Module Catalog M.Sc. Computational Science

CS-M-F

1. Module title:	**CS-M-F: Specialization**
2. Field / responsibility of:	Physics / department, Dean of Studies
3. Module contents:	Investigating the current state of research in the chosen area of specialization. Specific sources will be provided by the research phase supervisor. Exact planning of the master's thesis and acquiring the necessary experimental and theoretical specialized methods. At the end of the module, acceptance of the subject is compulsory.
4. Qualification objectives of the module / competencies to be acquired:	Familiarization with the research phase subject area.
5. Prerequisites for participation:	
a) Recommended knowledge:	Subject-dependent
b) Prerequisite courses:	See examination regulations
6. Module can be used for:	MSc. in Computational Science
7. Module is offered:	At any time
8. Module can be completed in:	1 semester
9. Recommended semester of study:	3rd semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 30 CP x 30 = 900 hours Allocation: 1. Attendance: 50 hours 2. Independent study: 850 hours Credit points: 30

11. The module is successfully completed when the requirements below have been met:

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R		Specialization	50	Participation in seminar
2	R		Specialization	850	Seminar presentation

Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

No.	Competence / topic	Type of exam	Duration	Time / Comments	Weighting of module grade

14. Notes:
The supervisor will confirm that the topic was covered in the seminar presentation in a scientifically correct manner.

CS-M-P1

1. Module title:	**CS-M-P1: Applied Mathematics I**
2. Field / responsibility of:	Mathematics / Faculty of Mathematics
3. Module contents:	Topics of applied mathematics that are relevant to the field of computational science.
4. Qualification objectives of the module / competencies to be acquired:	In-depth knowledge of applied mathematics
5. Prerequisites for participation:	
a) Recommended knowledge:	Analysis I – III, linear algebra
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Computational Science
7. Module is offered:	Each semester
8. Module can be completed in:	1 semester
9. Recommended semester of study:	1st semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 9 CP x 30 = 270 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study, exam preparation: 180 hours Credit points: 9

11. The module is successfully completed when the requirements below have been met:

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture Practical course	See below See below	4 2	 Practical exercises

Elective participation in the following courses: Introduction to Probability Theory and Statistics, Numerics II, Analysis IV, Partial Differential Equations I, Partial Differential Equations II, Functional Analysis, Optimization, Optimal Control, Mathematical Modeling, Numerics of Partial Differential Equations, Linear Algebra II, Algebra. In addition, all courses of the module Intensification - Bachelor of the bachelor program in mathematics and all courses of the master program in mathematics may be attended. Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

Competence / topic/area	Type of exam	Duration	Time	Weighting of module grade
Topic from 12.	Oral or written	Written: 90-180 min. Oral: 20-45 min.	Lecture period to end of semester	Graded, 100%

14. Notes: The module cannot be completed as part of a bachelor's degree.

CS-M-P2

1. Module title:	**CS-M-P2: Applied Mathematics II**
2. Field / responsibility of:	Mathematics / Faculty of Mathematics
3. Module contents:	Topics of applied mathematics that are relevant to the field of computational science.
4. Qualification objectives of the module / competencies to be acquired:	In-depth knowledge of applied mathematics
5. Prerequisites for participation:	
a) Recommended knowledge:	Analysis I – III, linear algebra
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Computational Science
7. Module is offered:	Each semester
8. Module can be completed in:	1 semester
9. Recommended semester of study:	1st semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 9 CP x 30 = 270 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study, exam preparation: 180 hours Credit points: 9

11. The module is successfully completed when the requirements below have been met:

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture Practical course	See below See below	4 2	Practical exercises

Elective participation in the following courses: Introduction to Probability Theory and Statistics, Numerics II, Analysis IV, Partial Differential Equations I, Partial Differential Equations II, Functional Analysis, Optimization, Optimal Control, Mathematical Modeling, Numerics of Partial Differential Equations, Linear Algebra II, Algebra. In addition, all courses of the module Intensification - Bachelor of the studies program Bachelor in Mathematics and all courses of the master program Mathematics may be attended. Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

