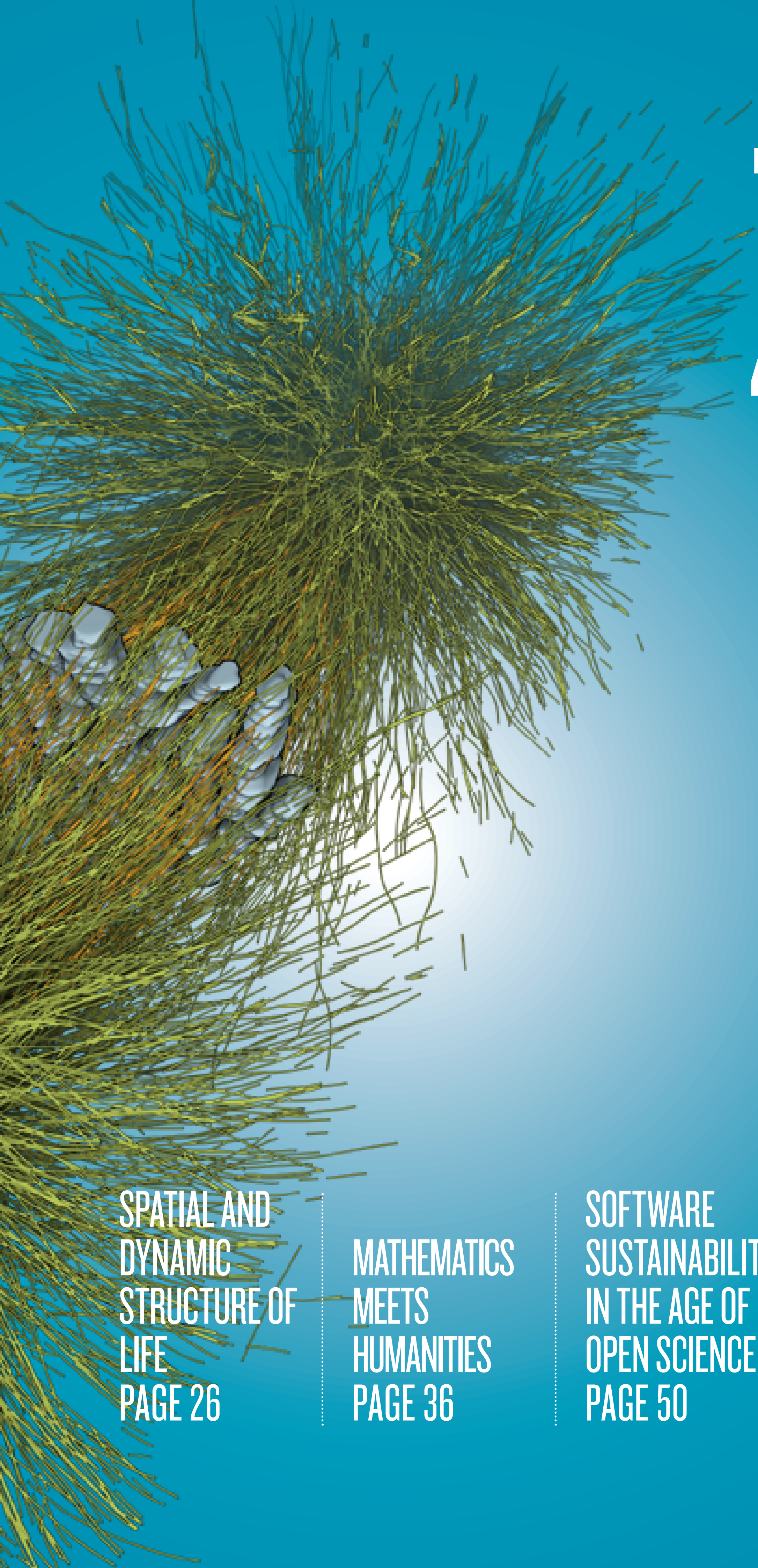
ZIB

2017 Annual Report



WWW.ZIB.DE

PREFACE

We are living in a rapidly changing world with enormous opportunities, but also many threats. Mastering complexity is becoming more and more important. The last decade has caused the digitization of almost every aspect of our daily lives and generated an avalanche of digital data. What looks like an immense gain in information for our networked society at first, quickly turns out to be a curse. Data per se still is not information, and certainly is not knowledge. On the contrary: intelligent questions about data diversity can only generate information in the true sense of the term, and thus allow for taming complexity. However, even the most reliable information is not sufficient for decision-making, which has to be based on exploring several options and trying to predict their consequences (costs and benefits) in order to select the best option or create new solutions to grand challenges. The prediction of complex processes, however, requires massive simulation based on efficient algorithms and high-performance computing infrastructures.

