Amtliche Bekanntmachungen der TU Bergakademie Freiberg

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Modulhandbuch

für den

Masterstudiengang

Computational Materials

Science

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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

Data:	ADVTCMS. MA. Nr. 3587 / Examination number: 44511	Version: 16.02.2022	Start Year: WiSe 2018
Module Name:	**Atomistic Simulation Methods**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with the most recent developments in computational materials science and current state-of-the-art simulation methods for atomistic problems. They will learn the theoretical background of advanced methods on the nanoscale and will be able to apply those to new problems.		
Contents:	This course will cover atomistics subjects such as atomic interactions, validation of potential functions, structure generation, surface energies as well as simulation and critical assessment of three-dimensional nanoscale specimens. Students will get an overview over current developments and will also be able to study such phenomena by hands-on simulations using open source software. Theoretical background and application of advanced methods for data analysis and visualization of atomic defect structures complement this course. The main emphasis of the exercises is on applying the methods from the lecture to problems with materials scientific relevance.		
Literature:			
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** 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: 40912	Version: 15.06.2016	Start Year: WiSe 2016
Module Name:	**Ceramic Engineering**		
(English):			
Responsible:	Aneziris, Christos G. / Prof. Dr.-Ing.		
Lecturer(s):	Aneziris, Christos G. / Prof. Dr.-Ing.		
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 / 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:	3		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 90h. It is the result of 30h attendance and 60h 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: 16.02.2022	Start Year: SoSe 2019
Module Name:	**Crystal Plasticity, Texture and Anisotropy**		
(English):	Crystal Plasticity, Texture and Anisotropy		
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will be exposed to the materials scientific fundamentals of plasticity in single and polycrystals. They will learn mathematical and conceptual 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 synthesis of polycrystalline materials, for testing and characterization. Students will be introduced to different types of representing the particular deformation behaviour in polycrystalline materials, i.e., mean field and full field approaches. They will be able to understand positive and negative aspects of these models and can transfer their knowlege to new models. An other 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 be able to apply them to new problems.		
Contents:	• Mathematical concepts of orientation distributions, description and characterization of grain distributions • Texture: Definition, typical textures • Experimental methods for synthesis, testing and characterization • Basics of most commonly used crystal plasticity models • Grain boundaries, 5-parameter description, experimental and modeling aspects The above topics will be extended in the hands-on tutorial/exercise/programming sessions, where the emphasis will be on applying the methods learnt in the lecture.		
Literature:	1. Crystal Plasticity Finite Element Methods: In Materials Science and Engineering; F. Roters, P. Eisenlohr, T. Bieler and D. Raabe, 2010, Wiley Publishers 2. Texture and Anisotropy; U.F. Kocks, C. Tomé and H.-R. Wenk, 1998, Cambridge University Press 3. The measurement of grain boundary geometry; V. Randle, 1993, CRC Press 4. Texture Analysis in Materials Science, H.-J. Bunge, 1983, Elsevier 5. Grain Boundary and Crystalline Plasticity, L. Priester, 2013, Wiley Publishers		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Mechanics of Materials, 2022-02-16 Minimum requirements are scientific programming skills (as, e.g., aqcuired during "Software Tools for Computational Materials Scientists 1") and a basic understanding of plasticity (as, e.g., aqcuired from "Fundamentals of Microstructures").		
Frequency:	yearly in the summer semester		
Requirements for Credit	For the award of credit points it is necessary to pass the module exam.		

Points:	The module exam contains: PVL: Calculation and simulation MP/KA (KA if 6 students or more) [MP minimum 30 min / KA 90 min] PVL have to be satisfied before the examination.
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: PVL: Berechnungen und Simulation MP/KA (KA bei 6 und mehr Teilnehmern) [MP mindestens 30 min / KA 90 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. Der Zeitaufwand beträgt 150h und setzt sich zusammen aus 60h Präsenzzeit und 90h Selbststudium.