Competence / topic/area	Type of exam	Duration	Time	Weighting of module grade
Topic from 12.	Oral or written	Written: 90-180 min. Oral: 20-45 min.	Lecture period to end of semester	Graded, 100%

14. Notes: The module cannot be completed as part of a bachelor's degree.

CS-M-P3

1. Module title:	**CS-M-P3: Applied Mathematics III**
2. Field / responsibility of:	Mathematics / Faculty of Mathematics
3. Module contents:	Topics of applied mathematics that are relevant to the field of computational science.
4. Qualification objectives of the module / competencies to be acquired:	Acquiring in-depth knowledge of applied mathematics
5. Prerequisites for participation:	
a) Recommended knowledge:	Analysis I – III, linear algebra
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Computational Science
7. Module is offered:	Each semester
8. Module can be completed in:	1 semester
9. Recommended semester of study:	1st semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 9 CP x 30 = 270 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study, exam preparation: 180 hours Credit points: 9

11. The module is successfully completed when the requirements below have been met:

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture Practical course	See below See below	4 2	 Practical exercises

Elective participation in the following courses: Introduction to Probability Theory and Statistics, Numerics II, Analysis IV, Partial Differential Equations I, Partial Differential Equations II, Functional Analysis, Optimization, Optimal Control, Mathematical Modeling, Numerics of Partial Differential Equations, Linear Algebra II, Algebra. In addition, all courses of the module Intensification - Bachelor of the studies program Bachelor in Mathematics and all courses of the master program Mathematics may be attended. Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

Competence / topic/area	Type of exam	Duration	Time	Weighting of module grade
Topic from 12.	Oral or written	Written: 90-180 min. Oral: 20-45 min.	Lecture period to end of semester	Graded, 100%

14. Notes: The module cannot be completed as part of a bachelor's degree.

CS-M-P4

1. Module title:	Biochemistry
2. Field / responsibility of:	Biochemistry / Prof. Dr. R. Sterner
3. Module contents:	• Chromatin structure • RNA biology • Ribosome biology • Protein structure • Biophysics
4. Qualification objectives of the module / competencies to be acquired:	Advanced knowledge of current topics in experimental biochemistry; presentation and discussion of scientific results
5. Prerequisites for participation:	
a) Recommended knowledge:	Knowledge from bachelor's degree
b) Prerequisite courses:	None
6. Module can be used for:	M.Sc. in Computational Science
7. Module is offered:	Each semester
8. Module can be completed in:	2 semesters
9. Recommended semester of study:	1st and 2nd semester of study
10. Module workload / number of credit points:	300 hours (60 hours of attendance, 210 hours of independent study, 30 hours of exam preparation) / 10 credit points

11. Module components:

No.	R / RE / E	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture	The students choose the lecture from a given set of lectures. If in doubt, please consult with an academic advisor.	2 credit hours / 30 hours	
4	R	Lecture	The students choose the lecture from a given set of lectures. If in doubt, please consult with an academic advisor.	2 credit hours / 30 hours	

Notes:

12. Module exam:

ME / PME*	Contents of exam	Type of exam	Duration	Time	Type of evaluation
T	Biochemistry	Oral exam	45 min.	At the end of semester	10 CP

13. Notes:

The module cannot be completed as part of a bachelor's degree.

