HGS MathComp

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

The Future of Simulation

14th Annual Retreat
of the Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences

September 5–7, 2022
Speyer, Germany

Last updated 1st of September 2022.
The latest version of this booklet can be found at:
https://www.mathcomp.uni-heidelberg.de/fellows/annual-retreat-2022

The open-source LATEX template, AMCOS_booklet,
used to generate this booklet is available at:
https://github.com/maximelucas/AMCOS_booklet

HGS MathComp

14th Annual Retreat

Book of Abstracts

Speyer 2022

Contents

About

The latest information about the event can be found at
https://www.mathcomp.uni-heidelberg.de/fellows/annual-retreat-2022

HGS MathComp

excerpt from https://www.mathcomp.uni-heidelberg.de/home

The Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences (HGS MathComp) at Heidelberg University is the only graduate school in Germany to focus on the complex topic of Scientific Computing. Placed in a vibrating research environment, the school is funded by the German Excellence Initiative and offers a uniquely structured interdisciplinary education for PhD students. The program enables students to pursue innovative PhD projects with a strong application-oriented focus anywhere from mathematics, physics and chemical engineering sciences to cultural heritage.

Members of HGS MathComp are top experts in their fields and work on projects that combine mathematical methodology with topical research issues. Individual mentoring and career-building programs ensure that graduates acquire all qualifications for top positions in industry and science.

Annual Retreat

The Annual Retreat (formerly Annual Colloquium) is an event organized by members of the HGS MathComp (the fellow speakers) for members of the HGS MathComp. It features talks from researchers both academic and from the industry as well as talks and posters from the members themselves. The Retreat generally takes place at a remote location to foster a more intimate environment for the attending members and encourage discussions both scientific and personal.

Organizing committee

Manuel Weiß Masoumeh Hashemi Nils Oberhof
Sarah Steinbach Michael Winckler

Timetable

CT: Contributed Talk, IT: Invited Talk.

Monday, 5th of September

13:00–14:00	**Arrival and Registration**		
14:15–14:30	**Welcome remarks by Fellow Speakers**		
14:30–15:30	IT	**Benjamin Stamm** RWTH Aachen	Acceleration of Quantum Mechanical Simulations by Exploiting Similarity
15:30–16:00	CT	**Marcel Meyer** IWR	Invertible Neural Networks for Molecular Interactions
16:00–16:30	**Coffee Break**		
16:30–17:30	IT	**Gerit Brandenburg** Merck	Future of Simulation in Industry: Physics or Data Driven Approaches
17:30–18:00	CT	**Jonathan Teuffel** HITS	Learning the Determinants of Interprotein Electron Transfer From Combined Quantum Mechanics and Molecular Mechanics Simulations
18:30–19:00	**Walk to Dinner Venue**		
19:00–open end	**Dinner at Loi Xua**		
late night (optional)	**Board Games in the Common Room**		

Tuesday, 6th of September

7:00–9:30	**Breakfast**		
09:30–10:30	IT	**René Haber** BASELABS	Challenges in Automotive Sensor Fusion
10:30–11:00	**Coffee Break**		
11:00–11:30	CT	**Tom Rix** DKFZ	Photoacoustic Image Synthesis with Deep Learning
11:30–12:00	CT	**Da Eun Kang** IMPRS-HD	Emission-Line Diagnostics of HII Regions Using Conditional Invertible Neural Network
12:00–13:30	**Lunch**		
13:30–14:00	IT	**Florian Krellner** SAP	Quantum Optimization SAP
14:00–14:30	CT	**Eric Hartmann** HITS	Developing a Reactive Molecular Dynamics Scheme for Protein Mechanochemistry
14:30–15:00	**Break**		
15:00–16:00	IT	**Johannes Fieres** Volume Graphics	Physics Simulation Based on Industrial Computed Tomography Images
16:00–16:30	**Coffee Break**		
16:30–17:00	IT	**Lisa Koeppel** Denkinger Group Global Dx	Statistical Modelling of Infectious Diseases
17:00–18:00		**HGS Fellow Speakers & Participants**	**Discussion:** Not Simulation But Reality: Moving the HGS MathComp Forward
18:00	**Dinner at Jugendherberge Speyer – Free Evening**		
late night (optional)	**Board Games in the Common Room**		

