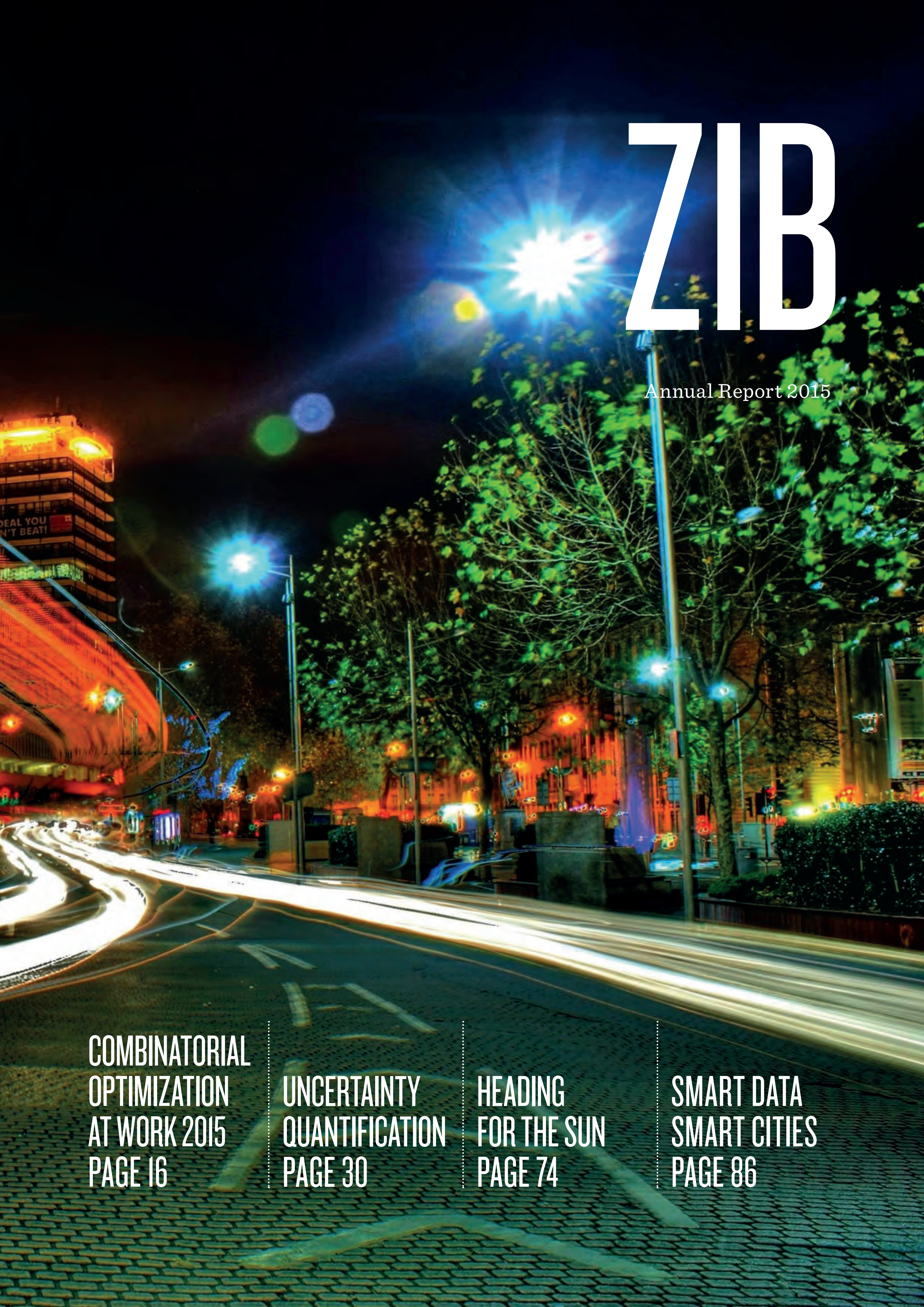

ZIB

Annual Report 2015

COMBINATORIAL OPTIMIZATION AT WORK 2015
PAGE 16

UNCERTAINTY QUANTIFICATION
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HEADING FOR THE SUN
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SMART DATA SMART CITIES
PAGE 86

ZIB

WWW.ZIB.DE

PREFACE

2015 was a year of change for ZIB: one era has ended, and a new one has started. All-time records were achieved, and limits were reached.

After 30 very successful years, the era of leadership by Peter Deuflhard and Martin Grötschel ended with Martin stepping down as President of ZIB on September 30, 2015, after having taken over from Peter in 2012.

Peter Deuflhard became President of ZIB 30 years ago. He formed ZIB into one of the first and most successful institutes for Scientific Computing in Europe. Under his leadership the institute became a driving force in research and service in computing, and established itself as an institution working at the forefront of Numerical Mathematics and Visualization. In the early 1990s, Martin Grötschel was appointed Vice-President of ZIB and started the Discrete Mathematics division with the aim of solving very large practical combinatorial optimization problems which were unsolvable by then-existing methods. Research in Discrete Mathematics was complemented by activities in Computer Algebra and Scientific Information. At the end of the 1990s, with the arrival of Alexander Reinefeld, the new head of ZIB supercomputing, research activities were broadened again. In addition to the divisions of Numerical Analysis and Discrete Mathematics, a third scientific division, Computer Science, was created. This division combined research in Applied Computer Science with all computer-related service aspects under one umbrella, and this led to an even closer link between research and service.

With Peter and Martin no longer in the driving seat, ZIB now takes the next step in the continuing advancement of the institute, and enters a new era by claiming the role of Berlin's Competence Center for the Digital Sciences. Computer-aided research has become an indispensable third pillar of science alongside theory and experiment. The cores of this pillar, which has established itself in recent years with great vigor, are the fields of Computing, including Modeling, Simulation and Optimization, and Data Science, which are now starting to merge into one new field, "Digital Science". ZIB, with its rich portfolio of collaborative projects in Applied Mathematics and Applied Computer Science, with regional, national and international partners and its expertise and capacities in data and information science, seems to be ideally placed for this endeavor, both scientifically as well as location-wise, as a part of Berlin's thriving research and technology landscape.

Despite these major changes, ZIB continues to be a place booming with excellent research and first-rate scientific services and infrastructure. 2015 broke several all-time records, an achievement made possible by the strong commitment of all of ZIB's members: in total, almost 8 million Euros' worth of third party funding were acquired, which marked an increase for the fourth year in a row and a new record in ZIB's history! With more than one hundred on-going research projects, ZIB grew to have over 220 employees, complemented by more than 60 research fellows and long-term guests. These numbers mean that we are reaching the capacity limit of our present building and infrastructure. Therefore, priority shifts leading to a concentration of activities around ZIB's main competence fields are expected to occur in the next years.

This annual report provides a general overview of ZIB's organization and key factors for its successful development. A few feature articles, which combine brief surveys of outstanding topics that highlight our own work - keeping global developments in mind – illustrate the progress made during the year.

The article on "Uncertainty Quantification" gives a general introduction to UQ and Bayesian Inverse Problems and describes ZIB's activities in these fields, with applications to system biology, parameter estimation, optical metrology, molecular design, computer vision, and geometry reconstruction, including the relation to uncertainty visualization.

"Systems Biology" features mathematical modelling and simulation in reproductive medicine, concerning the metabolism of high-performance dairy cows, as well as image analysis for understanding molecular signaling, and it also illustrates the software tools developed at ZIB in these fields.

"An Educated Guess" is a text about the ubiquity of difficult optimization problems in everyday life and how to solve them using heuristics. In a slightly modified form, this text won the Klaus Tschira Award 2015 for Achievements in Public Understanding of Sciences.

"New KOBV Portal" presents the relaunch of the web portal of the Collaborative Library Network Berlin-Brandenburg at ZIB, which enables discoveries in 60 libraries and handles more than 1 million individual queries per month.

Turning back to in-depth research, "Heading for the Sun" outlines the insight that quantum-mechanical coherence plays a role for efficient energy transfer in photoactive complexes. Here, the simulation of coherent energy transfer processes in complex molecules requires the design of new scalable algorithms for current and future many-core supercomputers.

Finally, the article "Smart Data, Smart Cities" illustrates how ZIB's expertise in scalable and distributed databases can be utilized and extended to establish reliable smart internet-enabled services within European cities.

Obviously, these feature articles can only be appetizers. The readers interested in the specifics of ZIB's activities can find further feature articles and the full technical details of our research and services, of our projects, and the statistics about publications, lectures, etc. on ZIB's web pages: the starting point is www.zib.de.

Last but not least, ZIB is grateful for having many supporters and friends. Thanks to all those who provide us with encouragement, assistance and advice.

Berlin, May 2016
Christof Schütte
ZIB President

CONTENTS

EXECUTIVE SUMMARY

MATHEMATICS FOR LIFE AND MATERIALS SCIENCES

The last year saw a surge of activities in the fields of data-intensive computing and uncertainty quantification in accordance with the priority shift initiated the year before.

Examples of these developments are the establishment of the new research group Uncertainty Quantification and the launch of a collaborative data analysis and management platform for scientists jointly with Freie Universität Berlin. Treatment of uncertainties also penetrates a multitude of other activities from optical metrology to visualization, as outlined in the feature article "Uncertainty Quantification."

These new developments are complemented by a successful continuation of activities in modelling, simulation, and optimization as well as visual data analysis, with the foundation of the Joint Lab for Optical Simulations for Energy Research together with Helmholtz-Zentrum Berlin for Materials and Energy and Freie Universität Berlin, the extension of the DFG-CRC 765 and graduate school SALSA, and new topics such as photoacoustic tomography. Another focus of research has been laid on joint diseases, with several projects in the BMBF Research Networks on Musculoskeletal Diseases and ECMath.

MATHEMATICAL OPTIMIZATION AND SCIENTIFIC INFORMATION

In its first year, the Research Campus MODAL has grown considerably. New industrial and academic partners joined the four labs to broaden the scope and to intensify the transfer of scientific insights and technological innovations, ranging from the construction of fully dated ICE rotations for DB Fernverkehr to the solution of general mixed-integer nonlinear optimization problems by the leading academic solver SCIP, which has recently successfully utilized 80,000 cores in parallel. On the educational edge, the third Combinatorial Optimization at Work summer school attracted more than 100 students and researchers from all over the world.

The Scientific Information department develops information systems and services for the sciences. During the year, a completely new search portal for the Berlin-Brandenburg library network went operational. It allows people to search for more than 25 million books in regional libraries. A major effort was put into building a trusted long-term archive system.

PARALLEL AND DISTRIBUTED COMPUTING

Supercomputers age fast. With the HLRN-III supercomputer only in its second year of full production, it was already time to plan for an even more powerful successor to be installed in 2018. Our proposal for the HLRN-IV was recently positively decided by the German Science Council. Of course, we are very happy about this decision because it sets green lights for the European procurement in 2016, vendor negotiations in 2017 and installation in 2018.

The research division is internationally renowned for its strong theoretical background on distributed algorithms. Now it is becoming more application-oriented. Just three examples: In the Smart Data – Smart Cities project (see feature article), we provide robust data management for mobile citizens. Fault-tolerant software in the automobile sector is a second focus. We started a research project on the verification of concurrent software that drives the many digital devices in modern cars. A third field is energy, where we are simulating the conversion process of solar energy in photosynthesis (feature article: "Heading for the Sun: Where Quantum Physics Meets Photosynthesis"). As usual, these are just three motivating examples of our wide research spectrum.

ADMINISTRATIVE BODIES

The bodies of ZIB are the President and the Board of Directors *(Verwaltungsrat)*.

President of ZIB was
PROF. MARTIN GRÖTSCHEL
until September 30, 2015

President of ZIB is
PROF. CHRISTOF SCHÜTTE
since December 1, 2015

Vice President of ZIB was
PROF. CHRISTOF SCHÜTTE
until November 30, 2015

Vice President is
N.N.

The Board of Directors was composed in 2015 as follows

PROF. PETER FRENSCH
Vice President, Humboldt-Universität zu Berlin (Chairman)

PROF. CHRISTIAN THOMSEN
President, Technische Universität Berlin (Vice Chairman)

PROF. BRIGITTA SCHÜTT
Vice President, Freie Universität Berlin

BERND LIETZAU
Senatsverwaltung für Wirtschaft, Technologie und Forschung

N.N.
Senatsverwaltung für Bildung, Jugend und Wissenschaft

PROF. MANFRED HENNECKE
Bundesanstalt für Materialforschung und -prüfung (BAM)

PROF. ANKE KAYSSER-PYZALLA
Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)

DR. HEIKE WOLKE
Max-Delbrück-Centrum für Molekulare Medizin (MDC)

The Board of Directors met on June 3, 2015, October 21, 2015, and December 11, 2015.

SCIENTIFIC ADVISORY BOARD

The Scientific Advisory Board advises ZIB on scientific and technical issues, supports ZIB's work, and facilitates ZIB's cooperation and partnership with universities, research institutions, and industry.

The Board of Directors appointed the following members to the Scientific Advisory Board:

PROF. JÖRG-RÜDIGER SACK
Carleton University, Ottawa, Canada

PROF. ALFRED K. LOUIS
Universität des Saarlandes, Saarbrücken

PROF. RAINER E. BURKARD
Technische Universität Graz, Austria

PROF. MICHAEL DELLNITZ
Universität Paderborn

LUDGER D. SAX
Grid Optimization Europe GmbH

DR. ANNA SCHREIECK
BASF SE, Ludwigshafen

DR. HORST D. SIMON
NERSC, Lawrence Berkeley National Laboratory, USA

DR. REINHARD UPPENKAMP
Berlin Chemie AG, Berlin

DR. KERSTIN WAAS
Deutsche Bahn AG, Frankfurt am Main

The Scientific Advisory Board met on June 22 and 23, 2015, at ZIB.

THE STATUTES

The Statutes, adopted by the Board of Directors at its meeting on June 30, 2005, define the functions and procedures of ZIB's bodies, determine ZIB's research and development mission and its service tasks, and decide upon the composition of the Scientific Advisory Board and its role.

ORGANIZATION

SCIENTIFIC ADVISORY BOARD

CHAIRMAN PROF. JÖRG-RÜDIGER SACK | *Ottawa*
PROF. RAINER E. BURKARD | *Graz*
PROF. MICHAEL DELLNITZ | *Paderborn*
PROF. ALFRED K. LOUIS | *Saarbrücken*
LUDGER D. SAX | *Essen*
DR. ANNA SCHREIECK | *Ludwigshafen*
DR. HORST D. SIMON | *Berkeley*
DR. REINHARD UPPENKAMP | *Berlin*
DR. KERSTIN WAAS | *Frankfurt am Main*

BOARD OF DIRECTORS

CHAIRMAN: PROF. DR. PETER FRENSCH
Humboldt-Universität zu Berlin (HUB)

PRESIDENT

PROF. CHRISTOF SCHÜTTE

VICE PRESIDENT

N.N.

MATHEMATICS FOR LIFE AND MATERIAL SCIENCES

Prof. Christof Schütte

MATHEMATICAL OPTIMIZATION AND SCIENTIFIC INFORMATION

Prof. Ralf Borndörfer
Prof. Thorsten Koch

PARALLEL AND DISTRIBUTED COMPUTING

Prof. Alexander Reinefeld

ADMINISTRATION AND LIBRARY

Annerose Steinke

MATHEMATICS FOR LIFE AND MATERIAL SCIENCES
C. Schütte

NUMERICAL MATHEMATICS
M. Weiser

- COMPUTATIONAL MEDICINE — *M. Weiser, S. Zachow*
- COMPUTATIONAL MOLECULAR DESIGN — *M. Weber*
- COMPUTATIONAL NANO-OPTICS — *F. Schmidt*
- COMPUTATIONAL SYSTEMS BIOLOGY — *S. Röblitz*
- UNCERTAINTY QUANTIFICATION — *T. Sullivan*

VISUAL DATA ANALYSIS
H. Hege

- VISUAL DATA ANALYSIS IN SCIENCE AND ENGINEERING — *H. Hege*
- IMAGE ANALYSIS IN BIOLOGY AND MATERIAL SCIENCE — *S. Prohaska, D. Baum*
- THERAPY PLANNING — *S. Zachow*
- BIOINFORMATICS IN MEDICINE — *T. Conrad*

MATHEMATICAL OPTIMIZATION AND SCIENTIFIC INFORMATION
R. Borndörfer, T. Koch

MATHEMATIC OPTIMIZATION
R. Borndörfer, T. Koch

- MATHEMATICS OF TRANSPORTATION AND LOGISTICS — *R. Borndörfer*
- MATHEMATICAL OPTIMIZATION METHODS — *A. Gleixner*
- MATHEMATICS OF TELECOMMUNICATION — *A. Werner*
- ENERGY NETWORK OPTIMIZATION — *J. Zittel*

SCIENTIFIC INFORMATION
T. Koch

- WEB TECHNOLOGY AND MULTIMEDIA — *W. Dalitz*
- INFORMATION-TECHNOLOGY TOOLS FOR MUSEUMS — *C. Saro*
- DIGITAL PRESERVATION — *W. Peters-Kottig*
- SERVICE CENTER DIGITIZATION BERLIN — *A. Müller*
- KOBV LIBRARY NETWORK - RESEARCH AND DEVELOPMENT — *B. Rusch*
- KOBV LIBRARY NETWORK - OPERATING — *S. Lohrum*
- FRIEDRICH-ALTHOFF-KONSORTIUM — *U. Kaminsky*

LEGEND

- SCIENTIFIC DIVISIONS AND DEPARTMENTS
- RESEARCH GROUPS
- RESEARCH SERVICE GROUPS

PARALLEL AND DISTRIBUTED COMPUTING
A. Reinefeld

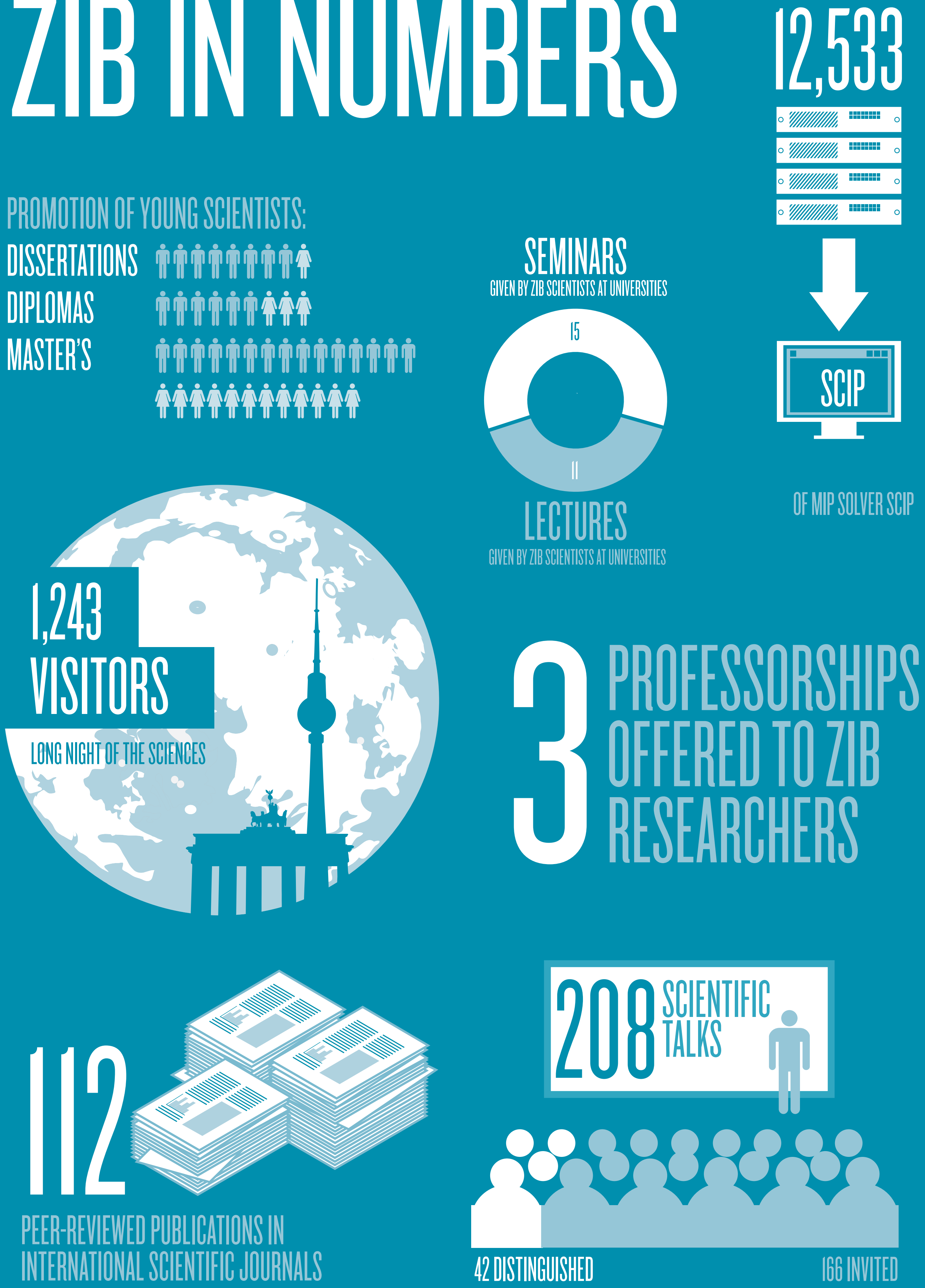
- **DISTRIBUTED ALGORITHMS AND SUPERCOMPUTING** — *F. Schintke, T. Steinke*
  - DISTRIBUTED DATA MANAGEMENT — *F. Schintke*
  - SCALABLE ALGORITHMS — *T. Schütt*
  - SUPERCOMPUTER ALGORITHMS AND CONSULTING — *T. Steinke*
  - SUPERCOMPUTER SYSTEMS — *C. Schimmel*
  - SOFTWARE SERVICE — *A. Löbel*
- **DATACENTER INFRASTRUCTURE** — *W. Pyszkalski*
  - DATA STORAGE AND ARCHIVES — *W. Pyszkalski, T. Pham*
  - SERVER AND LOCAL NETWORKS — *D. Krickel, S. Düring*
  - BERLIN METROPOLITAN NETWORK BRAIN — *W. Pyszkalski*

ADMINISTRATION AND LIBRARY
A. Steinke

ZIB is structured into four divisions, three scientific divisions, and ZIB's administration. Each of the scientific divisions is composed of two departments that are further subdivided into research groups. For further information on the broad spectrum of thematic and application foci of the research groups, please visit www.zib.de.

ZIB STRUCTURE

ZIB IN NUMBERS



AMIRA AVIZO

AMIRA AVIZO

AMIRA AVIZO

AMIRA AVIZO

5,500 LICENSES OF AMIRA AND AVIZO INSTALLED WORLDWIDE IN 2015

54 OUTREACH EVENTS FOR SCHOOL CLASSES AND THE GENERAL PUBLIC

€7,829,000

€5,723,000 PROJECT-RELATED, PUBLIC, THIRD-PARTY FUNDS

€2,106,000 INDUSTRIAL THIRD-PARTY PROJECTS

THIRD-PARTY FUNDING MARKED A NEW RECORD IN ZIB'S HISTORY

18 AWARDS

6,275 INTERNATIONAL GUESTS AT ZIB IN 2015

117 CONFERENCES AND WORKSHOPS AT ZIB

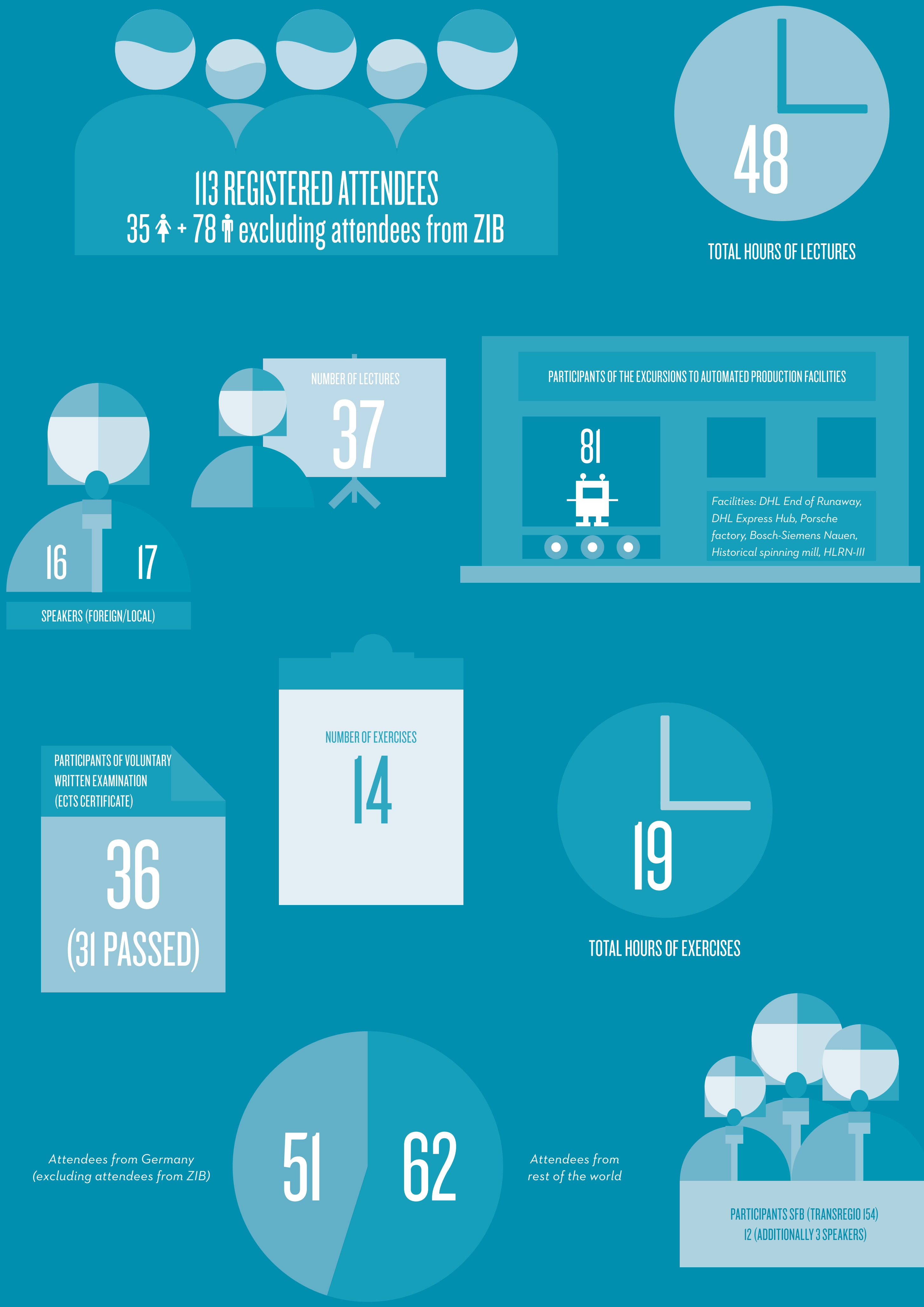
IN JUNE 2015: ZIB SUPERCOMPUTER IS NO. 69 IN TOP-500 LIST

COMBINATORIAL OPTIMIZATION AT WORK 2015

A two-week intensive block lecture on the use of combinatorial optimization and mathematical programming techniques (LP/MIP/MINLP) in real-world industrial applications held at Zuse Institute Berlin from September 28 to October 10, 2015.

CO@Work 2015 was the third lecture series of its kind the previous ones held in 2005 and 2009. Additionally, it has taken place once in Beijing in 2006. It consisted of eleven days of lectures with integrated exercises on the use of combinatorial optimization and mathematical programming techniques together with a nice social program and an excursion to industrial facilities.

CO@Work was organized by ZIB in cooperation with the Institute of Mathematics of TU Berlin, and it served as a summer school of the DFG Collaborative Research Center TRR 154 and of the Research Campus MODAL. It was supported by the Research Center MATHEON, the Berlin Mathematical School, the Research Campus MODAL, and the EU COST Action TD1207.

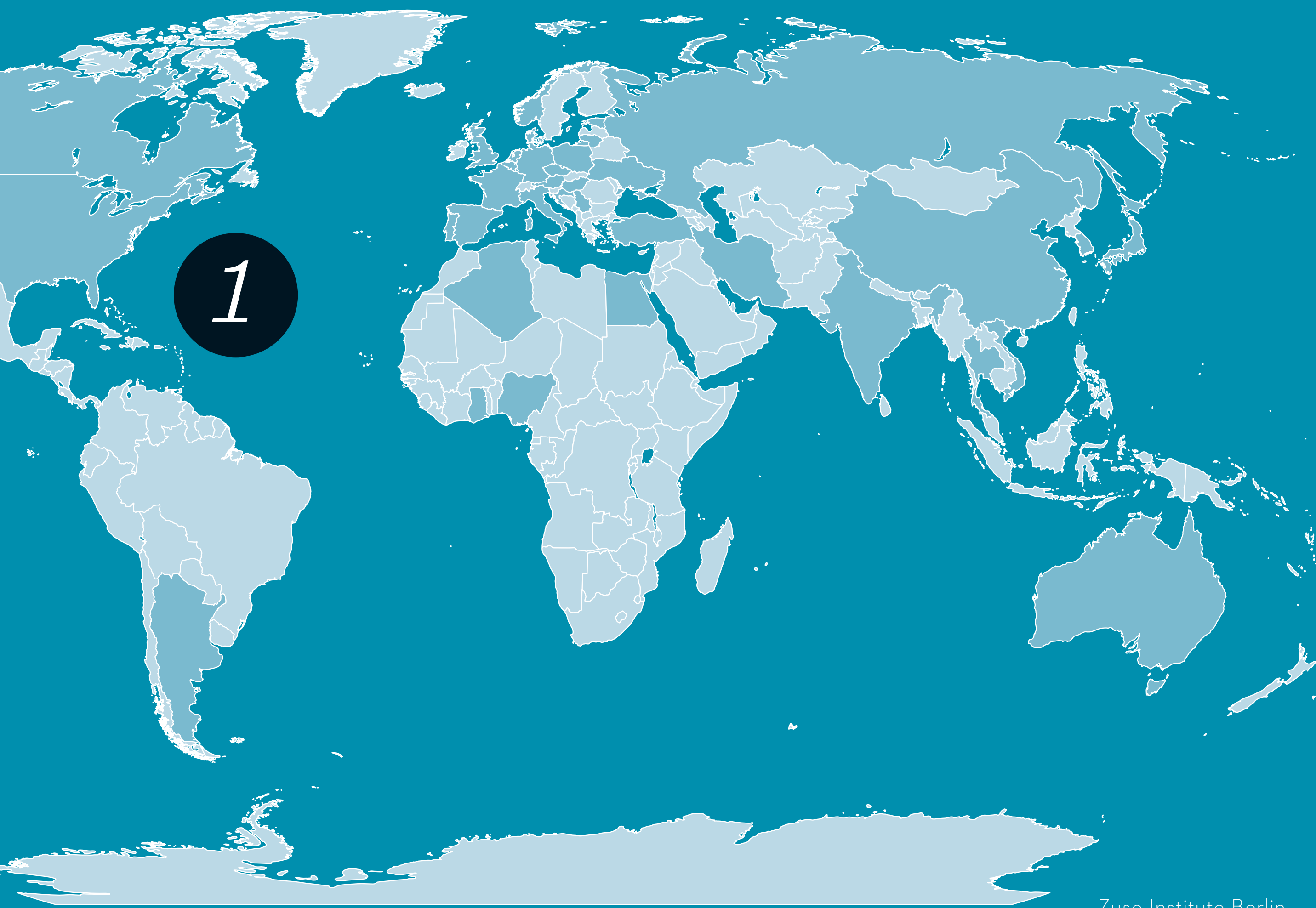

113 REGISTERED ATTENDEES
35 + 78 excluding attendees from ZIB
48
TOTAL HOURS OF LECTURES
NUMBER OF LECTURES
37
PARTICIPANTS OF THE EXCURSIONS TO AUTOMATED PRODUCTION FACILITIES
81
Facilities: DHL End of Runaway, DHL Express Hub, Porsche factory, Bosch-Siemens Nauen, Historical spinning mill, HLRN-III
16
17
SPEAKERS (FOREIGN/LOCAL)
NUMBER OF EXERCISES
14
PARTICIPANTS OF VOLUNTARY WRITTEN EXAMINATION (ECTS CERTIFICATE)
36
(31 PASSED)
19
TOTAL HOURS OF EXERCISES
Attendees from Germany (excluding attendees from ZIB)
51
62
Attendees from rest of the world
PARTICIPANTS SFB (TRANSREGIO 154)
12 (ADDITIONALLY 3 SPEAKERS)

FOREIGN LECTURES
DR. TOBIAS ACHTERBERG (GUROBI)
PROF. PIETRO BELOTTI (FICO XPRESS)
PROF. JOHANNES BISSCHOP (LITIC)
PROF. ROBERT BIXBY (GUROBI)
DR. PIERRE BONAMI (IBM CPLEX)
DR. CHRISTINA BURT (U MELBOURNE)
DR. JOACHIM DAHL (MOSEK)
PROF. KATSUKI FUJISAWA (IMI, KYUSHU UNIVERSITY)
DR. DANIEL JUNGLAS (IBM CPLEX)
PROF. SVEN LEYFFER (ARGONNE NATIONAL LABORATORY)
PROF. ALEXANDER MARTIN (FAU ERLANGEN-NÜRNBERG)
DR. DOMENICO SALVAGNIN (IBM CPLEX)
DR. FLORIAN SEIPP (SIEMENS AG)
DR. MARTIN SEYDENSCHWANZ (SIEMENS AG)
DR. STEFAN VIGERSKE (GAMS)
PROF. HAYATO WAKI (IMI, KYUSHU UNIVERSITY)

LOCAL LECTURES
PROF. RALF BORNDÖRFER (FU BERLIN)
DR. AMBROS GLEIXNER
PROF. MARTIN GRÖTSCHEL (BBAW)
GREGOR HENDEL KAI HENNIG
DR. JESCO HUMPOLA
PROF. MICHAEL JOSWIG (TU BERLIN)
PROF. THORSTEN KOCH (TU BERLIN)
RALF LENZ
DR STEPHEN MAHER
MATTHIAS MILTENBERGER
BENJAMIN MÜLLER
DR. FRANK PFEUFFER
ROBERT SCHWARZ
FELIPE SERRANO
DR. AXEL WERNER
JAKOB WITZIG

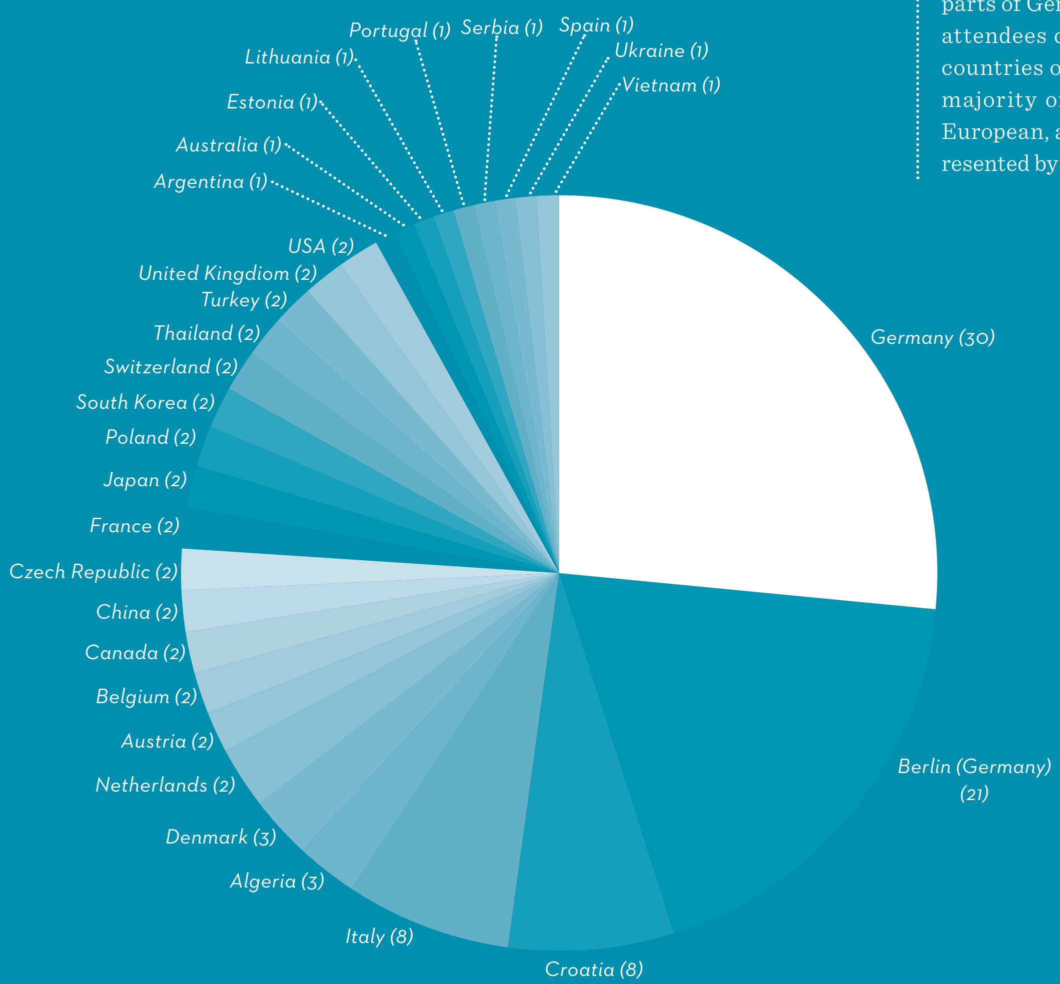
1 Outreach: All of the countries from which people applied for participation are colored in darker blue.