In its white paper SWD (2016) 106, the European Commission states: "High-performance computing (HPC) is at the core of major advances and innovation in the digital age. In the massively connected digital economy, the exponential growth of data, networking, and computing will continue to drive societal changes, scientific advances, and productivity gains. The nature of computing is changing with an increasing number of data-intensive critical applications, and the intertwining of HPC with a growing number of industrial applications and scientific domains makes HPC the engine to power the new global digital economy. Mastering HPC technologies has become indispensable for supporting policy making, maintaining national sovereignty, and economic competitiveness. The development of the next HPC generation has become a national strategic priority for the most powerful nations, including the USA, China, Japan, Russia, India, and Europe as well."

From a more scientific view, one has to add that MSO (modeling, simulation, and optimization) is equally important for the development of most innovations in technology, health, energy, and finance. Although HPC, data analytics, and artificial intelligence offer new opportunities, their impact on decision-making, technological and social innovation, and the improvement of products and services will be limited without a massive effort on the MSO axes. This statement is supported by various scientific studies that show that MSO methods have outpaced computational power in terms of capability over the past decades. It is well known that the performance of computing machines improves by a factor of two every 18 months. Moore's law describes this trend. In the period from 1990 to 2014, this resulted in a speedup of more than a factor of 1,000,000. What is not known to the general public is that MSO research has achieved similar or even higher speedups in algorithms needed for grand challenge simulations, so that the combined speedup is estimated to be larger than an expressive factor of 1,800,000,000,000. This means that computations that we can do in one second today would have needed more than 50,000 years in 1990.

At ZIB, we are guided by the belief that a high-level approach to modeling, simulation, and optimization (MSO), enriched by data analytics and high-performance computing (HPC), delivers a considerable contribution to solving the grand challenges, improving the scientific and industrial innovation capability, and allowing better services for citizens and better decision-making. Major opportunities rely on the connections at this interface across the whole spectrum of the sciences and humanities. Additionally, the convergence of MSO, HPC, and big data will enable traditional computational-intensive sectors to be more productive and move up into higher-value products and services, and will also pave the way for new science, businesses, and applications that we are far from being able to imagine now. ZIB is one of the places where this convergence is happening now.

In 2017, we worked frantically to open new horizons, for example, into computational social science and humanities, and we intensified our research activities in established application fields like life and materials sciences, nanophotonics, and traffic and transport networks. This annual report provides insights into a variety of other success stories and gives a general overview of ZIB's organization and key factors for its successful development. In particular, six feature articles highlight aspects of our work: "Mathematics Meets Humanities" provides an insight for new fruitful interactions between mathematics, facing new challenges by integrating the human factor into complex systems modeling, and the humanities, seeking possible solutions to otherwise unsolvable tasks. In "Spatial and Dynamic Structure of Life," we report on recent research results at ZIB that provide insight into fundamental principles of biological processes, such as cell division, protein regulation, and brain formation and activity. "20,000 Feet Above the Ground" sheds some light on one of ZIB's innovation projects with industry partners by showing how basic research leads to new navigation systems for aircraft that save both fuel and time. The article "Scalability and Concurrency" features joint research problems in two interdisciplinary projects in the fields of high-energy physics and the automotive industry. "Dusting off Cometary Surfaces" shows how simulation and data analytics can be combined to model the gas and dust cloud around the comet Churyumov–Gerasimenko in order to extract relevant information from the data gathered by a space mission to the comet. And, "Software Sustainability in the Age of Open Science" reports on research activities at ZIB regarding sustainability methods that form part of increasing efforts to conduct research in accordance with open-science principles, and demonstrates how these efforts may change the way research is done in the future.

In summary, ZIB continues to be a place booming with excellent research and first-rate scientific services and infrastructure. Against our own expectations, we again broke several all-time records in 2017, although present capacity limitation seemed to prevent this. For example, in total, €8 million worth of third-party funding was acquired, which marked an increase for the sixth year in a row and a new record in ZIB's history.