Wednesday, 7th of September

7:00–9:30	**Breakfast**		
9.30–10:30		**Fellow Speakers**	Closing Remarks
10:30	**Leaving the Premises**		

List of Abstracts – Talks

Monday 5th

Acceleration of Quantum Mechanical Simulations by Exploiting Similarity

Benjamin Stamm, RWTH Aachen **IT**

In this talk, we will present two examples of exploiting similarity of solu-tions to minimize the computational effort while maintaining accuracy for the simulation of approximation to quantum mechanical systems. In the first ex-ample, we present an alternative to extended Lagrangian Born-Oppenheimer molecular dynamics simulations at the level of theory of DFT or Hartree-Fock that is based on an extrapolation of previous solutions on the tangent space of the Grassmann manifold. The second example illustrates the performance of the reduced basis method for quantum-spin systems. We illustrate in examples that, surprisingly, while the dimension of the underlying Hilbert space increases exponentially with the number of particles, the Kolmogorov N -width for these parametrised examples only increases slightly. Further, the greedy-strategy to assemble the reduced basis only requires very few high-dimensional solutions to be computed.

Invertible Neural Networks for Molecular Interactions

Marcel Meyer, IWR **CT**

Protein-biomolecule-interactions are ubiquitous in life, from DNA-replication to regulating the heartbeat. The stability of biomolecular complexes depends heavily on the involved proteins' amino acid sequence. Changes in this sequence and their effects on complex formation are of interest in many diseases, but also in protein design. However, predicting how two molecules will interact remains a challenge due to the high degrees of freedom both within and between the interaction partners. In the recent past, deep neural networks have proved useful for structure prediction of biomolecules. We investigate the suitability of invertible neural networks (INNs) for predicting the structures of molecular complexes, as well as the effects of mutations in sequence. INNs are interesting candidates because they model the full probability distribution of molecular interactions. Also, they do not suffer from the curse of high dimensionality and can therefore be scaled to very large problems like protein-protein-interactions. Major tasks at hand are finding the right representation of the molecular structure and building suitable network architectures. Once we can reliably predict molecular interactions, we will integrate sequence information to learn how sequence alterations influence the structure of biomolecular complexes.

Future of Simulation in Industry: Physics or Data Driven Approaches

Gerit Brandenburg, Merck **IT**

Emerging technologies are based on molecules and materials with highly optimized properties. New materials are needed in an increasing pace, and thus material discovery has to as well. Approaches based on the fundamental laws of quantum mechanics combined with machine learning are nowadays integrated to many design initiatives in academia and industry, underpinning efforts such as the Materials Genome initiative or autonomous laboratories. The different driving forces for academic developments and industrial applications and the trade-off between physics and data driven approaches will be discussed. Two industry uses cases will focus on (i) application of simulated electronic spectra for identifying and quantifying impurities in OLED material production and (2) using a digitally enhanced materials kit for effective catalyst optimization.

Learning the Determinants of Interprotein Electron Transfer from Combined Quantum Mechanics and Molecular Mechanics Simulations

Jonathan Teuffel, HITS **CT**

Cytochrome P450 (CYP) is a family of heme-containing enzymes which catalyze reactions to increase solubility and reactivity of drug molecules and steroid hormones. As such, they determine the speed at which most drugs are metabolized by the human body. The net-reaction of CYPs requires supply of external electrons from complementary redox proteins such as NADPH-Cytochrome-P450 Oxidoreductase. Electron-transfer between the redox-centers happens over large distances of about 15-25 A and is hence, relatively slow. A quantitative understanding of the kinetic determinants of this process is desirable as it has been demonstrated to be rate-limiting for some CYPs and since different CYPs within a shared environment are assumed to compete for electrons from a limited number of redox-proteins. Within the CYP family the redox-protein binding mode and ET kinetics differ significantly between individual sequences. We are interested in identifying the sequence features steering these parameters. To increase accuracy of our current approach, we aim to develop a multiscale-simulation protocol to quantitatively describe the ET-kinetics between different CYPs and their redox-partners by combining molecular simulations with machine learning approaches. Once a reliable simulation protocol for computing ET-characteristics has been established, we intend to learn sequence-features within the CYP family, which determine the electron transfer kinetics using machine learning models.

