax and semantic of multi paradigm programming languages. Construction of suitable data structures and the choice of adequate algorithms are further skills to learn. Based on this, the students should be able to implement interactive programs having a graphical user interface.		
Contents:	Part programming language: Data types and variables, pointer and arrays, expressions, statements, operators, control structures, functions, objects and classes, encapsulation, access rights, inheritance, polymorphism, overloading of functions an operators, type casting, templates; Part algorithms: Iteration, recursion, special functions; Part GUI programming: User—software interaction, use of standard class libraries for programming graphical user interfaces.		
Literature:	Stroustrup, Bjarne . The C++ programming language Register, Andrew. A guide to MATLAB object oriented programming		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Practical Application (2 SWS)		
Pre-requisites:	**Recommendations:** Höhere Mathematik für Ingenieure 1, 2015-03-12 Höhere Mathematik für Ingenieure 2, 2015-03-12		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: KA [120 min] PVL: Programming Project PVL have to be satisfied before the examination. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [120 min] PVL: Programmierprojekt PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): KA [w: 1]		
Workload:	The workload is 120h. It is the result of 60h attendance and 60h self-studies.		

Data:	MLMS MA Nr. 3659 / Examination number: 44510	Version: 12.08.2024	Start Year: SoSe 2019
Module Name:	**Machine Learning for Materials Scientists**		
(English):	Machine Learning for Materials Scientists		
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will be exposed to fundamental knowledge in stochastics, statistics and combinatorics and will be able to apply this knowledge using the programming language Python. They will aqcuire an overview over machine learning approaches and algorithms and will be able to choose the appropriate algorithm for a specific problem. Furthermore, they will be able to use existing machine learning libraries and to independently solve problems of materials scientific relevance. Students will be able to judge the quality of their results.		
Contents:	• basics of stochastics and statistics: events, probability, conditional probability, variance, mean, median, likelyhood • fundamentals of machine learning: linear regression, principal component analysis • neural networks, Bayesian methods, convolutional networks, support vector machines • training validation, testing, overfitting • selection of appropriate algorithms • implementation, e.g., using PyTorch, scikit-learn, or TensorFlow/KERAS		
Literature:	1. M. P. Deisenroth, A.A. Faisal, Ch.S. Ong: Mathematics for Machine Learning, 2019, Cambridge University Press, UK 2. I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016, http://www.deeplearningbook.org		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Good foundation in mathematics and Python programming (as, e.g., acquired during "Software Tools for Computational Materials Scientists 1")		
Frequency:	yearly in the summer semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 5 students or more) [MP minimum 30 min / KA 90 min] PVL: Coding PVL have to be satisfied before the examination.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 5 und mehr Teilnehmern) [MP mindestens 30 min / KA 90 min] PVL: Programmierung PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	MaTheCMS. MA. Nr. / Examination number: -	Version: 01.07.2024	Start Year: SoSe 2025
Module Name:	**Master Thesis Computational Materials Science**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):			
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	6 Month(s)		
Competencies:	The objective of the master thesis is to give the students the opportunity to apply the knowledge acquired during their studies on a research project.		
Contents:	Not Applicable		
Literature:	Not Applicable		
Types of Teaching:	S1: Thesis (6 Mon)		
Pre-requisites:	**Mandatory:** Personal Programming Project, 2024-07-01 Masterarbeit: Abschluss aller Module des 1. u. 2. Semesters sowie Antritt aller Modulprüfungen des 3. Semesters und davon höchstens 12 offene Leistungspunkte, Kolloquium: Abschluss aller Module (Master Thesis: Compare to § 19 sup-paragraph 3 clause 5. Colloquium: Compare to § 19 sup-paragraph 10 clause 3 of the Examinations Regulations)		
Frequency:	constantly		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: AP*: Master Thesis AP*: Colloquium [40 to 60 min] * In modules requiring more than one exam, this exam has to be passed or completed with at least "ausreichend" (4,0), respectively.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: AP*: Masterarbeit AP*: Kolloquium [40 bis 60 min] * Bei Modulen mit mehreren Prüfungsleistungen muss diese Prüfungsleistung bestanden bzw. mit mindestens "ausreichend" (4,0) bewertet sein.		
Credit Points:	30		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): AP*: Master Thesis [w: 3] AP*: Colloquium [w: 1] * In modules requiring more than one exam, this exam has to be passed or completed with at least "ausreichend" (4,0), respectively.		
Workload:	The workload is 900h.		

