Book of Modules for the Elite Master's Programme

Scientific Computing

Faculty for Mathematics, Physics and Computer Science, University of Bayreuth, Germany

February 10, 2026

Preface

This Book of Modules describes all currently admissible modules for the elite master's programme *Scientific Computing* and their assignment to the module areas decribed in the examination regulations "Studien- und Prüfungsordnung". Each module description contains the frequency (and sometimes the term) with which the corresponding course is offered; the list of courses actually provided during the current semester is published via Campus Online. The coordinator of this master's programme will be glad to help you selecting suitable courses to satisfy the requirements formulated in the examination regulations.

The executive committee of the elite master's programme   February 10, 2026

Contents

1 Module Section A: Mathematical Foundation

1.1 Module A1: Numerical Methods for Partial Differential Equations

Title	Numerical Methods for Partial Differential Equations
Module Label	A1
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chairs of Applied and Numerical Analysis, Applied Mathematics, Scientific Computing
Learning Outcomes	This module lays ground to many modules of this programme. It should be attended during the first semester in order to be able to • understand the way numerical algorithms for the solution of partial differential equations work • choose a suitable algorithm for a given class of partial differential equations • adapt standard algorithms to new problems • implement the algorithms discussed in the lecture in MATLAB or in a higher programming language. In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	• finite difference methods for partial differential equations (transport, Poisson, heat, wave equation) • conforming finite element methods for elliptic PDEs (Galerkin method, convergence) and further subjects such as • adaptivity • multigrid methods
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	6
Work Load	4 h lectures plus 2 h post-processing per week = 90 h; 2 h discussion sections plus 3 h preparation/post-processing = 75 h; 15 h preparation for exam, in total: 180 h
Recommended Prerequisites	Introduction to Numerical Mathematics, Introduction to Iterative Methods; helpful but not required: Introduction to Advanced Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year during winter term
Can also be used as	module B-MP or C1 in bachelor Mathematics and module A1 in master Mathematics

1.2 Module A2: Applied Functional Analysis

Title	Applied Functional Analysis
Module Label	A2
Module Type	Lecture
Area of Research	Partial Differential Equations
Responsible	Chairs of Applied and Numerical Analysis, Applied Mathematics, Scientific Computing, Nonlinear Analysis and Mathematical Physics
Learning Outcomes	This module lays ground to many modules of this programme. It should be attended during the first semester. By the end of the course, a successful student should • know the basic solution spaces and understand their uses in the theory of partial differential equations; • master the concept of a weak solution; • be able to apply functional analysis methods to problems in partial differential equations; • understand how functional analysis concepts develop out of applications. In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	Basic solution spaces and methods from functional analysis which are used for analysing partial differential equations, in particular • Sobolev spaces, embedding theorems • weak solutions of elliptic equations, Lax-Milgram lemma, Fredholm alternative • regularity of weak solutions of elliptic equations • spectral theory for compact operators
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	Introduction to Advanced Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year during winter term
Can also be used as	module B-MP or C1 in bachelor Mathematics and module A1 in master Mathematics

2 Module Section B: Modeling and Simulation

2.1 Elective Modules B1: Advanced Topics in Numerical Mathematics

Title	Numerical Methods for General Types of PDEs
Module Label	B1.1
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chairs of Applied and Numerical Analysis, Scientific Computing
Learning Outcomes	- Understanding the way numerical algorithms for the solution of special partial differential equations work - Ability to choose a suitable discretization technique for a given partial differential equation - Ability to choose a suitable algorithm - Ability to implement the algorithms discussed in the lecture in a higher programming language In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	This module is the continuation of the module A1: *Numerical Methods for Partial Differential Equations*. It is focused on the numerical solution of more general types of partial differential equations arising from realistic applications such as fluid dynamics, electromagnetism, structural mechanics, etc. These require special discretization techniques: - non-conforming and mixed finite element methods - finite element methods for (Navier-)Stokes equations - finite volume methods - edge elements Special topics: - adaptivity - smoothed particle hydrodynamics - mortar methods - level-set methods
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module A1 in master Mathematics

Title	Discontinuous and Multiscale Methods for PDEs
Module Label	B1.2
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chair of Scientific Computing
Learning Outcomes	- Understanding of important analysis techniques for Sobolev spaces and their modifications for discontinuous approximation spaces - Ability to choose and apply a suitable discontinuous Galerkin discretization for standard linear and nonlinear advection–diffusion problems - Ability to implement various types of discontinuous Galerkin discretizations in 1D and 2D using a programming language - Understanding of key mechanisms and challenges in scale interaction for the PDE-based equations and systems in scientific and technical problems - Ability to identify and apply a suitable modeling and/or numerical technique for a wide range of multiscale problems - Ability to implement the mathematical methods and numerical algorithms introduced in the course using a programming language
Content	The module consists of two courses: 'Discontinuous Galerkin finite element methods' focusing on the formulation, analysis and application of discontinuous Galerkin (DG) finite element method for hyperbolic and parabolic PDEs 'Efficient Numerical Treatment of Multiscale Problems' which treats, among others, the following topics: - asymptotic analysis - homogenization - multiscale finite element method (MsFEM) - variational multiscale method - heterogeneous multiscale methods (HMM)
Duration	2 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	8
Work Load	2 h lectures plus 1,5 h post-processing per week = 52,5 h; 1 h discussion sections plus 2,5 h preparation/post-processing = 52,5 h; 15 h preparation for exam; in total (two semesters): 240 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis
Grading	Oral or written exam each semester; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	Constructive Approximation Methods
Module Label	B1.3
Module Type	Lecture
Area of Research	Advanced Analysis and Applications / Numerical Mathematics
Responsible	Chair of Applied and Numerical Analysis
Learning Outcomes	By the end of the course, a successful student should be able to • explain the most important concepts of modern, multivariate approximation methods • explain the problems inherent to the reconstruction of multivariate functions from scattered data • prove and analyse the existence, the uniqueness, the computability and the quality of discrete reconstruction techniques • explain and implement the associated numerical schemes • understand the underlying mathematical theory In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	• Jackson- and Bernstein theorems for classical univariate polynomial approximation • Multivariate reconstruction methods based upon radial basis functions, moving least-squares and partition of unity methods • Error and stability analysis of multivariate reconstruction methods • Development and implementation of efficient algorithms for such reconstruction methods • Optimal recovery for generalised interpolation with application to solving partial differential equations
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	Introduction to Advanced Analysis, Introduction to Numerical Mathematics
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B-MP or C1 in bachelor Mathematics and module A1 in master Mathematics

Title	**Mathematical Control Theory**
Module Label	B1.4
Module Type	Lecture
Area of Research	Optimization / Advanced Analysis and Applications
Responsible	Chair of Applied Mathematics
Learning Outcomes	• knowledge of methods and concepts of mathematical control theory • ability to solve selected problems from mathematical control theory • ability to apply these solution strategies to practical problem formulations In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.