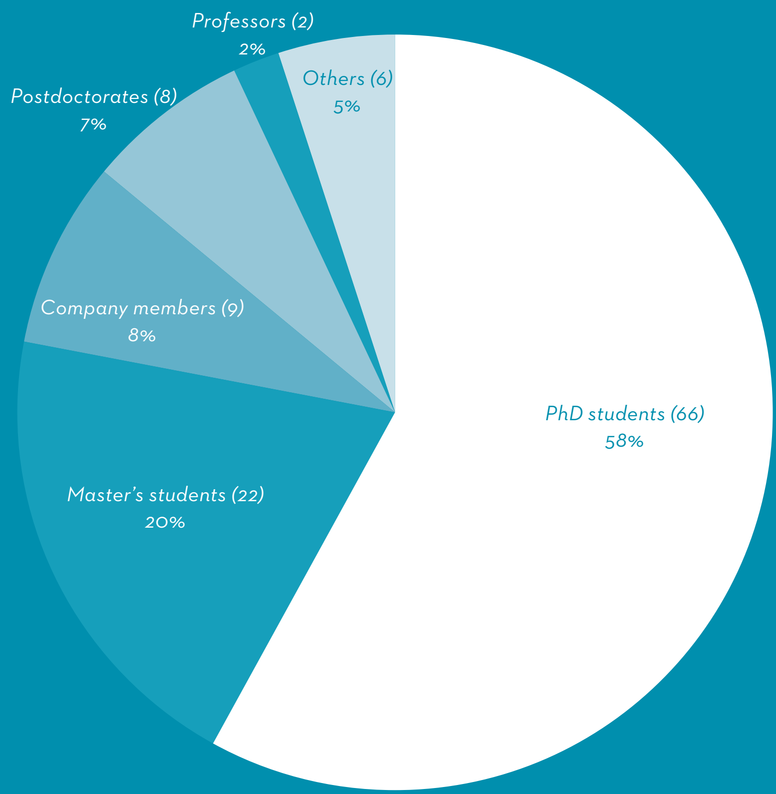
Although the application process had to be stopped early due to space restrictions, CO@Work 2015 attracted more than 160 applicants. In addition to applicants from the majority of the European countries and other developed countries such as Japan, Australia, and the United States, there was also a broad interest in CO@Work from developing countries such as Nigeria, Ghana, and Vietnam, as well as newly industrialized countries such as India, Thailand, and China.



ORIGIN OF ATTENDEES

While 51 of the 113 attendees of CO@work2015 came from Berlin and other parts of Germany, more than half of the attendees came from other European countries or from abroad. In total, the majority of the attendees have been European, and all continents were represented by at least one attendee.





EVALUATION

63 FOREIGN ATTENDEES RESPONDED

- **97%** FOUND THE LECTURES INTERESTING
- **35%** WOULD PREFER MORE TIME FOR EXERCISES
- **57%** ARE CONFIDENT WITH THE RATIO OF LECTURES AND EXERCISES
- **90%** WOULD RECOMMEND THE CO@WORK TO OTHERS
- **75%** WOULD COME AGAIN
- **76%** THINK THAT THE DURATION WAS APPROPRIATE
- **83%** SAID THERE WAS A GOOD BALANCE BETWEEN THEORY AND PRACTICAL APPLICATION

What did you like?

"This is the best summer school I have ever attended."

"Everything!"

"Great summer school! Great city! Great time! Thank you!"

"Lectures were well designed."

"Best thing is the attendance of the top researchers."

"High quality speakers!"

"I took *Bildungsurlaub* for two weeks. 'It was a great, but also a very demanding time. Great job!"

"A variety of content."

"Meeting the top developers of state-of-the-art solvers."

"Very good workshop with a lot impressions and ideas."

"It was well-constructed schedule; informative lectures, interesting topics, and applications."

"It is a very nice summer school."

"I was really impressed by the quality. I learned a lot in these two weeks."

In recent years, we have seen a dramatic increase in digitized data from many different kinds of sources, including imaging, sequencing, and simulation.

RESEARCH-DATA MANAGEMENT

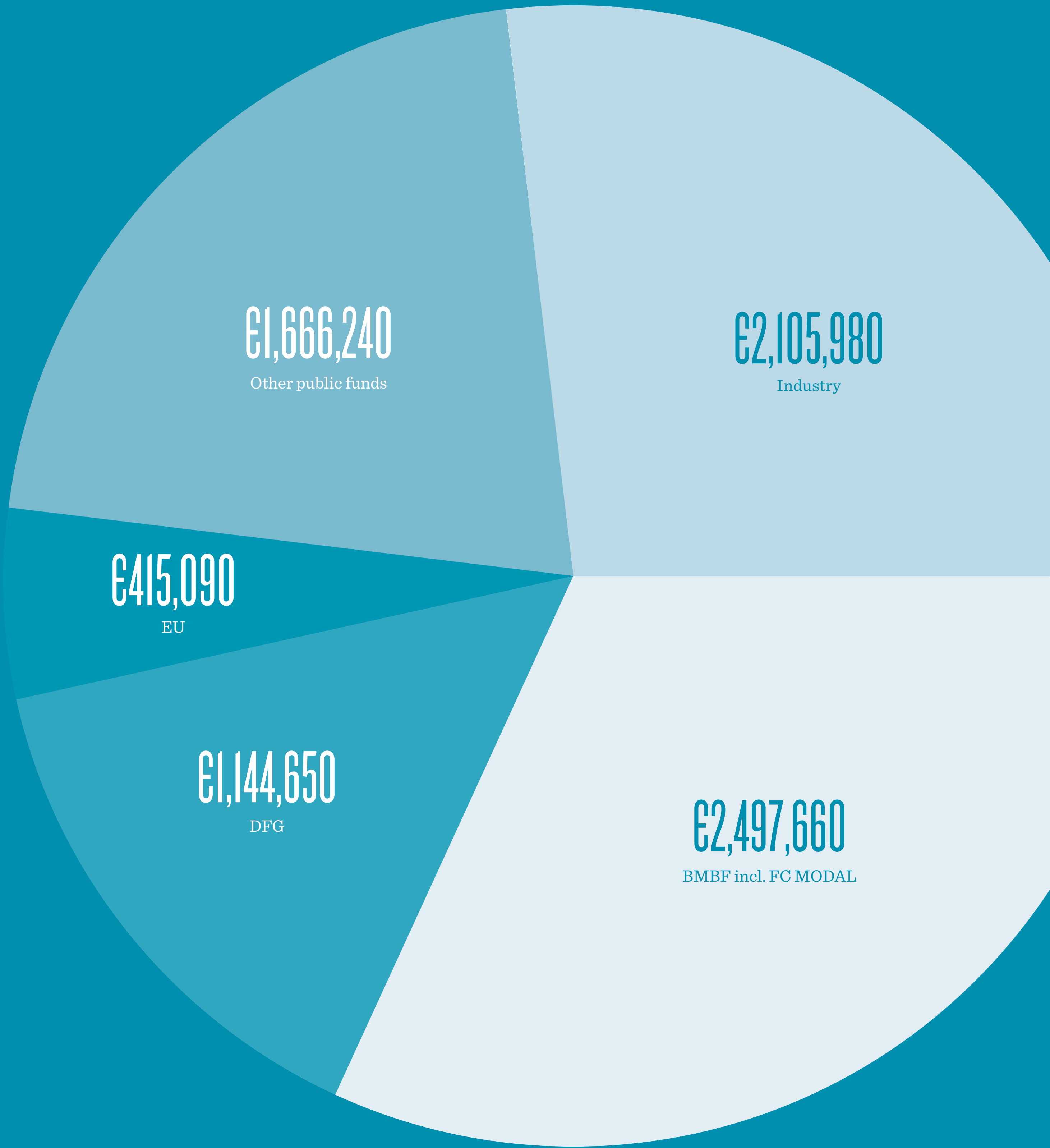
Although data arise from fields as different as natural sciences, medicine, and humanities, a common theme is that, apart from the original data, it is also important to store additional information, called metadata, describing the content and context of the data. Because the creation of data is often expensive, the data, both original and metadata, need to be preserved for a long time so that they can be reused by the data creator, as well as other scientists. For the latter purpose, it is advisable to make data publicly available. Research-data management (RDM) concerns the whole process of handling data from their creation throughout processing, to the dissemination of results and data archiving.

With its data storage and archiving facilities hosted by the research group Data Storage and Archives, ZIB offers unique conditions for research-data management. In addition, ZIB's high-throughput computing facilities run by the departments Distributed Algorithms and Supercomputing and Datacenter Infrastructure, as well as the associated research teams, provide the necessary computational power and competencies regarding database techniques for handling and processing large and distributed data. This is complemented by expertise in digitization and long-term preservation provided by the Service Centre Digitisation Berlin (digiS) and the research group Digital Preservation, respectively. Ensuring availability, readability, and comprehensibility of data in the long run is an ongoing research issue. Additional expertise exists in the Cooperative Library Network Berlin-Brandenburg (KOBV) that is also based at ZIB. KOBV has lengthy experience in providing information infrastructure services to researchers and cultural institutions inside and outside ZIB.

Another very important part of the research-data life cycle is data analysis. At ZIB, research in data analysis spans the whole range from method development in visualization, image processing, mathematical data analysis, and machine learning to uncertainty quantification, with applications in many different fields, including individualized and precision medicine, molecular and biological processes, materials and optical processes, and digital humanities.

Even though RDM should be part of all projects dealing with data, it is particularly important for projects in which large amounts of data are being handled. One example is the Collaborative Data Analysis for Microscopy project run in the research group Image Analysis in Biology and Materials Science. In this project, a collaborative data analysis platform is being developed that will eventually provide a full pipeline from intuitive data management to the analysis and computation of large microscopy image data sets. Managing many large data sets on one platform will also enable more powerful analyses in a larger context, using the collected metadata. The massive amount of data to be analyzed by this platform can only be handled using research-data management tools.

Another example in this area is the MODAL - MedLab project in the Bioinformatics in Medicine research group. The focus here is on high-throughput *omics* mass data, such as genomics data acquired from genome sequencers, proteomics data from mass spectrometry machines, or data from other biological high-throughput experiments. Typical data-set sizes range from several gigabytes up to terabytes for one experiment. Additional metadata is collected from the acquisition process of the machine (machine parameters, SOP variables, etc.) and patient-specific clinical data, such as disease information, age, results from medical checkups, etc. Data security and data privacy are important issues to be addressed in this context. The data are stored on secured servers in the ZIB and FU intranet using the LabKey platform and are being analyzed with advanced sparse data analysis techniques aiming at finding novel diagnostic tools or therapy response monitoring. If patients allow publication of their data, it will be made available in an anonymized form.


€1,666,240
Other public funds
€2,105,980
Industry
€415,090
EU
€1,144,650
DFG
€2,497,660
BMBF incl. FC MODAL

ECONOMIC SITUATION IN 2015

ZIB THIRD-PARTY FUNDS BY SOURCE

- 5% EU
- 15% DFG
- 21% Other public funds
- 27% Industry
- 32% BMBF incl. FC MODAL

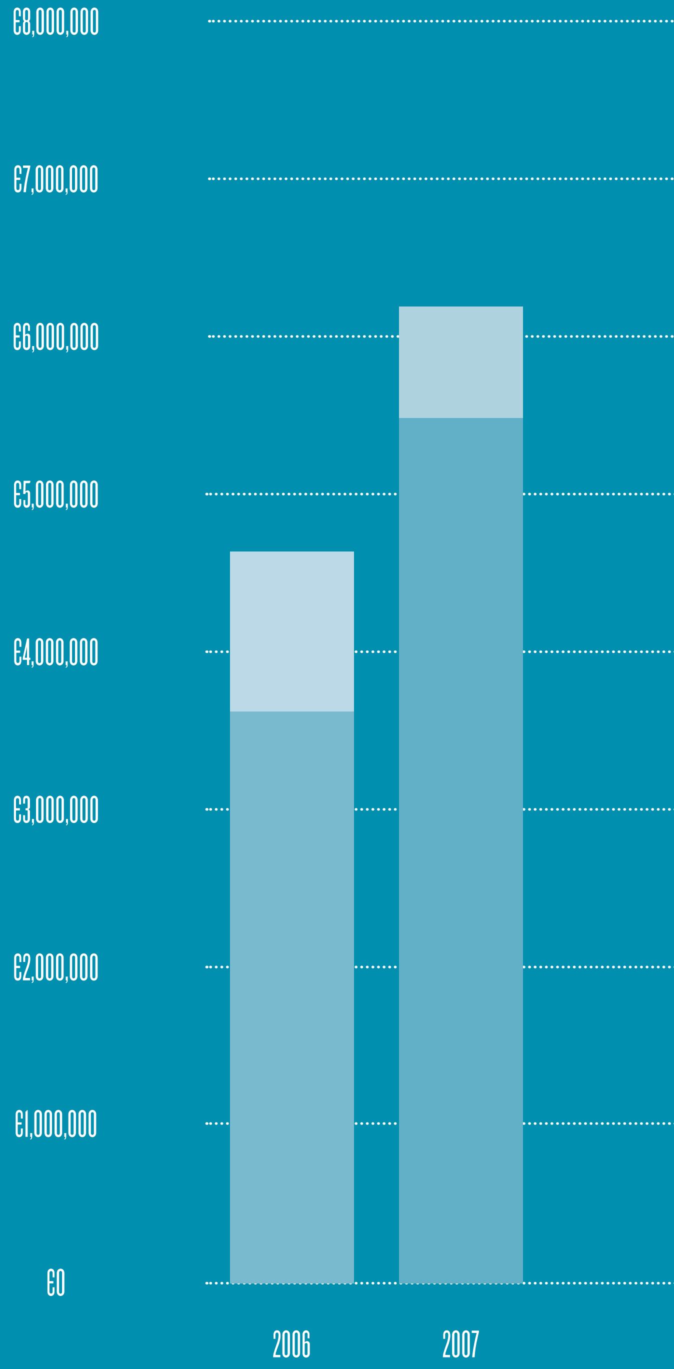
The Zuse Institute Berlin finances its scientific work via three main sources: the basic financial stock of the Federal State of Berlin and third-party funds of public sponsors as well as of industrial cooperation contracts.

In 2015, ZIB raised third-party funding by a large number of projects. Project related public third-party funds increased from € 4,339,000 in 2014 to € 5,723,000 in 2015; industrial third-party projects decreased from € 2,905,000 to € 2,106,000. The significant reduction of funds raised in the industrial sector results from the reassignment of funds in the context of our private-public partnership program Research Campus (Forschungscampus) MODAL: within MODAL, industry funds complement public funding by the German Ministry of Research and Education (BMBF), and together they are combined into one large project that is listed as publicly funded.

In total, € 7,829,000 third-party funding marked a new record in ZIB's history - an increase for the fourth year in a row!

Based on these success stories, the number of employees at ZIB increased from 208 to 224 employees despite the fact that many highly qualified scientists were offered attractive careers in academia or industrial research elsewhere.

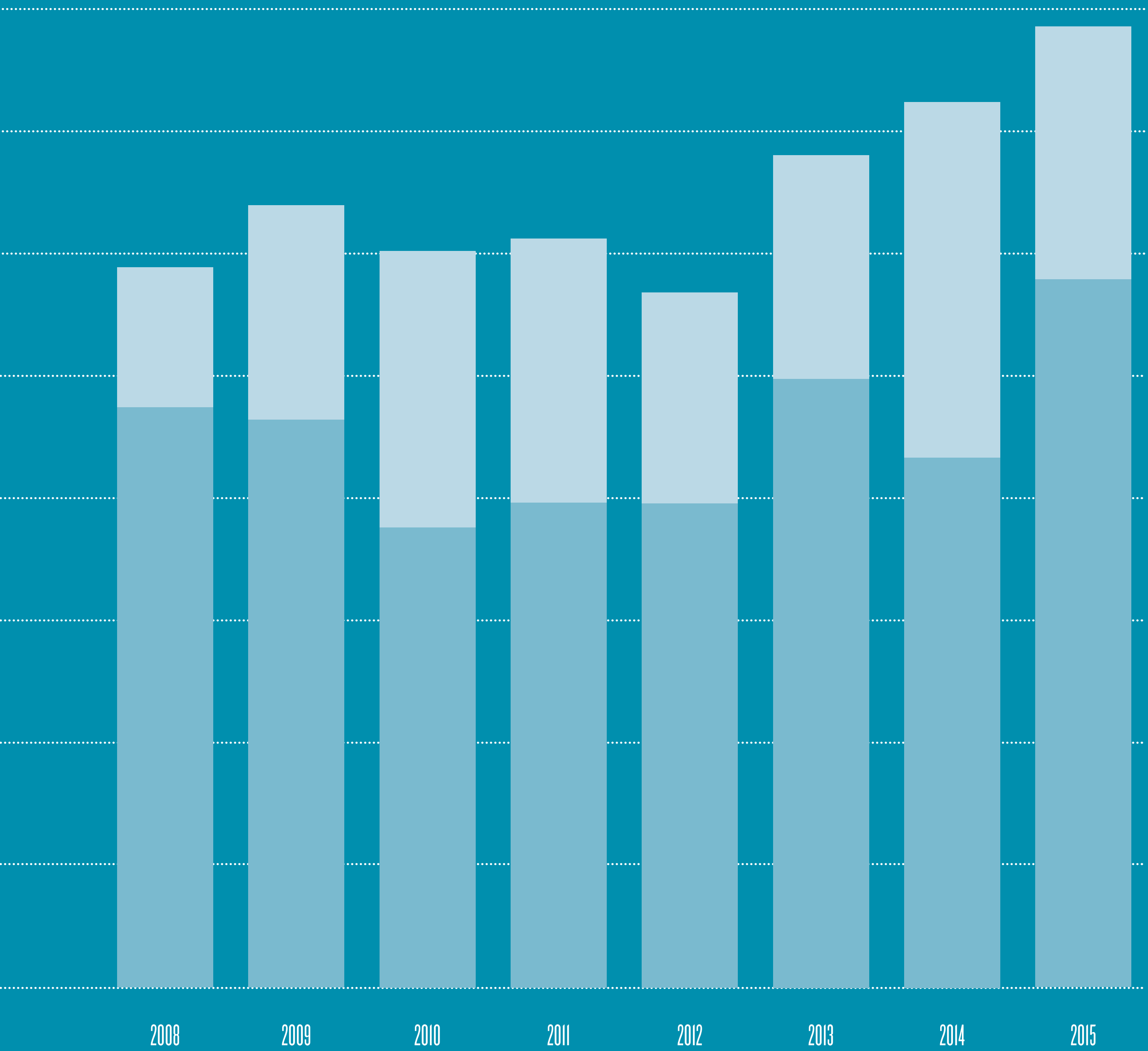
The new HLRN-III high-performance computer at ZIB performed well in 2015. And again, the institute's long-term data storage was further expanded. As a consequence, a large number of new research collaborations with Berlin-based, national, and international institutions in this area could be initiated. With these developments, ZIB strengthened its position as a competence center for computing and data science.



ZIB THIRD-PARTY FUNDS IN EUROS

INDUSTRY

PUBLIC FUNDS



COMPUTING IN TECHNOLOGY GMBH (CIT)
1992 | www.cit-wulkow.de
Mathematical modeling and development of numerical software for technical chemistry

RISK-CONSULTING PROF. DR. WEYER GMBH
1994 | www.risk-consulting.de
Database marketing for insurance companies

INTRANETZ GMBH
1996 | www.intranetz.de
Software development for logistics, database publishing, and e-government

AKTUARDATA GMBH
1998 | www.aktuardata.de
Development and distribution of risk-evaluation systems in health insurance

VISAGE IMAGING GMBH (Originating from a spin-off of Visual Concepts GmbH)
1999 | www.visageimaging.com
Visualization and data analysis (Amira etc), especially medical visualization

ATESIO GMBH
2000 | www.atesio.de
Development of software and consulting for planning, configuration, and optimization of telecommunication networks

BIT-SIDE GMBH
2000 | www.bit-side.com
Telecommunication applications and visualization

DRES. LÖBEL, BORNDÖRFER & WEIDER GBR
2000 | www.lbw-berlin.de
Optimization and consulting in public transport

LENNÉ3D GMBH
2005 | www.lenne3d.com
3-D landscape visualization, software development, and services

JCMWAVE GMBH
2006 | www.jcmwave.com
Simulation software for optical components

ONSCALE SOLUTIONS GMBH
2006 | www.onscale.de
Software development, consulting, and services for parallel and distributed storage and computing systems

LAUBWERK GMBH
2009 | www.laubwerk.com
Construction of digital plant models

1000SHAPES GMBH
2010 | www.1000shapes.com
Statistical shape analysis

TASK – Berthold Gleixner Heinz Koch GbR
2010
Distribution, services, and consulting for ZIB's optimization suite

QUOBYTE INC.
2013 | www.quobyte.com
Quobyte develops carrier-grade storage software that runs on off-the-shelf hardware

KEYLIGHT GMBH
2015 | www.keylight.de
keylight develops scalable real-time web-services and intuitive apps. The focus is on proximity, marketing, iBeacon as well as Eddystone for interactive business models.

SPIN-OFFS

NUMBER OF EMPLOYEES

In the year 2015, 208 people were employed at ZIB; of these, 145 positions were financed by third-party funds.

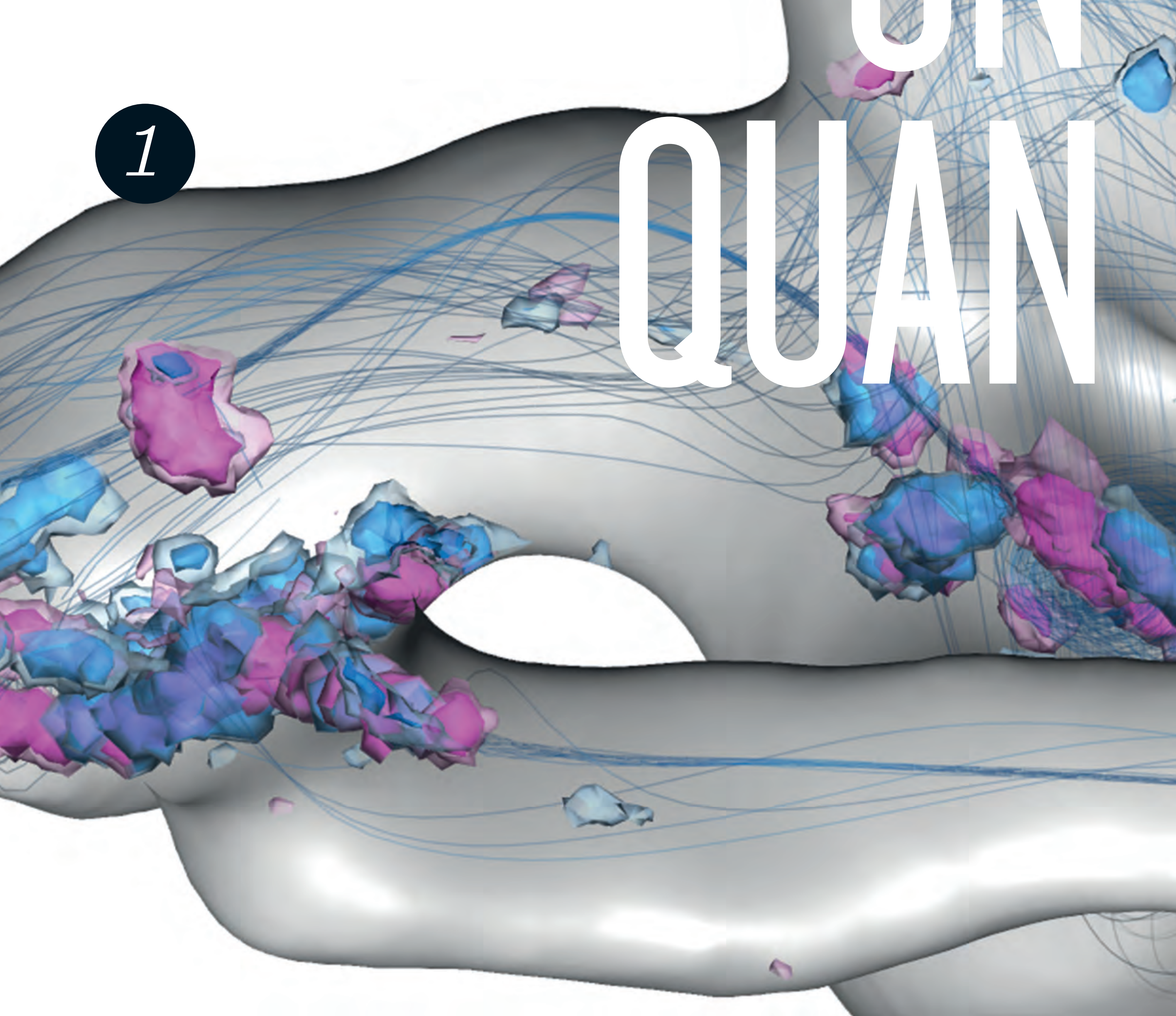
	1/1/2015 Permanent	1/1/2015 Temporary	1/1/2015 TOTAL	1/1/2016 Permanent	1/1/2016 Temporary	1/1/2016 TOTAL
MANAGEMENT	4	0	4	3	0	3
SCIENTISTS	18	85	103	18	87	105
SERVICE PERSONNEL	34	14	48	34	13	47
KOBV HEADQUARTERS	7	8	15	7	8	15
STUDENTS	0	38	38	0	54	54
TOTAL	63	145	208	62	162	224

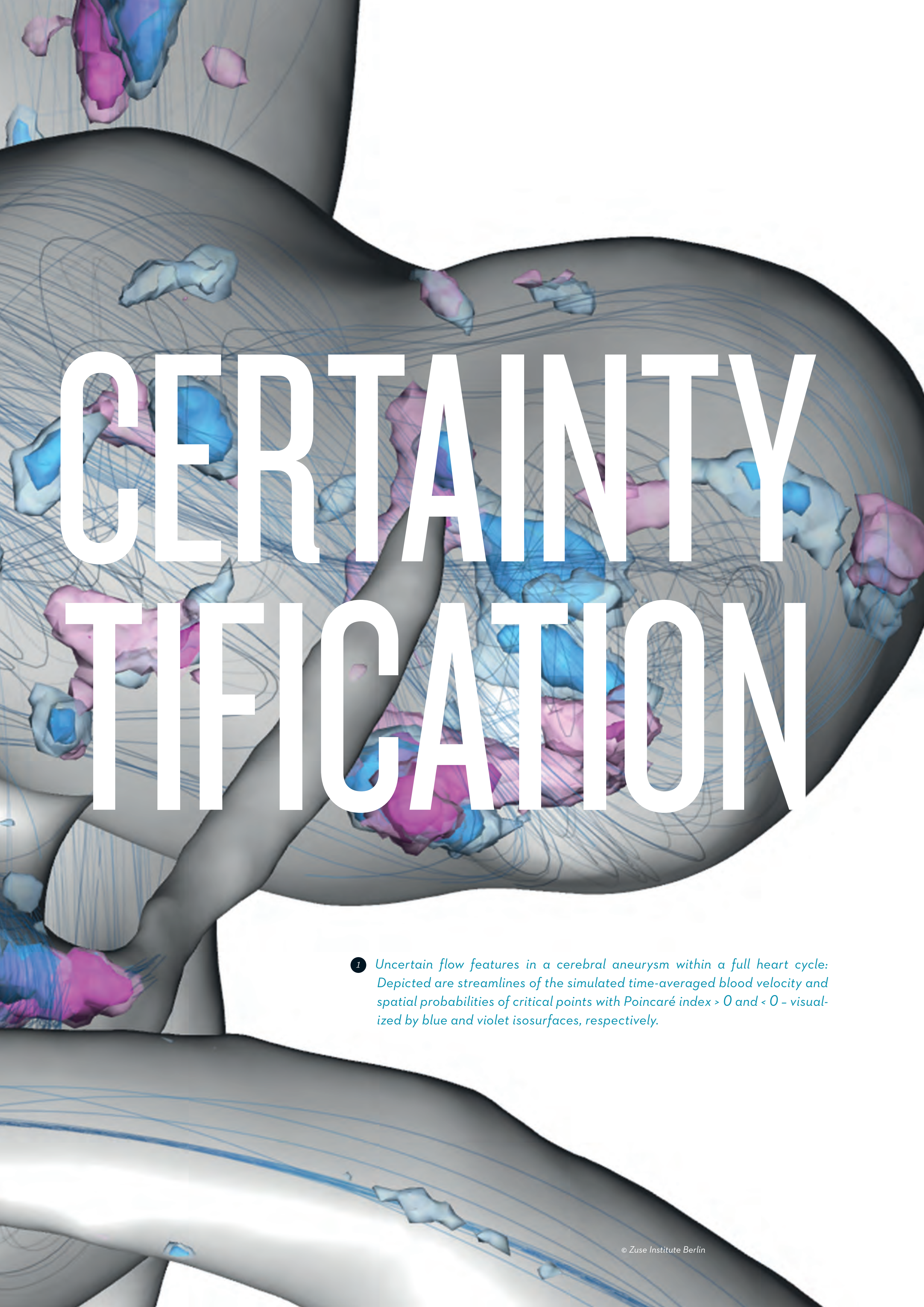
Martin Weiser | weiser@zib.de | +49-30-84185-170

How accurate are numbers inferred from measurements and simulations?

“Uncertainty quantification” (or “UQ” for short) is a research area that has sprung to prominence in the last decade at the interface of applied mathematics, statistics, computational science, and many applications, usually in physical sciences and engineering, but also in biology, finance, and insurance.

1





CERTAINTY TIFICATION

1 *Uncertain flow features in a cerebral aneurysm within a full heart cycle: Depicted are streamlines of the simulated time-averaged blood velocity and spatial probabilities of critical points with Poincaré index > 0 and < 0 – visualized by blue and violet isosurfaces, respectively.*

UNCERTAINTY QUANTIFICATION

In all these applications, there is a real and growing demand to synthesize complex real-time data sets and historical records with equally complex physically-based computational models for the underlying phenomena, in order to perform tasks as diverse as extracting information from novel imaging techniques, designing a new automobile or airplane, or predicting and mitigating the risks arising from climate change.