Data:	Examination number: 50120	Version: 11.06.2024	Start Year: SoSe 2025

Module Name:	**Materials Science and Mechanical Properties of Metals**
(English):	
Responsible:	Biermann, Horst / Prof. Dr.-Ing. habil Leineweber, Andreas / Prof. Dr. rer. nat. habil.
Lecturer(s):	Weidner, Anja / Dr.-Ing. habil. Martin, Stefan / Dr.-Ing.
Institute(s):	Institute of Materials Engineering Institute of Materials Science
Duration:	1 Semester(s)
Competencies:	The student is able to relate problems from engineering practice to fundamental concepts from Materials Science. Further the student is able to relate technological aspects of processing of metallic materials to changes in microstructure, the mechanical parameters and further properties.
Contents:	The first part of the lectures deals with the basics of materials science (structure, classes of materials), the main properties and the application of materials. The second part of the lecture deals with the (micro-)structure - properties relations of metallic materials. Focus is given to plastic deformation and failure, particularly to following metal alloy types: • Ferrous metals (plain carbon steels, high-alloyed steels, cast irons); • Non-ferrous metals (e.g. copper, nickel) • Light metals (aluminum, titanium, magnesium) • High-temperature alloys (superalloys, intermetallic alloys)
Literature:	Askeland, D.R., The Science and Engineering of Materials, Chapman and Hall, London etc.Schatt, W.; Worch, H., Werkstoffwissenschaft, Deutscher Verlag für Grundstoffindustrie.W. D. Callister, jr. Materials Science and Engineering – An Introduction, New York etc.: John Wiley & Sons. Inc. M. F. Ashby, D.R.H. Jones, Engineering materials 2, 2nd ed., Butterworth-Heinemann, Oxford, 1998 James F. Shackelford, Introduction to Materials Science for Engineers, 7th ed. Addison Wesley., 2009
Types of Teaching:	S1 (SS): Lectures (4 SWS) S1 (SS): Exercises (1 SWS)
Pre-requisites:	**Recommendations:** Basic fundamentals of physics, chemistry and solid materials
Frequency:	yearly in the summer semester
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: KA [120 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [120 min]
Credit Points:	7
Grade:	The Grade is generated from the examination result(s) with the following weights (w): KA [w: 1]
Workload:	The workload is 210h. It is the result of 75h attendance and 135h self-studies.

Data:	MHP. MA. Nr. 3615 / Examination number: 41913	Version: 06.06.2018	Start Year: WiSe 2018
Module Name:	**Micromechanics and Homogenization Principles**		
(English):			
Responsible:	Kiefer, Björn / Prof. PhD.		
Lecturer(s):	Kiefer, Björn / Prof. PhD. Kozinov, Sergii / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Successful participants of this course are able to apply fundamental concepts of micromechanics to determine effective properties of multiphase elastic solids such as composite materials. They understand the theoretical foundations as well as the advantages and shortcomings of classical micromechanics techniques. The students are also familiar with advanced homogenization principles—both analytical and numerical in nature—that incorporate the influence of micro-defects (inclusions, cavities, cracks) and inelastic behavior. They have further acquired first experience with numerical implementation of these modeling concepts through simple programing examples.		
Contents:	The main ingredients are: • Micromechanics techniques for computing effective elastic properties of composite media • Fundamental Eshelby solutions, inclusions, inhomogeneities • Dilute distribution, Mori-Tanaka, and self-consistent approaches • Energetic bounds on effective properties • General averaging theorems, Hill-Mandel Principle, periodic homogenization, asymptotic expansions • Direct numerical homogenization schemes, including the FE^2-method • Numerical examples (programing in Matlab /Mathematica/Python • Strength and failure, localization		
Literature:	• S. Nemat-Nasser and M. Hori, Micromechanics: *Overall Properties of Heterogeneous Materials*, Second Edition, North-Holland Series in Applied Mathematics and Mechanics, 1999 • Christensen, *Mechanics of Composite Materials*, Dover Publications, 2005 • D. Gross and T. Seelig, *Bruchmechanik — mit einer Einführung in die Mikromechanik*, Springer-Verlag Berlin Heidelberg, 2016		
Types of Teaching:	S1 (WS): Lectures / Lectures (2 SWS) S1 (WS): Excercises / Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Continuum Mechanics, 2017-05-18		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 10 students or more) [MP minimum 30 min / KA 120 min]		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 10 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w):		

	MP/KA [w: 1]
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies. To help deepen the understanding of the subject matter, (voluntary) homework problems are given out along with the exercise sheets.