CS-M-P5

1. Module title:	Experimental Genomic Science
2. Field / responsibility of:	Functional Genomics / Dr. Reinders, Dr. Dettmer, Prof. Dr. Oefner
3. Module contents:	Detailed review of current experimental techniques from the fields of sequence, transcription, proteome and metabolome analysis. Topics include next-generation sequencing, microarray analysis, mass spectrometric proteome analysis, and metabolome analysis using coupled mass spectrometric techniques as well as multidimensional and multinuclear NMR spectroscopy. In addition, fundamental aspects of the experimental design will be discussed. We will address, for example, the necessary number of experiments to answer a particular question, the necessity of replicas, avoiding batch effects, and timing. The aspects covered in the lecture will be deepened in small groups in a laboratory course.
4. Qualification objectives of the module / competencies to be acquired:	Theoretical and practical insight into current analysis methods in genomic science.
5. Prerequisites for participation:	
a) Recommended knowledge:	B.Sc. Bioanalytics (module CS-B-P2b Part 1), genomic data analysis (module CS-B-P2b Part 2)
b) Prerequisite courses:	Biochemistry (CS-B-Med3 or course with related contents)
6. Module can be used for:	M.Sc. in Computational Science
7. Module is offered:	Every winter semester
8. Module can be completed in:	2 semesters
9. Recommended semester of study:	1st and 2nd semester of study
10. Module workload / number of credit points:	300 hours (180 hours of attendance, 90 hours of independent study, 30 hours of exam preparation) / 10 credit points

11. Module components:

No.	R / RE / E	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture	Experimental Genomic Science Part 1	2 credit hours / 30 hours	
2	R	Seminar	Introduction to Experimental Genomic Science Laboratory (1st sem.)	1 credit hour / 15 hours	
3	R	Course	Methods in Experimental Genomic Science (1st sem.)	4 credit hours / 60 hours	Experiment reports
4	R	Lecture	Experimental Genomic Science Part 2	1 credit hour / 15 hours	
5	R	Seminar	Literature Seminar in Experimental Genomic Science	1 credit hour / 15 hours	Lecture
6	R	Seminar	Introduction to Experimental Genomic Science Laboratory (2nd sem.)	1 credit hour / 15 hours	
7	R	Course	Methods in Experimental Genome Science (2nd sem.)	4 credit hours / 30 hours	Experiment reports

Notes:

12. Module exam:

ME / PME*	Contents of exam	Type of exam	Duration	Time	Type of evaluation
PME	Experimental Genome Science Part 1 & 2	Exam	120 min.	End of 2nd semester	Graded

Notes: PME = partial module exam. The module grade is derived in equal parts from the partial module exams of Experimental Genome Science Part 1 (1/2) and Part 2 (1/2).

13. Miscellaneous/remarks:

a) Literature:
Lottspeich & Engels, Bioanalytik, Spektrum-Verlag
Rehm & Letzel, Proteinbiochemie / Proteomics, Spektrum-Verlag
Brown, Genome und Gene, Spektrum-Verlag
Villas-Boas et al., Metabolome Analysis, WILEY-VCH

b) The module cannot be completed as part of a bachelor's degree.

CS-M-P6

1. Module title:	Bioinformatics
2. Field / responsibility of:	Prof. Dr. Spang
3. Module contents:	Specific topics of both algorithmic and statistical bioinformatics
4. Qualification objectives of the module / competencies to be acquired:	Understanding of current research topics in bioinformatics
5. Prerequisites for participation:	
a) Recommended knowledge:	Knowledge from bachelor's degree
b) Prerequisite courses:	Genomic Science & Bioinformatics, Genomic Data Analysis, corresponding to modules CS-B-P2b (Genomic Science B) or CS-P2 (Genomic Science and Bioinformatics), or modules with related contents.
6. Module can be used for:	M.Sc. in Computational Science
7. Module is offered:	Every winter semester
8. Module can be completed in:	2 semesters
9. Recommended semester of study:	1st and 2nd semester of study
10. Module workload / number of credit points:	300 hours (210 hours of attendance, 60 hours of independent study, 30 hours of exam preparation) / 10 credit points

11. Module components:

No.	R / RE / E	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Seminar	Algorithmic Bioinformatics	2 credit hours / 30 hours	2
2	R	Seminar	Statistical Bioinformatics	2 credit hours / 30 hours	2
3	R	Laboratory	Block laboratory course	10 credit hours / 150 hours	6

Notes:

12. Module exam:

ME / PME*	Contents of exam	Type of exam	Duration	Time	Type of evaluation
PME	Bioinformatics	Oral	45 min.	At the end of semester	Graded

13. Notes:

The module cannot be completed as part of a bachelor's degree.