Tuesday 6th

Challenges in Automotive Sensor Fusion

René Haber, Project Manager Dynamic Grid, BASELABS GmbH **IT**

In the last ten years the detection density of automotive sensors has increased enormously. Where a radar sensor delivered one detection per object back then, it may now provide 50 detections or more. The same holds for the resolution of lidars and cameras. With the increasing capabilities of the sensors and the increasing expectations of driving functions, sensor fusion has become challenging. In this talk, an overview of the algorithms which BASELABS uses to tackle these problems will be presented and an outlook to still unsolved problems will be given.

Photoacoustic Image Synthesis with Deep Learning

Tom Rix, DKFZ **CT**

Advances in machine learning techniques have yielded breakthrough successes in various domains, but the lack of a gold standard method for obtaining labelled ground truth training data in vivo has been a great obstacle in transferring state-of-the-art methodology to spectral image quantification. Synthetic training data generation has been proposed as a means for overcoming this bottleneck, but while state-of-the-art methods for generating synthetic data such as Monte Carlo simulations are physically accurate, they are very time consuming. In the talk, it will shown that deep learning methods can be leveraged for spectrally accurate and fast image synthesis. Within the talk a focus will specifically be set on the task of optical simulation of the absorbed light energy in photoacoustic imaging (PAI) given the optical absorption and scattering.

Emission-line Diagnostics of HII Regions Using Conditional Invertible Neural Network

Da Eun Kang, IMPRS-HD **CT**

The stellar feedback is an energetic interaction between star clusters and the surrounding interstellar medium (ISM), activated by young massive stars. Energy injected by massive stars disrupts the surrounding environment and regulates further star formation. Information on young star clusters and their birthplace inhere in emission lines observed from star-forming regions. However, inferring the physical properties of star-forming regions from observations is difficult for the following two reasons. First, the forward process from nature to observation is so complicated and non-linear that it is not easy to understand this overall process by ordinary forward modeling methods. Second, information loss during the forward process leads to degeneracy in observations, making it hard to solve the inverse problem. On this account, we develop a novel method that estimates the physical properties of star-forming regions directly from spectral observations by coupling a conditional invertible neural network (cINN, Ardizzone et al. 2021) with the WARPFIELD-emission predictor (WARPFIELD-EMP, Pellegrini et al. 2020). In this talk, I will present a cINN that predicts the posterior distribution of seven physical parameters (cloud mass, star formation efficiency, cloud density, cloud age which means age of the first generation stars, age of the youngest cluster, the number of clusters, and the evolutionary phase of the cloud) from the luminosity of 12 optical emission lines, and test result of our network with synthetic models that are not used during training.

Quantum Optimization @ SAP

Florian Krellner, SAP **IT**

Mathematical optimization is in the backbone of automated intelligent decision making. Being NP-hard in general, the solving methods often suffer from bad performance. After its (theoretical) success in factorizing the product of two prime numbers and solving sparse linear systems of equations, quantum computing is applied with great hope to mathematical optimization to speed up the solution process. Currently, both, the quantum hardware and quantum optimization methods are still in the early phases and much research is needed to develop production-ready quantum solutions. In this talk we will show, first, how mathematical optimization is used in SAP solutions and, second, how we approach the challenges we face in developing quantum optimization methods. We will focus on quadratic unconstraint binary optimization problems (QUBOs) and quantum annealing due to the hardware being the most mature quantum technology currently available on which it is possible to solve a bit bigger academic (toy) problems of interest.

Implementing Reactions for Classical Molecular Dynamics Simulations

Eric Hartmann, HITS **CT**

It has been established nearly a century ago that mechanoradicals originate from homolytic bond scission in polymers. Recently, formation of radicals through mechanical stress has been shown in the protein collagen, indicating a role for mechanoradicals in biology. Classical Molecular Dynamics simulations could serve as a tool to understand the mechanisms behind radical formation and propagation but reach their limit because of their non-reactive nature. To push this limit of classical Molecular Dynamics, we are developing a reactive scheme. Here, reactions are treated separately by using the kinetic Monte Carlo method. This allows for long simulations in which reactions could occur in any part of the system. The implementation is open source, modular and extensible with user friendliness in mind.