Daten:	MSMOM / Prüfungs-Nr.: -	Stand: 16.07.2024	Start: WiSe 2024
Modulname:	**Microstructures and Mechanics of Materials**		
(englisch):			
Verantwortlich(e):	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Dozent(en):	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institut(e):	Institut für Mechanik und Fluiddynamik		
Dauer:	1 Semester		
Qualifikationsziele / Kompetenzen:	For the **microstructure part**, students will learn theoretical aspects of microstructural elements in real crystalline materials and their links to different physical properties. They will become able to solve problems of materials scientific relevance. Furthermore, students will be able to transfer their knowledge to new problems. During the practical part of this module, students will additionally learn to apply computational methods that can be used to visualize, analyze and model chosen aspects of microstructures. For the part on **Mechanics of Materials**, students will develop an understanding of the deformation behavior and failure mechanisms of engineering materials; they get familiar with elastic, plastic, viscous, viscoelastic and viscoplastic behaviors of materials; students learn to apply tensor algebra as the language of continuum mechanics; development of the ability to assess the behavior of materials and to design structures accordingly.		
Inhalte:	For the **microstructure part**, the most important topics are: Atomic interactions, crystallography, point defects, dislocations, grain boundaries, strengthening mechanisms, diffusion characteristics and the characteristic length scale associated with each of these elements. Further topics of relevance are dimensional analysis and scaling laws in nature, materials science and mechanics. For the **Mechanics of Materials** part, the most important ingredients are: • vector and tensor algebra • continuum mechanics foundations of stress, strain and displacements • rheological models for elastic, plastic, viscous, viscoelastic, and viscoplastic deformation behavior • time integration algorithms for the inelastic constitutive laws • multi-axial continuum laws for anisotropic elasticity and plasticity, extended strength and failure theories / criteria for multiaxial loading		
Typische Fachliteratur:	W.D. Callister and D.G. Rethwisch: Materials Science and Engineering, an introduction D. Hull and D.J. Bacon: Introduction to dislocations R. Phillips: Crystals, Defects and Microstructures, Modeling across length scale. A.S. Argon: Strengthening Mechanisms in Crystal Plasticity J. Lemaitre and J.-L. Chaboche: Mechanics of Solid Materials, Cambridge University Press,2000		
Lehrformen:	S1 (WS): Fundamentals of Microstructures / Vorlesung (2 SWS) S1 (WS): Fundamentals of Microstructures / Übung (2 SWS) S1 (WS): Mechanics of Materials / Vorlesung (2 SWS) S1 (WS): Mechanics of Materials / Übung (2 SWS)		
Voraussetzungen für die Teilnahme:	**Empfohlen:** Basic knowledge in engineering mechanics. Basic programming/scripting		

	experience in Python. This is satisfied by simultaneously participating in the module „Software Tools for Computational Materials Scientists“.
Turnus:	jährlich im Wintersemester
Voraussetzungen für die Vergabe von Leistungspunkten:	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [240 min] PVL: Home work assignments PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.
Leistungspunkte:	10
Note:	Die Note ergibt sich entsprechend der Gewichtung (w) aus folgenden(r) Prüfungsleistung(en): KA [w: 1]
Arbeitsaufwand:	Der Zeitaufwand beträgt 300h und setzt sich zusammen aus 120h Präsenzzeit und 180h Selbststudium.

Data:	TAFEM. MA. Nr. 3219 / Examination number: 42605	Version: 08.06.2017	Start Year: SoSe 2018

