Module Catalog M.Sc. Computational Science

CS-M-F

1. Module title:				CS-M-	CS-M-F: Specialization				
2. F	ield /	responsib	ility of:		Physics	Physics / department, Dean of Studies			
3. N	3. Module contents:				Investic area of by the master experir At the is comp	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:					/ Familia	rization \	with the research phas	e subject area.	
5. P	rerec	quisites for	particip	pation:					
	a) Re	commende	ed know	/ledge:	Subject	-depend	ent		
	b) Pr	erequisite	courses	:	See exa	aminatio	n regulations		
6. Module can be used for:				MSc. ir	n Compu	tational Science			
7. Module is offered:				At any	time				
8. N	8. Module can be completed in:				1 seme	ster			
9. F	lecon	nmended s	emestei	r of study:	3rd ser	3rd semester or higher			
10.	Mod point	ule worklo s:	ad / nur	nber of credit	Worklc Total n Allocat 1. Atte 2. Inde Credit	Workload: Total number of hours: 30 CP x 30 = 900 hours Allocation: 1. Attendance: 50 hours 2. Independent study: 850 hours Credit points: 20			
11.	The	module is s	successf	ully completed	when the	require	ments below have b	een met:	
12.	Mod	ule compo	nents:						
No.	R / RE	Form of teaching	S	ubject area/topic	2	Credit hours	Coursework		
1	R	R Specialization				50	Participation in seminar		
2 R Specialization				850 Seminar presentation					
Furt	her in	formation v	vill be pr	ovided by the in	structors at	the beg	inning of the course.		
13.	Mod	ule exam:						1	
No.	No. Competence / topic Type of exam			Durati	Duration Time / Comments Weighting of module grade				
14. The	Note super	s: visor will co	onfirm th	at the topic was	covered in	the sem	inar presentation in a	scientifically	

correct manner.

						CC M D1. Applied Mathematics			
					CS-M-P1: Applied Mathematics I				
2. Field / responsibility of:					Mathematics / Faculty of Mathematics				
3. N	Nodule	contents:			Topic field	cs of applie of comput	ed mathemati tational science	ics that are relevant to the ce.	
4. C con	4. Qualification objectives of the module / competencies to be acquired:				In-de	epth know	ledge of appli	ied mathematics	
5. F	Prerequi	sites for p	participation:						
	a) Reco	mmendec	l knowledge:		Anal	ysis I – III, I	linear algebra	l	
	b) Prere	quisite co	ourses:		None	5			
6. N	Nodule	can be us	ed for:		MSc.	in Compu	itational Scier	nce	
7. N	//odule i	s offered	:		Each	semester			
8. N	Nodule	can be co	mpleted in:		1 ser	nester			
9. F	Recomm	ended se	mester of stu	ıdy:	1st s	emester or	^r 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.	Module	compone	ents:	inpleted wr				w have been met.	
No.	R / RE	Form of teaching	Subject	t area/topic		Credit hours	Coursework		
1	R	Lecture Practical course	See below See below			4 2	Practical exerc	ises	
Elective participation in the following courses: Intro II, Analysis IV, Partial Differential Equations I, Partia Optimization, Optimal Control, Mathematical Mod Algebra II, Algebra. In addition, all courses of the r program in mathematics and all courses of the matinformation will be provided by the instructors at t					roduc ial Dif deling modu aster the b	tion to Pro fferential E g, Numeric ule Intensi program in peginning c	bability Thec quations II, F s of Partial D fication - Bach n mathematic of the course.	bry and Statistics, Numerics unctional Analysis, ifferential Equations, Linear nelor of the bachelor as may be attended. Further	
13.	13. Module exam:								
Competence / Type of Duratio			n	Т	īme	Weighting of module grade			
Торі	c from 12		Oral or written	Written: 90-180 min. Oral: 20-45 r	nin.	Lecture per end of sem	iod to ester	Graded, 100%	

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

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1. Module title:					CS-M	CS-M-P2: Applied Mathematics II			
2. Field / responsibility of:				Mathematics / Faculty of Mathematics					
3. Module contents:				Topic field o	Topics of applied mathematics that are relevant to the field of computational science.				
4. C con	4. Qualification objectives of the module / competencies to be acquired:					oth know	ledge of appl	lied mathematics	
5. Prerequisites for participation:									
	a) Reco	mmende	d knowledge:		Analy	sis I – III,	linear algebra	3	
	b) Prere	equisite c	ourses:		None				
6. I	Nodule	can be us	sed for:		MSc.	in Compu	utational Scier	nce	
7. N	Nodule	is offered	l:		Each	semester			
8. N	Nodule	can be co	ompleted in:		1 sem	lester			
9. F	Recomm	ended se	mester of stu	ıdy:	1st se	mester o	r higher		
10. Module workload / number of credit points:			f credit	Work Total Alloca 1. Att hou 2. Ind	 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 				
12.	Module	e compon	ients:						
No.	R / RE	Form of teaching	Subject area/to	opic		Credit hours	Coursework		
1	R	Lecture Practical course	See below See below			4 2	Practical exer	cises	
Elective participation in the following courses: InII, Analysis IV, Partial Differential Equations I, ParOptimization, Optimal Control, Mathematical MeAlgebra II, Algebra. In addition, all courses of theBachelor in Mathematics and all courses of the rinformation will be provided by the instructors a 13. Module exam: Competence / topic/areaType of examDuratiTopic from 12.				troduct tial Diff odeling e modu naster p t the be	tion to Pro ferential E , Numeric le Intensi program I eginning o	obability Theo equations II, F s of Partial D fication - Bac Mathematics of the course Time	ory and Statistics, Numerics Functional Analysis, ifferential Equations, Linear helor of the studies program may be attended. Further Weighting of module grade Graded, 100%		
Topic from 12. Oral or written Written: 90-180 min Oral: 20-45		90-180 min. Oral: 20-45	min.	end of se	emester				
14.	Notes:	The modu	ile cannot be c	ompleted as	part o	f a bache	lor's degree.		