Simply put, UQ is the end-to-end study of the impact of all forms of error and uncertainty in the models arising in the applications. The questions considered range from fundamental, mathematical, and statistical questions to practical questions of computational accuracy and cost [1]. Research into these questions takes place at ZIB in the Uncertainty Quantification group, and finds applications in other working groups such as Computational Medicine, Computational Molecular Design, and Visualization.

A GENERAL INTRODUCTION TO UQ AND BAYESIAN INVERSE PROBLEMS

$P(X|Y) = P(Y|X) P(X) / P(Y)$

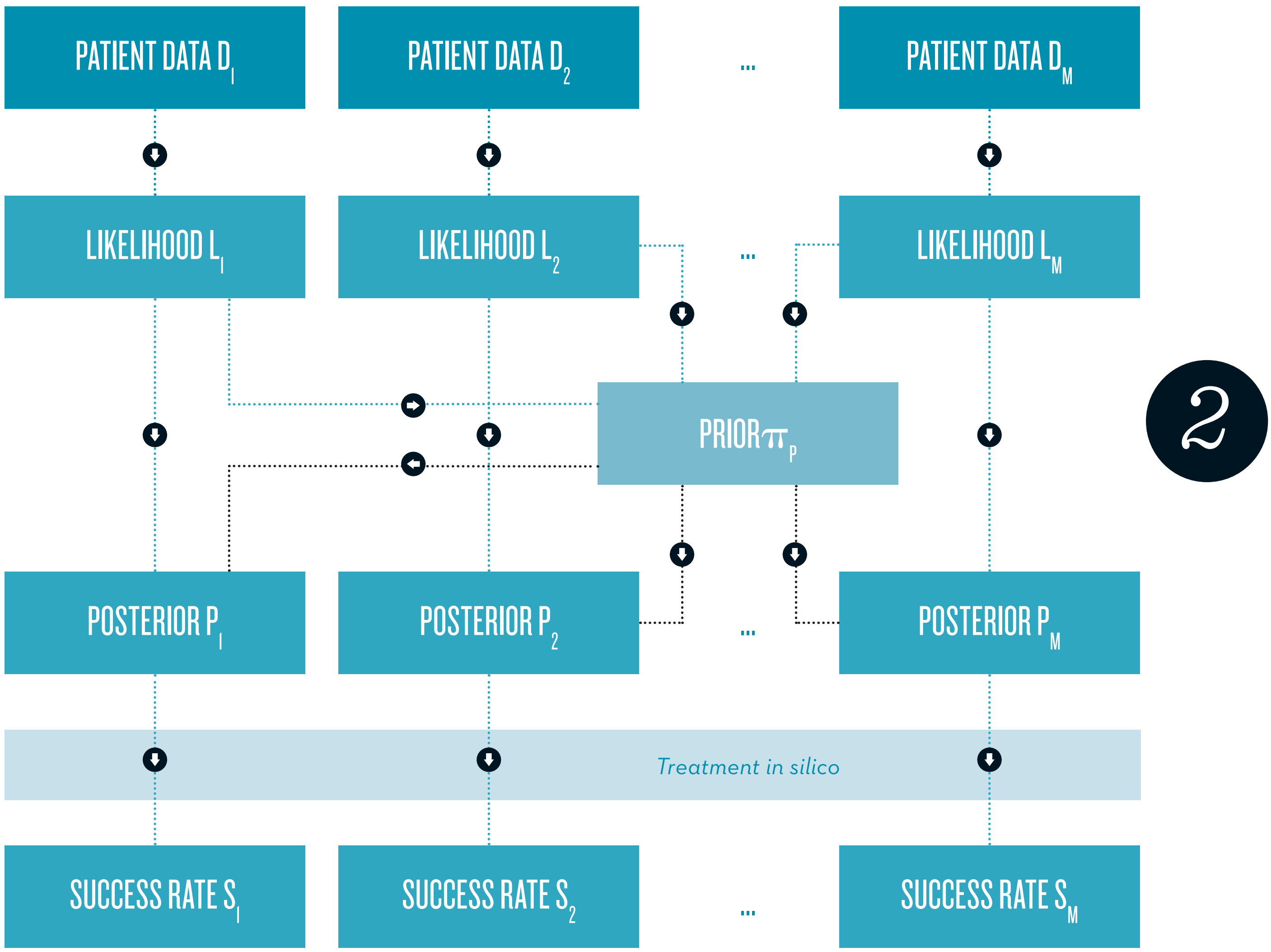
Roughly speaking, UQ divides into two major branches, forward and inverse problems. In the forward propagation of uncertainty, we have a known model F for a system of interest. We model its inputs X as a random variable and wish to understand the output random variable Y = F(X), sometimes denoted Y|X, read as "Y given X." There is a substantial overlap between this area and sensitivity analysis, since the random variations in X probe the sensitivity of the forward model F to changes of its inputs. In the other major branch of UQ, inverse problems, F is still the forward model, but now Y denotes some observed data, and we wish to infer inputs X so that F(X) = Y; that is, we want not Y|X but X|Y. Here, there is substantial overlap with statistical inference and with imaging and data analysis.

Inverse problems typically have no solutions in the literal sense, because our models F are only approximate, there is no X for which F(X) agrees exactly with the observed data Y. Therefore, it becomes necessary to relax the notion of a solution, and often also to incorporate prior or expert knowledge on what a "good" solution X might be. In recent years, the Bayesian perspective on inverse problems has received much attention, because it is powerful and flexible enough to meet these requirements, and because increased computational power makes the Bayesian approach more feasible than in decades past [2].

In the Bayesian perspective, we again regard X and Y as random variables and encode our prior expert knowledge about X into a prior probability distribution p(X), which we condition with respect to Y using Bayes' rule p(X|Y) = p(Y|X) p(X) / p(Y) to produce a so-called posterior distribution for X|Y, which is the mathematical representation of all knowledge/uncertainty about X, given the observed data Y and the expert knowledge encoded in the prior p(X). However, the posterior p(X|Y) is typically a very complicated distribution on a large space (the space of unknown Xs that we are trying to infer), so there are major mathematical and computational challenges in implementing this fully Bayesian approach, and in producing appropriate simplifications for end users.

UQ IN SYSTEMS BIOLOGY AND PARAMETER ESTIMATION

The Systems Biology group at ZIB deals with the computational and mathematical modeling of complex biological systems: metabolic networks or cell signaling networks, for example. Usually, the models consist of large systems of ordinary differential equations that describe the change of concentrations of the involved species over time. Such models involve a huge number of model parameters representing, for example, reaction rate constants, volumes, or effect concentrations. Only a few of these parameters are measurable, sometimes their approximate range of values is known, but often their order of magnitude is completely unknown. The aim is to estimate parameter values in such a way that simulation results match with given experimental data and that predictions can be made about the system's behavior under external influences: thus, these problems fall under the general heading of *inverse problems*.



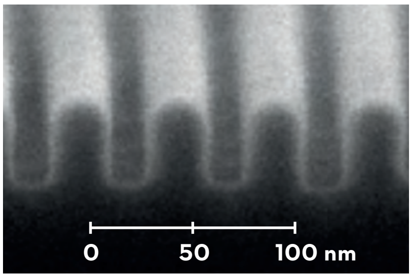
The data, however, are prone to measurement errors and are therefore uncertain. Given a fixed set of data and a statistical model for the error, one can solve an optimization problem to compute a single set of parameter values that make the observed data the most probable given the model [3]. The function to be optimized is called likelihood function. In practice, this optimization problem is often difficult to solve, because its solution is not unique. In other words, there exist several different sets of parameter values that all lead to equally good fits to the data.

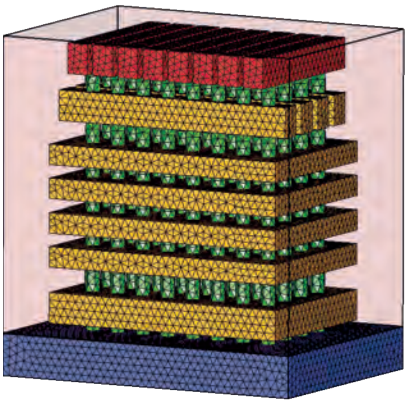
Alternatively, when prior knowledge about the parameters is postulated, parameters can be treated as random variables in the framework of Bayesian statistics. This allows you to compute a joined probability distribution for the parameters, called the posterior. Performing model simulations with parameters sampled from this posterior distribution gives insight into the variability and uncertainty of the model output.

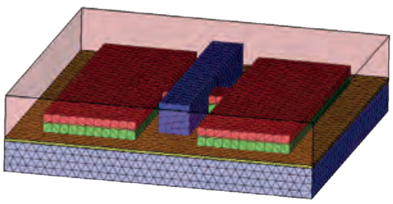
A possible application is the prediction of patient-specific treatment success rates based on a physiological model for a specific disease or health status. Given some measurement data from a large group of patients, one can construct a prior distribution that reflects the variability of parameters within the patient population [4]. Using this prior and a patient-specific data set, an individual posterior can be computed. Running model simulations including the treatment with parameters sampled from the posterior then allows us to quantify the failure probability of the treatment and to analyze under which conditions a treatment fails for a specific patient.

2 *Schematic representation of the Bayesian approach to the construction of patient-specific physiological models for the prediction of individual treatment success rates, for example.*

UQ IN OPTICAL METROLOGY

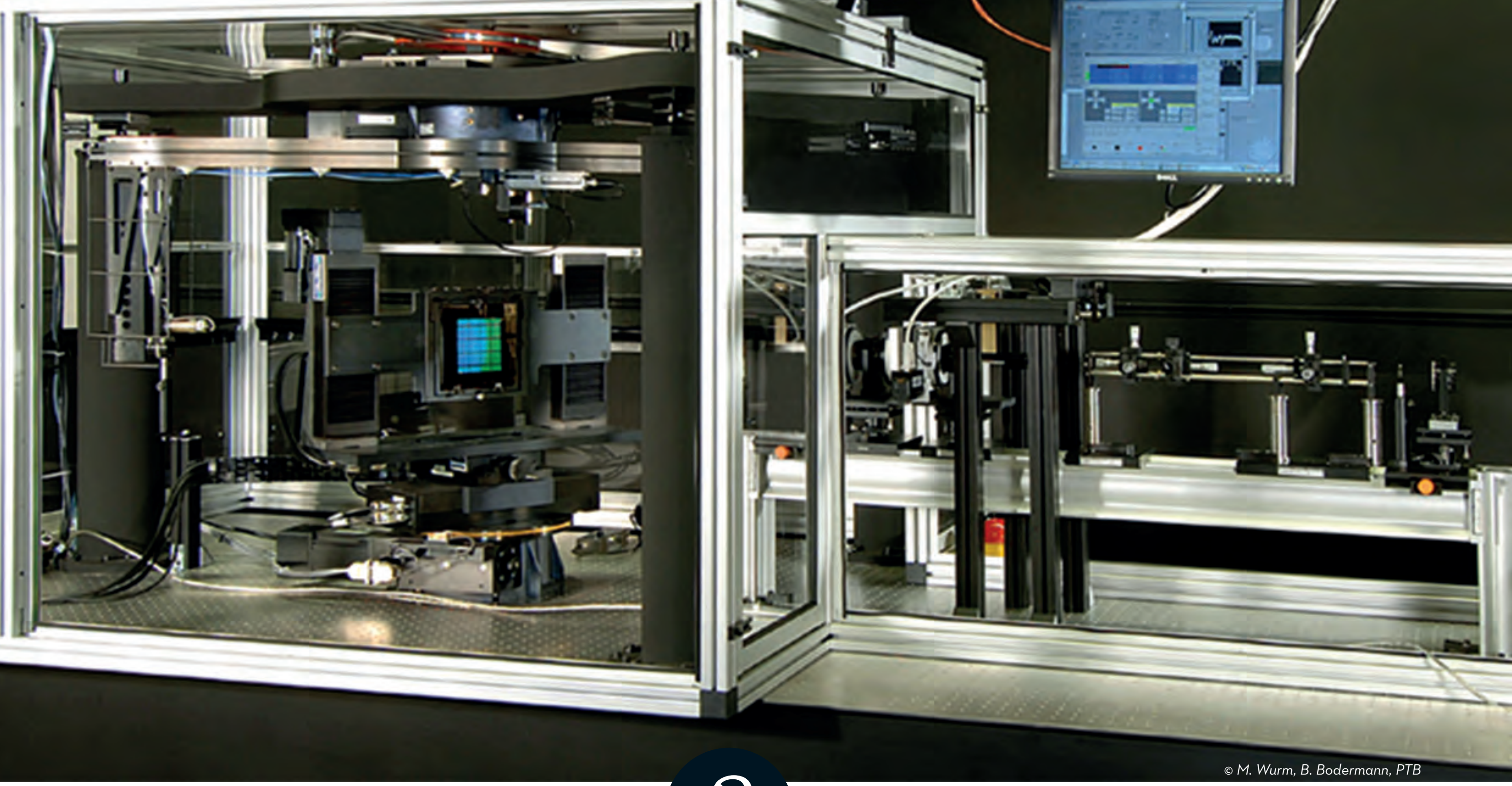






Optical metrology uses the interaction of light and matter to measure quantities of interest, like geometry or material parameters. Reliable measurements are essential preconditions in nanotechnology. For example, in the semiconductor industry, optical metrology is used for process control in integrated circuit manufacturing, as well as for photomask quality control. In this context, measurements of feature sizes need to be reliable down to a sub-nanometer level. As the measurement amounts to solving an inverse problem for given experimental results, methods for both simulating light-matter interaction in complex 3-D shapes and uncertainty quantification are required.

A typical experimental setup consists of a well-defined light source, the scattering object, and a detector for the scattered light. Figure 3 shows a setup with fixed illumination wavelength and variable settings for polarization and direction of incident and detected light components. However, wavelength-dependent measurements are also typical in optical metrology. The detected spectra are used to reconstruct the scattering structure. The choice of illumination and detection conditions directly impacts the measurement sensitivity. The scatterers to be analyzed are manifold in the semiconductor industry, for example. Gratings, as well as active components like FinFETs or VNANDs, are of interest.



3

In a collaborative study of Physikalisch-Technische Bundesanstalt (PTB) and ZIB's research group on Computational Nano Optics, the grating shown in Figure 4 (top) has been studied. Its geometric parameters, as shown in Figure 5, have been identified by a Gauß-Newton method. Reconstruction results are summarized in Table 1. The simulated spectral reflection response for the reconstructed parameters matches the experimental data very closely. Estimating the posterior covariance by local Taylor approximation reveals a satisfactory accuracy and indicates the high quality of the implemented models [5]. Hence, the approach is a promising candidate for investigations of far more complex semiconductor structures, as exemplarily shown in the center and bottom parts of Figure 4.

3 Goniometric deep ultraviolet scatterometer of Physikalisch-Technische Bundesanstalt.

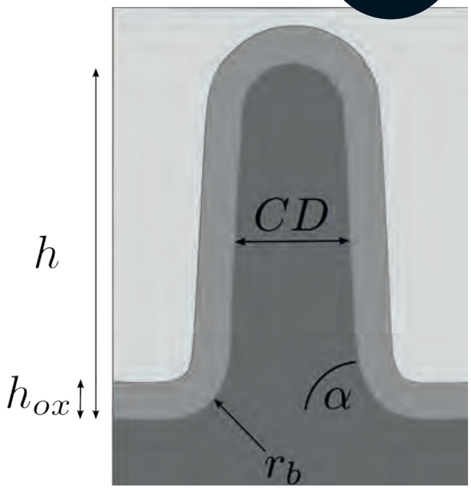
4 Top: Microscopic image (SEM) of a prototype of a scatterometry reference standard sample, manufactured at Helmholtz-Zentrum, Berlin. Center: Simplified geometry model of a 3-D NAND structure for memory chips. Bottom: Simplified geometry model of a FinFET semiconductor component.

5 Geometry model for the sample shown in Figure 2.

TABLE 1

Parameter	CD [nm]	h[nm]	α	h_{ox}	r_b
Admissible interval	(10,20)	(45,55)	(82,96)	(3,6)	(5,13)
Reconstructed value and deviation	16.05 (0.25)	48.94 (1.0)	87.0 (1.4)	4.95 (0.19)	10.45 (3.0)

5



MOLECULAR DESIGN

THE CHALLENGE FOR COMPUTATIONAL MOLECULAR DESIGN

Molecular systems have metastable states with low transition probabilities between these states. For the optimal design of interacting molecules (drugs, analytes, sensors) it is often very important to adjust some of these transition probabilities by redesigning parts of the molecular system, in order to increase affinity or specificity, for example. The Computational Molecular Design group predicts the essential transition probabilities of molecular systems on the basis of molecular dynamics (MD) simulations. To save on computational costs, one aims at extracting the essential transition probabilities from as few as possible short MD simulations. The trajectories that result from each of these simulations can be considered as observed data that are used to infer the desired transition probabilities.

UNCERTAINTY OF TRANSITION PROBABILITIES

The challenge for the Computational Molecular Design group is to compute the long-term behavior of molecular systems on the basis of only a few short-time molecular simulations. Molecular systems exhibit a multiscale dynamical behavior: they undergo rare transitions between metastable states, for example. If the statistical analysis of these transitions is based on a few short-time simulations (the observed data Y) only, then the correct transition probabilities (the inferred unknowns X) are uncertain. In this case the posterior distribution for $X|Y$ is a distribution on transition matrix space that reflects the uncertainty about the transition matrix X, given the observed simulation data Y and the expert knowledge encoded in the prior p(X). Applying appropriate UQ algorithms leads to an ensemble of transition matrices. This ensemble of transition matrices allows us to compute the uncertainty in the quantities extracted from the transition matrices, the dominant timescales of the system, for example. It was recently demonstrated how to utilize the insight into these uncertainties for understanding the physical/chemical meaning of the indeterminacy of metastable states [6] which led to new design principles for synthetic chemistry [7].

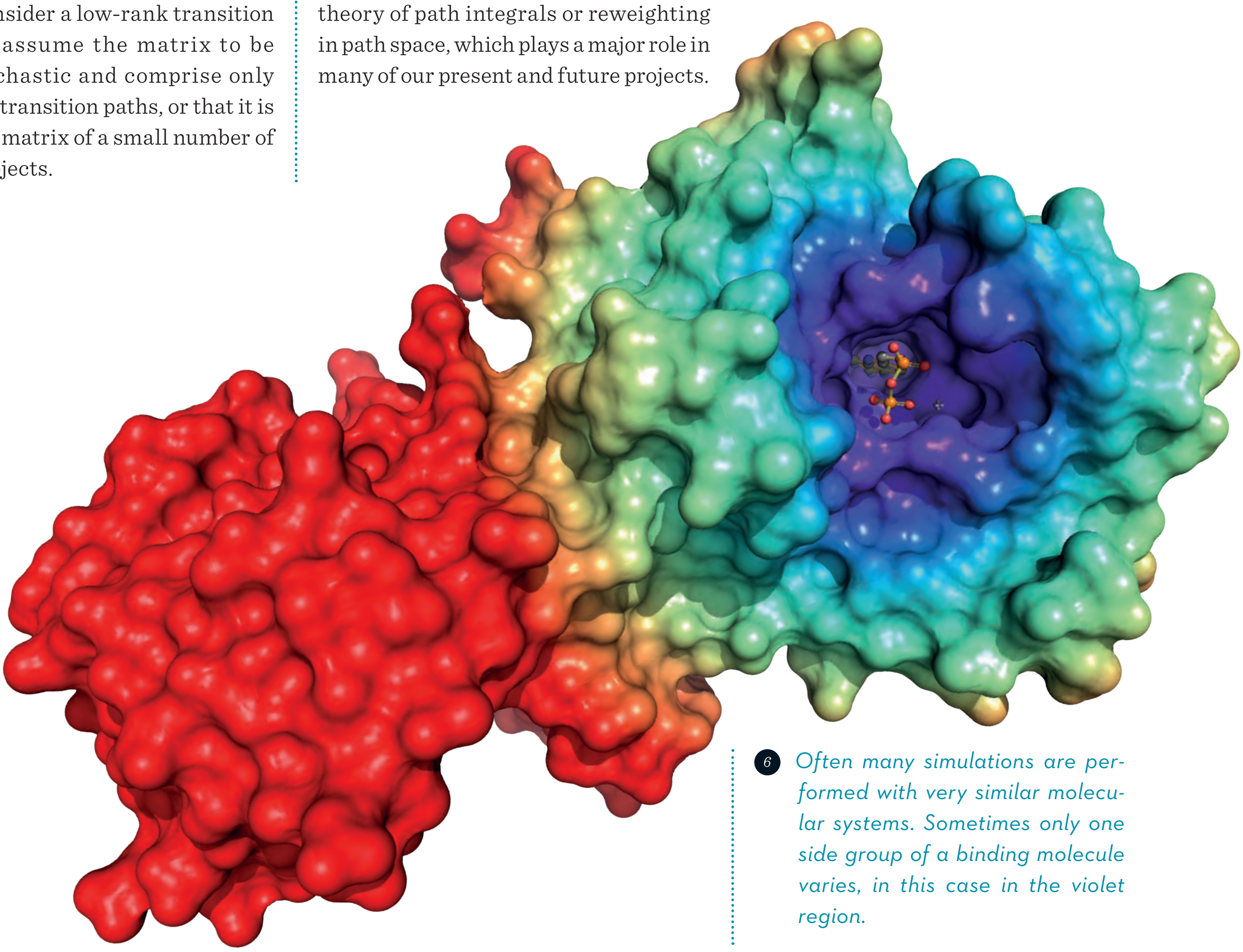
INCOMPLETE SIMULATION DATA

If only some and not all of the essential transition probabilities are known, then the corresponding transition matrix is incomplete, or some entries are missing. We have constructed matrix completion algorithms for estimating these entries on the basis of the given simulation data without performing further simulations, which saves a lot of computational effort. In order to estimate the unknown entries, different assumptions are useful. One can consider a low-rank transition matrix, or assume the matrix to be doubly-stochastic and comprise only some major transition paths, or that it is a similarity matrix of a small number of clustered objects.

CHANGING THE MOLECULAR STRUCTURE

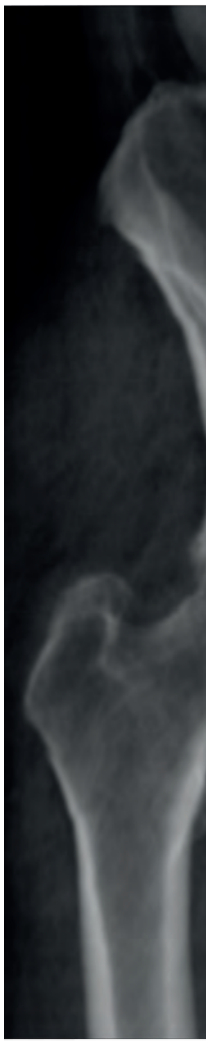
Another important question is how to reduce computational costs when simulating various molecular systems which only differ in some part of the molecular system that is small (Figure 6) compared to the size of the entire system. We investigated methods that allow for the prediction of transition matrices for a changed molecular system on the basis of the simulated original system [8, 9]. The mathematical background is based on the theory of path integrals or reweighting in path space, which plays a major role in many of our present and future projects.

6



6 *Often many simulations are performed with very similar molecular systems. Sometimes only one side group of a binding molecule varies, in this case in the violet region.*

UQ IN COMPUTER VISION AND GEOMETRY RECONSTRUCTION



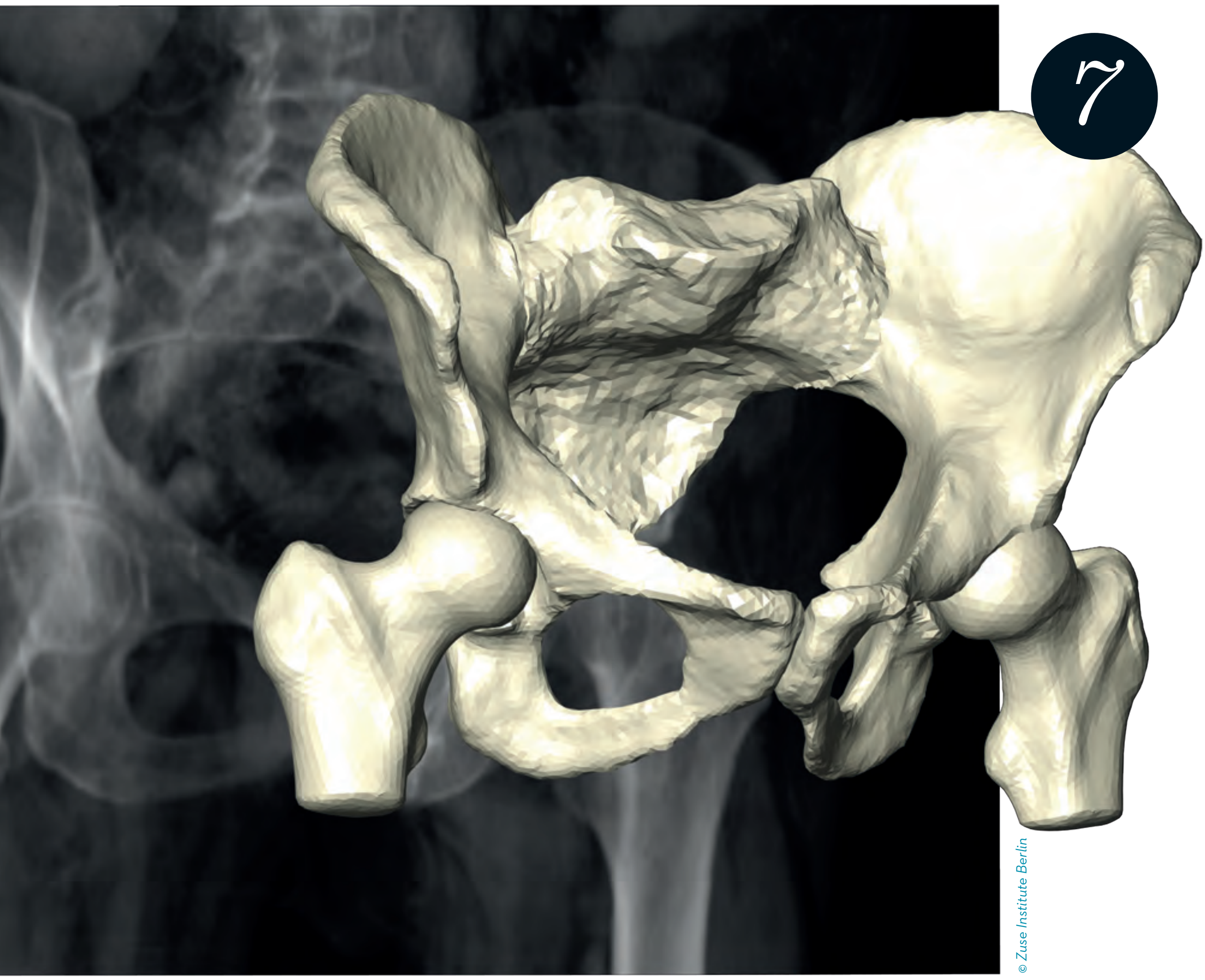
COMPUTER VISION

Computer vision extracts numerical or symbolic information from image data, using methods for acquiring, processing, analyzing, and understanding images. If decisions are based on such information, it is important to know how reliable it is. Thus, UQ becomes necessary for processing pipelines in computer vision.

This is illustrated by the following three examples: 1) An orthopedic surgeon has to decide, based on a computed tomography (CT) scan of a patient, whether a bone is solid enough to permit fixation of a screw that holds a certain maximum load. Such a decision requires extraction of the bone's thickness and material density – including error bounds – from the CT scan. 2) In pathology, many conclusions are drawn, based on frequencies of cell types in biopsies. Reliable diagnoses require knowledge not just of cell counts in microscopic images, but also of the uncertainties related to the identification and classification of cells. 3) In self-driving cars, potentially far-reaching decisions have to be taken based on information from video images; examples are the route and speed of the car, considering estimated trajectories of vehicles and pedestrians, for example. The uncertainty of such image-based information needs to be estimated to be taken into account.

Obviously, a wealth of research topics arises. At ZIB, research has started concerning UQ in image segmentation. In a first approach, images are considered as random fields, and spatial probabilities for membership functions are computed. This works for basic segmentation techniques that utilize only local information, like thresholding, for example. Consideration of non-local information renders UQ into a much more difficult problem. A fundamental problem is to capture the modeling uncertainty in image segmentation.

7 *Reconstruction of pelvic bone and hip joints on the basis of few X-ray projections.*



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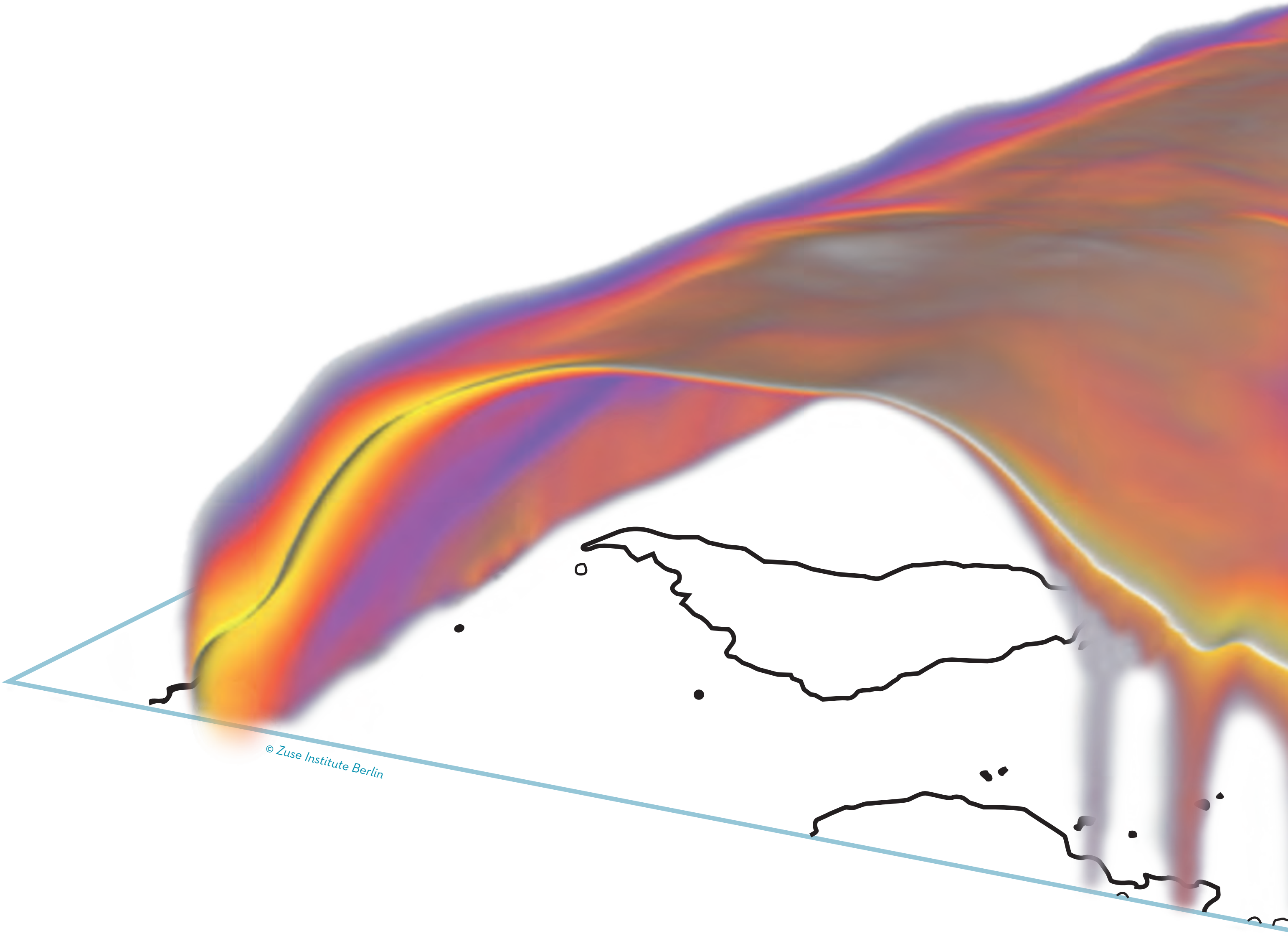
GEOMETRY RECONSTRUCTION

The 3-D shape of human anatomy, as needed in particular for surgery and therapy planning tasks, is usually extracted from 3-D image stacks provided by CT scans. Dose reduction requires a limit on the number of X-ray projections entering the CT to very few, but these do not contain enough information to reconstruct 3-D image stacks. The anatomy, however, can be described by statistical shape models in terms of a small number of parameters. Using such shape models as priors renders the Bayesian inverse problem well-posed and allows an efficient computation of maximum posterior estimates [10]. The research groups on Therapy Planning, Computational Medicine, and Visual Data Analysis in Science and Engineering investigate the properties of the posterior density and the design of X-ray acquisition to minimize the uncertainty.

Due to the nonlinear impact of shape changes on the projection images, the posterior density is a mixture of Gaussian and Laplacian distributions. This makes UQ by local Gaussian approximation unreliable and requires the use of sampling techniques or a more accurate modeling of the impact of nonlinearities.