Content	• definition and classification of control systems
	
	• qualitative analysis of control systems
	
	• methods for controller design, e.g.
	
	   – methods from linear algebra
	   – methods from optimal control
	   – methods based on Lyapunov functions

Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	Introduction to Numerical Mathematics, A1: Numerical Methods for Partial Differential Equations
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module A1 in master Mathematics

Title	Nonlinear Optimization
Module Label	B1.5
Module Type	Lecture
Area of Research	Optimization
Responsible	Chairs of Applied Mathematics, Scientific Computing
Learning Outcomes	- understanding of optimatlity conditions for nonlinear optimization - understanding of the most important algorithms for the numerical solution of nonlinear optimization problems - ability to model and solve given practical problems in nonlinear optimization - ability to use and develop software for nonlinear optimzation In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	- modeling of nonlinear optimization problems - advanced algorithms for unconstrained optimization - optimality conditions for nonlinear optimization problems - algorithms for constrained optimization - outlook on further problem classes
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	Introduction to Numerical Mathematics, Higher Skills in Numerical Mathematics
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B-MP or C1 in bachelor Mathematics and module A1 in master Mathematics

Title	**Optimization of Partial Differential Equations**
Module Label	B1.6
Module Type	Lecture
Area of Research	Numerical Mathematics / Optimization
Responsible	Chairs of Applied Mathematics, Scientific Computing
Learning Outcomes	- ability to derive and analyse optimality conditions - ability to apply theory to concrete applications - ability to solve the arising problems numerically In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	- Introductory examples and concepts - General existence theory and first order optimality conditions - Linear-quadratic problems - Introduction to some non-linear problems - Basic numerical methods - Examples from applications
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	A2: Applied Functional Analysis, A1: Numerical Methods for Partial Differential Equations
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module A1 in master Mathematics

2.2 Elective Modules B2: Modeling and Simulation

Title	Partial Differential Equations and Integral Equations
Module Label	B2.1
Module Type	Lecture
Area of Research	Partial Differential Equations
Responsible	Chair of Nonlinear Analysis and Mathematical Physics
Learning Outcomes	By the end of the course, a successful student should • understand the origin of the treated equations in the modeling process; • know fundamental results on existence and uniqueness of their solutions; • understand qualitative properties of their solutions; • master key methods of their analysis. In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	Existence, uniqueness, and properties of solutions for integral equations and for various types of partial differential equations that are eminent for modeling in the sciences, in particular • parabolic equations • wave equations and symmetric hyperbolic systems • Schrödinger equations • integral operators related to elliptic equations
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam, in total: 240 h
Recommended Prerequisites	Introduction to Advanced Analysis, A2: Applied Functional Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module A1 in master Mathematics

Title	**Modeling with Differential Equations**
Module Label	B2.2
Module Type	Lecture
Area of Research	Partial Differential Equations
Responsible	Chairs of Applied Mathematics, Scientific Computing
Learning Outcomes	• Ability to identify suitable mathematical models for a given application • Knowledge about important modeling principles • Ability to apply modeling techniques to basic practical applications In contrast to students who have passed bachelor module C1, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.

Content	• General modeling principles
	
	• Mathematical Models based on Ordinary Differential Equations from, e.g.,
	  – Mathematical Biology
	  – Mechanics
	
	• Mathematical Models based on Partial Differential Equations from, e.g.,
	  – Mathematical Physics
	  – Mathematical Finance

Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	A2: Applied Functional Analysis, A1: Numerical Methods for Partial Differential Equations
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	module B1 in master Mathematics

Title	**Mathematical Modeling for Climate and Environment**
Module Label	B2.3
Module Type	Lecture
Area of Research	Partial Differential Equations
Responsible	Chair of Scientific Computing
Learning Outcomes	• Knowledge of important physical principles and their representation in mathematical models for main types of climate and environmental models • Ability to identify the key interactions between different compartments of a climate model and to express them in mathematical form • Ability to formulate simple environmental and climate models and skills to implement them using e.g. Matlab
Content	• Physical principles, mathematical models, and selected numerical methods in climate and environmental sciences • Earth system: Main components, driving forces, scales, feedbacks • Hierarchy of climate models, regional and global focus • Environmental modeling: Main applications and problem settings
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 2 h post-processing per week = 90 h; 120 h practical course; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	A2: Applied Functional Analysis, A1: Numerical Methods for Partial Differential Equations, basic programming skills in Matlab
Grading	Oral exam; active participation in the tutorials
Frequency	Once per year, summer term
Can also be used as	module A1 in master Mathematics

Title	Ergodic Theory and Data Science
Module Label	B2.4
Module Type	Lecture
Area of Research	Dynamical systems, Data Analysis
Responsible	Chair of Dynamical Systems and Data
Learning Outcomes	• Presentation of methods and concepts of ergodic theory • Ability to analyze dynamical systems from a measure-theoretic perspective • Ability to apply domain-specific numerical methods and to interpret their results • Ability to read research papers
Content	Ergodic theory in concerned with the behavior of dynamic systems on the long run and provides statistical statements thereof. It delivers a statistical forecast for systems which are otherwise unpredictable (e.g., chaotic or genuinely stochastic). This course discusses the mathematical characterization of this situation. A central role is going to be played by the so-called transfer operator, which describes the action of the dynamics on a distribution of states. We are also going to highlight its importance in applications, when it comes to the numerical and data-driven approximation of quantities of interest. Topics covered: • Measure theory and L^p spaces • Measure-preserving transformations, Poincaré recurrence theorem • Ergodicity, mixing, Birkhoff ergodic theorem and von Neumann's mean ergodic theorem • Functional characterization, transfer operator, Koopman operator • Data-based approximation • Entropy
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	Basic knowledge in calculus, linear algebra, and probability theory. Helpful, but not required is basic knowledge on functional analysis (A2: Applied Functional Analysis).
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	**Pattern Recognition**
Module Label	B2.5
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Applied Computer Science III
Learning Outcomes	This course imparts advanced, systematic comprehension and methods to recognize or classify patterns in a set of data. E. g. applications are in the fields of object recognition, recognition of hand writing, speech, or gestures, and facial recognition.
Content	Bayesian classification, Parameter estimation, Nonparametric techniques, Linear classification, Feedforward neural networks, Feedback neural networks, Nonmetric methods, Supervised Learn- ing, Unsupervised Learning
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1 h post-processing per week = 45 h; 60 h practical course; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	none
Grading	Oral exam
Frequency	Once per year, winter term
Can also be used as	