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. C con	4. Qualification objectives of the module / competencies to be acquired:					iring in-de	epth knowlec	lge of applied mathematics
5. Prerequisites for participation:								
	a) Reco	mmendeo	d knowledge:		Analy	vsis I – III,	linear algebra	a
	b) Prere	equisite co	ourses:		None)		
6. I	Module	can be us	ed for:		MSc.	in Compu	utational Scie	nce
7. N	Module	is offered	:		Each	semester		
8. N	Module	can be co	mpleted in:		1 sen	nester		
9. F	Recomm	ended se	mester of stu	ıdy:	1st se	emester o	r higher	
 10. Module workload / number of credit points: 11. The module is successfully completed w 				f credit mpleted w	 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 hen the requirements below have been met: 			
No.	R / RE	Form of teaching	Subject area/to	opic		Credit hours	Coursework	<u> </u>
1	R	Lecture Practical course	See below See below			4 2	Practical exer	cises
Elective participation in the following courses: Introduction to Probability Theory and Statistics, Numerica II, Analysis IV, Partial Differential Equations I, Partial Differential Equations II, Functional Analysis, Optimization, Optimal Control, Mathematical Modeling, Numerics of Partial Differential Equations, Linea Algebra II, Algebra. In addition, all courses of the module Intensification - Bachelor of the studies progra 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.						ory and Statistics, Numerics Functional Analysis, Differential Equations, Linear chelor of the studies program may be attended. Further		
13.	Module	e exam:	1					1
Competence / Type of Duratic topic/area exam			n	n Time Weighting of module grade		Weighting of module grade		
Topic from 12. Oral or Written: written 90-180 min. Oral: 20-45			min.	Lecture per end of sem	riod to lester	Graded, 100%		
14.	Notes:	The modu	le cannot be c	ompleted as	part o	of a bache	lor's degree.	

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	Subjec	Subject area/topic		Coursev	vork		
1	R	Lecture	The students c from a given se doubt, please o academic advis	hoose the lecture et of lectures. If in consult with an cor.	2 credit hours / 30 hours				
4	R	Lecture	The students c from a given se doubt, please o academic advis	The students choose the lecture from a given set of lectures. If in doubt, please consult with an academic advisor.					
Not	Notes:								
12.	Modu	le exam:							
ME PM	/ Cor E*	itents of exam	Type of exam	Duration	Time		Type of evaluation		

At the end of semester

45 min.

10 CP

' 13. N	otes:	Uldi exalli
TI		

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

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 a	rea/topic	Credit hour	s Co	oursework		
1	R	Lecture	Experimental G	enomic Science Part	1 2 credit hours 30 hours	s /			
2	R	Seminar	Introduction to Experimental Genomic Science Laboratory (1st sem.)		1 credit hour 15 hours	. /			
3	R	Course	Methods in Exp Science (1st ser	perimental Genomic m.)	4 credit hours 60 hours	s / Exp	periment reports		
4	R	Lecture	Experimental G	enomic Science Part	2 1 credit hour 15 hours	. /			
5	R	Seminar	Literature Semi Genomic Scien	nar in Experimental ce	1 credit hour 15 hours	/ Lee	cture		
6	R	Seminar	Introduction to Genomic Scient sem.)	troduction to Experimental 1 credit hour / enomic Science Laboratory (2nd 15 hours m.)		. /			
7	R	Course	Methods in Exp Science (2nd se	erimental Genome em.)	4 credit hours 30 hours	s / Exp	periment reports		
Not	es:								
12.	Modu	le exam:							
ME PM	/ Co E*	ntents of exam	Type of exam	Duration	Time		Type of evaluation		
PME	Exp (Sc	oerimental Genome ience Part 1 & 2	Exam	120 min.	End of 2nd seme	ester	Graded		
Not exa	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.	Misce	llaneous/re	marks:						
a) L Lott Reh Brov Villa	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) T	he moo	dule cannot	be completed a	as part of a bachel	or'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
Not	es:				

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 m	odule cannot be	e completed as	part of a bacheld	or's degree.					