CS-M-P7

1. Module title:	**CS-M-P7: Lattice QCD I**
2. Field / responsibility of:	Physics / department, Dean of Studies
3. Module contents:	**Lattice QCD I:** • Path integral quantization • Scalar field theory on the lattice • Monte Carlo methods • Gauge theories • Strong-coupling expansion • Continuum limit and phase transition • Fermions on the lattice • Chiral symmetry on the lattice • Numerical methods for fermions • Hadron spectroscopy
4. Qualification objectives of the module / competencies to be acquired:	Acquiring a fundamental knowledge of lattice QCD. The ability of independent transfer, generalization and abstraction of the studied description and solution methods to a new problem.
5. Prerequisites for participation:	
a) Recommended knowledge:	Basic knowledge of at least one of the programming languages Fortran, C and C++; basic knowledge of quantum field theory
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Computational Science, MSc. in Physics
7. Module is offered:	On a yearly basis
8. Module can be completed in:	1 semester
9. Recommended semester of study:	1st semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 8 CP x 30 = 240 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study, exam preparation: 150 hours Credit points: 8
11. The module is successfully completed when the requirements below have been met:	
12. Module components:	

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture Practical course	Lattice QCD I Lattice QCD I	4 2	 Practical exercises

Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

Competence / topic/area	Type of exam	Duration	Time	Weighting of module grade
a) Area 1	Exam or oral	Exam: 105 min. or 135 min. or 210 min. (if it consists of two parts) Oral: 25-35 min.	At the end of semester	Graded (100%)

14. Notes: The module cannot be completed as part of a bachelor's degree.

CS-M-P8

1. Module title:	**CS-M-P8: Lattice QCD II**
2. Field / responsibility of:	Physics / department, Dean of Studies
3. Module contents:	**Lattice QCD II:** • Decay constants • Chiral extrapolation • Perturbative and non-perturbative renormalization • Hadronic structure • Electroweak matrix elements • QCD at non-zero temperature • QCD for finite baryon density • Lattice gauge theories beyond QCD
4. Qualification objectives of the module / competencies to be acquired:	Acquiring advanced knowledge of lattice QCD as well as the ability to independently apply to a new problem the description and solution methods studied by means of transfer, generalization and abstraction.
5. Prerequisites for participation:	
a) Recommended knowledge:	Basic knowledge of at least one of the programming languages Fortran, C and C++; basic knowledge of quantum field theory, lattice QCD I
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Computational Science, MSc. in Physics
7. Module is offered:	On a yearly basis
8. Module can be completed in:	1 semester
9. Recommended semester of study:	2nd semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 8 CP x 30 = 240 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study, exam preparation: 150 hours Credit points: 8

11. The module is successfully completed when the requirements below have been met:

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture Practical course	Lattice QCD II Lattice QCD II	4 2	 Practical exercises

Further information will be provided by the instructors at the beginning of the course.

13. Module exam:				
Competence / topic/area	Type of exam	Duration	Time	Weighting of module grade
a) Area 1	Exam or oral	Exam: 105 min. or 135 min. or 210 min. (if it consists of two parts) Oral: 25-35 min.	At the end of semester	Graded (100%)