Title	**Mechanics of Continua**
Module Label	B2.6
Module Type	Lecture
Area of Research	Fluid Mechanics
Responsible	Theoretical Physics
Learning Outcomes	• Understand fundamental concepts of continuum mechanics such as stress tensors, dynamic equations • Assess which physical effects are relevant/irrelevant for a given situation • Propose a theoretical description and solution approach for a given continuum mechanical problem

Content	• Fundamental concepts in fluid mechanics: pressure, stress tensor
	
	• Euler, Stokes and Navier-Stokes equations
	
	• Dimensionless numbers
	
	• Applications to
	
	   – Turbulence
	
	   – Microfluids

Duration	1 semester
Language	German / English on demand
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	Understanding of classical Newtonian mechanics
Grading	Oral or written exam
Frequency	Every year
Can also be used as	

Title	**Molecular Dynamics Simulations of Biophysical Systems**
Module Label	B2.7
Module Type	Lecture
Area of Research	Physics
Responsible	Biofluid Simulation and Modeling
Learning Outcomes	• Understanding of the theoretical background in biophysical simulations • Practical application to example problems, e.g. protein folding
Content	Molecular Dynamics computer simulations have become an invaluable tool in many areas of the natural sciences. Their widespread applications range from protein folding and membrane dynamics in biological physics, solute-solvent interactions in theoretical chemistry to nanofluidics in process engineering. The aim of this course is (i) to understand the physics behind frequently employed simulation methods and (ii) to gain practical experience in using these methods for a range of sample prob-lems. We will start by considering the basic ingredients for atomistic simulations such as Verlet integration, force fields, long-range electrostatistic interactions, thermostating, etc. We will then move on to cover more advanced topics such as free energy methods and sampling techniques for rare events. Finally, we will discuss systematic coarse-graining methods which allow the simulation of larger and more complicated processes, e.g. the unfolding of a protein in shear flow. The course includes a lab part in which actual simulations with the GROMACS package are conducted.
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and additional practical project
Credit Points	4
Work Load	2 h lectures plus 2 h post-processing per week = 60 h; Practical project = 40 h; 20 h preparation for exam; in total: 120 h
Recommended Prerequisites	Knowledge of statistical mechanics is helpful
Grading	Oral or written exam
Frequency	Approximately every two years
Can also be used as	

Title	Bioinformatics: Molecular Modeling
Module Label	B2.8
Module Type	Lecture with practical course
Area of Research	Biochemistry
Responsible	Bioinformatics / Structural Biology
Learning Outcomes	Knowledge on modeling and analysis of biomolecular processes such as enzymatic reactions In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	The lecture treats the theoretical foundations of molecular modeling (molecular force fields, biomolecular electrostatics, classical and statistical mechanics), their numerical designs (molecular dynamics simulations, energy minimization and normal mode analysis, Monte Carlo simulations), fundamentals quantum chemical methods as well as the modeling of biochemical reactions and ligand binding. In the practical course, various techniques (including analysis of biomolecular structures, computation of electrostatic properties of biomolecules, normal-mode analysis) will be exemplified by selected case studies to provide students with practical demonstrations of these methods.
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and practical course (3 weeks)
Credit Points	4
Work Load	2 h lectures plus 1 h post-processing per week = 45 h; 60 h practical course; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Basic knowledge of chemistry and some biochemistry
Grading	Oral or written exam; active participation in the practical course
Frequency	Every year during winter term
Can also be used as	

Title	**Foundations of Bioinformatics**
Module Label	B2.9
Module Type	Lecture with practical course
Area of Research	Biochemistry
Responsible	Bioinformatics / Structural Biology
Learning Outcomes	Students should acquire the basics of bioinformatics and get to know them in theory and practice. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	The lecture covers the basic bioinformatic applications. Namely, the application of various theoretical methods in the analysis of molecular biological data in the foreground (databases and database search, sequences and sequence alignments, phylogenetic trees) as well as fundamentals of molecular modeling, structure prediction and drug design. In the practical course, the students have hands-on sessions for the different methods, the use of internet tools for sequence data analysis, web-based databases and creation of sequence alignments. Moreover some basic introduction to molecular visualization and an introduction to the UNIX operating system are provided.
Duration	1 semester
Language	German
Teaching Method	Lectures (2 h/week) and practical course (3 h/week)
Credit Points	4
Work Load	2 h lectures plus 2 h post-processing per week = 60 h 3 h practical course = 45 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Basic knowledge of chemistry and some biochemistry
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year during summer term
Can also be used as	

Title	**Quantum Chemistry: Methods and Algorithms**
Module Label	B2.10
Module Type	Lecture with practical course
Area of Research	Chemistry
Responsible	Chair of Physical Chemistry 5
Learning Outcomes	Knowledge on quantum chemical methods and algorithms for predicting the electronic properties of molecules. Participants will learn how to implement important algorithms and how to use these methods in example problems of molecular design or computational chemistry.
Content	This lecture treats the theoretical foundations of modern quantum chemistry, including the LCAO approach to molecular electronic structure, density functional theory (DFT) for exchange and correlation, basis sets, molecular integrals, density fitting, self-consistent field algorithms (solvers, convergence acceleration, direct methods), energy gradients, exact exchange and hybrid DFT, many-body methods for electron correlation (CI, MP2, CC), and property prediction. The practical course will cover the implementation of a self-consistent field and MP2 code, and the use of this code in examplary applications.
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and practical course (3 weeks)
Credit Points	4
Work Load	2 h lectures plus 1 h post-processing per week = 45 h; 60 h practical course; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Basic knowledge of chemistry and one programming language.
Grading	Oral or written exam; active participation in the practical course
Frequency	Every year during winter term
Can also be used as	