Physics Simulation Based on Industrial Computed Tomography Images

Johannes Fieres, Volume Graphics GmbH, Heidelberg **IT**

Computed tomography (CT) has developed to be a standard inspection tool in industry, used throughout the entire manufacturing workflow, in research, production, and quality control. Classical inspection tasks aim at assessing geometric parameters of the scanned object, like, for example, measuring dimensions, quantifying internal porosity, or comparing the object to a reference shape. Often, the geometric parameters are used to infer about functional aspects, like stability of a part, based on experience and statistical heuristics. Image-based simulation aims at recovering the functional aspects directly from the CT scans, by performing physics simulations based on models extracted from the CT data. Volume Graphics GmbH is a developer of software for the analysis of industrial CT data. In this talk, we will first learn about the basics of industrial CT and then visit some recent projects involving image-based simulation.

List of Participants

Andreas Dreuw	IWR, Heidelberg
Anna Weidlich	IWR, Heidelberg
Arne Strehlow	IWR, Heidelberg
Benjamin Thomitzni	IWR, Heidelberg
Da Eun Kang	IMPRS-HD, Heidelberg
Eric Hartmann	HITS, Heidelberg
Freya Bretz	IWR, Heidelberg
Hridya Vinod Varma	IWR, Heidelberg
Jonathan Teuffel	HITS, Heidelberg
Josephine Westermann	IWR, Heidelberg
Maike Rees	DKFZ, Heidelberg
Manuel Weiß	IWR, Heidelberg
Marcel Meyer	IWR, Heidelberg
Marco Bauer	IWR, Heidelberg
Marco Hübner	DKFZ, Heidelberg
Masoumeh Hashemi	IWR, Heidelberg
Michal Tóth	IWR, Heidelberg
Nils Oberhof	IWR, Heidelberg
Pau Badia i Mompel	EMBL, Heidelberg
Reyhaneh Majidi	IWR, Heidelberg
Robert Kutri	IWR, Heidelberg
Santiago Ospina De Los Rios	IWR, Heidelberg
Sebastian Thielen	IWR, Heidelberg
Sophia Müller-Dott	EMBL, Heidelberg
Stefan Meggendorfer	IWR, Heidelberg
Tobias Kaczun	IWR, Heidelberg
Tom Rix	DKFZ, Heidelberg
Tristan Ranff	GSK, Heidelberg
Invited Speakers:	
Benjamin Stamm	RWTH Aachen
Florian Krellner	SAP
Gerit Brandenburg	Merck
Johannes Fieres	Volume Graphics
Lisa Koeppel	Denkinger Group
René Haber	BASELABS

Useful Information

The Annual Retreat will be held at the Jugendherberge Speyer (`https://www.diejugendherbergen.de/jugendherbergen/speyer`).

How to get to the Jugendherberge Speyer

The Jugendherberge Speyer is located at Geibstraße 5, 67346 Speyer.

It can be reached by **car** coming from the A61 Exit "Speyer", via the B9 and B39 in the direction "Dom/Museum". You cross the intersection towards "Jugendherberge". Afterwards turn right at the Technik Museum towards "Freibad und Jugendherberge".

It can also be reached by **public transport** by arriving at Speyer (line Ludwigshafen-Karlsruhe). From there you can take the buses 564 and 565 towards "Flugzeugwerke" and exit at the bus stop "Bademaxx/DJH".

Heidelberg Graduate School
of Mathematical and Computational Methods
for the Sciences

Chairman

Prof. Dr. Robert Scheichl
Institute of Applied Mathematics
Mathematikon
Im Neuenheimer Feld 205
69120 Heidelberg

Administrative Director

Dr. Michael J. Winckler
Heidelberg Graduate School
of Mathematical and Computational Methods
for the Sciences (HGS MathComp)
Mathematikon
Im Neuenheimer Feld 205
69120 Heidelberg