Module Name:	**Nonlinear Finite Element Methods**
(English):	
Responsible:	Kiefer, Björn / Prof. PhD.
Lecturer(s):	Hütter, Geralf / Dr. Ing. Kiefer, Björn / Prof. PhD. Roth, Stephan / Dr. Ing.
Institute(s):	Institute of Mechanics and Fluid Dynamics
Duration:	1 Semester(s)
Competencies:	This course will enable students to understand and apply the theoretical foundations of Finite Elements Methods (FEM) for geometrically and physically nonlinear problems, with a particular focus on solid mechanics. Hands-on experience will be obtained in the exercises and practical application sessions regarding the coding of custom finite element routines as well as using commercial FE-analysis software packages. The students will thus be capable of selecting appropriate FE formulations for specific nonlinear mechanics problems, of developing and implementing the associated algorithms, and of verifying and analysing the numerical results. This knowledge is transferable to a broad spectrum of nonlinear problems described by partial differential equations in engineering and the natural sciences.
Contents:	Most important ingredients are: • Weak form of the equilibrium conditions • FEM for physically nonlinear problems • FEM for coupled problems • FEM for dynamic problems • FEM for finite deformations • Programming of FEM codes with MATLAB.
Literature:	Belytschko, Liu, Moran: Nonlinear Finite Elements for Continua and Structures, John Wiley & Sons, 2000 Bonet, Wood: Nonlinear Continuum Mechanics for Finite Element Analysis, Cambridge University Press, 2008 Reddy: An Introduction to Nonlinear Finite Element Analysis, Oxford University Press, 2015 Wriggers: Nonlinear Finite Element Methods, Springer, 2008 Zienkiewicz, Taylor: The Finite Element Method, Butterworth-Heinemann, 2000
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Taught in English and German. / Exercises (1 SWS) S1 (SS): Taught in English and German. / Practical Application (1 SWS)
Pre-requisites:	**Recommendations:** Einführung in die Methode der finiten Elemente, 2017-06-08 Numerische Methoden der Mechanik, 2017-06-08 Basic knowledge in engineering mechanics
Frequency:	yearly in the summer semester
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 10 students or more) [MP minimum 30 min / KA 120 min] PVL: Preparation of an FEM coding assignment in MATLAB/Octave Possible in German. PVL have to be satisfied before the examination.
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen

	der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 10 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: FEM-Programmieraufgabe in MATLAB/Octave In Deutsch möglich. PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.
Credit Points:	4
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]
Workload:	The workload is 120h. It is the result of 60h attendance and 60h self-studies. The time needed for the preparation and reworking of lectures and exercises is rather extensive due to the complexity of the topics addressed within this course and because of the programming exercises involved.

Data:	NADE. MA. Nr. 3214 / Examination number: 11109	Version: 29.01.2024	Start Year: WiSe 2024
Module Name:	**Numerical Analysis of Differential Equations**		
(English):			
Responsible:	Aland, Sebastian / Prof. Dr.		
Lecturer(s):	Rheinbach, Oliver / Prof. Dr. Aland, Sebastian / Prof. Dr.		
Institute(s):	Institute of Numerical Mathematics and Optimization		
Duration:	1 Semester(s)		
Competencies:	Students shall understand fundamental concepts of numerical analysis of ordinary and partial differential equations, such as discretization, consistency, stability, and convergence. They can apply discretization methods to compute the numerical solution of a given differential equation. They can compare various methods and evaluate their efficiency for a given problem. The students know relevant terms in English.		
Contents:	ODEs: Euler methods, Runge Rutta Methods, Linear Multistep Methods, Stability, Stiffness; PDEs: Finite Difference techniques, time stepping, von Neumann stability analysis. Brief introduction to FEM. International literature and relevant terms in English are explained.		
Literature:	Finite Difference Methods for Ordinary and Partial Differential Equations von Randy Leveque, University of Washington		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Solid knowledge in computer programming. Advanced mathematics course for scientists and engineers. Some familiarity with the theory or applications of differential equations is helpful		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: KA [120 min]		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [120 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	PINSM. MA. Nr. 3589 / Examination number: 41910	Version: 05.08.2024	Start Year: SoSe 2025
Module Name:	**Parameter Identification in Nonlinear Solid Mechanics**		
(English):			
Responsible:	Kiefer, Björn / Prof. PhD.		
Lecturer(s):	Kiefer, Björn / Prof. PhD. Abendroth, Martin / Dr. Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Successful participation will enable students to apply concepts of nonlinear optimization to the problem of parameter identification for complex material models. In this context, they will be able to code, test and use classical optimization methods - as well as employ more advanced tools available in standard libraries (matlab, python) - and to combine them with algorithmic materials models and experimental data sets. The knowledge obtained in this course is transferrable to a broad spectrum of inverse problems in technology and the natural sciences.		
Contents:	The calibration of parameters plays a central role in establishing predictively accurate constitutive models for complex, nonlinear material responses. In numerical optimization-based approaches to parameter identification an objective function that measures deviations between simulation results and experimental data is minimized to compute optimal parameter sets. After motivating the inverse problem of parameter identification the course provides an introduction to fundamental theoretical and algorithmic concepts of (constrained) nonlinear optimization. The lectures are accompanied by programing exercises that lead to hands-on experience with implementing and testing such optimization methods. In the second part of the course students learn to apply these numerical tools to the specific problem of parameter identification for nonlinear (elasto-plastic, visco-elastic etc.) material models. To obtain the necessary experimental data, students will help conduct experiments in the materials characterization laboratory of the solid mechanics group. The lectures will further address advanced concepts, such as the parameter identification via inhomogeneous deformation processes by combining digital image correlation and finite element analysis. Lastly, it is demonstrated that very similar numerical concepts can be employed in solving structural optimization problems of nonlinear solid mechanics.		
Literature:	• D. P. Bertsekas, *Nonlinear Programming*, Athena Scientific, Belmont, MA, 2nd edition, 1999. • D. G. Luenberger, *Linear and Nonlinear Programming*, Addison-Wesley, Reading, MA, 2nd edition, 1984. • R. Mahnken, *Identification of Material Parameters for Constitutive Equations*, In Encyclopedia of Computational Mechanics, chapter 19, pages 637-655. John Wiley & Sons, New York, 2004. • J. Nocedal and S. J. Wright, *Numerical Optimization*, Springer-Verlag, Berlin, 2nd edition, 2006.		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Continuum Mechanics, 2017-05-18 Mechanics of Materials, Basic Knowledge of Numerical Methods		
Frequency:	yearly in the summer semester		

Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 10 students or more) [MP minimum 30 min / KA 120 min] Possible in German.
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 10 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] In Deutsch möglich.
Credit Points:	4
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.

Data:	PP. MA. Nr. 3215 / Examination number: 44504	Version: 01.07.2024	Start Year: WiSe 2024
Module Name:	**Personal Programming Project**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil. Prüger, Stefan / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	22 Week(s)		
Competencies:	The students will develop, test and document their own software tool for a subject relevant to the Course Computational Materials Science.		
Contents:	Most important ingredients of the programming project are: Search for resources (existing codes, libraries, etc.). Developing the software tool, commenting the source code. Code verification and documentation. Report about the project following the guidelines. Final presentation and defense.		
Literature:	None		
Types of Teaching:	S1 (WS): The seminar takes place in two blocks, (i) at the beginning of the semester: presentation and defense of the project in content, goals and schedule in front of the committee with individual feedback shaping the final form of the PPP, and (ii) at the end of the 22 week period: presentation and defense of the project results. / Seminar (6 d) S1 (WS): In between the seminar blocks the students are guided in practical application-type sessions. / Practical Application (3 SWS)		
Pre-requisites:	**Recommendations:** None		
Frequency:	each semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: AP: Final Report (source code, documentation, analysis of an example solved with their numerical tool) AP: Presentation and defending of the project [30 to 45 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: AP: Abschlussbericht (Quellcode, Dokumentation, Analyse eines mit ihrem numerischen Tool gelösten Beispiels) AP: Präsentation und Verteidigung des Projekts [30 bis 45 min]		
Credit Points:	12		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): AP: Final Report (source code, documentation, analysis of an example solved with their numerical tool) [w: 4] AP: Presentation and defending of the project [w: 1]		
Workload:	The workload is 360h. It is the result of 93h attendance and 267h self-studies.		

Data:	PLAS. MA. Nr. 3216 / Examination number: 44701	Version: 05.06.2018	Start Year: WiSe 2018
Module Name:	**Plasticity**		
(English):			
Responsible:	Kiefer, Björn / Prof. PhD.		
Lecturer(s):	Kiefer, Björn / Prof. PhD.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students understand theoretical concepts and fundamental ideas that are important for an advanced treatment of nonlinear constitutive laws for solids from the viewpoint of thermomechanics. Particular emphasis is placed on the formulation of rate-independent inelasticity. They can apply this knowledge to the development of new constitutive material behavior. They further acquire the relevant knowledge for the numerical implementation of such constitutive laws.		