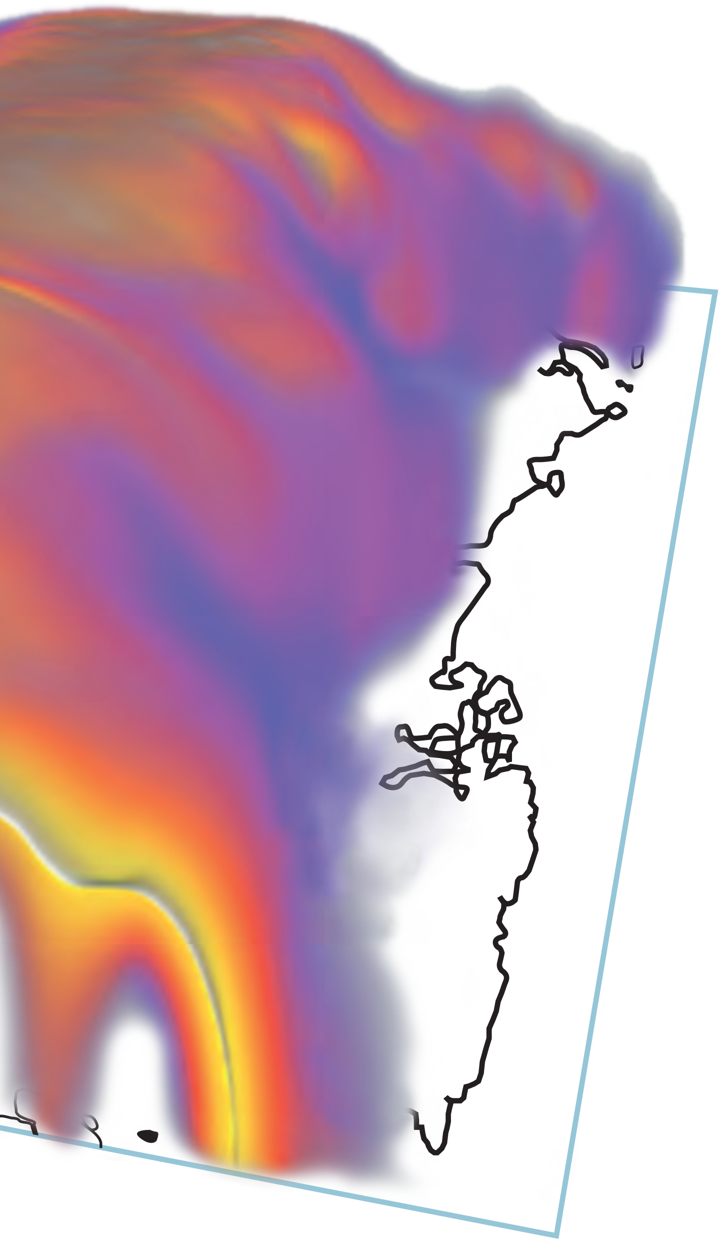
UNCERTAINTY VISUALIZATION



In many applications of information processing, humans are (still) involved; examples are explorative data analysis where humans try to gain understanding or making decisions based on computed information. In such cases, information must be conveyed to humans, ideally by visualization. If the information is subject to uncertainty, this should also be communicated visually.

Research in the group Visual Data Analysis in Science and Engineering at ZIB focuses on the visualization of uncertainties in spatial and spatiotemporal data, particularly on cases where certain "features" in the data are of interest. Examples of such features are level sets, critical points, and ridges in scalar fields, or critical points in vector fields. For uncertain data that can be represented as random fields, an approach has been developed to compute and depict the resulting spatial or spatiotemporal uncertainties of such features [11, 12]. Here, expectation values of feature indicators are computed with Monte Carlo methods; these can be interpreted as probabilities of the presence of a feature at some point in space or space-time.

In Scientific Computing, uncertainties are often captured by ensemble computations, where instead of a single computation many computations are performed, with varying parameters or even mathematical models. This approach is used in meteorology and climatology, for example. If the results of such ensemble computations can be summarized in random fields, our methods for uncertainty visualization apply directly.



8

8 Color-coded spatial probabilities of the 0°C isotherm in the earth's atmosphere at some specific date. The white surface represents the isotherm of the ensemble average.

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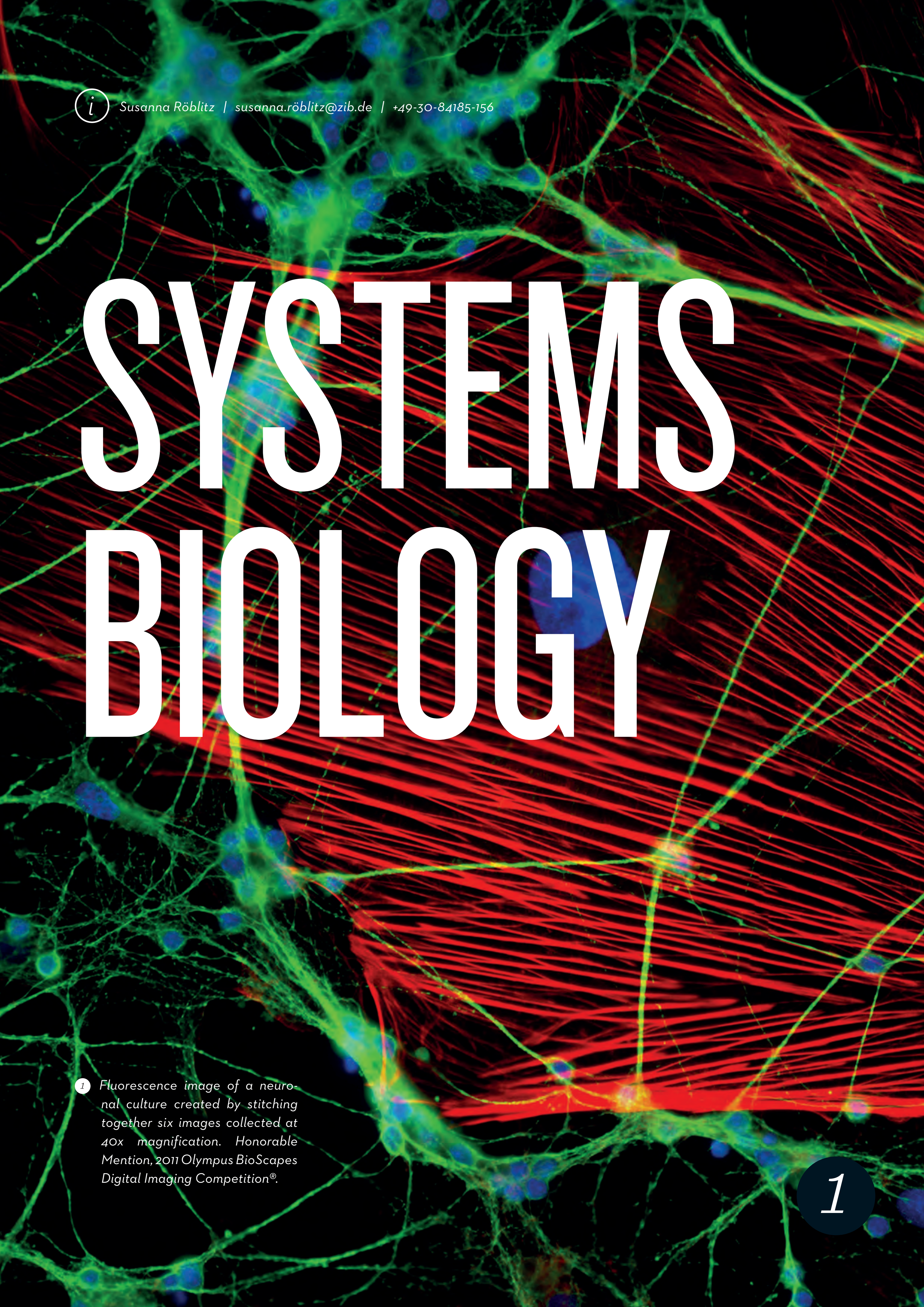
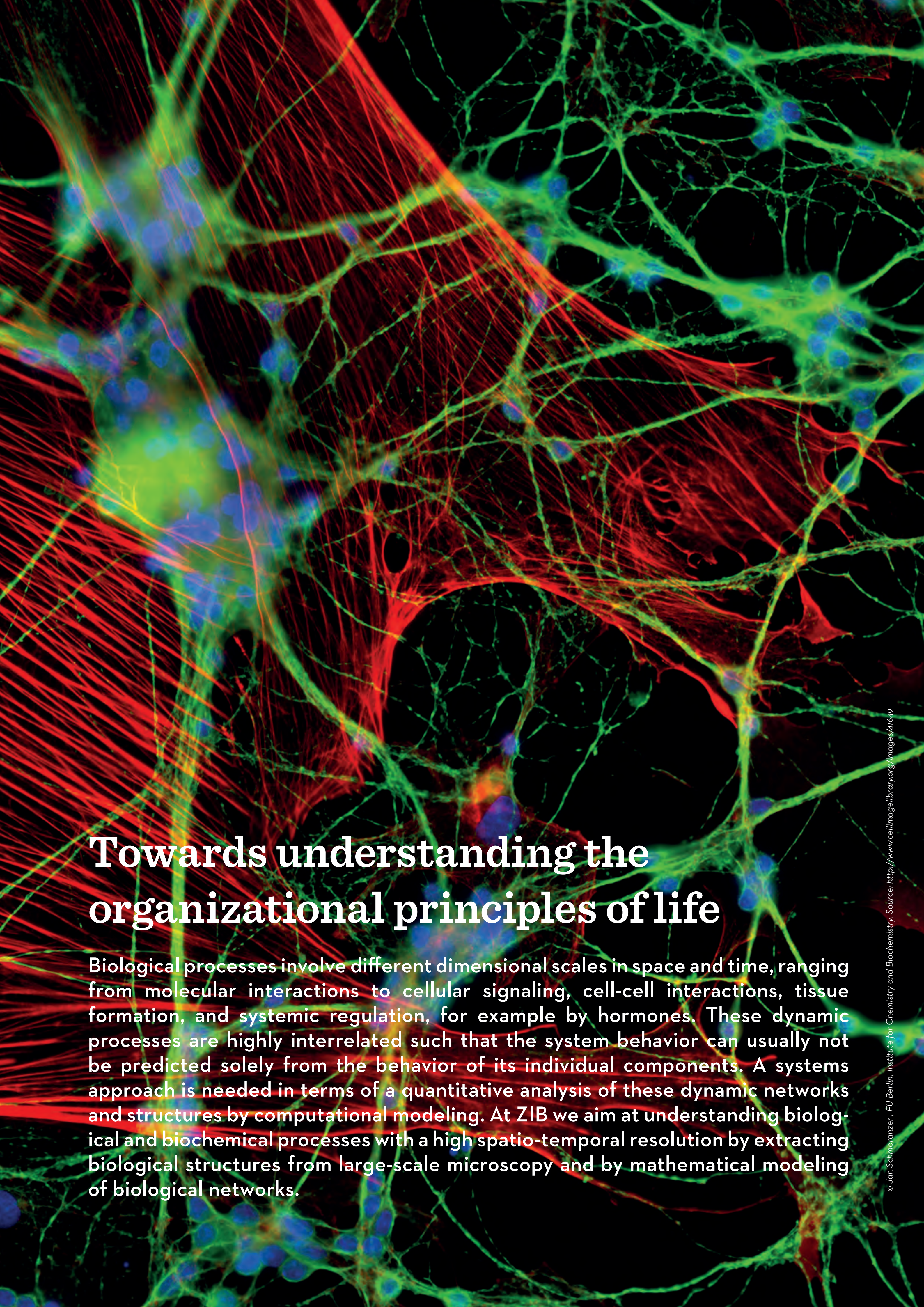
SYSTEMS BIOLOGY



1 Fluorescence image of a neuronal culture created by stitching together six images collected at 40x magnification. Honorable Mention, 2011 Olympus BioScapes Digital Imaging Competition®.



Towards understanding the organizational principles of life

Biological processes involve different dimensional scales in space and time, ranging from molecular interactions to cellular signaling, cell-cell interactions, tissue formation, and systemic regulation, for example by hormones. These dynamic processes are highly interrelated such that the system behavior can usually not be predicted solely from the behavior of its individual components. A systems approach is needed in terms of a quantitative analysis of these dynamic networks and structures by computational modeling. At ZIB we aim at understanding biological and biochemical processes with a high spatio-temporal resolution by extracting biological structures from large-scale microscopy and by mathematical modeling of biological networks.

A VIRTUAL HOSPITAL FOR REPRODUCTIVE MEDICINE

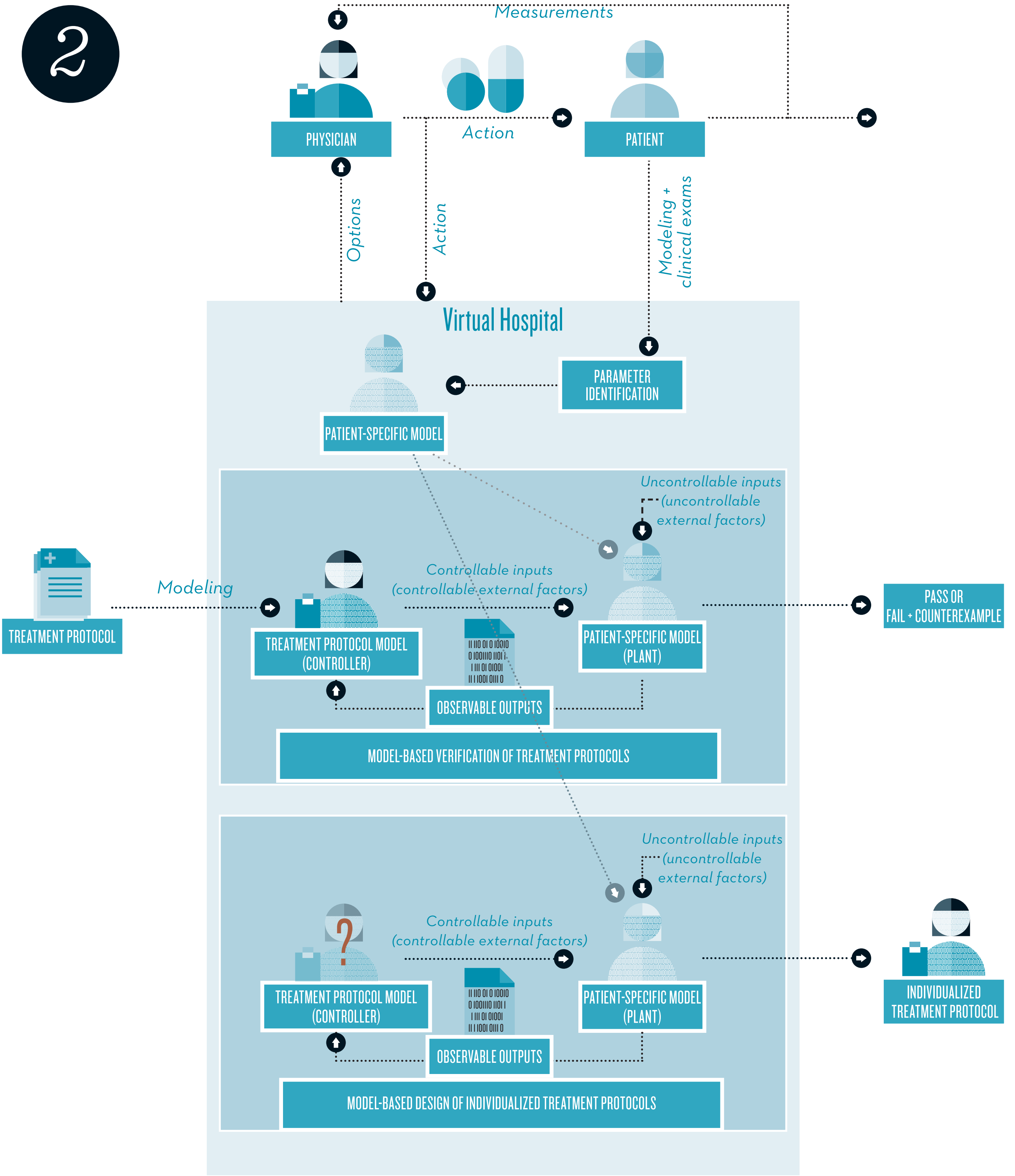
For many couples, having children is one of the major aims of life. Failure is associated with guilt, inadequacy, and loss of the sense of purpose in life, bearing an increased risk for negative psycho-social functioning. Furthermore, changes in population demographics and greater focus on education and careers among women have resulted in greater numbers of women attempting pregnancy at more advanced ages when they are inherently less biologically fertile. In Europe, for example, infertility affects 10% to 15% of couples at the reproductive age.

Human fertility is based on physiological events like adequate follicle maturation, ovulation, ovum fertilization, corpus luteum formation, as well as endometrial implantation, proceeding in a chronological order. Diseases such as endometriosis or polycystic ovary syndrome seriously disturb menstrual cycle patterns, oocyte maturation, and, consequently, fertility. Besides endocrine diseases, several environmental and lifestyle factors, especially smoking and obesity, also have a negative impact on fertility.

Modern assisted reproductive technologies have dramatically increased the chances for successful pregnancy. Nevertheless, current success rates have only reached 35%, even in leading clinical centers. The main reason is a limited understanding of the large inter- and intra-individual variability in hormonal regulation. We tackle this problem within the collaborative research project PAEON – Model Driven Computation of Treatments for Infertility Related Endocrinological Diseases, which has been funded by the European Commission since 2013. Partners of the Computational Systems Biology group at ZIB are the Sapienza University of Rome, the Lucerne University of Applied Sciences and Art, the Hannover Medical School, and the University Hospital Zurich.

Within this project the problem is addressed with a systems biology approach that aims at integrating clinical data with mathematical modeling of the complex biological system [1]. Although the relevant components and feedback mechanisms have been identified from experiments and have been described qualitatively for many years, dynamic mathematical models for the periodic changes in hormone levels and follicular function started being developed only a few years ago. From a mathematical point of view, the challenge is to represent a single real patient or a patient population with virtual patients, whereby a virtual patient is characterized by a specific parametrization of the model equations [2]. For this purpose, statistical model checking and Bayesian methods for parameter inference are applied.

The goal of the mathematical approach is to develop a model-based clinical decision support system for physicians [3]. As part of a software called "virtual hospital," such a system contributes to a better understanding of the highly complex processes in the female cycle and provides the opportunity to simulate and optimize treatment strategies on the computer, thus finding patient-specific treatments with the highest expected success rates.



2 In the virtual hospital a physician enters real patient data into the system and proposes an action, a specific treatment strategy, for example. The system then predicts a patient-specific success rate for the proposed treatment (model-based verification of treatment protocols) or even proposes a modified treatment with a higher expected success rate (model-based design of individualized treatment protocols). The output contains options to be performed on the patient, like dosing recommendations or days where measurements should be taken. Note that the output is just a recommendation, the final decision is made by the physician.

HIGH-PERFORMANCE DAIRY COWS – A METABOLIC CHALLENGE

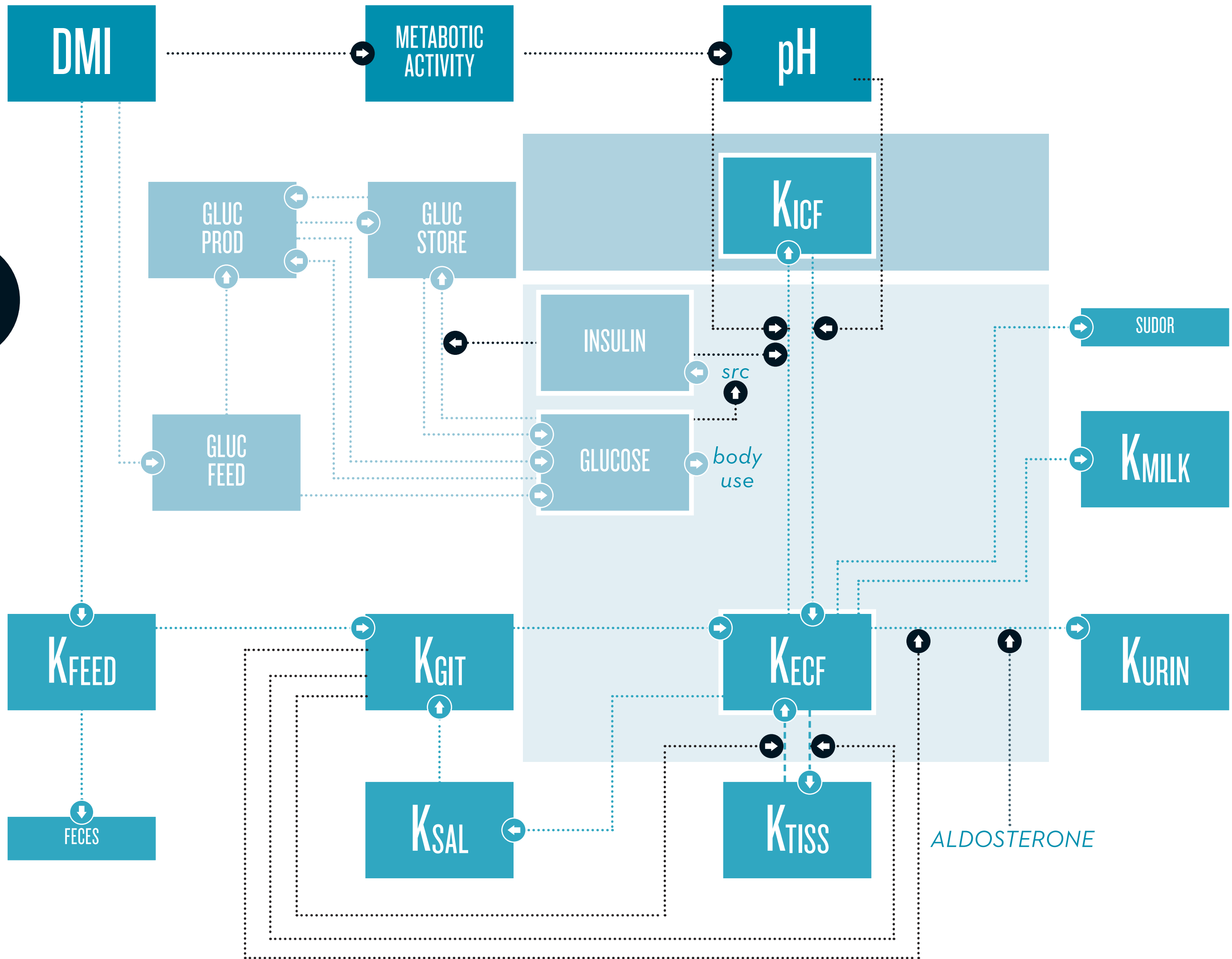
Modern dairy cows produce up to 50 litres of milk per day. This is an enormous challenge for the organism that needs to provide the substrates and the energy. Therefore, high-producing dairy cows often suffer from prevalent diseases which affect their metabolism and, as a consequence, lead to reduced fertility. Over the last few decades, animal scientists have studied the complex interplay between energy balance, nutrition, milk yield, and fertility, and collected large amounts of data, in vitro as well as in vivo. In order to find and understand the biological mechanisms that arise from the dynamic interactions of the different components, a systems biology approach is needed to analyze and integrate these data into predictive mathematical models in silico.

We are facing this challenge within the Junior Research Group project BovSys, which is funded for five years by the Federal Ministry of Education and Research (BMBF). Our aim is the development of a dynamic, mechanistic, mathematical model of genetic, nutritional, and physiological control of reproductive processes in dairy cattle. Integrated into larger models and software for herd or farm management, this research contributes to a sustainable production of food and a predictive veterinary practice, including an early warning for disease and the identification of new targets for diagnosis and treatment.

Currently, we are working with two major models of physiological networks that are related to the hormonal regulation, energy, and mineral metabolism of dairy cows: a model for the bovine estrous cycle [4], named BovCycle, and a model for potassium balance [5]. Both models are linked by a model for the glucose-insulin interaction [6] that is known to influence both networks. There are pharmaceutical interventions frequently performed in veterinary practice, like application of glucocorticoids, whose effects on potassium balance and reproduction have not yet been studied in detail. We are particularly interested in conducting in-silico simulations of such interventions. Studying the systems' behavior gives new insights into short- and long-term effects and interactions of drug administrations, without the need for new animal experiments.

3 Potassium balance in dairy cows is the result of dry matter intake (DMI), distribution inside the organism, and excretion, mainly via urine, milk, feces, and sudor. Distribution between the extracellular fluid (ECF) and intracellular fluid (ICF) is influenced by the glucose-insulin metabolism and pH.

3



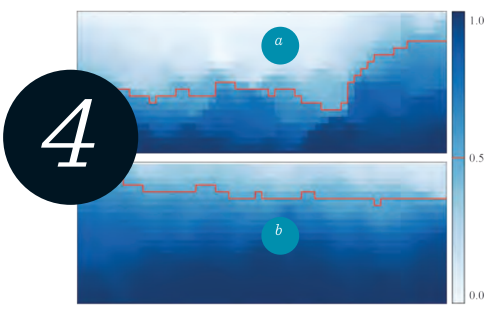
MICROSCOPY IMAGE ANALYSIS FOR UNDERSTANDING MOLECULAR SIGNALING

Many processes in systems biology depend on molecular signals. Such signals can control the behavior of cells. The signals can, for example, stimulate growth or cell migration. The effect of signal proteins is important for many processes in the human body. It is also crucial for understanding diseases like cancer. One of the main characteristics of cancer is an increased angiogenesis, the attraction of blood vessels. Tumors can emit signal proteins like Vascular Endothelial Growth Factor (VEGF) to attract the formation of new blood vessels towards it in order to grow even faster.

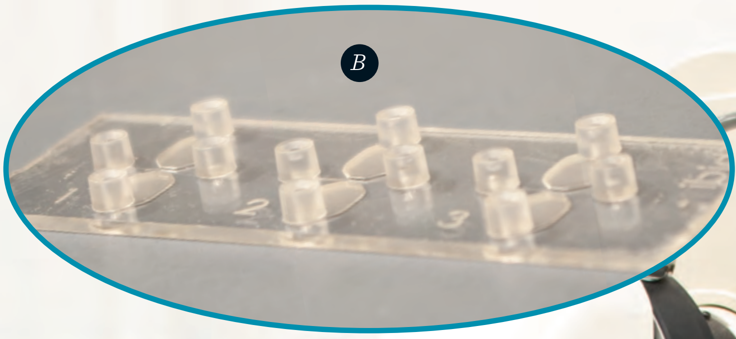
In collaboration with the Institute of Chemistry and Biochemistry at FU Berlin, we have been working on understanding molecular signaling in cells experimentally. We develop analysis methods and software that enable biologists to investigate cell behavior under various conditions. One example are factors that control cell migration, which can be identified using chemotaxis migration assays. Therefore, hundreds of epithelial cells from the human umbilical vein (HUVECs) are seeded in the middle of a two-chamber glass slide. In one condition, both chambers are filled with a nutrition-free medium. In a second condition, low doses of VEGF are added to the lower chamber. Cell migration is then monitored using a phase-contrast microscope, acquiring a sequence of images over 16 hours with a five-minute interval, in order to detect the preferred migration direction. To analyze and quantify the migration behavior objectively, we developed a method to track the movement of individual cells robustly. The exact position for around 500 cells for almost 200 time points alone, however, is not sufficient to understand the migration behavior, because cell migration is a complex biophysical process, and the migration appears chaotic at first glance. When a growth factor like VEGF is present, cells are only expected to have a preferred migration direction, although they do not migrate straight towards the growth factor.

In this example, we applied Markov State Models (MSM) to model, analyze, and visualize the relevant migration patterns. One of these analyses is the Committor Analysis, which calculates the probability for a cell to migrate to the lower image border before reaching the upper border.

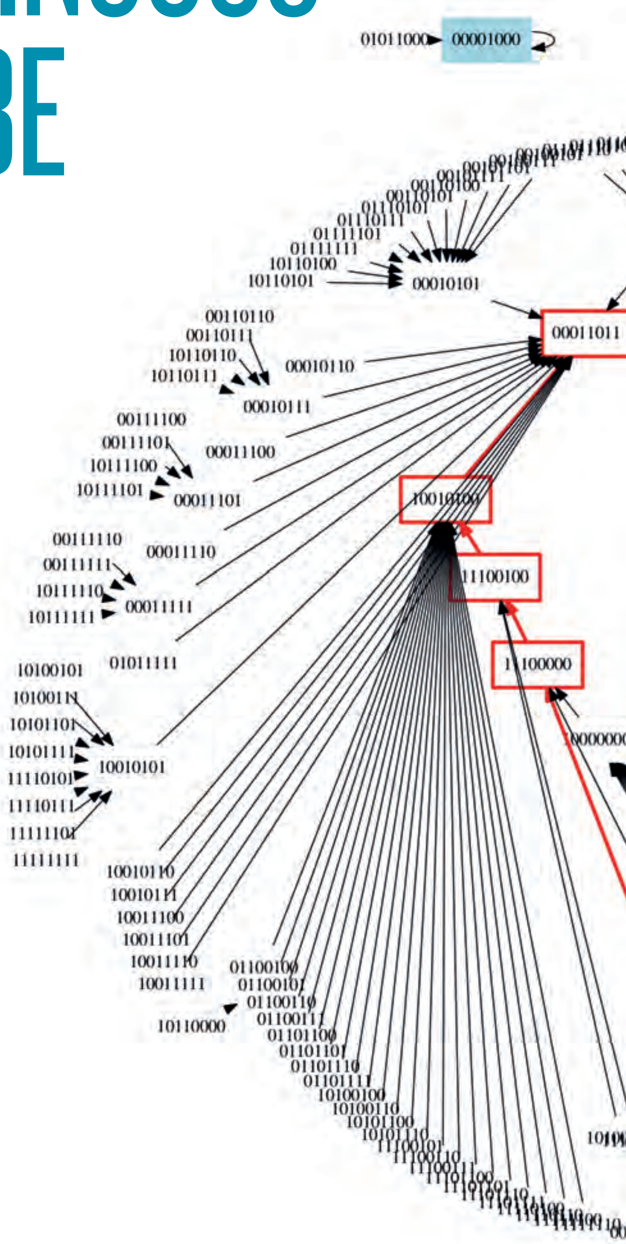
4 Results of the committor analysis. The color represents the probability for a cell to migrate towards the lower image border rather than the upper image border, and the 0.5 isoline indicates that all cells below are more likely to migrate downwards and vice versa. Figure a below depicts the results from the experiment without a gradient. The isoline is located around the image center, thus cells will most likely migrate towards their nearest chamber. The results from the VEGF experiment are depicted in Figure b, where the isoline is clearly shifted upwards. This indicates that cells on most of the image area will probably migrate downwards, where the VEGF-filled chamber is located.



5 *Cells are most likely to migrate towards their closest chamber when no growth factor is present* A. *But in the presence of VEGF in the lower chamber, most cells tend to migrate towards the VEGF* B. *Our analysis allows us to detect and quantify such effects.*



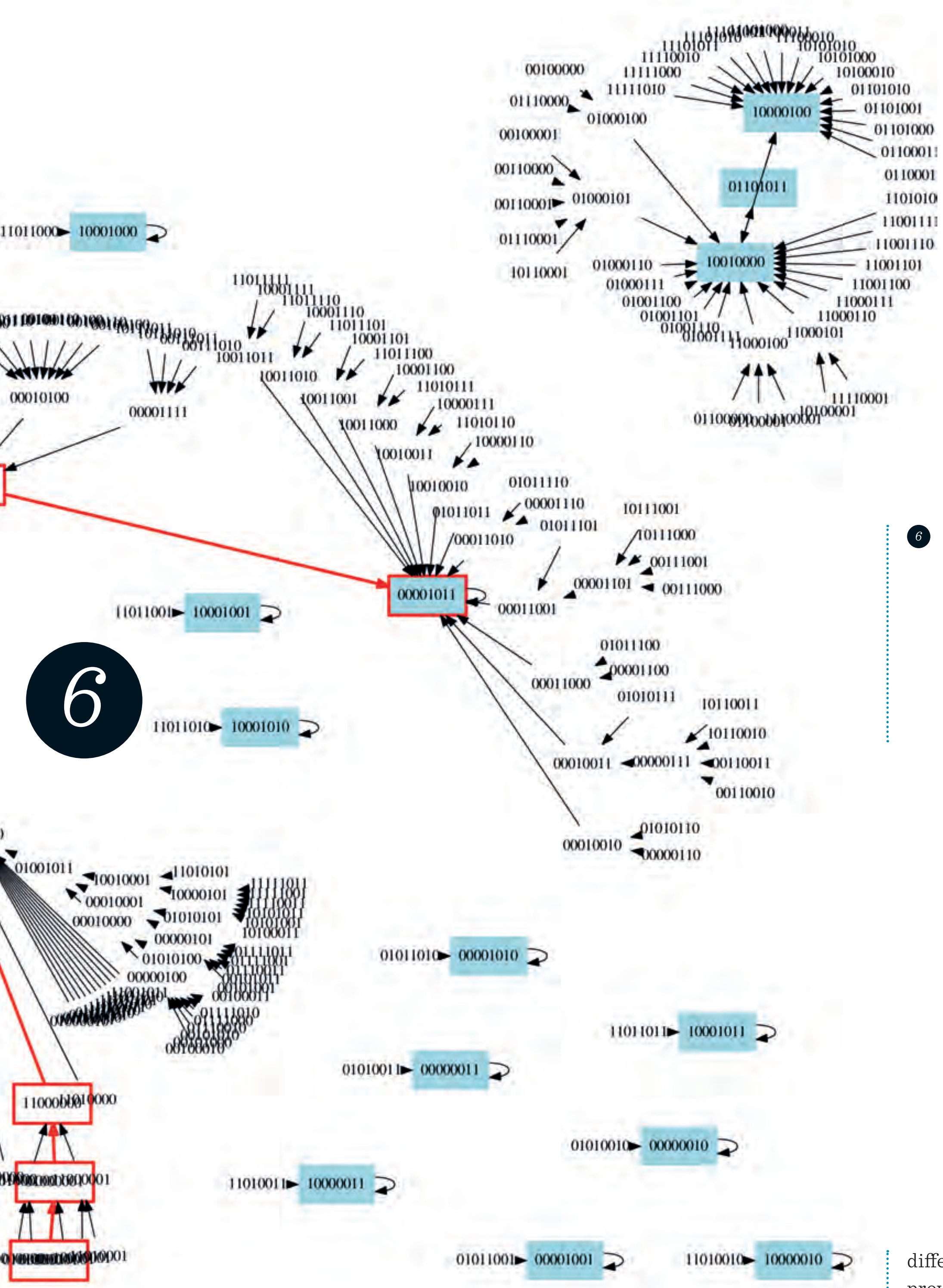
DISCRETE OR CONTINUOUS – HOW TO DESCRIBE BIOLOGY WITH MATHEMATICAL EQUATIONS



Typical experiments on single cells or tissue involve measurements of gene expression levels or the identification and quantification of certain molecules, proteins, for example, as well as techniques for analysing the dynamics and interactions between the measured components. The systems biology approach aims at creating, refining, and retesting mechanistic, mathematical models to accurately reflect the experimental observations and to make predictions about the system's behavior upon environmental changes.