Title	Advanced Strength of Materials
Module Label	B2.11
Module Type	Lecture
Area of Research	Engineering Science
Responsible	Chair of Design and CAD
Learning Outcomes	After successfully completing this module, students can: • Abstract components to appropriate mechanical models and deformations and to determine tensions, • Behavior of materials by taking suitable material laws into account to describe mechanical and thermal loads, • Design components in an elasto-plastic manner, • to determine stresses in the notch base, • to design components under cyclic stress, • Understand the principle of strength hypotheses and appropriate comparison stresses to select, • Also more sophisticated components on machines, devices and vehicles Type to be designed reliably and economically in terms of its rigidity and strength.
Content	Theory of elasticity: bending of straight beams, torsion of prismatic rods, axially symmetric Stress states (disks, plates, shells), energy methods elastostatics; Material models and their consequences for components, component flow curves and plastic support numbers, load-bearing methods and plastic joints, Strength hypotheses and comparative stresses, stress-strain cycles in notches; Operational strength: static load, oscillating load Stress (LCF, HCF), multi-stage vibration stress.
Duration	1 semester
Language	German
Teaching Method	Lectures (2 h/week) and tutorials (2 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 2 h discussion sections plus 1.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Basic engineering knowledge funding on Bachelor Engineering Science studies, especially in technical mechanics and strengths of materials.
Grading	Written examination
Frequency	Every year
Can also be used as	

Title	Computer Aided Engineering
Module Label	B2.12
Module Type	Lecture
Area of Research	Engineering Science
Responsible	Chair of Design and CAD
Learning Outcomes	CAE1: ability to create CAD models and generate design proposals using optimization algorithms. CAE2: mastery of modern methods of calculation of statics and their application to constructive tasks; knowledge of associated software In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	CAE1: mastery of modern calculation methods and their application to constructive tasks; knowledge of associated software. Ability to design independently using CAD. CAE2: theory and application of finite element methods to static problems with a focus on the constructive point of view and modeling.
Duration	2 semesters
Language	English
Teaching Method	CAE1: lectures (2 h/week) and CAE2: seminar (2 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 2 h seminar plus 1.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Basic technical understanding A1: Numerical Methods for Partial Differential Equations
Grading	Written examination and written report; For the admission to the written exam a vivid participation in the exercises is required.
Frequency	Every year
Can also be used as	

Title	Advanced Programming for Engineers
Module Label	B2.13
Module Type	Lecture
Area of Research	Engineering Science
Responsible	Chair of Design and CAD
Learning Outcomes	After successfully completing this module, students can: • Advanced concepts of engineering programming apply programs, • Design your own data containers using finite element data as an example, • The possibilities of parallel programming for engineering Analyze, evaluate and apply data.
Content	Advanced concepts of programming (data containers and algorithms, parallelization). Construction and programming of finite elements solvers.
Duration	1 semester
Language	German
Teaching Method	lectures (2 h/week) and seminars (2 h/week)
Credit Points	4
Work Load	45 h lecture + follow up work 45 h seminars + preparation and follow-up work; Examination: 30 h examination preparation; Module in total: 120 hours
Recommended Prerequisites	Basic engineering knowledge funding on Bachelor Engineering Science studies, especially in technical mechanics, construction design and mechanical engineering.
Grading	Oral examination
Frequency	Every year
Can also be used as	

Title	**Model Building and Simulation of Electrochemical Storage**
Module Label	B2.14
Module Type	Lecture
Area of Research	Engineering Science
Responsible	Chair of Electrical Energy Systems
Learning Outcomes	Knowledge of the fundamentals and theories of the processes taking place in an electrochemical storage unit; Acquisition of skills in the methods and approaches of modeling and simulation of electrochemical storage systems.
Content	Theory of the basics of electrochemical storage: electrochemical potential and thermodynamics, mass transport in electrolyte and electrode electrode, double layer and electrode kinetics; Methods of modeling and simulation of electrochemical storage in theory and practice: modeling concepts, model classes; Modeling approaches are used for the following topics: concentrated equivalent circuit models, discretized conductor models, Newman model for simplifying porous structures, finite element method for the solution of partial differential equations, thermal modeling, electrochemical impedance models (EIS) with in-depth study of distributed relaxation times (DRT). Finally, there is an outlook on further modeling approaches such as Gaussian process models or neural networks as well as a classification and evaluation of the models discussed.
Duration	1 semester
Language	German
Teaching Method	lectures (2 h/week) and seminars (2 h/week)
Credit Points	4
Work Load	45 h lecture + follow up work 45 h seminars + preparation and follow-up work; Examination: 30 h examination preparation; Module in total: 120 hours
Recommended Prerequisites	Modules BBP and BB
Grading	Oral examination and written report; participation in the tutorials
Frequency	Every year
Can also be used as	

Title	Foundations of Data Management
Module Label	B2.15
Module Type	Lecture
Area of Research	Data Management, Data Science
Responsible	Chair of Theoretical Computer Science
Learning Outcomes	Students will learn the mathematical foundations of data management (which includes databases and data science). They will understand the connections between logic, expressivity, computational complexity, and efficient algorithms in this area. They will learn the formal tools to be able to understand and interpret recent scientific developments in the area.
Content	The lecture starts with formal definitions of databases and query languages. After showing that there is a deep connection between first-order logic and SQL when it comes to querying relational databases, it investigates the computational complexity (or efficient algorithms) for evaluating and analyzing SQL or first-order logic queries on databases. We then investigate conjunctive queries as a practically relevant special case, treat their evaluation and optimization problems, and connections with graph theory. (Knowledge of SQL is helpful but is not required.)
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h exercises plus 1 h post-processing per week = 30 h; 37.5 h preparation for the exam; in total: 120 h
Recommended Prerequisites	Theoretische Informatik 1 or mathematical skills equivalent to those obtained in a BSc degree in mathematics or physics
Grading	Oral or written exam; participation in the tutorials
Frequency	Every year
Can also be used as	

2.3 Elective Modules B3: Complexity Reduction

Title	**Efficient Treatment of Non-local Operators**
Module Label	B3.1
Module Type	Lecture
Area of Research	Scientific Computing
Responsible	Chair of Scientific Computing
Learning Outcomes	- Understanding the way numerical algorithms for the solution of partial differential and integral equations work - Understanding that non-local operators may contain redundancies which can be used to reduce their asymptotic complexity - Ability to choose a suitable algorithm for a given class of partial differential and integral equations - Ability to implement the algorithms discussed in the lecture in a higher programming language on a parallel computer
Content	State-of-the-art linear complexity treatment of partial differential and integral operators and parallelization techniques: - fast multipole methods for the efficient treatment of multi-source potentials (one of the TOP10 algorithms from the 20th century) - hierarchical matrices (for the treatment of non-local operators with linear complexity) - Schwarz methods (additive and multiplicative) - BPX preconditioner - Domain decomposition (overlapping and non-overlapping), BPS and Neumann-Neumann preconditioners, FETI
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	module B-MP or C1 in bachelor Mathematics and module A1 in master Mathematics