Contents:	The most important ingredients are:
	• thermomechanics of solids:
	  ◦ thermodynamics with internal state variables
	  ◦ thermoelasticity
	• small-strain elastoplasticity:
	  ◦ particular models of elastoplasticity, evolution laws for internal state variables, hardening
	• elastoplasticity at finite deformations:
	  ◦ kinematics, thermodynamics, general principles		

Literature:	J. Lubliner: Plasticity Theory G. A. Maugin: The Thermomechanics of Plasticity and Fracture H. Ziegler: An Introduction to Thermomechanics P. Haupt: Continuum Mechanics and Theory of Materials Ottosen and Ristinmaa: ”The Mechanics of Constitutive Modeling” J. Lemaitre and J.-L. Chaboche: “Mechanics of Solid Materials”		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	**Mandatory:** Continuum Mechanics, 2017-05-18 or equivalent		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: PVL: Mid-Term Exam [60 min] MP/KA: Final Exam (Oral/Written) (KA if 10 students or more) [120 min] PVL have to be satisfied before the examination.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: PVL: Test [60 min] MP/KA: Final Exam (Oral/Written) (KA bei 10 und mehr Teilnehmern) [120 min] PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA: Final Exam (Oral/Written) [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	STSSP. MA. Nr. 3218 / Examination number: 42604	Version: 13.07.2016	Start Year: SoSe 2012
Module Name:	**Selected Topics of Solid State Physics**		
(English):			
Responsible:	Rafaja, David / Prof. Dr. rer. nat. habil.		
Lecturer(s):	Rafaja, David / Prof. Dr. rer. nat. habil.		
Institute(s):	Institute of Materials Science		
Duration:	1 Semester(s)		
Competencies:	Basic principles of solid state physics, correlation between the crystal structure, real structure and the electronic, magnetic, optical and thermal properties of solids. Absolving the course, the students should be able to recognise the effect of the structure on materials properties and to apply their knowledge in materials design		
Contents:	Drude model of electrical conductivity; temperature dependence of electrical resistivity in metals and semiconductors; Schottky contact; p-n contact; superconductivity (Landau theory); magnetic susceptibility; dia-, para-, ferro-, antiferro- and ferrimagnetism; optical properties of solids; complex index of refraction; dispersion curves for systems with free and bound electrons; Kramers-Kronig relationship; colour of metals; optical theory of reflection for multilayer systems; thermal expansion; specific heat (Einstein and Debye models); heat conductivity		
Literature:	R.E. Hummel: Electronic properties of materials C. Kittel: Introduction in solid state physics		
Types of Teaching:	S1 (SS): Lectures (3 SWS)		
Pre-requisites:	**Recommendations:** Höhere Mathematik für Ingenieure 1, 2015-03-12 Fundamental of Microstructures, 2010-12-02 Höhere Mathematik für Ingenieure 2, 2015-03-12 Allgemeine, Anorganische und Organische Chemie, 2009-09-02 Einführung in die Kristallographie, 2009-10-14 Physik für Naturwissenschaftler I, 2012-05-10 Physik für Naturwissenschaftler II, 2012-05-10		
Frequency:	yearly in the summer semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 10 students or more) [MP minimum 30 min / KA 120 min]		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 10 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min]		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Data:	SEMIC. MA. Nr. 3213 / Examination number: 22306	Version: 20.07.2016	Start Year: WiSe 2016
Module Name:	**Semiconductors**		
(English):			
Responsible:	Gumeniuk, Roman / Prof.		
Lecturer(s):	Gumeniuk, Roman / Prof.		
Institute(s):	Institute of Experimental Physics		
Duration:	1 Semester(s)		
Competencies:	The module conveys basic knowledge on the principles of semiconductor materials and devices based on their crystallographic and electronic structures. Students will get familiar with the electronic properties of semiconductors and should be able to calculate charge carrier concentrations and to describe and understand semiconductor devices based on energy band schemes.		
Contents:	The lecture is divided in four consecutive parts: • Structure of solids: crystal structure in general, examples of element structures and compound structures. • Electrons in matter: energy bands, zone schemes, Brillouin zones, band structures, Fermi distribution, density of states, population density, effective mass, conductivity. • Semiconductors: intrinsic vs. extrinsic semiconductors, band schemes, conductivity, possible defects. • Semiconductor devices: metal-semiconductor contact, p-n junction, diodes, transistors, memory devices, device fabrication.		
Literature:	Standard references on solid state physics and semiconductors for physicists, e.g.: • R. E. Hummel: Electronic Properties of Materials (Springer) • N. W. Ashcroft, N. D. Mermin: Solid State Physics (Brooks Cole) • S. M. Sze: Physics of Semiconductor Devices (Wiley)		
Types of Teaching:	S1 (WS): Semiconductors / Lectures (2 SWS)		
Pre-requisites:	**Recommendations:** Fundamentals of physics, chemistry and solid materials		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: KA [120 min] Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [120 min]		
Credit Points:	3		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): KA [w: 1]		
Workload:	The workload is 90h. It is the result of 30h attendance and 60h self-studies.		