14. Notes: The module cannot be completed as part of a bachelor's degree.

NS-M-4

1. Module title:	**NS-M-4 Computational Nanoscience**
2. Field / responsibility of:	Physics / department, Dean of Studies
3. Module contents:	1. Fundamentals • Introduction and overview • Multi-electron systems and Born-Oppenheimer approximation • Periodic and finite nanostructures 2. Density functional theory (DFT) • Interacting electron gas • Hartree-Fock approximation • Basic theorems of DFT • Exchange-correlation functionals 3. Numerical aspects of DFT • Basis set development • Implementation for periodic and finite systems 4. Applications • Theoretical spectroscopy • Quantum molecular dynamics
4. Qualification objectives of the module / competencies to be acquired:	Learning the fundamentals of modern methods of electron structure theory as well as their computational implementation. Acquiring an overview of potential application areas and limits of these methods in the field of nanostructured materials.
5. Prerequisites for participation:	
a) Recommended knowledge:	Quantum mechanics II
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Nanoscience, BSc. in Physics, BSc. in Nanoscience, BSc. in Comp. Science, MSc. in Physics, MSc. in Computational Science
7. Module is offered:	On a yearly basis
8. Module can be completed in:	1 semester
9. Recommended semester of study:	1st semester (master) or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 8 CP x 30 = 240 hours Allocation: 1. Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours 2. Independent study and exam preparation (including exam): 150 hours Credit points: 08

11. The module is successfully completed when the requirements below have been met.

12. Module components:

No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture	Computational Nanoscience	4	
2	R	Labs	Computational Nanoscience	2	

Further information will be provided by the instructors at the beginning of the course.

13. Module exam:

Competence / topic	Type of exam	Duration	Time / notes	Weighting of module grade
Computational Nanoscience	Laboratory report	---	End of lecture period to end of semester	Graded, 100%

14. Notes:
Following the lecture, a computer-based block laboratory course will take place, in which the knowledge acquired during the lecture will be practically applied. A meaningful report that includes an evaluation must be produced and handed in electronically according to the instructor's specifications, which ensures that the report was indeed written by the candidate.

NS-M-7

1. Module title:	**NS-M-7: Molecular Dynamics Simulations in Chemistry, Physics and Biology**
2. Field / responsibility of:	Prof. Horinek, Faculty of Chemistry
3. Module contents:	1. Fundamentals: Simulation methods, forces in molecular systems, electrostatics, thermostats, barostats 2. Determining structural, thermodynamic and dynamic characteristics 3. Free energy simulations 4. Classical force fields 5. Applications: Water, polymeres, proteins 6. Advanced methods
4. Qualification objectives of the module / competencies to be acquired:	After successful participation in this module, the student will be able 1. to describe the fundamental methods of molecular dynamics. 2. to understand and explain the approximations made in a classical molecular dynamics simulation. 3. to interpret simulation results with respect to experimental data by means of statistical mechanics. 4. to evaluate which simulation approaches are necessary to describe a given experimental problem. 5. to independently conduct simple simulation projects.
5. Prerequisites for participation:	
a) Recommended knowledge:	Basic knowledge of statistical mechanics, basic knowledge of Linux
b) Prerequisite courses:	None
6. Module can be used for:	MSc. in Nanoscience, BSc. in Nanoscience, BSc. in Comp. Science, MSc. in Comp.
7. Module is offered:	On a yearly basis
8. Module can be completed in:	2 semesters
9. Recommended semester of study:	1st semester or higher
10. Module workload / number of credit points:	Workload: Total number of hours: 8 CP x 30 = 240 hours Allocation: 1. Attendance: 2 sem. x 15 weeks x 6 credit hours = 180 hours 2. Independent study and exam preparation: 60 hours Credit points: 08

11. The module is successfully completed when the requirements below have been met.					
12. Module components:					
No.	R / RE	Form of teaching	Subject area/topic	Credit hours	Coursework
1	R	Lecture	Introduction to Molecular Dynamics I	2	
2	R	Lecture	Introduction to Molecular Dynamics II	2	
3	R	Practical course	Introduction to Molecular Dynamics	2	
Further information will be provided by the instructors at the beginning of the course.					

13. Module exam:				
Competence / topic	Type of exam	Duration	Time / notes	Weighting of module grade
Molecular Dynamics	Oral exam	20 min.	End of lecture period to end of semester	Graded, 100%
14. Notes:				