Title	**Fast Methods for Differential and Integral Equations**
Module Label	B3.2
Module Type	Lecture
Area of Research	Scientific Computing
Responsible	Chair of Scientific Computing
Learning Outcomes	• Understanding the way numerical algorithms for the solution of partial differential and integral equations work • Detection of suitable structures which can be exploited for the complexity reduction of solution operators of elliptic boundary value problems • Ability to choose a suitable algorithm for a given class of partial differential or integral equations • Ability to implement the algorithms discussed in the lecture in a higher programming language
Content	Numerical analysis of optimal complexity solvers for the treatment of boundary value problems; efficient treatment of parameter-dependent problems: • subspace correction methods • hierarchical bases and BPX preconditioners • geometric and algebraic multigrid methods (convergence and implementation aspects) • reduced bases methods • analysis of hierarchical matrices
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	module A1 in master Mathematics

Title	**Numerical Methods for Uncertainty Quantification**
Module Label	B3.3
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chair of Scientific Computing
Learning Outcomes	
Content	This is a cutting-edge area of Scientific Computing. In addition to Monte Carlo methods, stochatic collocation, polyonomial chaos expansions, stochastic Galerkin methods, the Karhunen-Loève expansion, model order reduction, and multilevel quadrature recent developments in this area are to be discussed.
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	4
Work Load	2 h lectures plus 3 h post-processing per week = 52,5 h; 1 h discussion sections plus 2,5 h preparation/post-processing = 52,5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	module B1 in master Mathematics

Title	High-dimensional Approximation
Module Label	B3.4
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chairs of Applied and Numerical Analysis, Scientific Computing
Learning Outcomes	By the end of the course, a successful student should • understand the curse of dimensionality • know several concepts to reduce the complexity in high-dimensional problems • be able to apply such concepts to typical examples from finance, physics and engineering
Content	• Introduction to problems from finance, physics and engineering leading to high-dimensional partial differential equations, such as Black-Scholes and Fokker-Planck • Modern concepts for high-dimensional problems including tensor product methods, sparse grids, kernel-based methods, Monte-Carlo and Quasi-Monte-Carlo methods • Error and stability analysis of such methods • Efficient algorithms for and implementations of such methods
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1,5 h post-processing per week = 52,5 h; 1 h discussion sections plus 2,5 h preparation/post-processing = 52,5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	Data Analytics
Module Label	B3.5
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair for Databases and Information Systems
Learning Outcomes	Conceptual foundation of development of large databases (Big Data) and information systems with focus on modeling. Deepening of proficiency in databases in the context of large and complex database and web applications; imparting of interdisciplinary, analytical competences for reconstructing and modeling complex applications (mostly stemming from the application fields); technological competence for selecting and integrating heterogeneous modeling and implementation concepts for the design and realization of data and process based applications. Deepening of proficiency in the fields of data analytics. Realization of complex architectures in the application fields Bio Informatics, Environmental Informatics and Engineer Informatics will be discussed in all courses. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	first semester: Data Warehousing, Data Mining second semester: Data Visualisation, Machine Learning, Ontologies, NoSQL, Distributed Computing Concepts (MapReduce, Hadoop, etc.)
Duration	2 semesters
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	Datenbanken und Informationssysteme I
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year during winter and summer term
Can also be used as	

Title	Complexity Reduction in Control
Module Label	B3.6
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chair of Applied Mathematics
Learning Outcomes	• Understanding why many numerical approaches to control problems suffer from the curse of dimensionality • Recognition of redundancies, such as the turnpike property in optimal control problems, and their use for complexity reduction • Knowledge about state-of-the-art model order reduction methods for linear and nonlinear control systems and how they rely on the particular input-output-structure • Ability to identify suitable techniques for particular applications

Content	• State-of-the-art techniques for the reduction of complexity in control problems, as for instance
	
	    – Model predictive control and its use as a complexity reduction technique
	    – Sparse grid and parallel computing approaches for Hamilton-Jacobi-Bellman equations
	    – Model order reduction methods for control systems, such as balanced truncation or proper orthogonal decomposition
	
	• Implementation of selected algorithms in the tutorials

Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	B1.4: Mathematical Control Theory, A1: Numerical Methods for Partial Differential Equations
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	**Meshfree Methods**
Module Label	B3.7
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chair of Applied and Numerical Analysis
Learning Outcomes	By the end of the course, a successful student should • know fundamental techniques to reduce the complexity in meshfree discretisations for solving partial differential equations numerically • be able to choose a suitable meshfree method for a given problem • master key methods of their analysis and implementation

Content	• Short review of kernel-based collocation and particle methods for solving partial differential equations
	
	• Discussion of various cost reducing methods including:
	
	    – Fast summation techniques based on far field expansions of radial basis functions (RBF) and completely monotone functions
	    – Local Lagrangian methods, RBF-FD
	    – Generalised alternating projection methods
	    – multilevel methods for compactly supported RBF
	    – Adaptive and greedy variants of the above methods
	
	• Discussion of data structures and implementational details for meshfree methods

Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam, in total: 120 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis, B1.3: Constructive Approximation Methods
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	Boundary Element Methods
Module Label	B3.8
Module Type	Lecture
Area of Research	Numerical Mathematics
Responsible	Chair of Scientific Computing
Learning Outcomes	Exterior boundary value problems are difficult to treat via finite element discretizations due to the unboundedness of the computational domain. This lecture presents a different approach by which the boundary value problem is reformulated as an integral equation on the boundary. In particular, this offers the advantage that only a lower-dimensional set has to be discretized. As a consequence, the resulting linear systems are significantly smaller but fully populated in general. The latter difficulty can be treated by local low-rank approximation. By the end of the course, a successful student should • know fundamental techniques to reduce suitable boundary value problems to boundary integral equations • master key methods of the analysis and implementation of boundary integral methods • be able to reduce the complexity of suitable discrete non-local operators
Content	• Sobolev spaces on manifolds • fundamental solutions of partial differential operators • boundary integral operators and their properties • boundary integral equations and their finite element discretization • generating the matrix coefficients • fast boundary element methods • applications: potential equation, linear elasticity, Stokes equations
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam, in total: 120 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, A2: Applied Functional Analysis
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