Data:	STCMS. MA. Nr. 3586 / Examination number: 44506	Version: 16.07.2024	Start Year: WiSe 2025
Module Name:	**Software Tools for Computational Materials Scientists**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	The students will learn the basics of the Linux operating system and how to interact through the shell with the computer, in particular with the file system. Students achieve competencies on how to set up a work environment for their needs, how to monitor system resources and to connect securely to remote computers. Moreover, they are trained to apply shell programming and advanced tools for usage with the shell. Participants will learn and understand elements and techniques of the Python programming language and are empowered to carry out structured software development using the language. This includes basic design patterns, data structures, object-oriented programming, file handling, among others. Students obtain competencies to write code for scientific computing using specific packages and features for the purpose and to carry out scientific visualizations. Finally, participants will be able to operate version control systems for working in a collaborative fashion.		
Contents:	The course is divided into two parts: In the first part, students learn to communicate with the computer through the Linux operating system including its tools, whilst in the second part they learn the Python programming language and aspects of scientific programming with this language. Subsequently, version control systems for collaborative working and usage of repositories will be introduced. Additionally, aspects of software testing and nuances pertaining to visualization of scientific data will be outlined.		
Literature:	https://www.tldp.org/LDP/intro-linux/intro-linux.pdf https://python.org https://numpy.org https://matplotlib.org https://gitref.org		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (2 SWS)		
Pre-requisites:			
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 8 students or more) [MP minimum 30 min / KA 120 min] PVL: Programming project PVL have to be satisfied before the examination. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 8 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: Programmierprojekt PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	5		
Grade:	The Grade is generated from the examination result(s) with the following		

	weights (w): MP/KA [w: 1]
Workload:	The workload is 150h. It is the result of 60h attendance and 90h self-studies.

Data:	STOMATE. MA. 3221 / Examination number: -	Version: 21.05.2023	Start Year: WiSe 2023
Module Name:	**Stochastic Methods for Materials Science**		
(English):	Stochastic Methods for Materials Science		
Responsible:	van den Boogaart, Gerald / Prof. Dr. Sprungk, Björn / Prof. Dr.		
Lecturer(s):	van den Boogaart, Gerald / Prof. Dr. Sprungk, Björn / Prof. Dr.		
Institute(s):	Institute of Stochastics Faculty of Mathematics and Computer Science		
Duration:	1 Semester(s)		
Competencies:	The students understand the fundamental concepts of probability theory and statistics. They can apply basic statistical tools to analyze given data sets. Moreover, they know important stochastic models for random materials, stochastic algorithms to simulate them for computational purposes, and are able to select and use appropriate stochastic models in an applied context		
Contents:	• Concepts of probability theory (e.g., random variables, common distributions, limit theorems) • Fundamentals of statistics (empirical characteristics, statistical graphics, parameter estimation, and hypothesis testing) • Regression analysis (linear and nonlinear regression) • Stochastic models for random materials (e.g., random fields, Poisson point process, Boolean models, random packings, and mosaics)		
Literature:	• D. Montgomery, G. C. Runger: *Applied Statistics and Probability for Engineers*. Wiley, 2018. • J. Ohser, F. Mücklich: *Statistical Analysis of Microstructures in Materials Science*. Wiley, 2000. • S. N. Chiu et al.: *Stochastic geometry and its applications*. Wiley, 2013 • J. Ohser, K. Schladitz: 3D Images of Materials Structures. Wiley, 2009.		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:			
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP*: Oral exam [20 to 30 min] AP: Programming Project * In modules requiring more than one exam, this exam has to be passed or completed with at least "ausreichend" (4,0), respectively. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP*: Mündliche Prüfung [20 bis 30 min] AP: Programmierprojekt * Bei Modulen mit mehreren Prüfungsleistungen muss diese Prüfungsleistung bestanden bzw. mit mindestens "ausreichend" (4,0) bewertet sein.		
Credit Points:	5		
Grade:	The Grade is generated from the examination result(s) with the following weights (w):		

	MP*: Oral exam [w: 1] AP: Programming Project [w: 1] * In modules requiring more than one exam, this exam has to be passed or completed with at least "ausreichend" (4,0), respectively.
Workload:	The workload is 150h. It is the result of 45h attendance and 105h self-studies.