CS-M-P7

1. Module title:					CS-M-P7: Lattice QCD I			
2. F	ield / r	responsibili	ty of:	Physics / department, Dean of Studies				
3. N	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:					ring a fun of indepo ction of t ods to a n	damental knowledge of lattice QCD. The endent transfer, generalization and the studied description and solution ew problem.		
5. P	Prerequ	uisites for p	articipation:					
a) R	Recomr	mended kn	owledge:	Basic knowledge of at least one of the programming languages Fortran, C and C++; basic knowledge of quantum field theory				
b) F	Prerequ	uisite cours	es:	None				
6. N	Module	e can be use	ed for:	MSc. in Computational Science, MSc. in Physics				
7. N	Module	is offered:		On a yearly basis				
8. N	Module	e can be co	npleted in:	1 semester				
9. F	Recomr	mended ser	mester 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 m	odule is su	ccessfully completed w	hen th	e require	ements below have been met:		
12.	Modu	le compone	ents:					
No. R / RE Form of teaching Subject area/topic			5	Credit hours	Coursework			
1	R	Lecture Practical course	Lattice QCD I Lattice QCD I		4 2	Practical exercises		
Furt	ther info	ormation wi	l be provided by the instru	uctors a	at the beg	inning 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. N	/Iodule ti	tle:		CS-M-P8: Lattice QCD II			
2. F	ield / res	ponsibility	of:	Physics / department, Dean of Studies			
3. N	Aodule co	ontents:		 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:					ng advai ity to ind tion and r, genera	nced knowledge of lattice QCD as well as dependently apply to a new problem the solution methods studied by means of alization and abstraction.	
5. P	Prerequisi	tes for par	ticipation:				
a) R	lecomme	nded knov	vledge:	Basic knowledge of at least one of the programming languages Fortran, C and C++; basic knowledge of quantum field theory, lattice QCD I			
b) F	Prerequisi	te courses	:	None			
6. N	Aodule ca	an be used	for:	MSc. in Computational Science, MSc. in Physics			
7. N	Aodule is	offered:		On a ye	arly bas	is	
8. N	/lodule ca	an be com	oleted in:	1 semester			
9. F	Recomme	nded seme	ster of study:	2nd ser	nester o	r higher	
10. Module workload / number of credit points:					 Workload: Total number of hours: 8 CP x 30 = 240 hours Allocation: Attendance: 1 sem. x 15 weeks x 6 credit hours = 90 hours Independent study, exam preparation: 150 hours Credit points: 8 		
11.	The mod	lule is succ	essfully completed w	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	Lattice QCD II Lattice QCD II		4 2	Practical exercises	

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 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	Exam: 105 min. or 135 min. or 210 min. (if it consists of two parts)	At the end of semester	Graded (100%)				
	oral	Oral: 25-35 min.						
14. Notes: The module cannot be completed as part of a bachelor's degree.								

NS-M	-4
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Nanoscience			
Physics / department, Dean of Studies			
 Fundamentals Introduction and overview Multi-electron systems and Born- Oppenheimer approximation Periodic and finite nanostructures Density functional theory (DFT) Interacting electron gas Hartree-Fock approximation Basic theorems of DFT Exchange-correlation functionals Numerical aspects of DFT Basis set development Implementation for periodic and finite systems Applications Theoretical spectroscopy Quantum molecular dynamics 			
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.			
Quantum mechanics II			
None			
MSc. in Nanoscience, BSc. in Physics, BSc. in Nanoscience, BSc. in Comp. Science, MSc. in Physics, MSc. in Computational Science			
On a yearly basis			
1 semester			
1st semester (master) or higher			
 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.	12. Module components:								
No.	R / RE	Form of teaching	Subject are	ea/topic	Credit hours	Coursework			
1	R	Lecture	Computation Nanoscience	onal ce	4				
2	R	Labs	Computation Nanosciene	onal ce	2				
Further information will be provided by the instructors at the beginning of the course.									
13.	Mod	ule exam		-			-		
Cor	Competence / topic Type of exam Duration Time / notes Weighting of module grade								
Cor Nar	Computational NanoscienceLaboratory reportEnd of lecture period to end of semesterGraded, 100%								
14. Foll kno an e	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.

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:	 Fundamentals: Simulation methods, forces in molecular systems, electrostatics, thermostats, barostats Determining structural, thermodynamic and dynamic characteristics Free energy simulations Classical force fields Applications: Water, polymeres, proteins 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 successf	ully completed when	n the requirements	below have been met.
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12. Module components:									
No.	R / RE	Form of teaching	Subject are	a/topic		Credit hours	Coursework		
1	R	Lecture	Introductic Molecular	on to Dynamics I		2			
2	R	Lecture	Introduction to Molecular Dynamics II			2			
3	R	Practical course	Introduction to Molecular Dynamics			2			
Furt	her in	formation	will be prov	vided by the i	nstructors at	the beg	ginning of the course.		
13.	Mod	ule exam							
Competence / topic Type of Duration Time / notes						Time / notes	Weighting of module grade		
Molecular Dynamics				Oral exam	20 mi	n.	End of lecture period to end of semester	Graded, 100%	
14.	Note	s:			•		·		