Title	Optimization in Data Science
Module Label	B3.9
Module Type	Lecture
Area of Research	Optimization, Data Analysis
Responsible	Chair of Applied Mathematics
Learning Outcomes	• Knowledge about the special nature of optimization problems in machine learning • Understanding of optimization algorithms in machine learning • Ability to apply optimization algorithms in machine learning properly
Content	• Introduction to machine learning • Stochastic gradient methods • Proximal gradient methods • Acceleration techniques
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	Basic knowledge in numerics and optimization
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every two years
Can also be used as	module B1 in master Mathematics

3 Module Section C: High-Performance Computing

3.1 Elective Modules C1: High-Performance Computing

Title	Algorithms and Data Structures II
Module Label	C1.1
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Algorithms and Data Structures
Learning Outcomes	This module teaches advanced techniques for the design and analysis of algorithms and data structures. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	Possible topics are: • design principles • graph algorithms • advanced data structures • approximation algorithms • parameterized algorithms • randomized algorithms
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	8
Work Load	4 h lectures plus 3 h post-processing per week = 105 h; 2 h discussion sections plus 5 h preparation/post-processing = 105 h; 30 h preparation for exam; in total: 240 h
Recommended Prerequisites	Elementary programming skills, Basic skills in the design and analysis of algorithms.
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	

Title	Algorithms and Data Structures III
Module Label	C1.2
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Algorithms and Data Structures
Learning Outcomes	This module teaches specialized techniques for the design and analysis of algorithms and data structures In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	Possible topics are: • geometric algorithms • algorithms for data analysis • streaming algorithms • external-memory algorithms
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Advanced programming skills, Advanced skills in the design and analysis of algorithms
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	

Title	**Parallel and Distributed Systems I**
Module Label	C1.3
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Parallel and Distributed Systems
Learning Outcomes	The goal of this course is to impart to the students basic techniques in parallel and distributed programming. By that, special methodical competences are acquired: By understanding basic problems such as load balancing and scalability and by learning synchronization and communication techniques, the students are enabled to design and, with the help of communication and thread libraries, to transform parallel algorithms into efficient parallel and distributed programs. By that, both shared and distributed address spaces are acquired. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	• Architecture and interconnection networks for parallel systems • Performance analysis and scalability of parallel programs • Programming and synchronization techniques for shared address space with multi-threading • Coordination of parallel and distributed programs • Application of programming techniques to complex examples from different areas • Programming techniques for distributed address spaces and message-passing
Duration	1 semester
Language	German
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	120 h in total (45 h presence, 60 h preparation/post-processing, 15 h preparation for exam)
Recommended Prerequisites	
Grading	Written exam; For the admission to the written exam a vivid participation in the exercises is required.
Frequency	Every year in winter term
Can also be used as	

Title	Parallel and Distributed Systems II
Module Label	C1.4
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Parallel and Distributed Systems
Learning Outcomes	The goal of this course is to give the students a deep understanding of important techniques in parallel and distributed programming. The emphasis lies on the acquiring of methodical and technical competences. Based on a deep understanding of standard protocols for computer networks such as IP or TCP/UDP, the students are enabled to design and implement distributed programs. The course covers message-passing approaches such as MPI, passiv communication mechanisms such as sockets, and also active mechanisms such as RPC, RMI, or CORBA. The course also imparts design and implementation competences by applying the techniques to a variety of examples. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	The course covers the basics of parallel and distributed systems with an emphasis on distributed systems. Based on the first part of the course, the following topics are covered: • Message-Passing programming (MPI) • Important communication protocols in distributed systems • Communication coordination and synchronization mechanisms in distributed systems (examples: Sockets, RPC, Java RMI) • Coordination with distributed objects (example: CORBA) • Security aspects and mechanisms in distributed systems
Duration	1 semester
Language	German
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	120 h in total (45 h presence, 60 h preparation/post-processing, 15 h preparation for exam)
Recommended Prerequisites	C1.3: Parallel and Distributed Systems I
Grading	Written exam; For the admission to the written exam a vivid participation in the exercises is required.
Frequency	Every year in summer term
Can also be used as	

Title	High-Performance Computing
Module Label	C1.5
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Parallel and Distributed Systems
Learning Outcomes	The goal of this course is to give the students a deep understanding of important techniques of program analysis and program transformation. The emphasis lies on the acquiring of analytical and technological competences: the students are enabled to analyse arbitrary programs by applying the techniques of data and control dependency analysis and to perform optimizing program transformation based on these analysis techniques. Examples are the vectorization and parallelization of program parts or optimization towards a given memory hierarchy. Methodical and algorithmis competences are acquired by learning scheduling and load balancing algorithms and the underlying principles. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	The following topics are covered: • Overview of current processor architectures and interconnection technologies • Control flow and data flow analysis, data flow equations and solution methods for data flow equations, optimizing transformations • Data dependency analysis, loop dependencies, data dependence equations and solution methods for them • Program transformations for vectorization, parallelization and cache optimization • Methods for scheduling and load balancing for instructions, loops, and tasks • OpenMP programming • Register allocation and program tranformations for reducing the register need of programs • CPU programming with CUDA
Duration	1 semester
Language	English
Teaching Method	Lectures (4 h/week) and tutorials (2 h/week)
Credit Points	8
Work Load	240 h in total (90 h presence, 150 h preparation/post-processing with processing of worksheets)
Recommended Prerequisites	C1.3: Parallel and Distributed Systems I
Grading	Written exam; For the admission to the written exam a vivid participation in the exercises is required.
Frequency	Every year in summer term
Can also be used as	

Title	Parallel Algorithms
Module Label	C1.6
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Parallel and Distributed Systems
Learning Outcomes	Students acquire in-depth knowledge about selected parallel algorithms from different fields of application. In particular, in connection with exercises, students gain analytical and methodological expertise, which empowers them to understand, implement, analyse, and design parallel algorithms. In contrast to students who have passed the corresponding bachelor module, students of this modules can apply the previous techniques more autonomously and can relate them to formerly acquired advanced skills.
Content	Selected parallel algorithms are presented. The range extends from basic, widespread algorithms (e.g., sorting) to complex algorithms from specific fields of application (e.g., computer graphics). Emphasis is put on algorithms from the field of scientific computing. The exercises cover theoretical problems as well as practical programming experience.
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	120 h in total (45 h presence, 60 h preparation/post-processing, 15 h preparation for exam)
Recommended Prerequisites	Algorithms and Data Structures I, C1.3: Parallel and Distributed Systems I
Grading	Oral or written exam
Frequency	Every year in summer term
Can also be used as	