Email: michael.winckler@iwr.uni-heidelberg.de

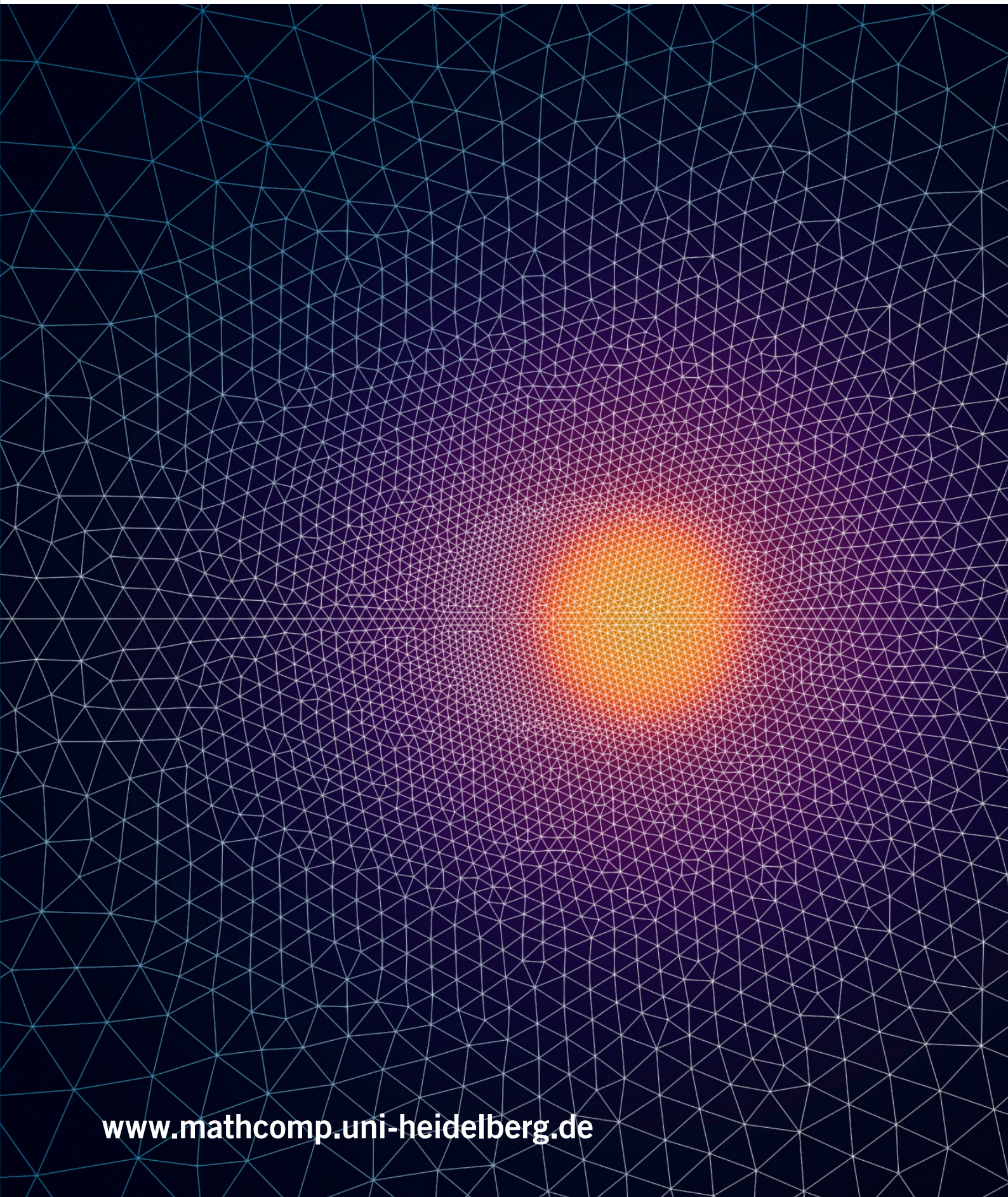
Office

HGS MathComp
Mathematikon · Room 5/214
Im Neuenheimer Feld 205
69120 Heidelberg

Phone: +49 (0) 6221 54 -14 410
Email: hgs@iwr.uni-heidelberg.de

Opening Hours
Monday & Thursday: 09:00–12:00 · 14:00–16:00
Wednesday: 10:00–12:00 · 14:00–16:00
Tuesday & Friday: closed

UNIVERSITÄT
HEIDELBERG
ZUKUNFT
SEIT 1386



www.mathcomp.uni-heidelberg.de