The first step in that process is to decide on a suitable mathematical formalism. That means, the modeler has to decide if the state space of the model (activation levels, molecule numbers, or concentrations, for example), the time variable, and the space variable are discrete (integers) or continuous (real numbers), and if there are stochastic fluctuations present or not. This choice depends on the quality of the available measurements and on the research question to be answered. Examples of modeling formalisms include Boolean networks, ordinary differential equations (ODEs), and the chemical master equation (CME) for spatially homogeneous systems, or partial differential equations (PDEs) and the spatio-temporal master equation (STCME) for inhomogeneous systems. Boolean networks, for example, were introduced as qualitative models of genetic regulatory networks, where genes are modeled as binary switches, whereas ODEs and CMEs can be used to describe chemical reaction networks.

Every modeling approach has its advantages and disadvantages. Generally, fine-scaled models allow more detailed statements about a system, but are often costly to solve, and the uncertainty in the prediction is much higher because the number of unknown model parameters is usually very large. Our



6 The state space and trajectories of a Boolean model of the cell cycle in fission yeast [10]. The red transitions represent the different phases of the cell cycle. In blue are other attractor states predicted by the model (Courtesy H. Klarner).

research focuses on the development of efficient algorithms for the numerical solution of such models [7] as well as on the quantification of uncertainty in model predictions.

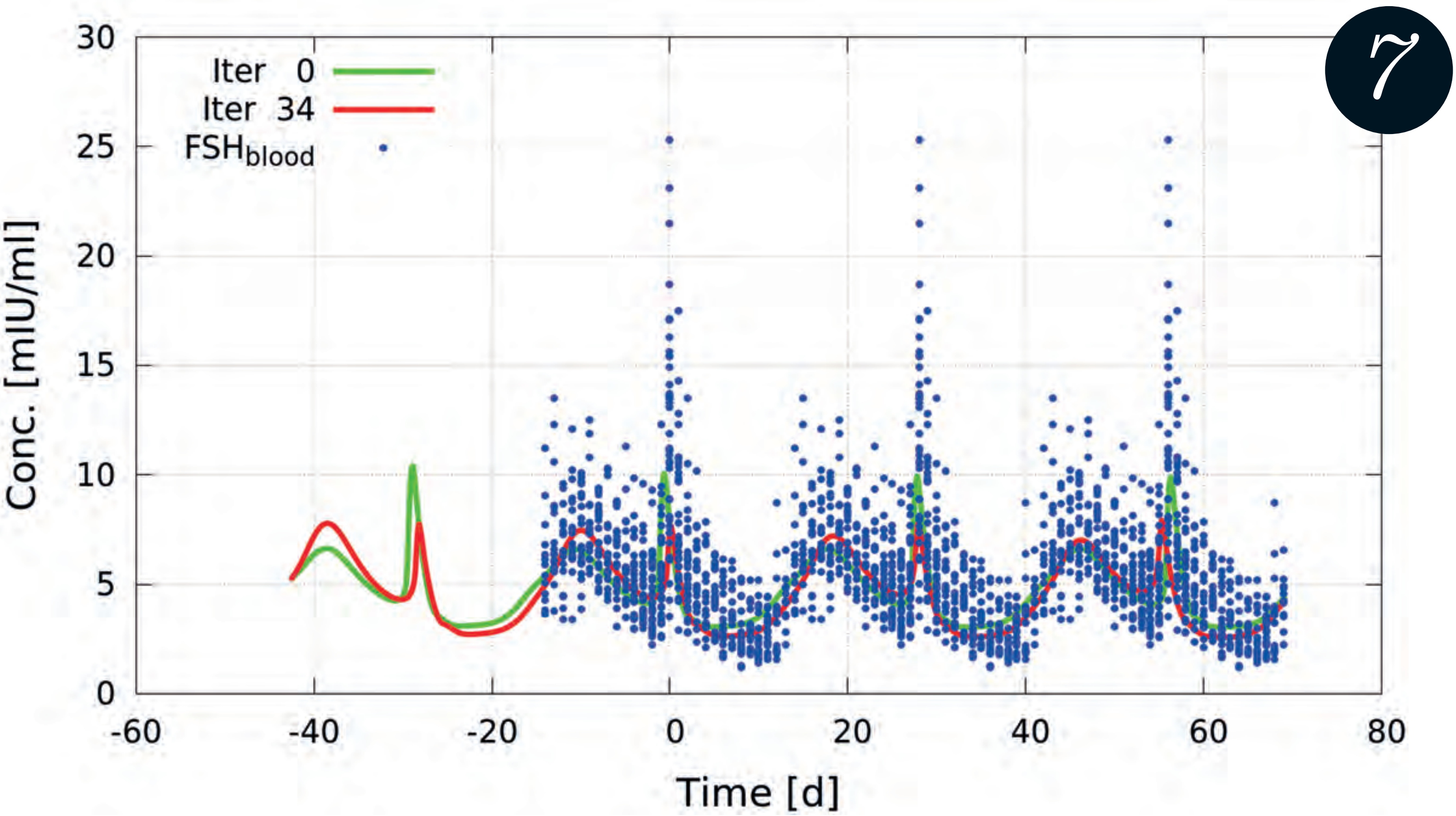
Coarse-grained models, on the other hand, are often easier to solve. They allow for a comprehensive analysis of the state and parameter space, but do not resolve all details of the underlying biological mechanisms. Common to all modeling formalisms is the fact that a model always constitutes a simplification of reality, focusing on particular aspects of interest and neglecting details either by design or simply due to a lack of knowledge.

Hence, our research at ZIB aims at combining different methods by using complementary modeling approaches and by building hybrid models. Utilizing different modeling approaches in parallel provides an alternative view on system characteristics and highlights modeling artifacts. For example, a complementary analysis of an ODE model for the bovine estrous cycle [8] using a Boolean network led to new insights regarding the regulation among the components, and also indicated strongly that the system is tailored to generate stable oscillations [9]. However, the mathematical questions of property conservation across formalisms, as well as the derivation of hybrid models in the presence of scaling cascades, are still largely unaddressed and will be in the focus of our future research.

SYSTEMS BIOLOGY SOFTWARE DEVELOPED AT ZIB

Modeling, parameter identification, and simulation play an important role in systems biology [13]. Computational system biology without efficient numerical software is hardly imaginable. Biological systems, the female menstrual cycle or cellular signaling processes, for example, are as diverse as they are complex. All these different systems, translated into the mathematical language, can be investigated and analyzed by our software: interactive, simple to use, and, most importantly, easily extensible for novel approaches. Our software is suitable not only for innovative research, but also for day-to-day teaching purposes. The software development process is done completely openly, accessible to everyone, as is all of our software.

To date, we have developed the software packages BioPARKIN[12] and ZIB_RubyExt[13], both publicly available at GitHub. Both packages involve long-standing mathematical codes for the numerical solution of ordinary differential equation systems, or simulation, and for parameter identification. In addition, they provide accurate and efficient numerical routines for solving the sensitivity equations; that is, for computing the sensitivity of the simulation results with respect to the model parameters. In our software, the effort for this computation only grows linearly with the number of model parameters, whereas the effort in standard implementations



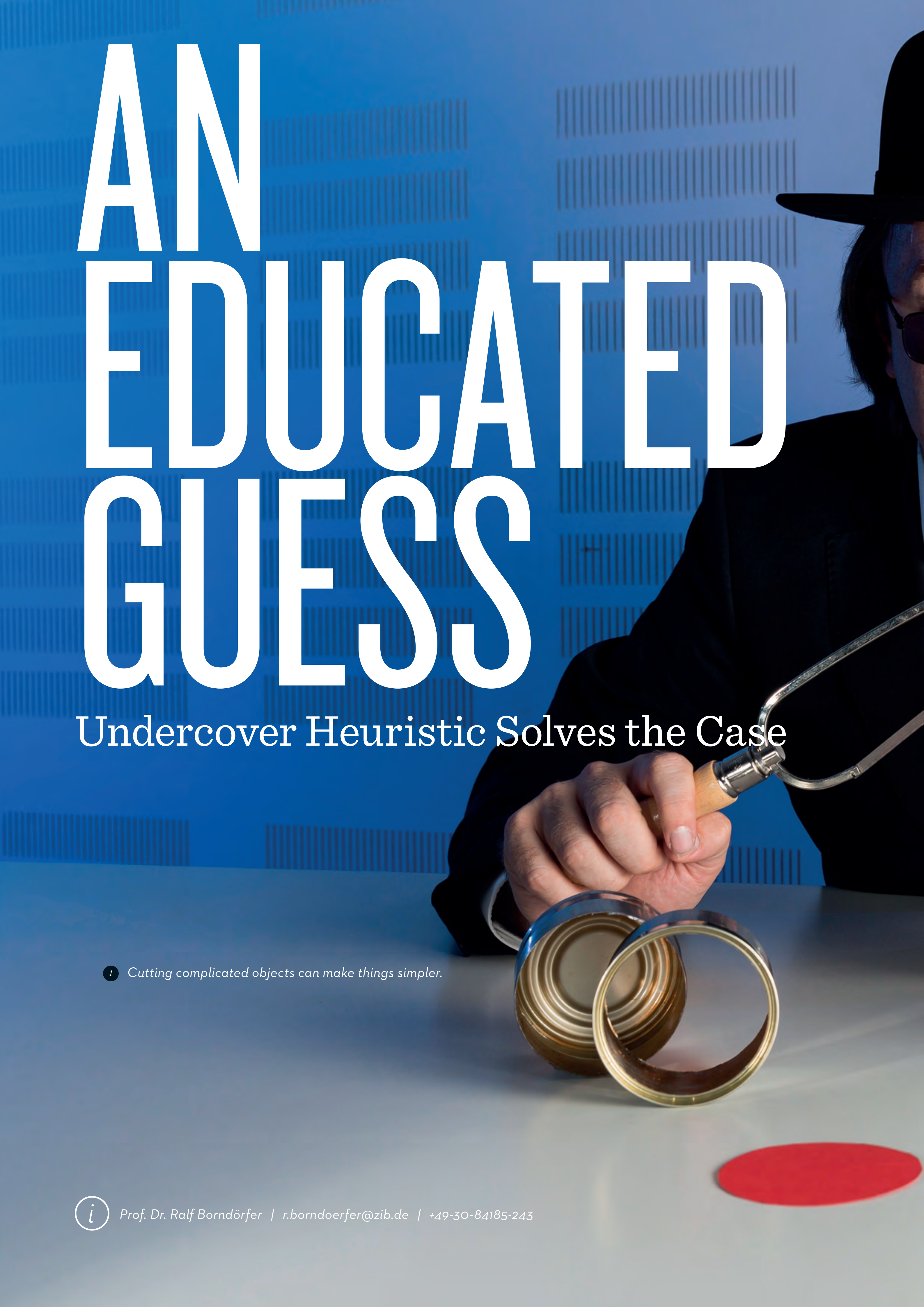
grows quadratically. Further speed-up in ZIB_RubyExt compared to BioPARKIN is obtained by making use of a library for automatic differentiation.

Both BioPARKIn and ZIB_RubyExt are compliant with the Systems Biology Markup Language (SBML), which has become the standard for representing models in systems biology. BioPARKIN consists of a computational core in C++ and a user-friendly graphical interface in Python, which hides the complicated math and makes it easy to use for non-mathematicians. Compared to BioPARKIN, ZIB_RubyExt is even more versatile, robust, and fast. ZIB_RubyExt makes use of numerical FORTRAN routines in Ruby. It is extremely easy to extend by the inheritance scheme of Ruby, similar to a plug-in mechanism. In addition, it is Web/mobile application ready, which paves the way for its use in clinical decision support systems or personal health records, for example.

7 Parameter identification result obtained by Gauss-Newton iteration in ZIB_RubyExt. Parameters in a model of the human menstrual cycle were estimated such that simulation results (solid lines) fit to measurements of hormone blood concentrations, including the follicle stimulating hormone FSH (blue dots).

AN EDUCATED GUESS

Undercover Heuristic Solves the Case



1 *Cutting complicated objects can make things simpler.*

Prof. Dr. Ralf Borndörfer | r.borndoerfer@zib.de | +49-30-84185-243

Buses, mobile phones, football: we encounter integer optimization problems in situations where we least expect them. In order to find solutions to such problems, you need good intuition – and also a bit of luck. This feature explains in plain text how this works. It won (in a slightly modified form) the Klaus Tschira Award 2015 for Achievements in Public Understanding of Sciences – KlarText! [3].

1

It's nice weather today and your favorite club is playing. You call your friends to arrange a meeting point and take the bus to the stadium. While having some cold drinks before kick-off, you discuss whether the roster of the upcoming opponent favors your club or not. You're having a great day with mathematics.

Mathematics? Yes, because bus timetables, the allocation of mobile radio frequencies to cell towers, and scheduling of sport leagues, are all so-called "integer optimization problems." Such a problem consists of three basic components: an objective function, constraints, and the restriction to integer solution values. Let's explain this using the examples provided above.

Passengers like to have short transfer times; for mobile communication, there should be little interference between adjacent transmission towers; and in professional sports, the revenue from broadcasting rights should be maximized. That is the objective function: something you aim to shrink within the feasible options, or something you are trying to expand. The constraints determine what the feasible options are; that is, constraints are like rules that have to be observed in any case. Bus drivers have to take breaks; there are location restrictions for the placement of transmission towers; and for many leagues, home and away games have to alternate. Such constraints can be formulated as a mathematical equation system – just as we remember it from school, but much, much larger. Instead of two or three variables and equations, there are often hundreds of thousands. For these equations we would like to find the best possible solution (concerning the objective function). Finally, there is the restriction to whole numbers, or integers. Half a bus driver or two-thirds of a football team – that doesn't work. Therefore, we need to find solutions that are in integers; hence, the variables take values such as zero, one, or two, but not five and three-sevenths.

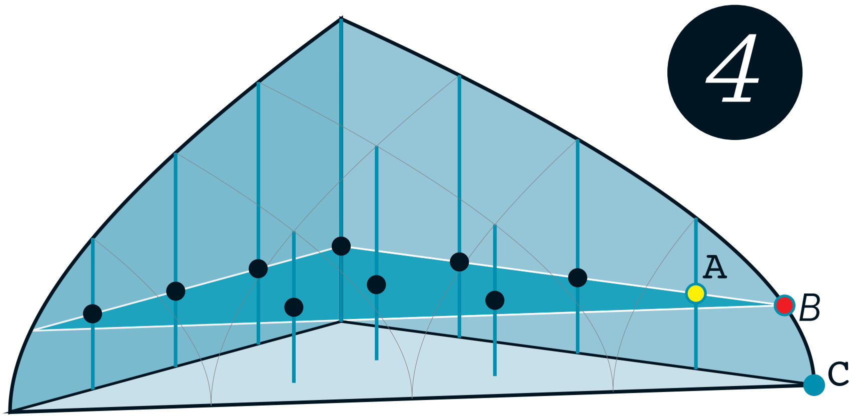
2 *A mathematician searching for a good solution.*

When the mathematicians at ZIB are faced with a new optimization problem, there are two major steps to be taken. The first step is to set up a suitable model; that is, a system of equations. This usually happens by utilizing a blackboard and chalk – and a duster! What are the variables? Did we consider all the constraints, and does the objective really represent what we want? Write down, dust off, start again. When we have a good model, step two follows: finding a solution for this model. No blackboard in the world is big enough for such a calculation. Instead, this is accomplished with computer programs. And the good news is: a very large class of such models, so called integer optimization problems, can often be solved these days by extremely powerful black-box software, like the optimization toolkit SCIP, which has been developed at ZIB.

A PROGRAM THAT FINDS THE SOLUTION – THE HEURISTIC

The magic component of such a program is the one that finds the solution – the heuristic (from the Greek word "heuriskein," which means "to discover, to find"). Heuristics are methods that attempt to quickly construct a relatively good solution for a given problem, yet often do not find the best possible solution. One could say that heuristics are intelligent guessing methods.

4



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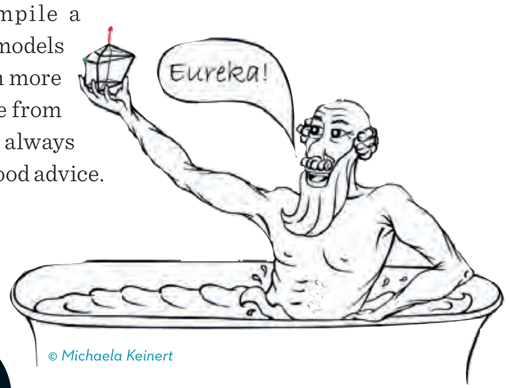
Heuristic decisions for optimization problems – this sounds complicated, but we all know heuristics from our daily lives. Imagine, for example, that you would like to buy a new smartphone. Theoretically, you could try to get a complete market overview and compare all of the available brands, models, versions, and all offers with each other. However, no one would do this, because it would take forever. Your favorite would probably be out of stock when you finally made your decision. Instead, you proceed in a much more focused and intuitive manner. You analyze some particularly relevant information, a test report, for example. You compile a shortlist of eligible models that you compare in more detail. You purchase from the retailer who has always provided you with good advice.



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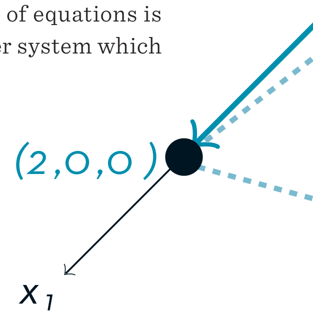
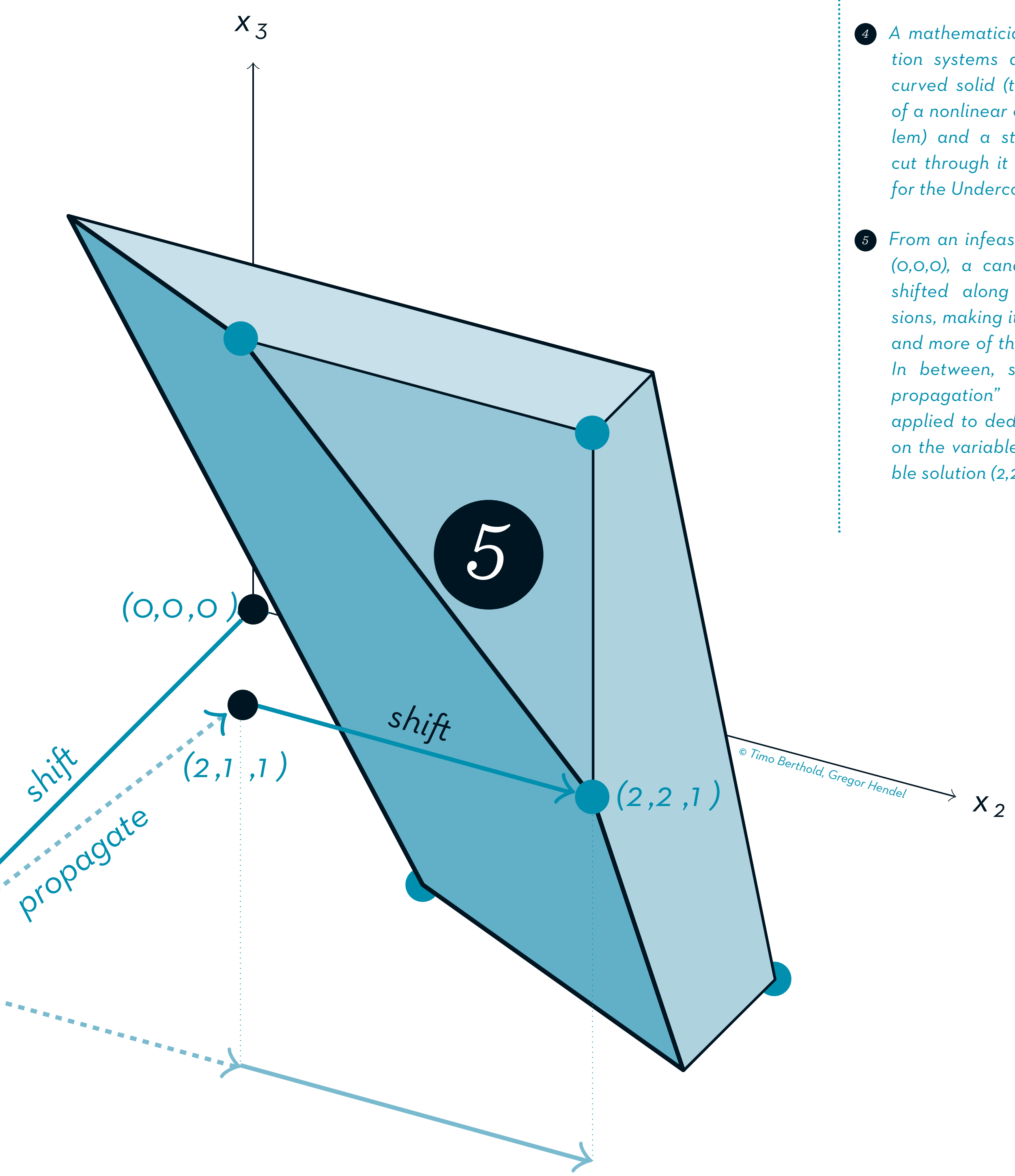
This is, more or less, how heuristics work. They collect statistics on which they base their decisions, try to fix a few variables, and recognize and exploit common patterns. Equation systems and the methods by which we solve them can often be interpreted and understood geometrically. Patterns can often be represented, moved, or divided geometrically. The set of feasible solutions of a system of equations might be a cube, a prism, a cone, or another solid. This object might be complex and multi-dimensional, but it is, literally, edgy. And at some point in this solid is the integer optimal solution that we are looking for.

One new heuristic of this type, which has been developed at ZIB and which has a nice geometric interpretation, is called "Undercover" [1,4]. It is based on the idea of finding an easy-to-handle solid within a much more complicated mathematical solid. Or to put it a different way: a huge, extremely hard system of equations is converted into a smaller system which is easier to solve.





3 Solutions can sometimes be found in strange places.

4 A mathematician's view of equation systems and algorithms: a curved solid (the solution space of a nonlinear optimization problem) and a straight, triangular, cut through it (the search space for the Undercover heuristic).

5 From an infeasible starting point (0,0,0), a candidate solution is shifted along different dimensions, making it feasible for more and more of the side constraints. In between, so-called "domain propagation" techniques are applied to deduce lower bounds on the variables. Finally, a feasible solution (2,2,1) is found.

Imagine a cylinder, or a solid in the shape of a tin can (see also Figure 1). If you cut a single, ultra-thin slice out of the cylinder, what do you get? Most people think of a circle, but that is not the only correct answer. If you cut through the cylinder along the height, then you get a rectangle as a cutting surface. The interesting part of this observation is that you have cut an object with straight sides from a round object with a single cut. In Figure 4, you can see a similar setup. The big, blue, "curved" object depicts the solution space of a nonlinear optimization problem. The Undercover heuristic restricts its search to the blue "straightly bounded" triangle, finding the solution corresponding to the yellow point A.

Mathematically, this cutting corresponds to the fixing of variables. The solid corresponds to the set of feasible solutions of an equation system. And interestingly, it is much easier to optimize over "straight-line-limited" objects than over curved objects. In math-speak: linear optimization is easier than non-linear. The Undercover heuristic proceeds exactly like this: determine the smallest possible set of variables of a given optimization problem that has to be fixed in order to obtain a simpler optimization problem. Then, solve this smaller problem. Any solution to it is a solution to the original problem, but not vice versa.

However, it may be that the optimal solution is not contained in our sub-problem, or worse that the sub-problem does not even have a feasible integer solution. After all, Undercover is just a heuristic. However, by an empirical analysis, three things could be demonstrated. First, it is often sufficient to fix relatively few variables to remove all non-linearities; that is, "straighten" the problem. Second, the resulting sub-problems can almost always be solved rapidly. Third, Undercover could find a feasible solution in more than half of the test cases. That's a very good value for a single heuristic.

Heuristics like Undercover or Shift-and-Propagate, see Figure 5, are generic; that is, they are not about a very specific application, but about the mathematics that are intrinsic to planning and the optimization of processes [1,5]. As a consequence, such methods can be utilized by a lot of different applications, though mostly behind the scenes. The mixed integer programming solver SCIP, which implements the named heuristics, was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6

6 This text (with some small changes) won a Klaus Tschira Award 2015 for Achievements in Public Understanding of Sciences – KlarText!. [3], see also http://www.klaus-tschira-preis.info/.

developed in cooperation with Siemens AG, SAP SE, and Open Grid Europe GmbH in the MODAL SynLab [2]. Methods developed at ZIB are nowadays employed by the three market leaders for mathematical optimization software – FICO Xpress, IBM Cplex, and Gurobi. As of today, such software is deployed in almost all blue-chip companies.

Final whistle. It was a really tight match with a well-earned win; that provides a nice buffer for the next few weeks. With your recently purchased smartphone, you check which bus is quickest for you. That's the beauty of integer optimization. We use its results, without having to think about it. If we encounter it in everyday life, then the optimal solution has already been found, maybe by one of the heuristics that were developed by researchers at ZIB.

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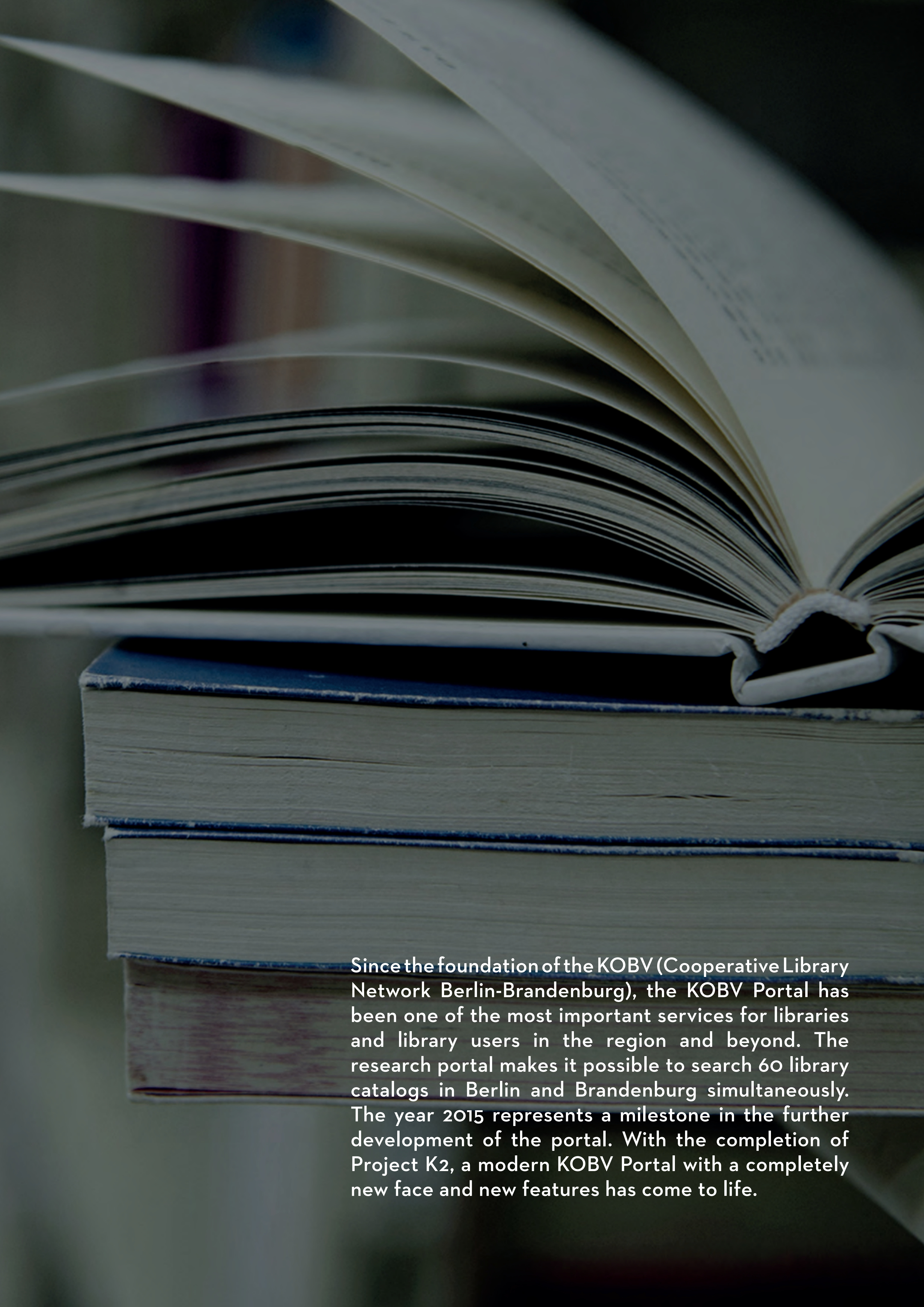
NEW KOBV PORTAL

DISCOVERY IN 60 LIBRARIES



Since the foundation of the KOBV (Cooperative Library Network Berlin-Brandenburg), the KOBV Portal has been one of the most important services for libraries and library users in the region and beyond. The research portal makes it possible to search 60 library catalogs in Berlin and Brandenburg simultaneously. The year 2015 represents a milestone in the further development of the portal. With the completion of Project K2, a modern KOBV Portal with a completely new face and new features has come to life.

KOBV PORTAL – FROM PROJECT TO SERVICE

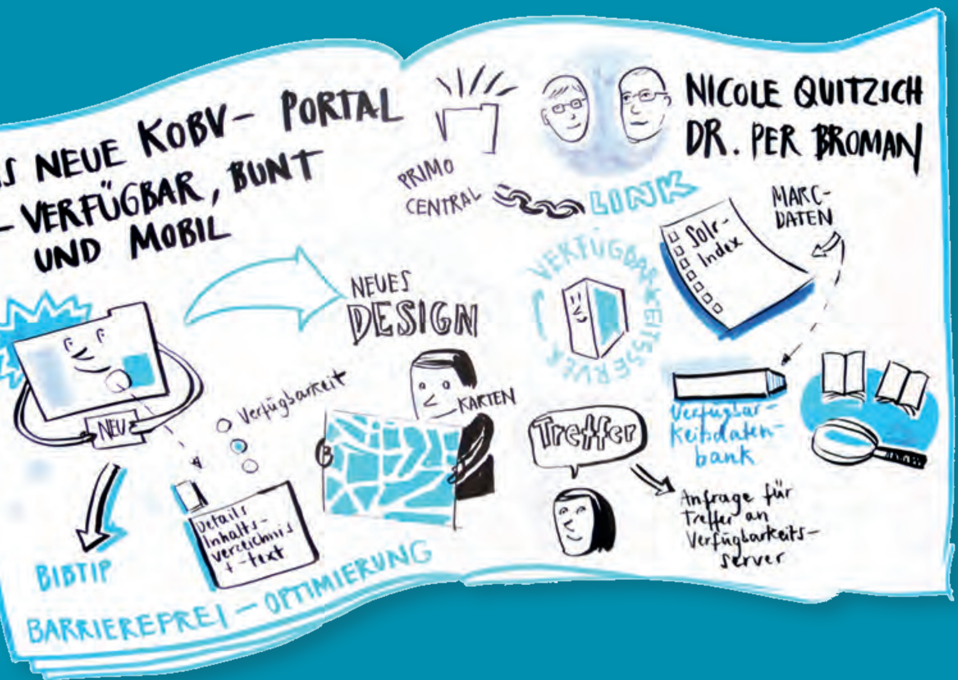
Abstract: The Cooperative Library Network Berlin-Brandenburg (KOBV) – located at ZIB since 1996 – benefits from the excellent technical infrastructure at Zuse Institute, which is paramount for the development of innovative information services for its customers. Since the foundation of the Library Network, the KOBV Portal has been one of the most important services for libraries and library users in the region and beyond. The research portal makes it possible to search 60 library catalogs in Berlin and Brandenburg simultaneously. About one million individual queries per month speak for themselves. The year 2015 represents a milestone in the further development of the portal. With the completion of Project K2, a modern KOBV Portal with a completely new face and new features has come to life.