Data:	TMSMICS. MA. Nr. 3588 / Examination number: 44507	Version: 01.07.2024	Start Year: SoSe 2025
Module Name:	**Theory, Modelling and Simulation of Microstructures**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will develop a fundamental understanding of computer-based simulations methods for modeling and simulation of microstructures. Of particular focus is the nanoscale where materials display significantly different properties in comparison to the macroscale. Participants learn to judiciously apply state-of-the-art methods for sample generation of crystalline matter. They are empowered to work independently with hands-on tutorials applying widely used simulation software towards specified goals. They are able to develop solution steps along with the choice of the appropriate numerical method in order to carry out simulation tasks based on their analysis of materials science problems. By virtue of their sound understanding of theory they are able to understand and analyze the driving mechanisms behind simulation results.		
Contents:	Key topics are: Structure generation of crystalline matter with and without defects, in particular point, line and planar defects; Boundary conditions in molecular dynamics/statics; Molecular statics and its implementation; Molecular dynamics; Methods for analysis and visualization of simulations in particular defect analysis; Application problems for molecular statics		
Literature:	• E. Tadmor, R. Miller. Modeling Materials: Continuum, Atomistic and Multiscale Techniques, Cambridge University Press • D. Raabe. Computational Materials Science, Wiley VCH • R. Lesar. Introduction to Computational Materials Science: Fundamentals to Applications, Cambridge University Press		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (2 SWS)		
Pre-requisites:	**Recommendations:** Lectures and exercises in Fundamentals of Microstructures. Programming experience in Python (which will be used in the exercises). This is satisfied by participating in the module „Software Tools for Computational Materials Scientists“.		
Frequency:	yearly in the summer semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 6 students or more) [MP minimum 30 min / KA 120 min] PVL: Home work assignments PVL have to be satisfied before the examination. Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 6 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: Hausarbeit PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	5		
Grade:	The Grade is generated from the examination result(s) with the following weights (w):		

	MP/KA [w: 1]
Workload:	The workload is 150h. It is the result of 60h attendance and 90h self-studies.

Data:	TM. MA. Nr. 3222 / Examination number: 51015	Version: 09.07.2024	Start Year: WiSe 2024
Module Name:	**Thermodynamics of Materials**		
(English):			
Responsible:	Leineweber, Andreas / Prof. Dr. rer. nat. habil.		
Lecturer(s):	Fabrichnaya, Olga / Dr.		
Institute(s):	Institute of Materials Science		
Duration:	1 Semester(s)		
Competencies:	The students understand thermodynamic properties of materials and are able to apply calculation methods of phase diagrams.		
Contents:	Most important topics are: Thermodynamic laws and quantities Thermodynamic properties of materials Calculation of complex equilibria in multiphase and multicomponent systems Optimization of phase diagrams		
Literature:	Mats Hillert, "Phase equilibria, phase diagrams and phase transformations", 2nd Ed., Cambridge (2009) Robert de Hoff, "Thermodynamics in Materials Science", 2nd Ed., Taylor & Francis (2006) Hans Leo Lukas, Suzana Fries, Bo Sundman, "Computational Thermodynamics, the CALPHAD method", Cambridge (2007)		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Seminar (1 SWS)		
Pre-requisites:	**Recommendations:** Background in physical chemistry and materials science		
Frequency:	yearly in the winter semester		
Requirements for Credit Points:	For the award of credit points it is necessary to pass the module exam. The module exam contains: MP/KA (KA if 6 students or more) [MP minimum 30 min / KA 120 min] PVL: task exercises (in the seminar) PVL have to be satisfied before the examination.		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP/KA (KA bei 6 und mehr Teilnehmern) [MP mindestens 30 min / KA 120 min] PVL: Übungsaufgaben PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 120h. It is the result of 45h attendance and 75h self-studies.		

Freiberg, den 26. September 2024

gez.
Prof. Dr. Klaus-Dieter Barbknecht
Rektor

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