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:	FUNMICRO. MA. Nr. 3209 / Examination number: 44501	Version: 28.03.2022	Start Year: WiSe 2018
Module Name:	**Fundamentals of Microstructures**		
(English):			
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:	The 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.		
Contents:	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.		
Literature:	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		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (2 SWS)		
Pre-requisites:	**Recommendations:** basic programming/scripting experience in Python (which will be used throughout the lecture and tutorials). This is satisfied by simultaneously participating in the module „Software Tools for Computational Materials 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 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:	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: 28.03.2022	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):	Prakash, Aruna / Dr.-Ing. 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 regression and classification • concepts of linear approaches, 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		
Literature:	1. M. P. Deisenroth, A.A. Faisal, Ch.S. Ong: Mathematics for Machine Learning, 2019, Cambridge University Press, UK 2. Sebastian Raschka, Vahid Mirjalili, Python Machine Learning, 2017, Packt Publishing, Birminham, UK 3. Phuong Vo. T. H, Martin Czygan, Getting Started with Python Data Analysis, 2015, Packt Publishing, Birminham, UK		
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:	MasThesis. MA. Nr. 3212 / Examination number: 9900	Version: 08.03.2022	Start Year: SoSe 2012
Module Name:	**Master Thesis Computational 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, 2016-07-11 Masterarbeit: Abschluss aller Module des 1. u. 2. Semesters sowie Antritt aller Modulprüfungen des 3. Semesters und davon höchstens drei offene Prüfungsleistungen, 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:	WERKMEC. BA. Nr. 253 / Examination number: 41906	Version: 16.02.2022	Start Year: WiSe 2018
Module Name:	**Mechanics of Materials**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Development of an understanding of the deformation behavior and failure mechanisms of technological materials; students will get familiar with elastic, plastic, viscous, viscoelastic and viscoplastic behaviors of materials; development of the ability to assess the behavior of materials and to design structures accordingly.		
Contents:	Most important ingredients are: • continuum mechanics foundations of stress, strain and displacements • rheological models for elastic, plastic, viscous, viscoelastic, and viscoplastic deformation behavior • multi-axial continuum laws for anisotropic elasticity and plasticity • extended strength and failure theories / criteria for multiaxial loading		
Literature:	J. Lemaitre and J.-L. Chaboche: Mechanics of Solid Materials, Cambridge University Press,2000		
Types of Teaching:	S1 (WS): Lectures (2 SWS) S1 (WS): Exercises (2 SWS)		
Pre-requisites:	**Recommendations:** Basic knowledge in engineering 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: 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: 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): KA [w: 1]		
Workload:	The workload is 150h. It is the result of 60h attendance and 90h self-studies.		

Data:	MetMat. MA. Nr. 3213 / Examination number: 50114	Version: 27.06.2016	Start Year: WiSe 2016
Module Name:	**Metallic Materials**		
(English):			
Responsible:	Biermann, Horst / Prof. Dr.-Ing. habil		
Lecturer(s):	Weidner, Anja / Dr.-Ing. habil.		
Institute(s):	Institute of Materials Engineering		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with metallic materials (ferrous materials, non-ferrous metals, light metals, high-temperature metals), their microstructure and mechanical properties as well as heat treatment. Focus is given to plastic deformation and failure. The module will enable the students to differentiate the different groups of metallic construction materials.		
Contents:	Most important topics are: 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:	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 (WS): Metallic Materials / Lectures (2 SWS)		
Pre-requisites:	**Recommendations:** Basic 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 [90 min]		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: KA [90 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:	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.

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: 10.05.2021	Start Year: SoSe 2012
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. 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 (SS): Lectures (2 SWS) S1 (SS): 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 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:	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 45h attendance and 45h self-studies.		