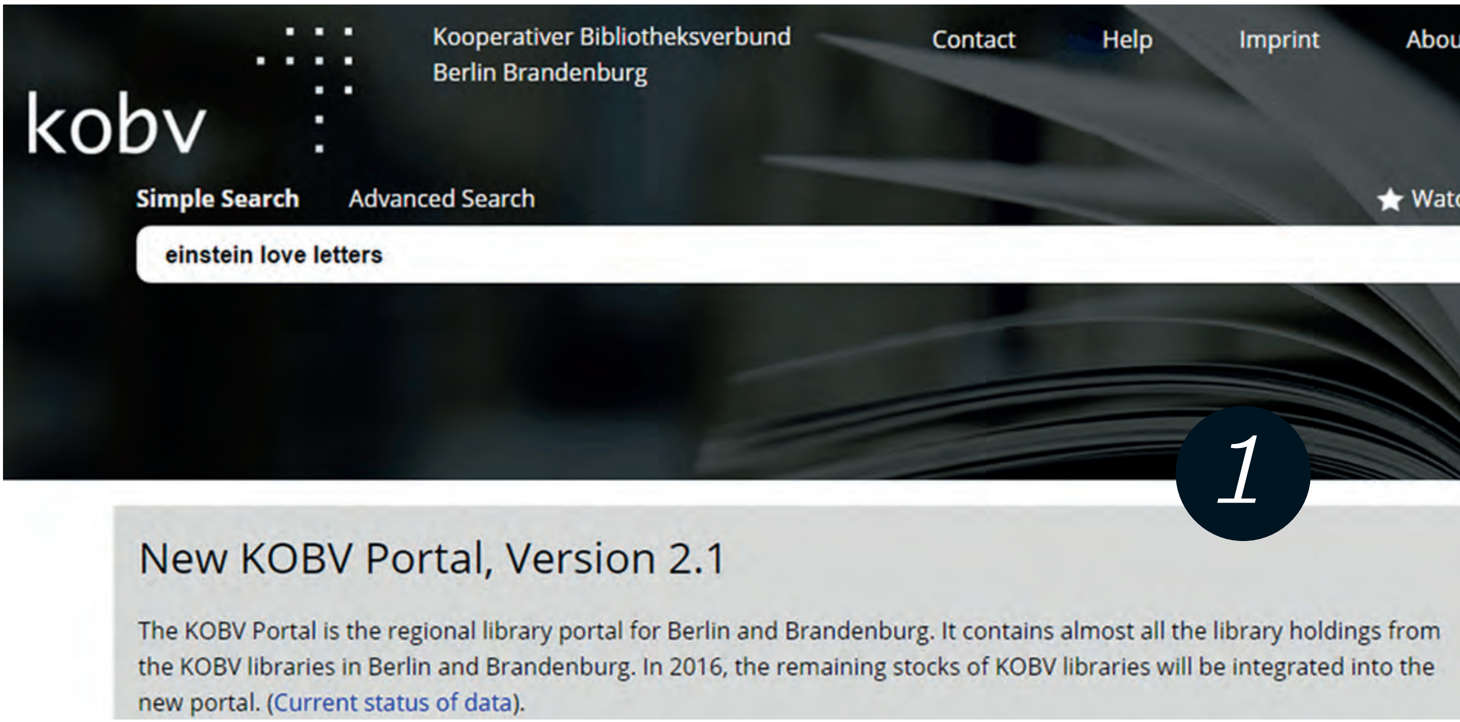
Those who do not only want to know which books and journal articles there are on a certain subject, but also where to get them without having to pull out their wallet, greatly appreciate being able to search library catalogs. The purpose of the KOBV Portal is to avoid having to sift through dozens of catalogs. Here, it is possible to search the library holdings of all university libraries, public libraries, and nearly 30 research and special libraries in the German federal states of Berlin and Brandenburg. These range from popular institutions to the small libraries of the Landesgeschichtliche Vereinigung der Mark Brandenburg, the Leibniz Centre for Agricultural Landscape Research, or the Haus der Wannseekonferenz, to name but a few. Unexperienced portal users frequently do not have the slightest notion that these precious collections exist. A search in the KOBV Portal regularly results in eye-opening experiences (we know this from surveys), when previously unknown collections of small libraries are discovered – in the true sense of the word – and surprising results are found.

In 2015, another milestone in the history of the KOBV Portal was achieved. We were able to complete the entire redevelopment following a two-year project period – “Project K2.” At the end of the year, the redevelopment, supported by the European Regional Development Fund (EFRE) of the Federal State of Berlin, was handed over to the KOBV operation (and, we are proud to say, in a well-documented way). In the future, the new KOBV Portal will be primarily geared toward mobile users in order to account for the worldwide trend toward permanent availability and the change in search habits.

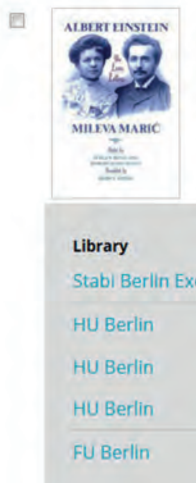
NEW AND ENHANCED FEATURES OF THE KOBV PORTAL

Besides a completely renewed design, the search experience and search performance in particular have been placed on a new footing by means of the ALBERT discovery software, which was developed in-house. In terms of functionality and usability, the portal has been comprehensively modernized in order to make the search experience more intuitive for the user (e.g. fewer clicks, clearer structure, personalized services). Furthermore, paramount to the success of the service, the search has become much quicker. Technically, an even better in-depth search of the collections of even the smallest libraries has been realized, and, for the first time, it is possible to also capture their unprinted ("born digital") materials. Now, several hundred million journal articles and other digital media, which have been licensed by different institutions, can be searched. Those looking for a particular book, however, should not be overwhelmed by millions of hits in the search results. Therefore, the search for journal articles is offered in a second menu tab that can be clicked separately.





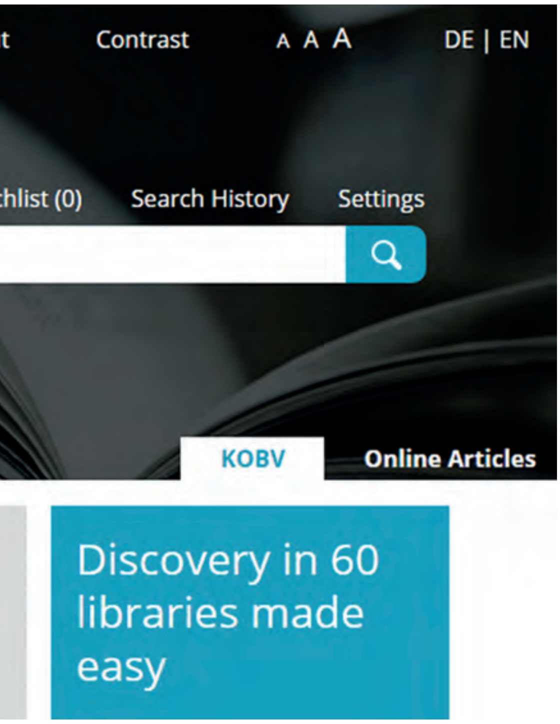
Faceted navigation using formal categories such as medium type, holding library, date of publication, or language helps users hone in on specific items of interest. For the first time, the search results also show whether a work can be borrowed in the relevant libraries at that particular moment or whether it may only be viewed in the reading room. This real-time item availability feature is intended to encourage users to visit the holding library, not least in order to reduce the number of unnecessary inter-library loans. By means of an internal link to the KOBV Bibliothekenführer, users can see the location of the holding library and the opening hours on an Open Street Map. In addition, for a lot of works, recommendations for related titles are displayed. This is done via a recommender function incorporating the widely used tool "BibTip." It seems that more relevant works are recommended compared to recommender systems known from sales platforms on the Internet ("customers who bought this item also bought ..."). Recommendations are based on statistical analyses of user behavior in various libraries. And, last but not least, we have invested in the improvement of Web accessibility pursuant to the W3C Web Content Accessibility Guidelines. Particularly in the field of (color) contrasts and the independent selection of font sizes, there was room for optimization. Web accessibility has been realized in detail by Webrunners GmbH in a separate development order dedicated entirely to



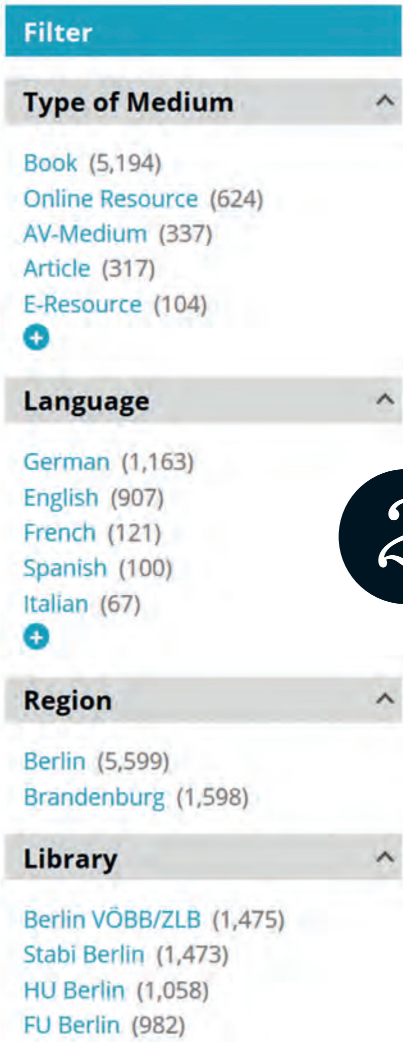
1 *Homepage of KOBV Portal (http://portal.kobv.de/).*

2 *Search filters to narrow down search results.*

3 *Representation of real-time item availability. Availability status is displayed using a traffic light metaphor.*



this purpose. For libraries, it is attractive to make their collections searchable in the KOBV Portal because, in this way, the collections become more visible to potential users. Since the beginning of the project phase in 2013, libraries' interest in becoming part of the portal has been consistently high – and by no means only KOBV member libraries. In the future, the KOBV Portal will continue to be open for experiments. It stands for agility and grows with the requirements of its users.



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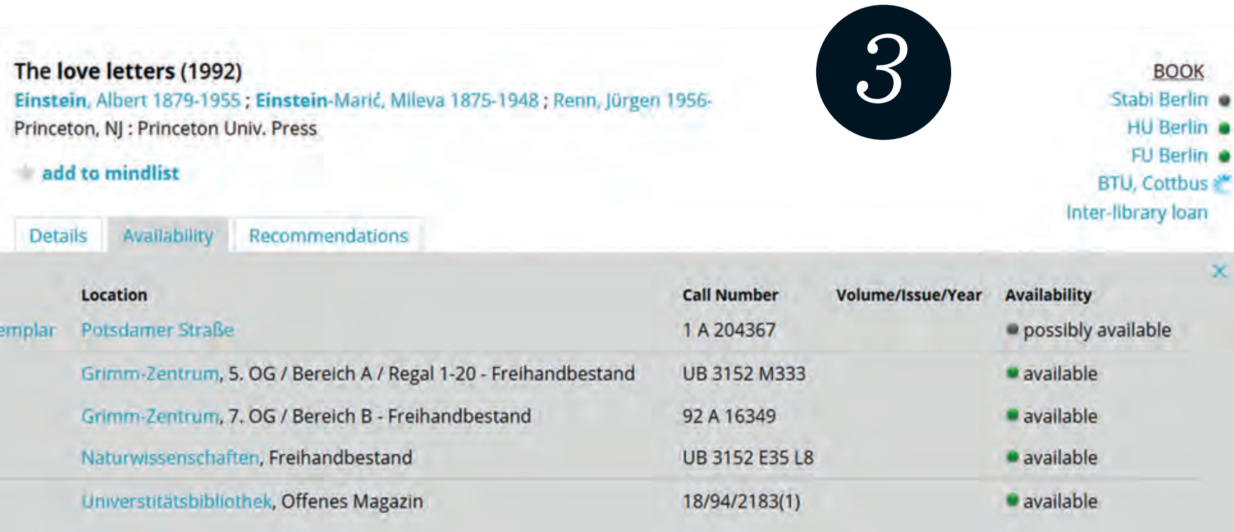
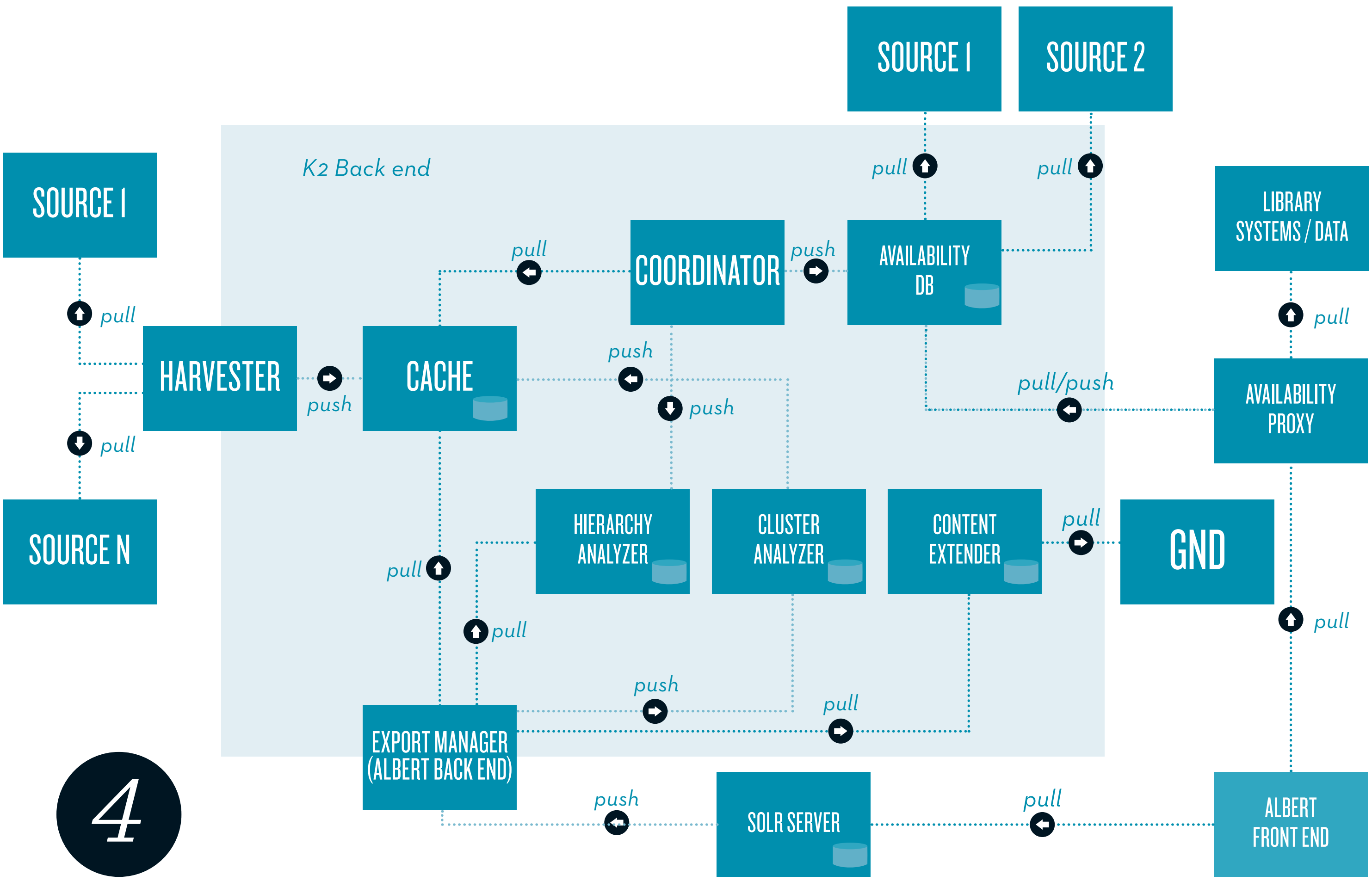


A LOOK BACK ON THE PROJECT PHASE 2013-2015

For the result to meet expectations, decisions about responsibilities had to first be made at the beginning of the project. In the Operation and Development project teams, more than ten librarians and developers were temporarily involved and cooperated very closely. For the search interface with integrated data management components, the required individual components were defined first and software decisions were made. Conceptually, the entire IT architecture consists of two more or less detached parts:

- Import, processing, and indexing to title sets; and
- Import and caching of item details and availability data.



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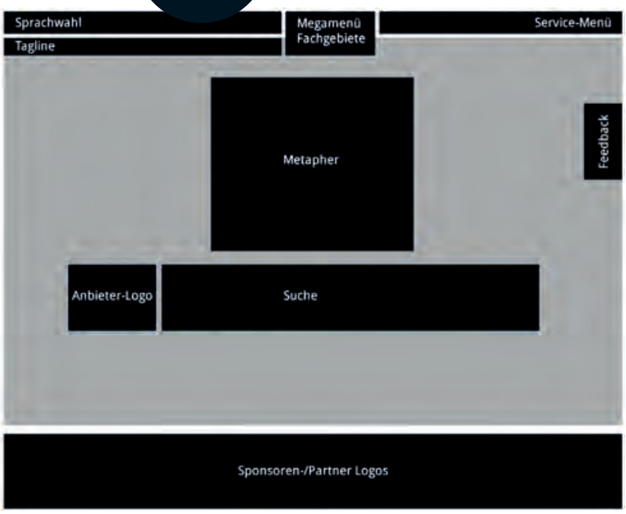


4 *Back-end architecture of KOBV Portal.*

5 *Exemplary mock-up of the search interface.*

6 *Initial KOBV Portal wireframe.*

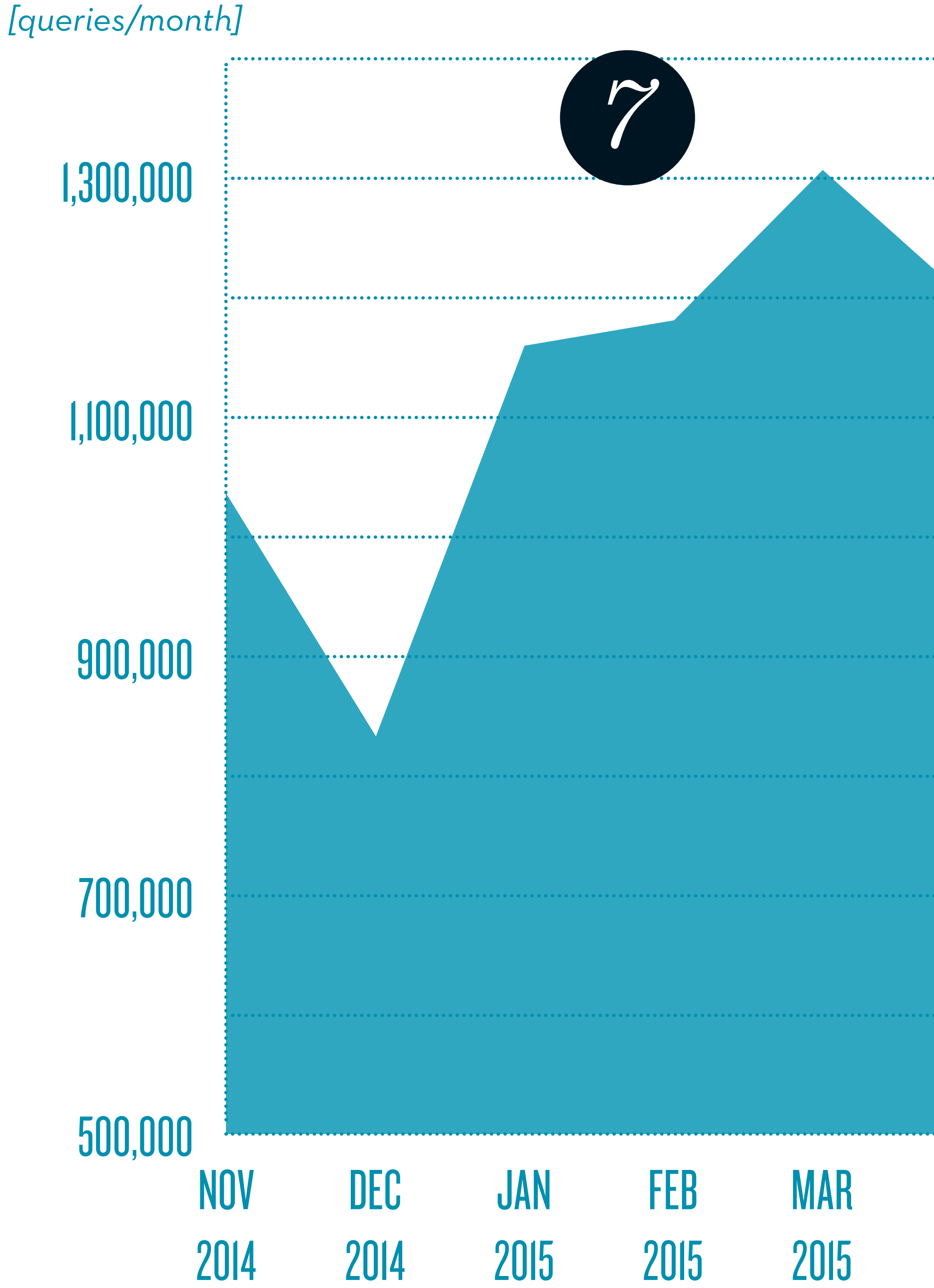
This is complemented by the Web applications for data retrieval: on the one hand, ALBERT as a front end for the search interface; on the other hand, the internally redeveloped "availability proxy". Parallel to software engineering tasks, librarians' expertise was a decisive factor in the implementation of the KOBV Portal. The initial project phase was characterized by considerable comparative evaluation (e.g. feature comparison, informal user testing) of library catalogs and similar discovery systems worldwide. All desirable functionalities of the discovery interface were formulated in the form of use cases and by means of a requirements specification, and the design was developed in the form of wireframes as well as mock-ups.

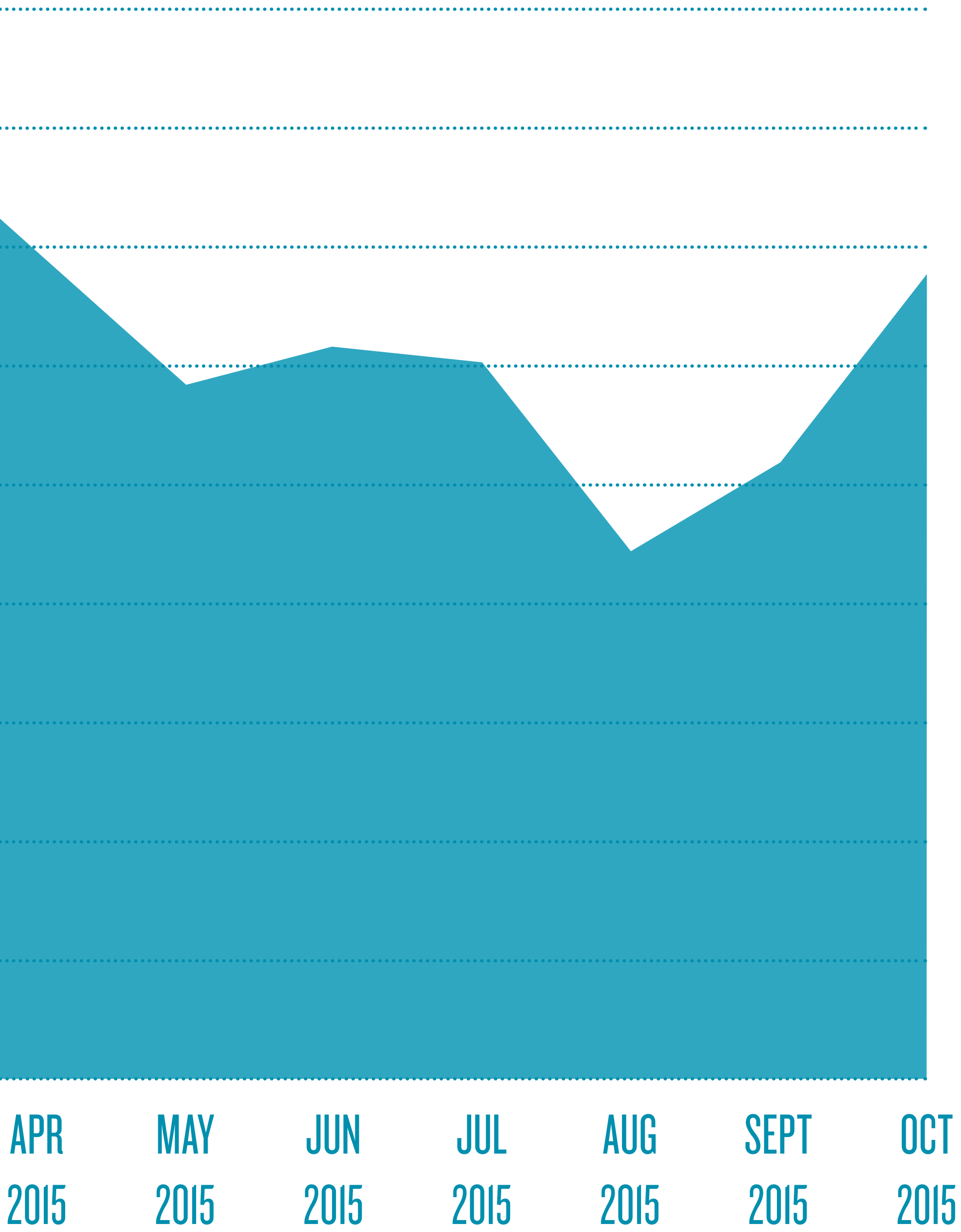
In addition, an expert library group with participants from KOBV libraries was established as project support. Already in the conceptual phase, users were actively included in the development process, and a co-design approach was taken. In this context, "users" refers to Humboldt University: the Berlin School of Library and Information Science of the Humboldt University conducted project-related user studies within the scope of two seminars. In this way, advances in development were continuously evaluated by users, e.g. by means of think-aloud protocols – captured with screen-cast software. In combination with task-based assessment, think-aloud techniques allow a better understanding of the choices made by test users. Testers were asked to participate in the assessment by explaining how they conducted their searches in the KOBV Portal and expressing whether they were satisfied with the search experience and search results. The overall evaluation of the KOBV Portal was consistently positive. The external testers, who were not familiar with the KOBV Portal before, intend to use it for their professional and private searches in the future because they are enthusiastic about the functions and scope of the portal. To the end of the project phase, monitoring of system uptime and performance of the back-end infrastructure was implemented using Pingdom. To monitor and report website usage, KOBV employs the Web analytics software Piwik.

The project had a sustained positive impact on the internal organization structure of the KOBV. Due to the EFRE Project, the development team of the KOBV has been strengthened in terms of staffing and concept and, at the same time, closely linked to the operational area in a matrix structure, which is reflected in ZIB's organization by the research groups KOBV – Research & Development and KOBV – Operating.

OUTLOOK – WHERE DOES THE JOURNEY GO?

Even prior to the end of the project, it became clear that the new KOBV Portal is very popular among users. About one million individual queries per month speak for themselves. Anyone in Berlin or Brandenburg searching for books, journals, videos, CDs, sheet music, etc. not only searches the OPAC of the local library, but of the entire region with the help of the KOBV Portal. The success can also be confirmed by internal measures. We had defined four quantifiable indicators for which the objective figures have been achieved successfully. We were able to reduce the previous average time until the display of search results from 15 seconds to about one second. The number of clicks until the display of the loan status has dropped from the initial four to five, to two. The proportion of searches resulting in zero hits has fallen from 17.5% to less than 10%, and the share of searches canceled by the user is now under 2% compared to 7.6% in the old version of the KOBV Portal. The KOBV Portal is a core service of KOBV and, as such, will be continually expanded and further developed. We intend to present new releases with minor design modifications, new availabilities, and new library collections every three months, on average. One aim is to display Judaica collections by way of an independent facet. Upon request of KOBV libraries in Brandenburg, we will potentially provide an individual search entry (library facet) for their own collections as a default setting.





7 *Access statistics (unique queries per month).*

The entire region profits from the new and further development of the KOBV Portal due to the modern, clearly structured bundling of all regional library resources, since hitherto unrecognized potential for regional, but also national and international efficient use of available media have been opened up. With the modern infrastructure, it is now possible to make the cultural heritage of Berlin and Brandenburg better and easier to find and thus strengthen it sustainably.

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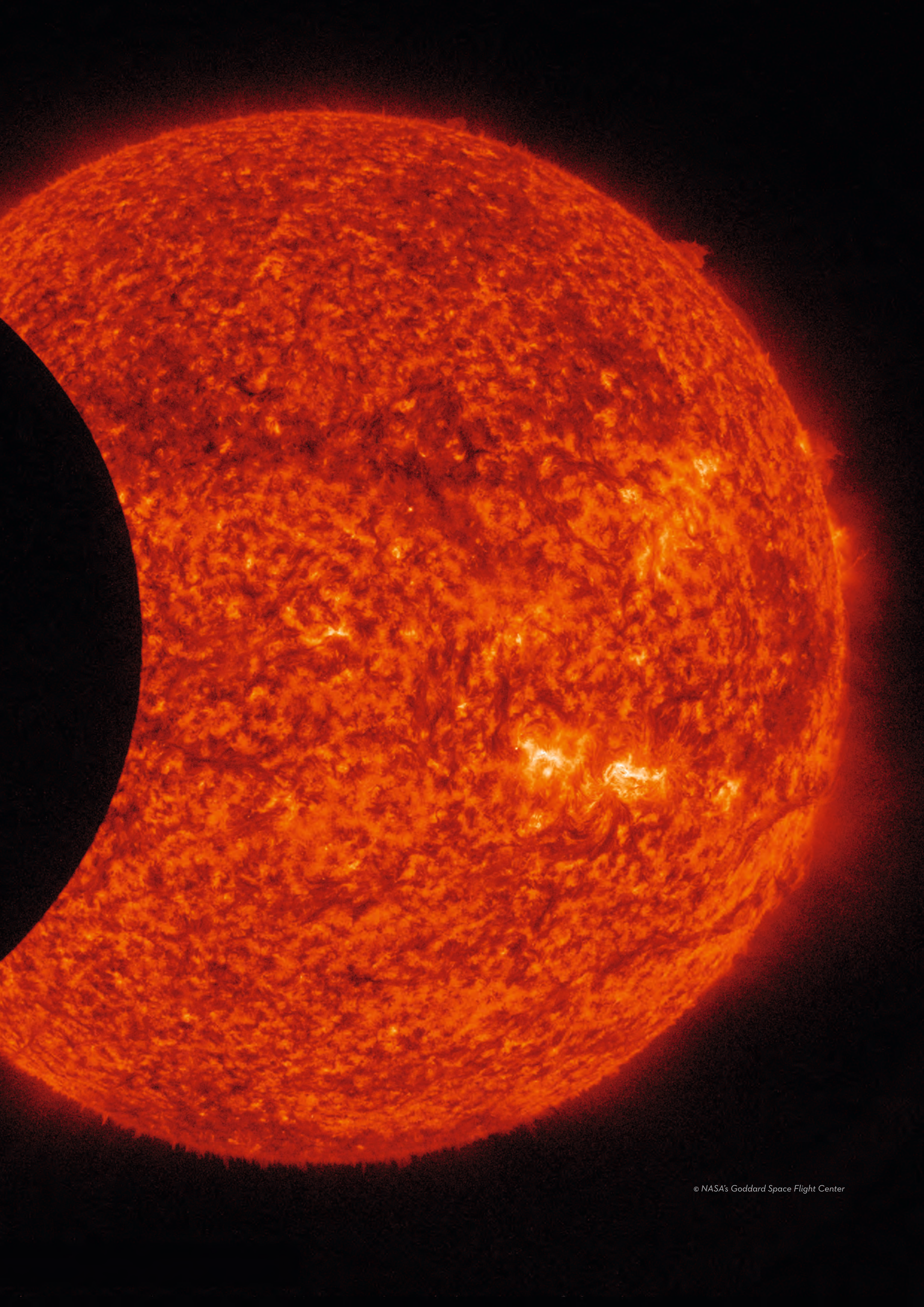
HEADING FOR THE SUN

Where Quantum Physics Meets Photosynthesis

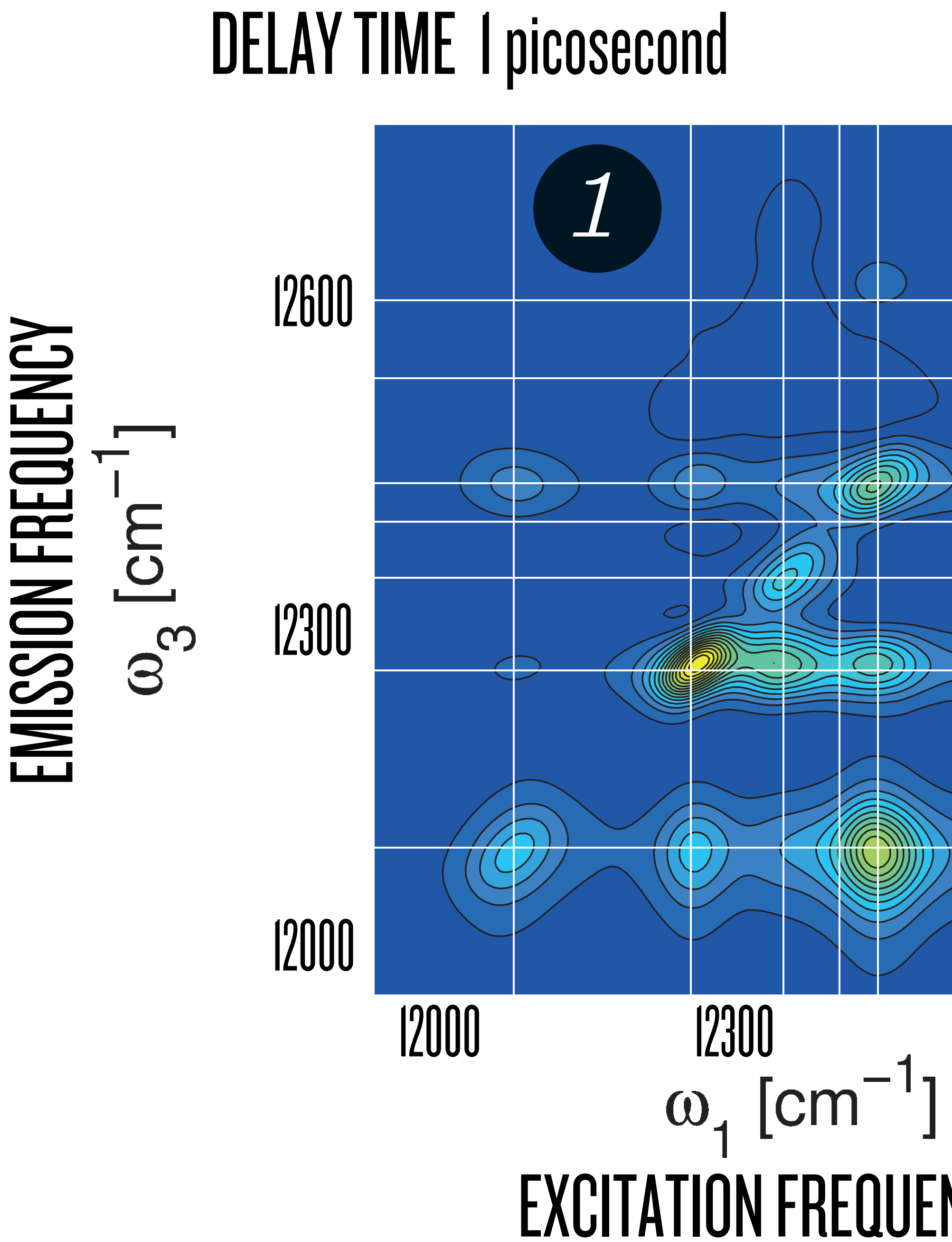
Recent experimental results suggest that quantum-mechanical coherence plays a role in efficient energy transfer in photoactive complexes. The physical simulation of energy pathways requires designing new scalable algorithms for current and future many-core supercomputers. ZIB tackles this challenge in interdisciplinary projects bridging physics, distributed scientific computing, and visual analysis.