Title	Programming and Data Analysis in Python
Module Label	C1.7
Module Type	Lecture
Area of Research	Computer Science
Responsible	Chair of Serious Games
Learning Outcomes	Students learn to quickly prototype and implement numerical programs in Python. They learn Python as a programming language and a scientific computing environment. They acquire knowledge of the basic programming language, as well as of important libraries for scientific computing, such as NumPy, SciPy, Matplotlib, Pandas, and TensorFlow/Keras. They develop practical and applied skills in exploratory computing, rapid prototyping, and implementation of numerical methods. In contrast to other environments, the Python scientific computing environment is open source, widely used, optimized for programmer productivity, and benefits from a large community and library ecosystem.
Content	The Python programming language: Programming philosophy in Python, data types, control structures, functions, object-oriented programming, debugging. Algorithms: Basic algorithms (e.g., searching and sorting), bisection, recursion, dynamic programming, Newton's method. Matrix methods: Linear Algebra with NumPy, matrix factorizations, eigenvectors and values, diagonalization, SVD, least squares and pseudoinverse. Data analysis: Pandas, clustering, plotting. Neural networks and deep learning.
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (2 h/week)
Credit Points	4
Work Load	120 h in total (45 h presence, 60 h preparation/post-processing, 15 h preparation for exam)
Recommended Prerequisites	None
Grading	Oral or written exam (85%), exercises (15%)
Frequency	Every year in winter term
Can also be used as	

3.2 Module C2: Practical Course on Parallel Numerical Methods

Title	Parallel Numerical Methods
Module Label	C2
Module Type	Lecture with practical course
Area of Research	Computer Science, Scientific Computing
Responsible	Chairs of Parallel and Distributed Systems, Scientific Computing
Learning Outcomes	• Implementation of parallel algorithms: select suitable efficient numerical methods choose data structures that are suitable for the respective problem implement the numerical methods on a parallel computer using standard libraries • Presentation and discussion: choose and master suitable presentation techniques speak freely about a subject and illustrate important structures instructively answer spontaneous questions from the audience in a reliable manner
Content	In this practical course, students implement manageable numerical problems (such as Gaussian elimination, finite element discretization of 2d Laplacian, etc.) on parallel computers using the programming language C/C++ and standard software libraries (LAPACK/BLAS, OpenMP, OpenMPI). The resulting parallel efficiency is observed depending on the chosen implementation (naive or advanced such as Schwarz methods).
Duration	2 weeks
Language	English
Teaching Method	Lecture with practical exercises or small projects
Credit Points	2
Work Load	30 h lecture; 30 h practicals and project preparation; in total: 60 h
Recommended Prerequisites	A1: Numerical Methods for Partial Differential Equations, C1.3: Parallel and Distributed Systems I, B3.1: Efficient Treatment of Non-local Operators; required: knowledge to the extent of G1: Preparation Course
Grading	Implementation and presentation of approaches; active participation and discussion
Frequency	Every year at the end of the winter term
Can also be used as	

4 Module Section D: Specialisation and Training

4.1 Module D1: Special Skills in Scientific Computing

Title	Special Skills in Scientific Computing
Module Label	D1
Module Type	Lecture
Area of Research	Numerical Mathematics, Scientific Computing
Responsible	Chairs of Applied and Numerical Analysis, Applied Mathematics, Scientific Computing
Learning Outcomes	The goal of this module is to provide students with special skills in the areas of Numerical Mathematics and Scientific Computing, relevant for current research activities.
Content	An active field of mathematical research, in which specialized techniques are applied or in which known techniques from different areas are combined in an original way. Examples are: 1. Fractional order differential operators 2. Optimization of nonsmooth problems 3. Advanced topics of optimization with partial differential equations 4. mathematical control theory for infinite-dimensional systems
Duration	1 semester
Language	English
Teaching Method	Lectures (2 h/week) and tutorials (1 h/week)
Credit Points	4
Work Load	2 h lectures plus 1.5 h post-processing per week = 52.5 h; 1 h discussion sections plus 2.5 h preparation/post-processing = 52.5 h; 15 h preparation for exam; in total: 120 h
Recommended Prerequisites	Advanced status of study
Grading	Oral or written exam; active participation in the tutorials
Frequency	Every year
Can also be used as	

4.2 Module D2: Industrial Internship

Title	Industrial Internship
Module Label	D2
Module Type	Internship
Area of Research	Scientific Computing
Responsible	Chair of Scientific Computing
Learning Outcomes	By the end of the internship, a successful student should have • gained hands-on experience in a non-academic environment • applied mathematical techniques and techniques from computer science to real applications • acquired new ideas for his/her own research • written a short report
Content	Industrial applications in the area of Scientific Computing
Duration	6 weeks
Language	English
Teaching Method	Practical course
Credit Points	8
Work Load	6 weeks of internship = 230 h 10 h preparation of report; in total: 240 h
Recommended Prerequisites	Basic lectures of this programme (after first year)
Grading	Written report of at least 10 pages (to be submitted not later than 4 weeks after the internship)
Frequency	Every semester
Can also be used as	

4.3 Module D3: Modeling and Status Seminar

Title	Modeling and Status Seminar
Module Label	D3
Module Type	Seminar
Area of Research	All areas
Responsible	Chair of Scientific Computing
Learning Outcomes	Successful students can • Modeling and numerical solution: transfer real-world problems to a mathematical model pave their way into a scientific topic; work in small groups select suitable efficient numerical methods and implement them on parallel computers • Talk: choose and master suitable presentation techniques speak freely about a subject and illustrate important structures instructively answer spontaneous questions from the audience in a reliable manner • Discussion: phrase appropriate subject-specific questions express constructive criticism for a talk exploit constructive criticism for their future talks • Handout: expose an advanced mathematical subject briefly, concisely, and memorably in writing efficient usage of scientific publication systems (e.g., LaTeX)
Content	Modeling Seminar: • Students receive real-world projects and work (in small groups) their way into them • Each group prepares a presentation for its subject (duration: 30–60 minutes) and talks about it in front of the plenum • Each group prepares and distributes a report (at least 10 pages) using a scientific text system (e.g., LaTeX) Status Seminar: • Each student prepares a presentation on the status of his/her studies and results of his/her research (duration: 15–30 minutes) and talks about it in front of the plenum For both seminars there will be a discussion on the subject and on the presentation.
Duration	4 semesters
Language	English
Teaching Method	Modeling seminar (1 week) and status seminar (2 days) each year
Credit Points	8
Work Load	70 h practical course and 30 h seminar each year = 200 h 40 h preparation/post-processing for seminar, in total: 240 h
Recommended Prerequisites	At least one module of A2 and D1, respectively; C2: Practical Course on Parallel Numerical Methods
Grading	Oral presentation and written report of at least 10 pages (to be submitted not later than 4 weeks after the seminar)
Frequency	Each year (modeling seminar during summer break, status seminar during winter break)
Can also be used as	