Data:	PINSM. MA. Nr. 3589 / Examination number: 41910	Version: 12.07.2017	Start Year: WiSe 2018
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 (WS): Lectures (2 SWS) S1 (WS): Taught in English and German. / Exercises (1 SWS)		
Pre-requisites:	**Recommendations:** Continuum Mechanics, 2017-05-18 Mechanics of Materials, Basic Knowledge of Numerical Methods		
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] 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: 08.03.2022	Start Year: WiSe 2018
Module Name:	**Personal Programming Project**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Rheinbach, Oliver / Prof. Dr. Kiefer, Björn / Prof. PhD. Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Numerical Mathematics and Optimization Institute of Mechanics and Fluid Dynamics		
Duration:	22 Week(s)		
Competencies:	The students will develop and document their own software tool for a subject relevant to the course Computational Materials Science (e.g., Dislocation or Molecular Dynamics, Finite Elements Method FEM, Discrete Element Method or advanced data analysis). Furthermore, they will use this method to simulate material behavior, to calculate a physical property or to analyze existing/own simulated data.		
Contents:	Most important ingredients are: Developing the tool, commenting the source file, documentation and running a successful example to verify the code.		
Literature:	None		
Types of Teaching:	S1 (WS): By the end of the second semester, the students decide on a topic. Then, the students design a concept for their project, which has to be discussed and approved by the responsible lecturer. After approval, the students register at examination office for the project. The final report has to be delivered within 22 weeks. / project (22 Wo)		
Pre-requisites:	**Recommendations:** None		
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: AP: Final Report (source code, documentation, analysis of an example solved with their numerical tool) AP: Presentation and defending of the project [20 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 [20 min]		
Credit Points:	7		
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 210h.		

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:	ResSem. MA. Nr. 3217 / Examination number: 44505	Version: 16.02.2022	Start Year: WiSe 2016
Module Name:	**Research Seminar and Journal Club**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	2 Semester(s)		
Competencies:	Students are able to use scientific methods for literature research. They acquire presentation skills for scientific presentations and are able to solve a general scientific problems based on softskills introduced during this module. Their scientific writing skills allow them to compose their own scientific abstracts and reviews.		
Contents:	Most important ingredients are: • Attending the seminar, where research results of CMS students are presented • Interacting / discussion with the speakers • 1. semester: Literature review on a general seminar topic • 2. semester: Literature review on an individual topic • written literature report and oral presentation		
Literature:	None		
Types of Teaching:	S1 (WS): Seminar (1,5 SWS) S2 (SS): Seminar (1,5 SWS)		
Pre-requisites:	**Recommendations:** None		
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: AP: Literatur report		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: AP: Literaturbericht		
Credit Points:	3		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): AP: Literatur report [w: 1]		
Workload:	The workload is 90h. It is the result of 45h attendance and 45h 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: 16.02.2022	Start Year: WiSe 2019
Module Name:	**Software Tools for Computational Materials Scientists**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	2 Semester(s)		
Competencies:	The students will be able to interact with their computer using a Unix shell. This includes monitoring their system resources, interacting with the file system, and setting up their work environment to their needs. Participants will know how to use a high-level general-purpose programming language and the fundamentals of software engineering within the scientific ecosystem of that language. This comprises basic design patterns, object-oriented programming, an introduction to modern file formats, efficient data serialization, data visualization, interfacing to other programs, and automated testing. The participants will be able to use modern version control systems for working in a collaborative fashion.		
Contents:	These courses will cover the software tools used within computational materials science. The Unix shell will be introduced as a mean to interact with the computer to promote automation of repetitive tasks and working on remote systems, both for monitoring and file system interaction purposes. Libraries and packages from the scientific community will be utilized to pre- and postprocess data for third-party simulation software and to write simulations from the ground up. The underlying data structures that enable a high-level language to be efficient enough for large-scale simulations will be introduced. Techniques for collaboration with other software contributors in form of modern version control systems in conjunction with repository hosting will be outlined.		
Literature:	http://www.tldp.org/LDP/intro-linux/intro-linux.pdf https://www.python.org https://matplotlib.org http://www.numpy.org		
Types of Teaching:	S1 (WS): Lectures (1 SWS) S1 (WS): Exercises (1 SWS) S2 (SS): Lectures (1 SWS) S2 (SS): 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: KA: 2nd Semester [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: 2. Semester [120 min] PVL: Programmierprojekt PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	6		
Grade:	The Grade is generated from the examination result(s) with the following		

	weights (w): KA: 2nd Semester [w: 1]
Workload:	The workload is 180h. It is the result of 60h attendance and 120h self-studies.