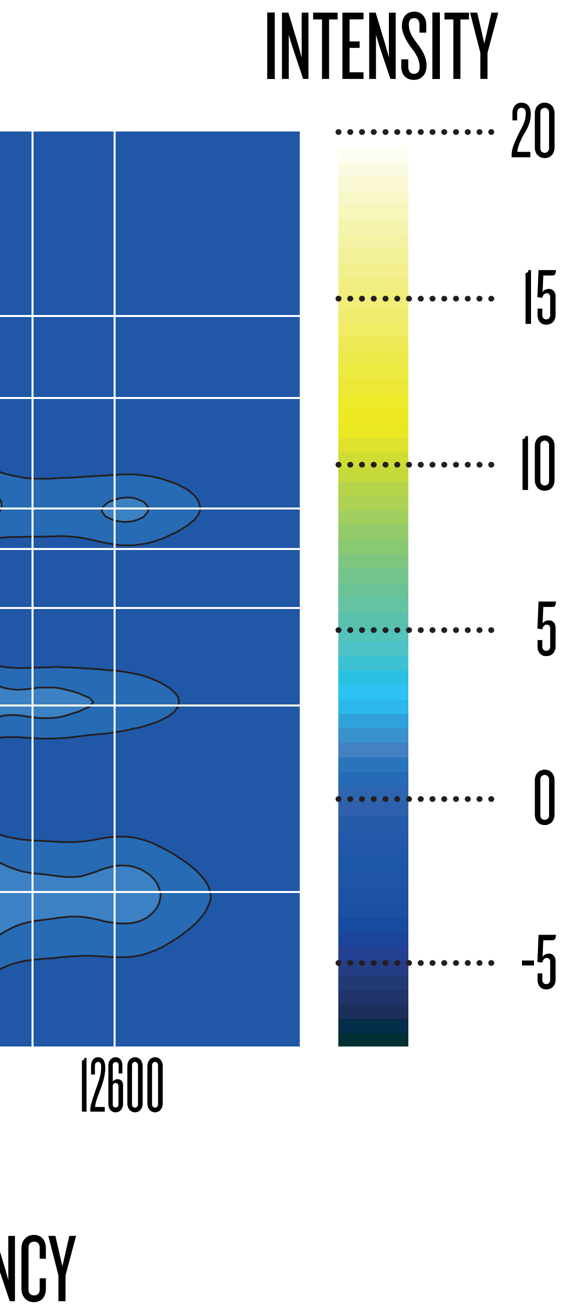


Photosynthesis fuels life on Earth by converting incoming solar radiation into chemical energy. Different strategies emerged during the evolution of natural photosynthesis to collect light in antenna systems and to guide it to the reaction center. Recent pulsed-laser experiments on parts of photosynthetic complexes reveal a time-resolved picture of the energy transport.

By tracking the frequency difference between absorbed and re-emitted light, the partial conversion of the excitation energy into heat has been demonstrated.

The heat generation guides the energy transfer to the reaction center, which lies energetically lower [Figure 1]. Unexpectedly, on top of the irreversible heating process, indications of intermolecular, quantum-mechanical coherences have been observed.





The presence of coherence suggests that classical transport models need to be revised to take into account quantum-mechanical effects that do assist the energy transfer [2]. The better understanding of quantum effects on the transfer through molecular networks at ambient room temperature will help to optimize OLEDs and organic photovoltaics.

1 Time-resolved spectroscopy of the Fenna-Matthews Olson complex computed with GPU-HEOM [1]. After one picosecond, intensity peaks below the diagonal of the two-dimensional frequency representation show the conversion of excitation energy into molecular vibrations.

FINDING ENERGY PHOTOSYSTEMS

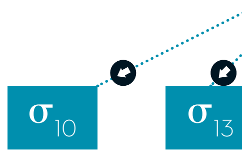
$$\frac{d}{dt}\sigma_{\vec{n}}(t) = -\frac{i}{h}[H,\sigma_{\vec{n}}(t)] + \sum_{i}^{n_{vibrations}} A_i\sigma_{\vec{n}^-}(t) + \sum_{i}^{n_{vibrations}} B_i\sigma_{\vec{n}^+}(t) + \sum_{i}^{n_{vibrations}} C_i\sigma_{\vec{n}}(t)$$

2

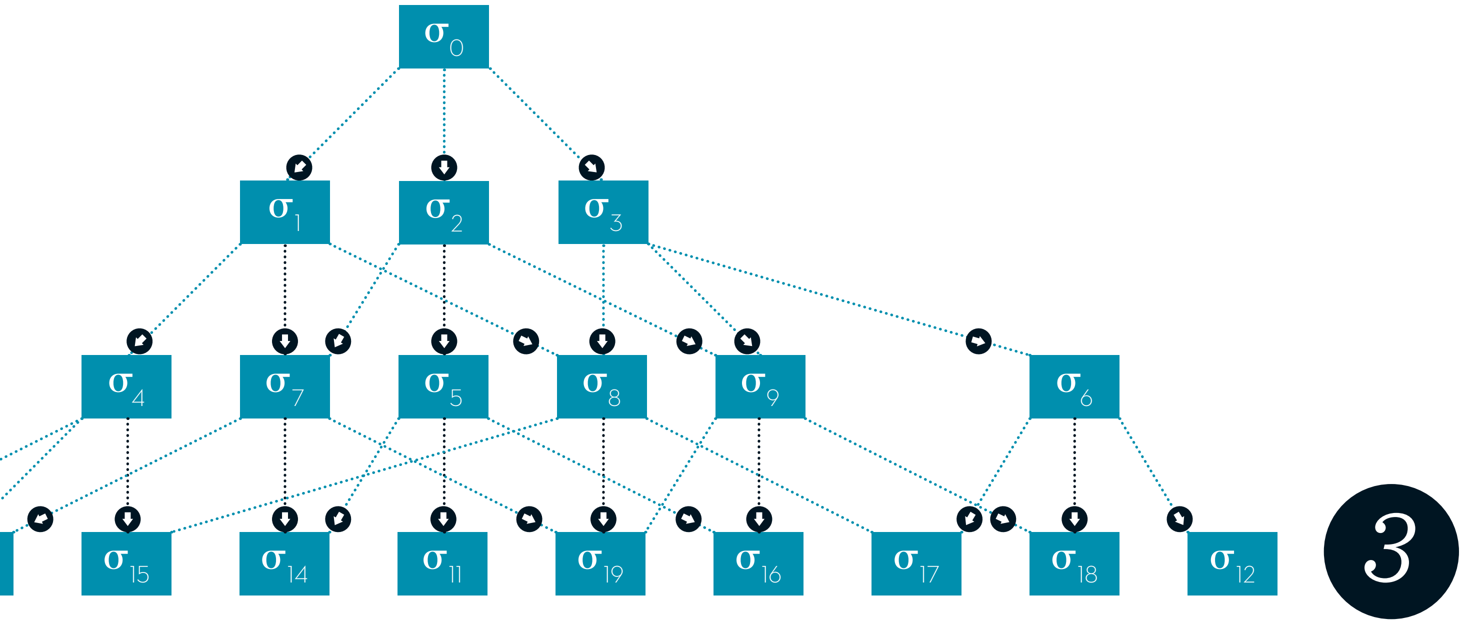
The major obstacle for analyzing the role of coherence in photosynthetic energy transport is the computational difficulty of obtaining an accurate numerical solution for the underlying quantum-mechanical dynamics.

Fully resolved quantum-dynamical models for complexes comprising hundreds of excited molecules are not feasible, but for smaller molecular units found in the Fenna-Matthews-Olson complex of green sulfur bacteria [3], computations of optical spectra have been performed [4].

In a coarse-grained description, the ensemble of quantum-mechanical states of the chlorophyll molecules is captured by the corresponding density matrix, which generalizes the concept of a wave function [5]. The forward time evolution of the density matrix is governed by the Liouville-von Neumann equation [Figures 2 + 3].

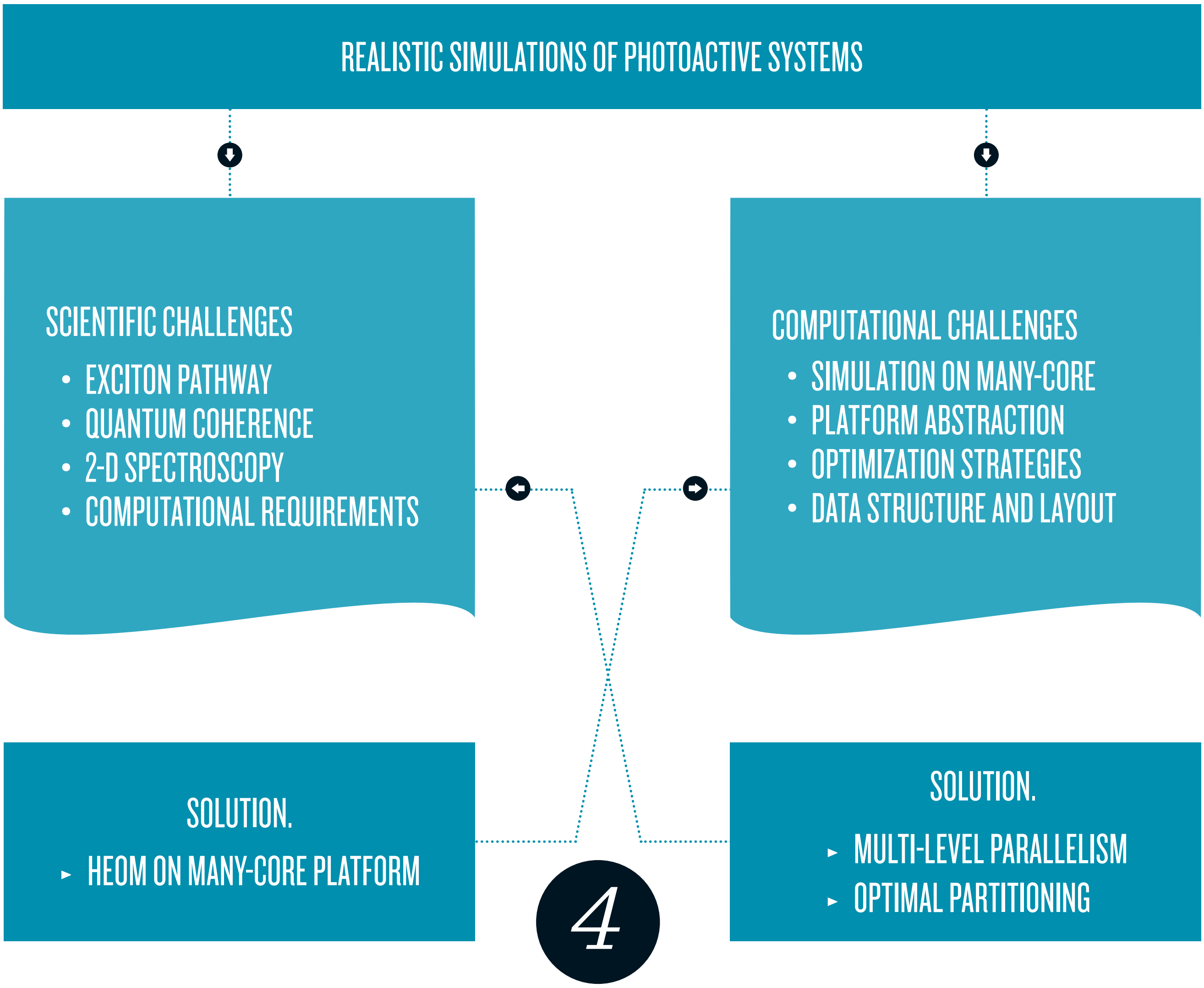


PATHWAYS IN



2 The quantum-mechanical time evolution of a density matrix is given by a hierarchy of Liouville-von Neumann equations.

3 The coupling of the different hierarchy elements is represented by a connectivity graph.



4 Realistic simulations of energy pathways through photoactive complexes require the design of new algorithms suitable for the variety of parallel computing devices used in today's and tomorrow's supercomputers.

Within the joint computer science/physics projects at ZIB, funded by the German Research Foundation (DFG), we design and apply distributed algorithms for calculating the excitonic energy flow in photoactive systems on massively parallel many-core computing platforms [Figure 4]. To obtain a solution for the Liouville-von Neumann equation, we have adapted the Hierarchical Equations Of Motion (HEOM) method introduced by Kubo and Tanimura to work on general purpose graphics processing units (GPGPUs). A demonstration tool for computing the excitation dynamics is installed as a ready-to-run cloud computing application on the open access nanoHUB.org simulation platform and has attracted a worldwide user base [6].

ALGORITHM DESIGN FOR NEXT GENERATION HPC SYSTEMS WITH MANY-CORES

Current state-of-the-art is the simulation of the optical response of the 7-8 bacteriochlorophyll network found in the Fenna-Matthews Olson complex (FMO). Larger systems exceed the capacity of a compute node with a single accelerator device like a GPGPU or many-core accelerator (e.g. Intel Xeon Phi). The incorporation of the molecular vibrations leads to high memory consumption and requires developing methods which scale across multiple accelerator devices and compute nodes. Figure 5 illustrates the increasing memory requirements for larger molecular complex sizes.

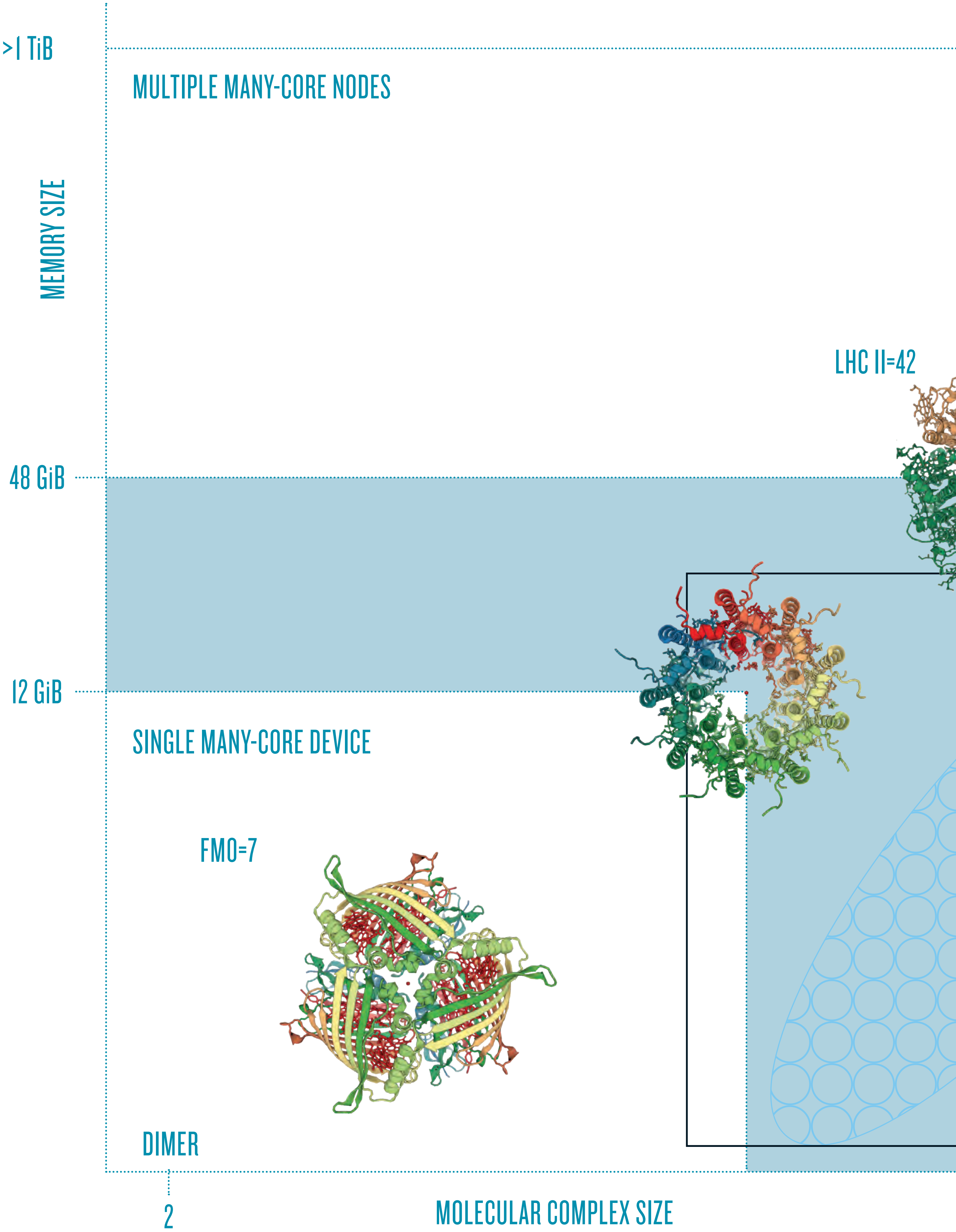
The increasing use of coprocessors in high-performance computers, as shown in the TOP 500 list, for example, and efforts by the leading vendors (Intel, Nvidia, AMD) to fuse multi-core CPUs and coprocessors into a single chip, both signal the transition from multi-core to many-core processors. Along with this development, existing optimization strategies and algorithmic designs need to be adapted to take advantage of the various levels of parallelism provided by the new architectures:

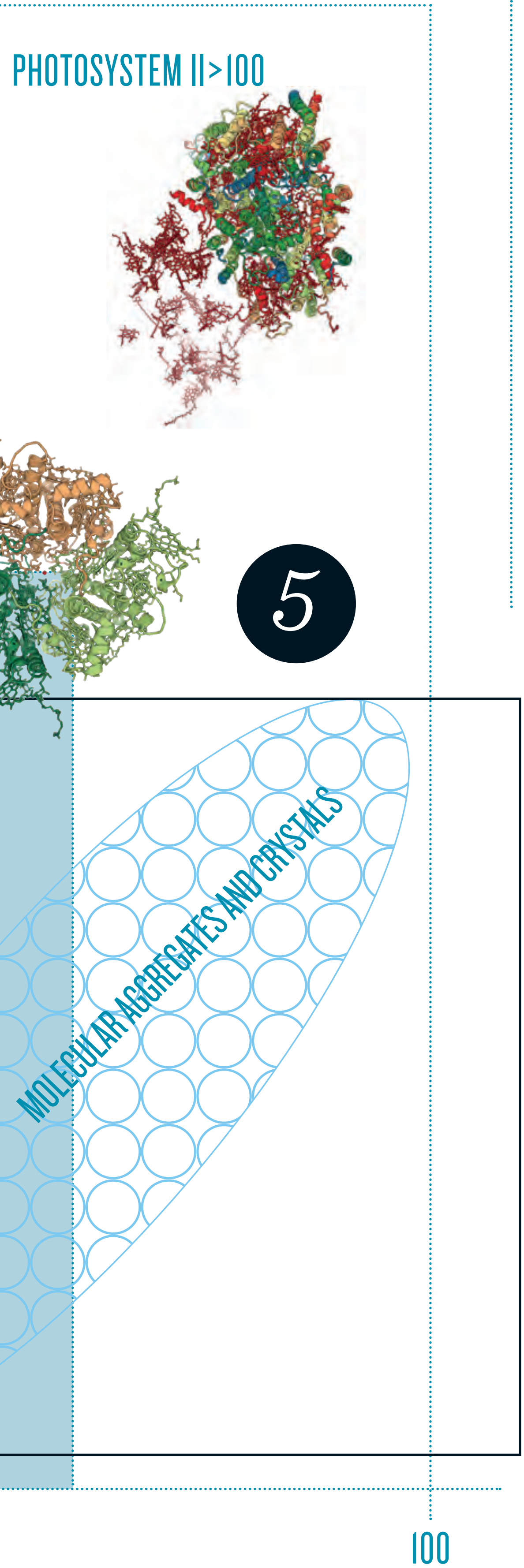
- Parallelism across hundreds to thousands of many-core processors;
- Parallelism within many-core processors; and
- Parallelism at the level of short-vector SIMD (single-instruction multiple-data) cores.

In addition, different characteristics of the architectures have to be considered, e.g. number and performance of processing elements, memory hierarchies and bandwidths, intranode and internode communication, and programming models. Due to the variety of hardware platforms, an important research goal is to find sweet spots between platform-specific optimizations and generic massively-parallel algorithms.

In this project, we take the GPGPU implementation of the HEOM density-matrix evolution as a baseline for researching various optimization strategies for various many-core platforms [7]. In addition, we evaluate current many-core programming models with respect to usability, portability, and performance. One immediate goal is to generalize the HEOM implementation to support GPGPUs, Intel Xeon Phi many-core and multi-core CPUs – across multiple compute nodes.

The program development across different platforms, along with the claim of retaining a similar program flow, can be addressed with the OpenCL programming framework, for example, which provides an open standard for cross-platform parallel programming within heterogeneous compute nodes. OpenCL aims at implementing the kernels just once, and to compile them at runtime for the particular platform detected in the


>1 TiB
MULTIPLE MANY-CORE NODES
MEMORY SIZE
LHC II=42
48 GiB
12 GiB
SINGLE MANY-CORE DEVICE
FMO=7
DIMER
2
MOLECULAR COMPLEX SIZE



computer system. This cross-platform portability is compromised by the performance guidelines of the device vendors, whose optimization recommendations are sometimes orthogonal. Even for the same hardware platform, OpenCL optimization strategies and techniques can be very different

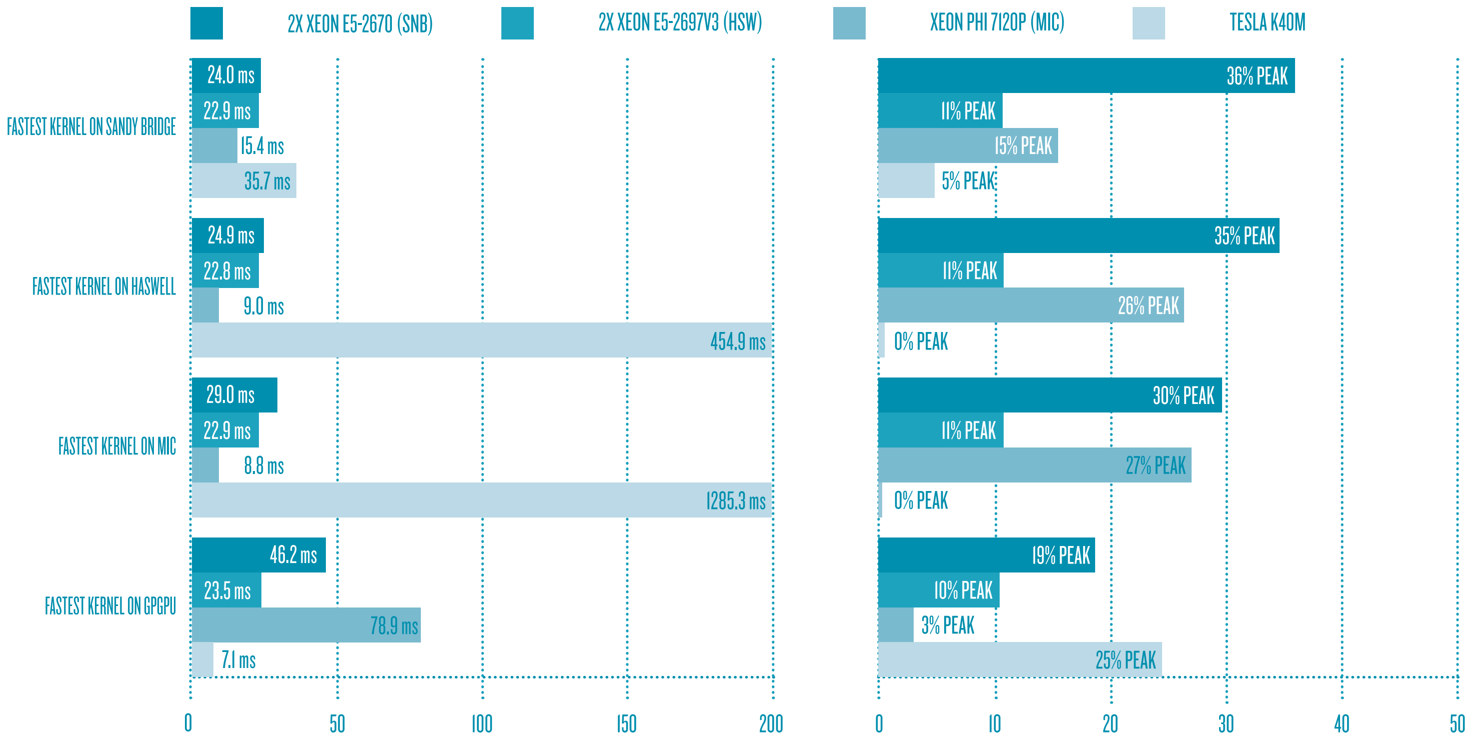
The limitations of cross-device performance demonstrate the need for additional close-to-hardware optimization, which requires the rewriting of relevant code sections for a particular hardware. A case study [8] for parts of the HEOM algorithm covering the coherent dynamics shows that different optimization techniques for every target hardware must be selected to achieve optimal performance. Figure 6 shows the performance portability of OpenCL across different computing devices.

Additional complexity arises from extending a parallel application across multiple compute nodes (possibly using PGAS or MPI). Future many-core systems require identifying generic optimization strategies which work across various many-core platforms and heterogeneous combinations thereof. Since direct porting of existing algorithms and workflows to these future architectures is not enough, the combined expertise and effort of computer science and user groups — biophysics and theoretical chemistry — is necessary to identify theoretical approaches with inherent parallelism and scalability.

We plan to develop configurable data layout templates that take the needed optimizations across all scales of massively parallel many-core HPC systems into account — from SIMD parallelism to distributed memory partitioning, based on connectivity graphs. Other contributions are theoretical upper and lower bounds for the communication costs of HEOM. The results are expected to be general enough to be applicable to other problem domains.

5 Molecular complex size vs. memory requirements for the HEOM method. Solutions for larger photosynthetic complexes found in the light harvesting system 2 [9] and photosystem II [10] can only be acquired by scaling up to many compute nodes.

PERFORMANCE PORTABILITY ACROSS DIFFERENT DEVICES IN OPENCL



6

6 *Runtime and device utilization of the best-performing kernels of each device across devices – performance is not portable.*

COLLABORATIONS

Prof. Alán Aspuru-Guzik, Harvard University, Department of Chemistry and Chemical Biology works on the quantum chemistry of photosynthetic complexes.

Prof. Thomas Renger, Johannes-Kepler Universität Linz, Institut für Physik, provides parameter sets for various photosystems.

Prof. Gerhard Klimeck is the Director of the Network for Computational Nanotechnology which powers nanohub.org at Purdue University.

VISUAL ANALYSIS OF ENERGY FLOW

The majority of methods for visual analysis of biomolecular systems is focusing on structural data, resulting from classical molecular dynamics simulations, for example. These methods need to be extended to reveal the extent of quantum-mechanical coherences shared between different chlorophylls. For this task, a ZIB-internal collaboration (bridge project) between the Distributed Algorithms and Supercomputing department and the Visual Data Analysis department was formed.

The goal is to develop novel visual methods and tools for analyzing:

a) Time-dependent quantities and flows through a molecular network; and

b) The spatiotemporal extent of quantum-mechanical coherence.

This includes:

- A combined visual representation of spatial molecular structure and a related directed graph with time-dependent attributes;
- The identification of dominant pathways and causes for delays by extracting flux information from time-dependent populations of network nodes; and
- Time-dependent tracers for revealing quantum-mechanical superposition states.

The resulting techniques will be integrated into the publicly available exciton dynamics tool previously developed by Kramer/Kreisbeck at nanoHUB.org.

The insights gained from the analysis of the energy flows are also expected to impact the simulation itself by revealing a pattern that allows to filter nodes inside the hierarchy graph that have a negligible impact on the result. This would help to further reduce the needed computational resources and allow for an improved time-to-solution or deeper hierarchies.

Digital Infrastructure for Public Participation

The IES Cities platform is a novel and practical way of building the digital identity of a city. Nine technical partners, from industry to research, and four city councils are creating a platform for Internet-enabled services for citizens in the form of mobile urban apps. These apps are based on an open platform which obtains information from open government data and enriches them through citizens' contributions. Companies, citizens, and councils interact and collaborate toward achieving a smarter city. ZIB performs research and development of the scalable, distributed storage back end.

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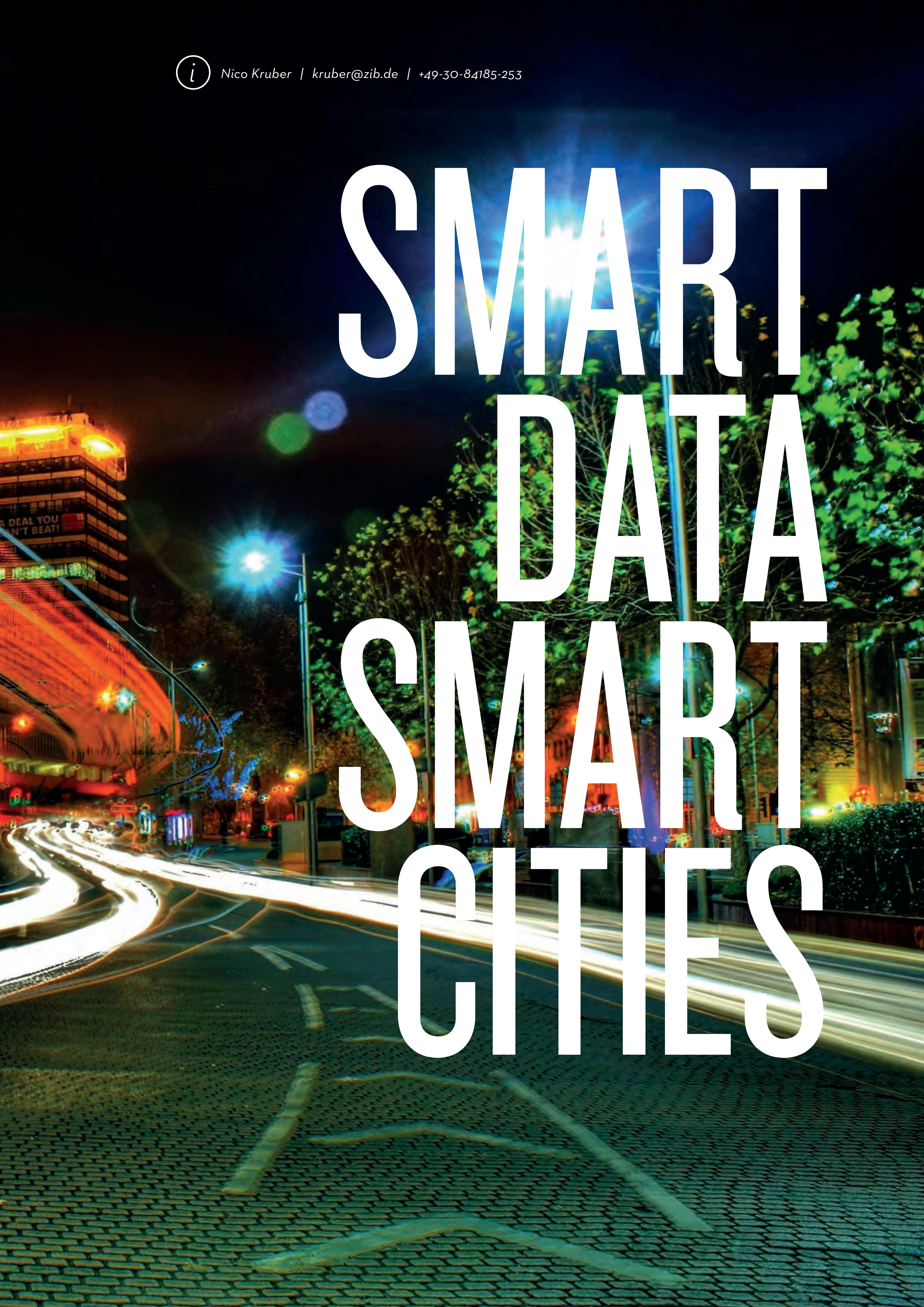
SMART DATA SMART CITIES



INTERNET-ENABLED SERVICES FOR CITIES ACROSS EUROPE

The EU-funded project IES Cities provides a novel and practical way of building the digital identity of a city. Nine technical partners, from industry to research, and four city councils are creating Internet-enabled services for citizens in the form of a mobile urban app. These apps are based on an open platform which obtains information from open government data and enriches them through citizens' contributions. Companies, citizens, and councils interact and collaborate towards achieving a smarter city. ZIB is responsible for research and development of the scalable, distributed storage back end.