5 Module Section E: Soft Skills

Title	Soft Skills
Module Label	E
Module Type	Seminar
Area of Research	
Responsible	Programme coordinator
Learning Outcomes	Key skills for personal development
Content	Participation in seminars devoted to presentation skills, data processing, literature research, handling of foreign-language literature, teamwork, etc.; for instance, the seminars *academic writing*, *embodied communication*, and *time- and self-management* are offered regularly by the Elite Network of Bavaria; the programme coordinator and your mentor will give individual recommendations
Duration	1 semester
Language	English
Teaching Method	Participation in seminars
Credit Points	2
Work Load	In total 60 h of seminars, i.e. 3–4 seminars
Recommended Prerequisites	None
Grading	Proof of attendance
Frequency	
Can also be used as	

6 Module Section F: Master's Thesis

Title	Master's Thesis
Module Label	F
Module Type	Thesis
Area of Research	all areas
Responsible	Programme coordinator
Learning Outcomes	Ability to prepare a scientific work (larger than a bachelor's thesis)
Content	Scientific work in the area of Scientific Computing that should have a connection with application-driven questions and with the focus of this master's programme. In particular, interdisciplinary problems should be treated.
Duration	2 semesters
Language	English or German
Teaching Method	
Credit Points	30
Work Load	900 h (editing time: at most 10 months)
Recommended Prerequisites	
Grading	Written thesis
Frequency	
Can also be used as	

7 Recommended Curriculum

The following recommended curriculum assumes that the studies start in winter term.

a) Full-time study

Sem.	Numerical Maths	SWS	ECTS	Modeling	SWS	ECTS	Computer Science	SWS	ECTS	ECTS
1	A1 Numerical Methods for PDEs	4+2	6	A2 Applied Funct. Analysis	4+2	8	C1-I	2+1	4	30
	B3-I	4+2	8	B2-I (non-math.)	2+1	4				
2	B1-I	4+2	8	B2-I (non-math.)	2+1	4	C1-II	4+2	8	30
	B1-II, B2-II, or B3-II	4+2	8				C2 Parallel Num. Methods	P 2 w.	2	
3	F Master's Thesis		14	D2 Industrial Internship or B3-IV	P 6 w.	8				30
	B3-III	4+2	8							
4	F Master's Thesis		16	D3 Modeling and Status Seminar	S	8	E Soft Skills	S 60h	2	30
	D1 Special Skills in Scientific Computing	2+1	4							
	Numerical Maths		72	Modeling		32	Computer Science		16	120

b) Part-time study

Sem.	Numerical Maths	SWS	ECTS	Modeling	SWS	ECTS	Computer Science	SWS	ECTS	ECTS
1	A1 Numerical Methods for PDEs	4+2	6	A2 Applied Funct. Analysis	4+2	8				14
2	B3-I	4+2	8				C1-I	4+2	8	16
3	B1-I	4+2	8	B2-I (non-math.)	2+1	4	C1-II	2+1	4	16
4	B1-II, B2-II or B3-II	4+2	8	B2-I (non-math.)	2+1	4	C2 Parallel Num. Methods	P 2 w.	2	14
5	B3-III	4+2	8	D2 Industrial Internship or B3-IV	P 6 w.	8				16
6	F Master's Thesis		15							15
7	F Master's Thesis		15							15
8	D1 Special Skills in Scientific Computing	2+1	4	D3 Modeling and Status Seminar	S	8	E Soft Skills	S 60h	2	14
	Numerical Maths		72	Modeling		32	Computer Science		16	120

The following recommended curriculum assumes that the studies start in summer term.

a) Full-time study

Sem.	Numerical Maths	SWS	ECTS	Modeling	SWS	ECTS	Computer Science	SWS	ECTS	ECTS
1	B1-I	4+2	8	B2-I (non-math.)	2+1	4	C1-I	4+2	8	30
	B3-I	4+2	8				C2 Parallel Num. Methods	P 2 w.	2	
2	A1 Numerical Methods for PDEs	4+2	6	A2 Applied Funct. Analysis	4+2	8	C1-II	2+1	4	30
	B1-II, I, B2-II or B3-II	4+2	8	B2-I (non-math.)	2+1	4				
3	F Master's Thesis		14	D2 Industrial Internship or B3-IV	P 6 w.	8				30
	B3-III	4+2	8							
4	F Master's Thesis		16	D3 Modeling and Status Seminar	S	8	E Soft Skills	S 60h	2	30
	D1 Special Skills in Scientific Computing	2+1	4							
	Numerical Maths		72	**Modeling**		32	**Computer Science**		16	120

b) Part-time study

Sem.	Numerical Maths	SWS	ECTS	Modeling	SWS	ECTS	Computer Science	SWS	ECTS	ECTS
1	B1-I	4+2	8				C1-I	4+2	8	16
2	A1 Numerical Methods for PDEs	4+2	6	A2 Applied Funct. Analysis	4+2	8				14
3	B3-I	4+2	8	B2-I (non-math.)	2+1	4	C2 Parallel Num. Methods	P 2 w.	2	14
4	B1-II, B2-II or B3-II	4+2	8	B2-I (non-math.)	2+1	4	C1-II	2+1	4	16
5	B3-III	4+2	8	D2 Industrial Internship or B3-IV	P 6 w.	8				16
6	F Master's Thesis		15							15
7	F Master's Thesis		15							15
8	D1 Special Skills in Scientific Computing	2+1	4	D3 Modeling and Status Seminar	S	8	E Soft Skills	S 60h	2	14
	Numerical Maths		**72**	**Modeling**		**32**	**Computer Science**		**16**	**120**