Data:	STOMATE. MA. Nr. 3221 / Examination number: 11709	Version: 05.07.2016	Start Year: WiSe 2016
Module Name:	**Stochastic Methods for Materials Science**		
(English):			
Responsible:	van den Boogaart, Gerald / Prof. Dr. Ballani, Felix / Dr. rer. nat.		
Lecturer(s):	van den Boogaart, Gerald / Prof. Dr. Ballani, Felix / Dr. rer. nat.		
Institute(s):	Institute of Stochastics		
Duration:	1 Semester(s)		
Competencies:	The student will understand the role of stochastic modelling and stochastic algorithms for computational material sciences. He/she will learn to select, implement and test stochastic algorithms and models in an applied context.		
Contents:	The lecture introduces examples of stochastic methods of material modeling, analysis and simulations: e.g. models and algorithms for the simulation of random structures (random mosaics, random composites, packing, ...) and random behavior (crack initiation, random loads, random fatigue, ...), statistical and stereological analysis of structural data and EBSD-crystal orientation measurements, Monte-Carle algorithms for material simulation, Markov-Chain-Monte-Carlo/Metropolis-Hastings algorithms for parameter estimation and structure reconstruction.		
Literature:	e.g. Chiu, Stoyan, Kendall, Mecke: Stochastic geometry and its applications, 3rd ed. Wiley, Chichester, 2013		
Types of Teaching:	S1 (WS): Lectures (2 SWS)		
Pre-requisites:	**Recommendations:** Basic knowledge of stochastic, statistic, geometry, continuum mechanics, computer programming, and either crystallography or basic group theory.		
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 [30 min] AP: Programming Project		
	Voraussetzung für die Vergabe von Leistungspunkten ist das Bestehen der Modulprüfung. Die Modulprüfung umfasst: MP [30 min] AP: Programmierprojekt		
Credit Points:	4		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP [w: 1] AP: Programming Project [w: 1]		
Workload:	The workload is 120h. It is the result of 30h attendance and 90h self-studies.		

Data:	TMSMICS. MA. Nr. 3588 / Examination number: 44507	Version: 16.02.2022	Start Year: SoSe 2020
Module Name:	**Theory, Modelling and Simulation of Microstructures**		
(English):			
Responsible:	Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Lecturer(s):	Prakash, Aruna / Dr.-Ing. Eidel, Bernhard / Prof. Dr.-Ing. habil.		
Institute(s):	Institute of Mechanics and Fluid Dynamics		
Duration:	1 Semester(s)		
Competencies:	Students will get familiar with some of the most relevant simulation methods for microstructures and will develop a fundamental understanding for the role of computer-based simulation methods in modern materials science. They obtain a detailed overview over the applications of most commonly used simulation together with their respective ranges of applicability. They learn the practical realization of simulation tasks based on analysis of materials science problems. Through fundamental understanding of theory they will understand the mechanisms behind simulation methods.		
Contents:	This course provides an overview of simulation methods operating on length scales from the atomistic to the meso scale scale. Simulation methods introduced include, e.g., Molecular Statics and Molecular Dynamics as well as mesoscopic methods such as the Dislocation Dynamics method. The introduction of methods operating on different scales is complemented by a discussion of multiscale approaches, i.e. how models operating on different scales can be linked for increasing the computational efficiency and/or the degree of detail. The lecture is accompanied by hands-on tutorials where the students will implement some simulation methods by themselves.		
Literature:	R. Lesar, Introduction to Materials Science, Cambridge University Press A. R. Leach, Molecular modelling – principles and applications, Pearson Education Ltd., Harlow		
Types of Teaching:	S1 (SS): Lectures (2 SWS) S1 (SS): Exercises (2 SWS)		
Pre-requisites:	**Recommendations:** Fundamentals of Microstructures, 2022-03-28 Knowledge of Python scripting, first Part of the Modul 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 20 min / KA 90 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 20 min / KA 90 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: 05.04.2018	Start Year: WiSe 2016
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): Practical Application (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: Successful completing of all practical courses 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: Erfolgreiche Teilnahme an den Praktika. PVL müssen vor Prüfungsantritt erfüllt sein bzw. nachgewiesen werden.		
Credit Points:	3		
Grade:	The Grade is generated from the examination result(s) with the following weights (w): MP/KA [w: 1]		
Workload:	The workload is 90h. It is the result of 45h attendance and 45h self-studies.		

Freiberg, den 30. April 2023

gez.
Prof. Dr. Klaus-Dieter Barbknecht
Rektor

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