1 Millenium Square in the center of Bristol.

2 Screenshot of the Bristol Healthy Office app.

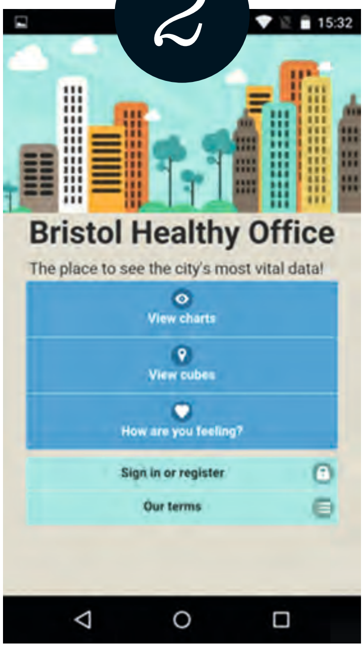
1

THE APPS

Each of the four pilot cities – Bristol, Majadahonda, Rovereto, and Zaragoza – developed four services available as apps for the Android platform. A common entry point into finding relevant apps is the IES Cities Player on Google Play. The individual cities' apps are available on Google Play as well, but with the IES Cities player, a user can browse through all available IES Cities apps and filter them based on the apps' descriptions and common tags, and also restrict search results to apps relevant for the user's location. Since the PhoneGap framework has been used to develop the apps, some of them are also available as pure HTML 5 services for other mobile or desktop platforms. Some of the apps are presented below. For the full set, please refer to the IES Cities Player.

BRISTOL HEALTHY OFFICE

2



This service allows citizens to record and monitor environmental parameters of their working space. For offices with the required sensors, it visualizes data such as temperature, humidity, noise, light, and air quality. Healthy Office [Figure 2] allows people to gain insight into what affects the quality of their working space. Additionally, this app allows employees to record and monitor their own levels of work-related stress indicators, providing valuable insight into how people deal with the demands of their everyday working life. Finally, if the user has access to one of the personal monitoring devices, Healthy Office can optionally record and display personal health-related metrics, such as heart rate and temperature. All these combined sources of information through the app provide a valuable tool for monitoring and improving one's working environment and conditions.

ROVERETO PERCORSI

This service allows citizens and tourists to organize tours and visit the city of Rovereto by following user-provided itineraries with points of interest worth seeing [Figure 3]. Visitors may search for new tours by duration, type, length, and other characteristics. Itineraries present tours on a map, as well as a brief summary of the tour. Each way point may also provide a detailed description, including photos of points of interest (POI). Locals can contribute by creating their own tours or add descriptions of new POIs with their own content, such as photos and comments. A civil servant of the city council will validate the added content.

ZARAGOZA VOTING

3 *Screenshot of the Rovereto Percorsi app.*

4 *View of Zaragoza.*

5 *Screenshot of the Zaragoza Voting app.*

6 *Screenshot of the Majadahonda Sports4U app.*

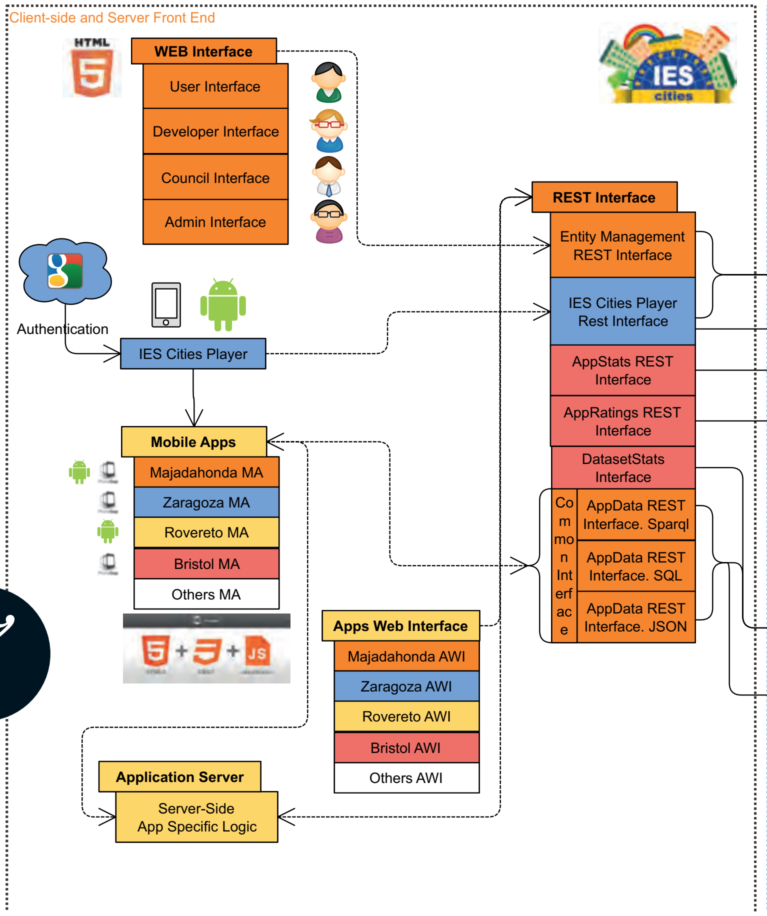
Zaragoza Voting enables citizens to add and vote on proposals to improve their neighborhood [Figure 5]. It is intended to assist in the process of regeneration of a neighborhood in the city, namely the Delicias neighborhood of Zaragoza. Through their contributions and votes, citizens have the opportunity to participate and co-decide how they want their neighborhood to be. It is an application of digital democracy and citizens' participation, which also meets a real social need. The app presents a list of all currently available polls and allows users who are logged on via a social network, for example, to cast a vote or create a new poll. Geo-referenced polls are also presented on a map.

MAJADAHONDA SPORTS4U

6

This service aims at increasing the dissemination of sports events organized by the city council and to foster the citizens' participation in the sportive life of the city [Figure 6]. It will also allow citizens to meet and organize joint events to practice sports. The app provides Majadahondas citizens with accurate information about different sports events in the city (with schedules, matches, competition scores, happenings, etc.) and about the city's sports facilities (with opening times, prices, availability, location, etc.). Registered users may also create groups of players in order to arrange matches with other players, to fix meetings, create leagues, etc. Majadahonda citizens will be able to search for events by different criteria such as the location on a map or the kind of sport they are interested in. Users can join events, add comments, add events to their own calendar, or share events on social networks. Citizens may also leave comments about the situation of the city facilities or questions related to practicing sports.

ARCHITECTURE

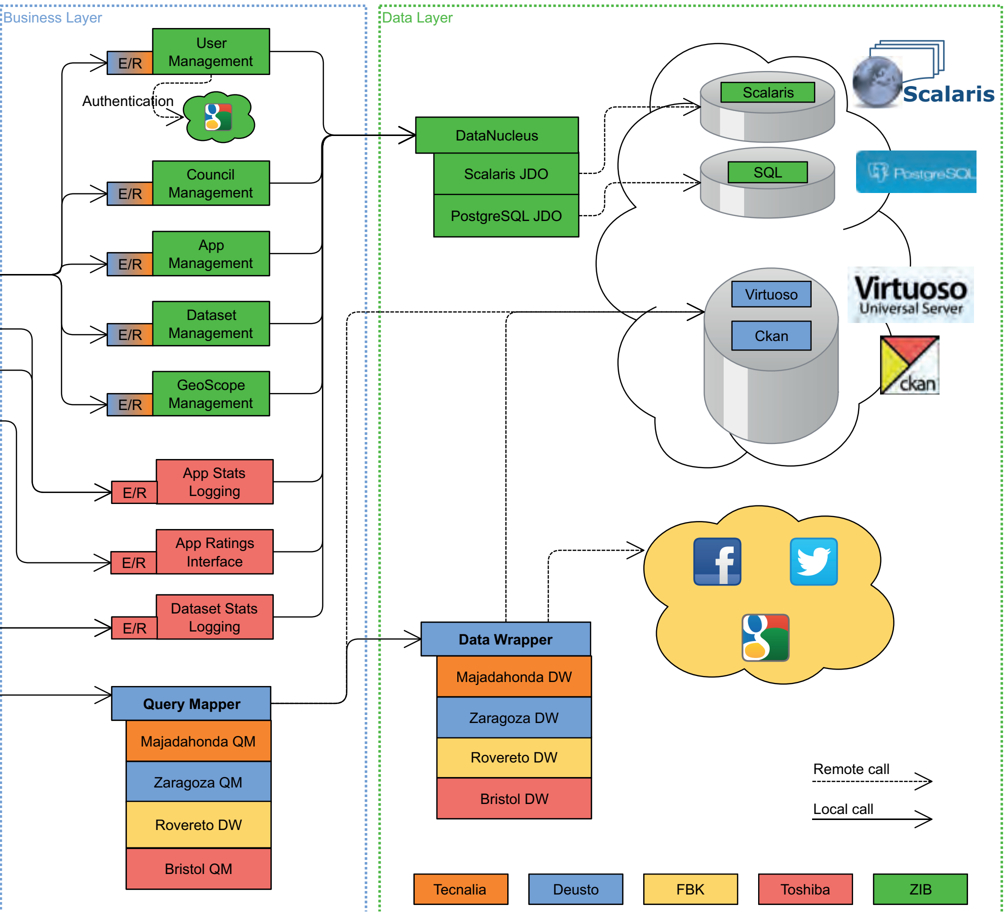


7

CLIENT-SIDE AND SERVER FRONT END

Mobile apps and Web interfaces (HTML5/CSS3-based) are developed in order to exploit urban data accessible through the back-end RESTful interface [Figure 7]. Responsive mobile apps are generated with the help of Apache Cordova (PhoneGap). A Web front end allows applying CRUD (Create, Read, Update, Delete) operations to IES Cities' main entities: users, councils, app metadata, datasets and geoscopes. This interface accounts for the different roles a user of the IES Cities platform may have: end users, application developers, city councils, and administrators.

A Jersey REST client is used for the apps to communicate with the IES Cities Framework's RESTful interface. Aside from access to entity management, apps can also collect application and dataset statistics which can be analyzed in the Web interface. App-specific data storage, as well as access to the city councils' datasets, external datasets and social media is provided by a common interface. Data queries for this functionality can be expressed in SPARQL, SQL, or JSON and are converted to the endpoint query format in the back end.



7 *Software component architecture of the IES Cities platform.*

SERVER BACK END (BUSINESS LAYER AND DATA LAYER)

The IES Cities server's back end is split into two layers [Figure 7]: a pure data layer for access and storage, and the business layer with application logic. The data layer for entity management and app and dataset statistics logging are implemented with the generic persistence framework DataNucleus. The business layer builds upon this but does not need to know the specifics of the data storage. Therefore, the actual storage engine can be changed at any time, depending on current needs. Currently, two data storage drivers are provided: a stable PostgreSQL-based storage for everyday use, and a highly scalable NoSQL solution using Scalaris, which we will detail later on.

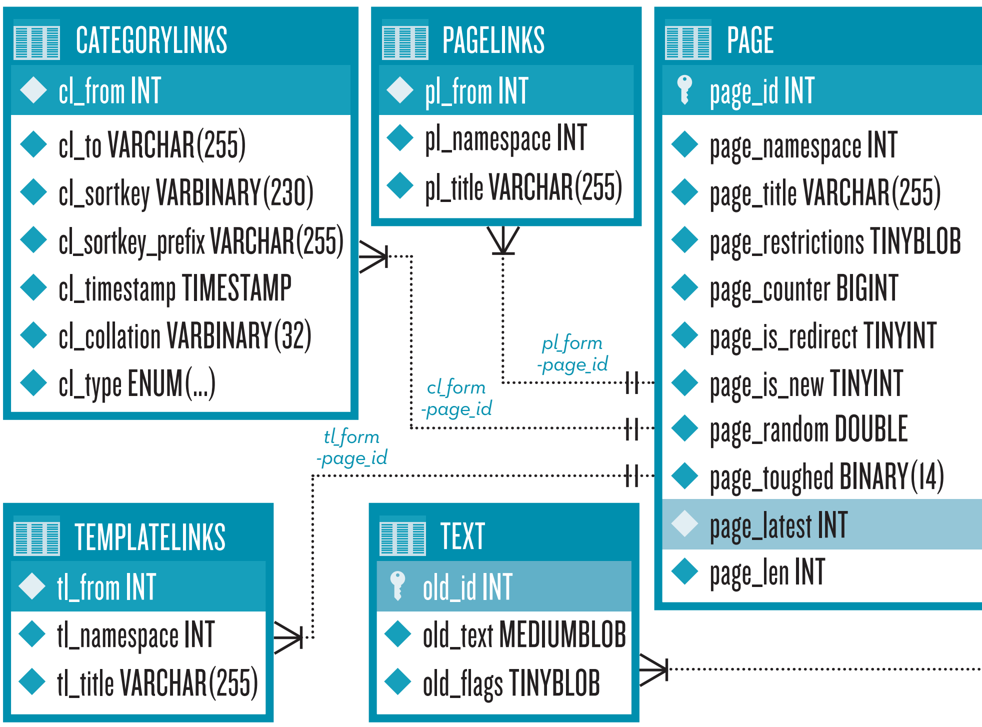
App-specific data as well as city council and external datasets are organized differently. The different datasets may be stored in different back ends with different APIs to access them. A Query Mapper translates app requests to data repository specific queries in SQL, JDOQL, SPARQL, or HTTP API calls with the help of the Data Wrapper, which gathers external data from social networks and Web pages. It adapts and stores this data to be accessible by the query mapper. Other dataset sources – open datasets offered by the city councils, for example – may be stored in Virtuoso or Ckan.

CREATING HIGHLY SCALABLE DATABASE BACK ENDS

FROM SQL TO NOSQL

Distributed key-value stores are horizontally scalable by design. However, most existing applications are developed with relational database schemes in mind, which generally do not scale horizontally in a cost-efficient way. These schemes represent objects and their relations, i.e. links between them. Even if an application is specifically designed for a scalable NoSQL data store, it is exactly these links (as well as indices of any kind) which can become hot spots or bottlenecks. These hot spots typically reduce the scalability of the key-value store and are especially prominent in cases where data needs to be modified. We have shown [1] that even the demanding Wikipedia database schema [Figure 8] can be mapped to the distributed transactional key-value store Scalaris. We show solutions for how to map dependent tables and secondary indices to a single key-value namespace and evaluate and identify hot spots and bottlenecks. These hot spots do not only arise from the aforementioned links between values, but also due to necessary work-arounds to cope with the limited expressibility of a typical key-value store.

PAGE TEXT AND ASSOCIATED INFORMATION



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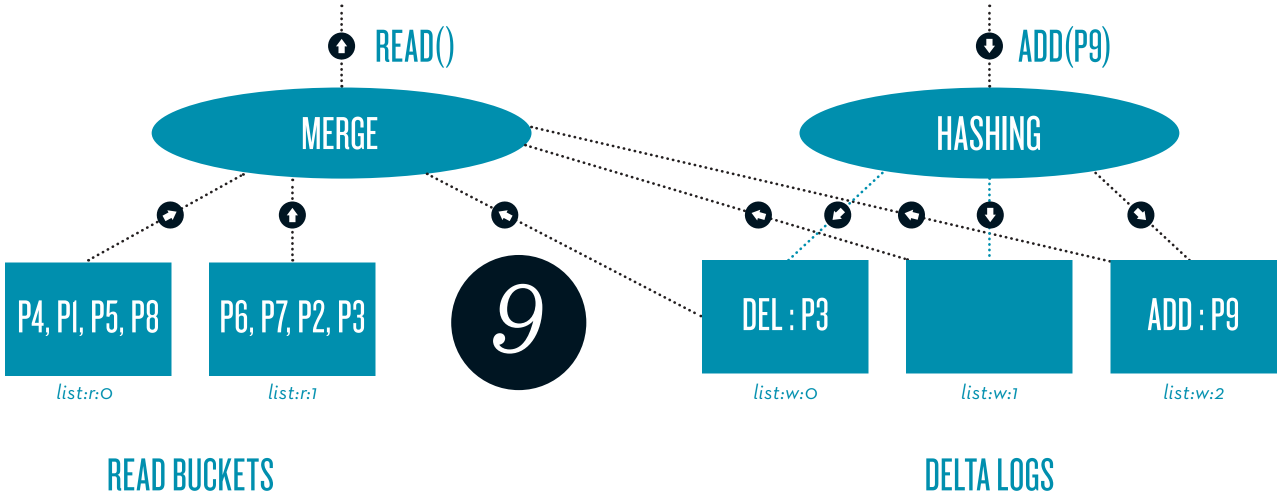
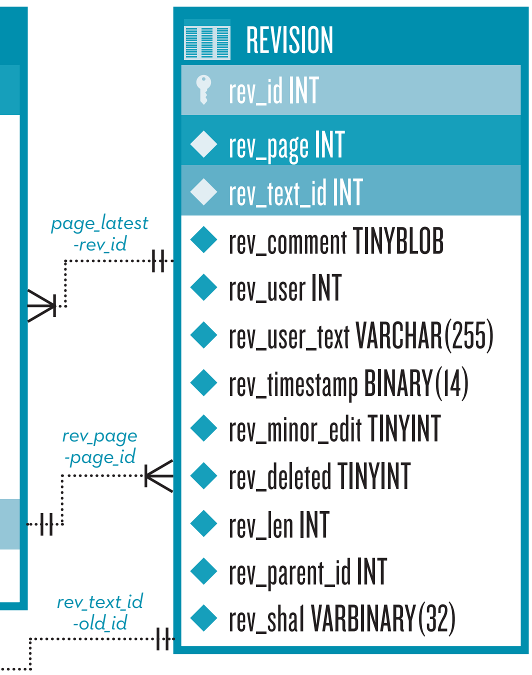




In a scenario with many more read operations than writes, such as the Wikipedia scenario, we denormalize and create redundant values holding the metadata of all revisions of a page, for example, to avoid having to look up indirections between objects during reads. In the absence of multiple namespaces and more advanced query types, such as efficient search and aggregation operations, we explicitly materialize indices and create aggregate objects to avoid expensive table traversals.

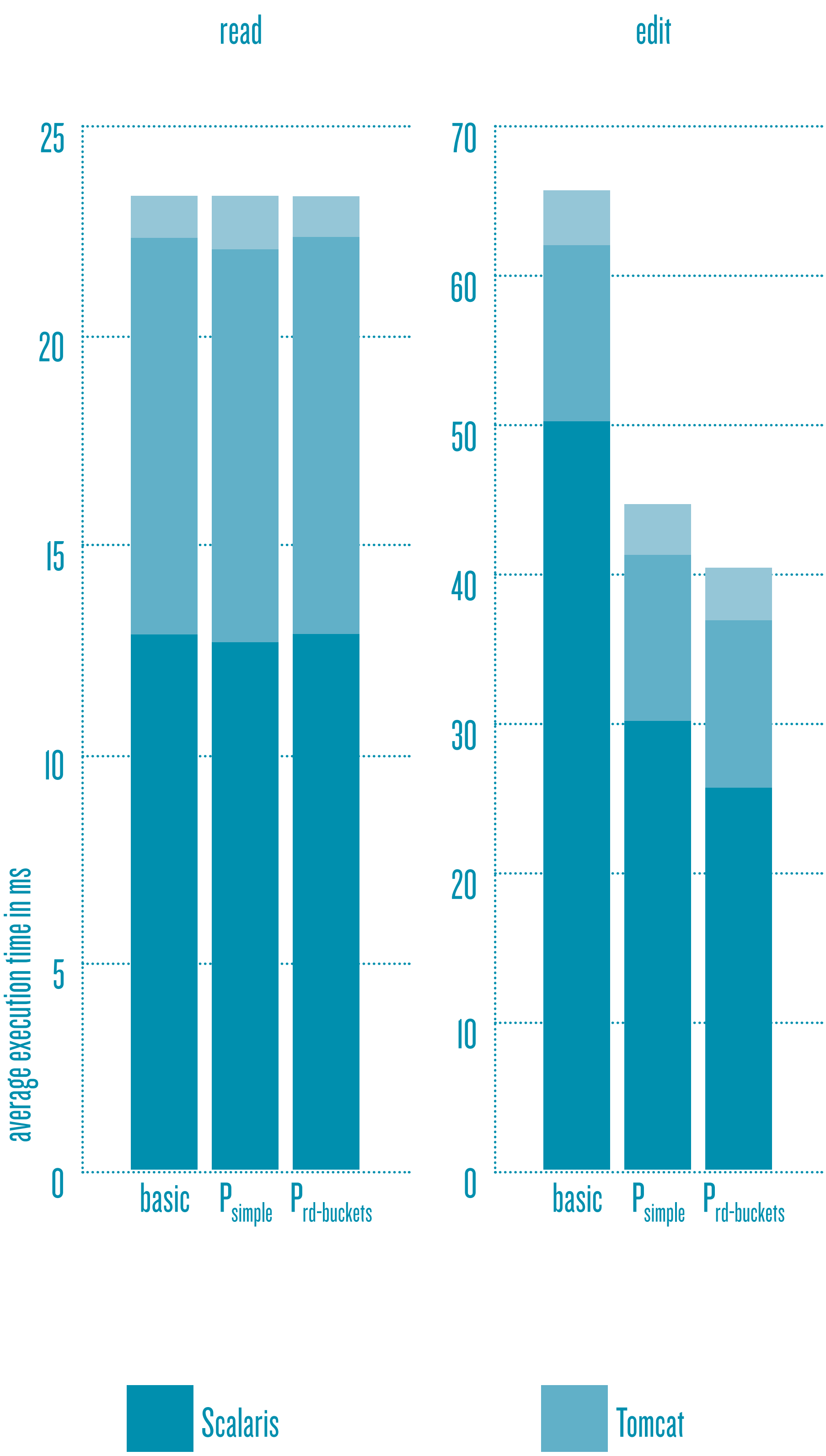
With these techniques, most prominent hot spots arise from the representation of primary and secondary indices. The solution is to find suitable partitioning schemes for such indices, which depend on the access pattern on the specific indices. An index can be represented as a list where simple partitioning schemes spread items randomly – or based on some hash function – into a number of sub-lists, i.e. the partitions. The overall size of a single partition is roughly the original size divided by the number of partitions. Since a partition's size influences the amount of data transferred during write operations and thus the length of a transaction, we propose a more advanced partitioning scheme using separate read and delta buckets [Figure 9]. During normal operation, only the delta buckets are touched and include a log of modifications to the index. These changes are periodically merged back into the read buckets. This allows independent tuning of the partition size (via read buckets) and write concurrency (via delta buckets) and reduces the payload for write transactions.

8 *SQL example schema (excerpt from MediaWiki 1.20).*

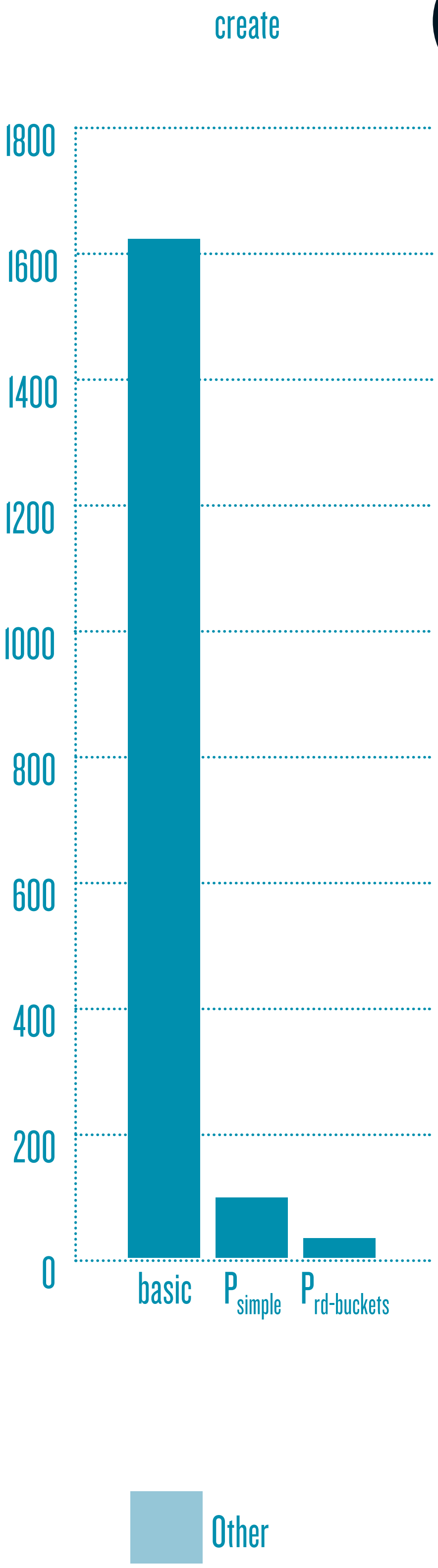
9 *Hot spot partitioning with delta buckets.*

WIKI BENCHMARK (1 BENCH THREAD, 28 NODES)

The effects of using these partitioning schemes on a Wiki application deployed with a Scalaris back end can be seen in the plot shown in Figure 10. We imported the Spanish Wikipedia dump, with roughly 700,000 pages, and used a real HTTP query trace from Wikipedia as a benchmark for different kinds of operations. In a single-threaded scenario, we can see the huge impact of partitioning schemes on the execution times of write operations. In a more concurrent scenario, we also show that these schemes do not only improve the execution times of write operations, but also considerably improve the read operations' speed due to the reduced network bandwidth used by the (very few) write operations [1]. This even holds for the typical back-end scenario where 95% of the read requests hit HTTP caches only. In the remaining requests, only 2.5% and 0.3% are edit and create operations, respectively.



10 *Benchmark results for the read, edit, and create operations with different data layouts of the Wiki on Scalaris.*



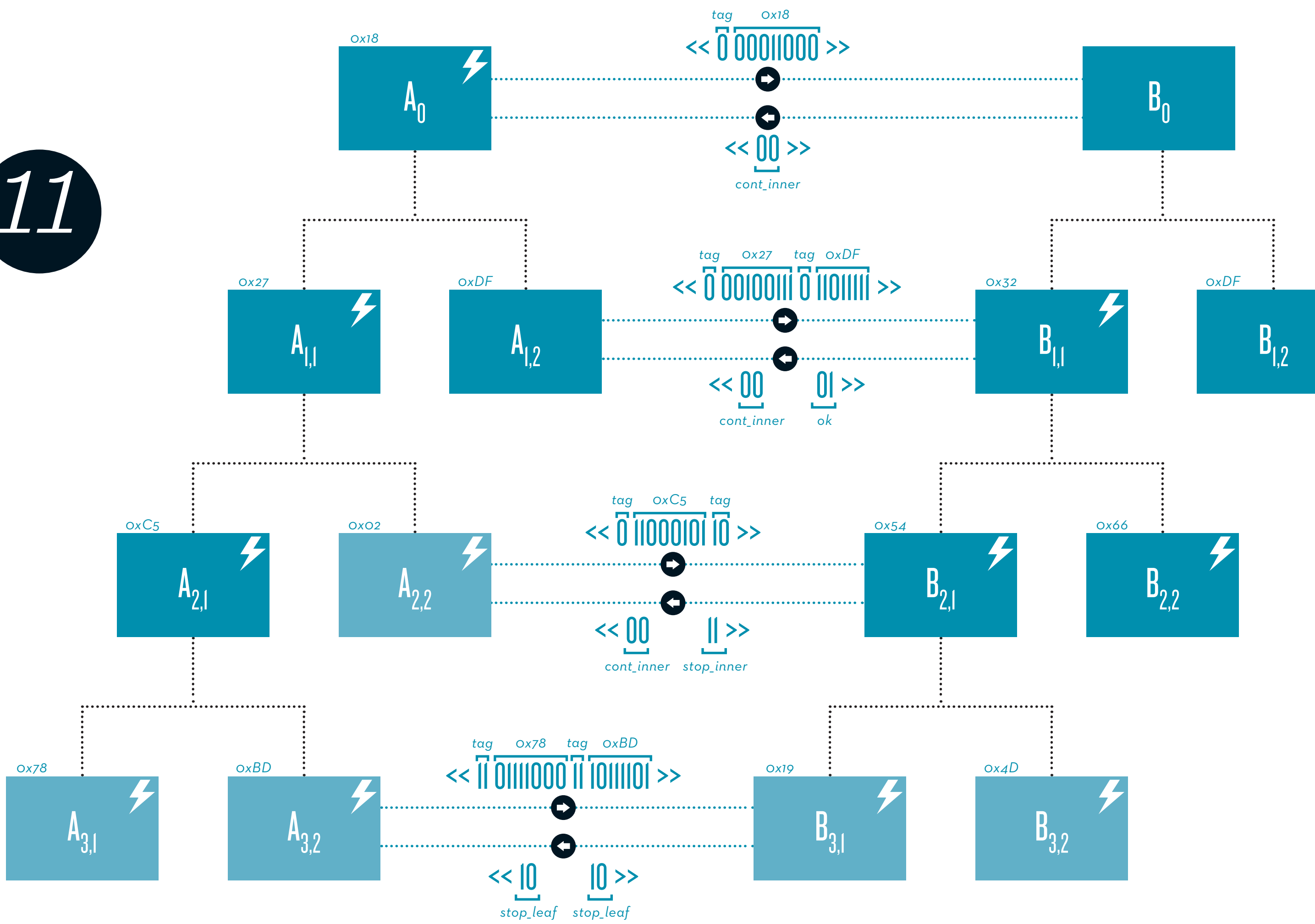
10

EFFICIENT REPAIR MECHANISMS

A distributed key-value store such as Scalaris may use replicated values to increase the reliability of stored data. In order to prevent faults, these systems need to have a mechanism to repair the replicated values in cases of node or network failures. Therefore, we need to compare the sets of two nodes' stored items by using at least an item's key and some version information associated with it. There is a number of set reconciliation algorithms to solve this task, both exact as well as approximate algorithms, with the latter promising lower transfer costs. The comparison of different approximate algorithms for distributed replica repair, however, is challenging. Each algorithm's behavior can be tuned for a given use case, such as low bandwidth or low computational overhead using different sets of parameters. These parameters often also influence the algorithm's accuracy in detecting differences between replicas and thus hinder objective comparisons.

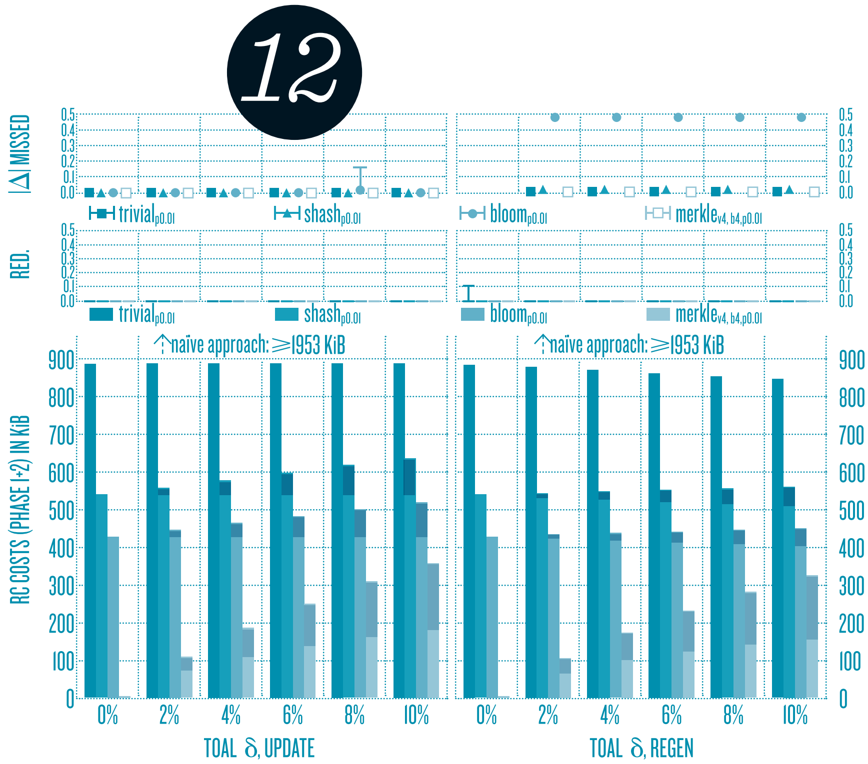
In [2], we develop models to deduce parameters for equally accurate (approximate) set reconciliation algorithms for replica repair in distributed systems. We compare equally accurate instances of two trivial hash-based algorithms, an algorithm using Bloom filters [3], and a newly developed approximate "Merkle-tree-based algorithm [4]" outlined in Figure 11 and described below.

11



11 *Merkle tree synchronization.*

12 *Performance comparision of different synchronization algorithms.*



In a Merkle tree, every inner node is labeled with the hash of the labels of its children and every leaf node is labeled with the hash of the data it represents, i.e. one or more items. This allows an effective recursive top-down comparison between two distributed trees. Instead of using a large fixed hash size for the nodes' labels, however, we use dynamic hash sizes to align the transfer overhead with the desired accuracy. To compare two nodes' item sets in a common synchronization interval I, we build a Merkle tree of degree v and bucket size b on each node using the key-version information of each stored data item. This is done recursively until the number of items is less than or equal to b. Finally, the hashes are created bottom-up. During synchronization, one node sends tagged Merkle tree node hashes to the other node which responds with result codes indicating hash matches (identical items below this tree) or mismatches (continue down to the next level) until no further mismatches occur [Figure 11].

As a result, this optimized Merkle tree reconciliation protocol is not only more efficient for a very low number of differences (as is usually the case), but also has lower transfer costs for differences up to 50% [2]. This is considerably higher than the 5.0% differences for which the original Merkle tree reconciliation was previously thought to still be efficient. The plot in Figure 12 shows how the four analyzed algorithms perform comparing two nodes' item sets in two scenarios: "update" with outdated items (left column) and "regen" with items lost on both nodes (right column). The two metrics shown in the upper two rows verify the configured accuracy differentiated by the number of items not found in the reconciliation and the redundantly transferred items where the algorithm suspected a difference, but there was none. RC costs reflect the transfer costs during different phases of the algorithm. It clearly shows the advantages of an adaptive algorithm like the Merkle tree. Note, however, that Merkle reconciliation is a multi-round algorithm bound by network latencies.

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PEER-REVIEWED (112)

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Amal Aboulhassan, Daniel Baum, Olga Wodo, Baskar Ganapathysubramanian, Aram Amassian, Markus Hadwiger (2015). A Novel Framework for Visual Detection and Exploration of Performance Bottlenecks in Organic Photovoltaic Solar Cell Materials. *Computer Graphics Forum*, 34(3):401-410.

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