Berlin, May 2018
Christof Schütte
President of ZIB

CONTENTS

EXECUTIVE SUMMARY

MATHEMATICS FOR LIFE AND FOR MATERIAL SCIENCES

This year was marked by the preparation of the Cluster of Excellence initiative MATH+, which fueled work on new application directions, in particular in the framework of collaborations with the existing excellence clusters TOPOI (digital humanities and computational social sciences) and Neurocure (analyzing and interpreting life microscopy data).

Many research activities that were started in previous years have been thematically extended, such as augmenting UQ by optimal design of experiments and empirical Bayesian approaches, or moving from linear to nonlinear shape manifolds. The investigation and utilization of machine-learning techniques has increased, with applications particularly in image segmentation and inverse problems, and massive simulation of particle-based and agent-based models allowed for novel insights in such diverse areas as biomedicine or archaeology.

These new developments are complemented by a successful continuation of activities in modeling, simulation, and optimization as well as visual data analysis. They resulted, for instance, in the development of a nonaddictive painkiller (with a publication in *Science* and emergence of a spin-off company), the first reconstruction and analysis of entire microtubule spindles of C. elegans (with a publication in *Nature Communication*), the acquisition of EU projects on optical metrology and scientific cloud computing, an industry project on cloth simulation and visualization, and the first prize in the worldwide MICCAI segmentation competition.

MATHEMATICAL OPTIMIZATION AND SCIENTIFIC INFORMATION

The ongoing digitization of industry and society continues to open up new opportunities for optimization in many applications, such as intermodal travel or computational biology, and brings up exciting mathematical challenges on the interfaces to data and computer science, as well as economics. The computation of a new line plan for the city of Karlsruhe (see the respective report below) and for the ICE rotations of Deutsche Bahn, as well as spectacular performance improvements in the general mixed-integer programming solver SCIP and the parallel computing framework UG were particular highlights.

Networking and outreach was also in the focus of the department in 2017. Together with Freie Universität Berlin's Department of Information Systems, ZIB's Optimization department co-organized the 55th International Conference on Operations Research (OR2017), in which more than 900 participants from 44 countries contributed almost 600 presentations in 21 parallel streams. Two international workshops in Tokyo and Berlin, jointly organized with the Institute of Statistical Mathematics in Tokyo, the Institute of Mathematics for Industry of Kyushu University, and MODAL AG, explored the fascinating interface of mathematical optimization and data analysis. Successful activities for the upcoming extension of the Research Campus MODAL focused on the acquisition of new partners from both industry and academia.

PARALLEL AND DISTRIBUTED COMPUTING

From the smallest structures at the sub-atomistic level to large-scale cosmic matter: supercomputers are indispensable tools to simulate important real-world phenomena. Our feature article "Dusting off Cometary Surfaces" describes how the beautiful dust corona of the comet 67P/Churyumov–Gerasimenko was investigated on the HLRN supercomputer. Taking the shape of the nucleus, the temperature distribution on the surface, the centrifugal, and the Coriolis forces into account, the dust distribution was predicted with a much higher accuracy than previously possible. This project is also a good example of the new breed of mixed HPC/big-data projects, since our simulation results had to be correlated with a great deal of observation data from the Rosetta mission.

The two interdisciplinary projects of the feature article "Scalability and Concurrency" also combine high-performance computing with data-stream processing. A scalable software for the real-time analysis of nucleus–nucleus collisions at the FAIR particle accelerator was developed and parallel algorithms were designed for testing and verifying software components that are used in cars for the real-time analysis of sensor data. As in the years before, research at ZIB was focused on improving scalability and fault tolerance in dynamic systems with failing components.

Our next supercomputer, the HLRN-IV, will make it much easier to conduct the most challenging research projects. The European procurement lead by ZIB was successfully finalized in 2017 and the contract signed in early 2018. With 244,000 processor cores, the new system will provide a six-fold increase in application performance. The supercomputer will be operated on behalf of the North German HLRN consortium by ZIB in Berlin and the University of Göttingen in Lower Saxony.

ADMINISTRATIVE BODIES

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

President of ZIB
PROF. DR. CHRISTOF SCHÜTTE

Vice President
N.N.

The Board of Directors was composed in 2017 as follows:

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

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

PROF. DR. BRIGITTA SCHÜTT
Vice President, Freie Universität Berlin

DR. JUTTA KOCH-UNTERSEHER
Der Regierende Bürgermeister von Berlin Senatskanzlei – Wissenschaft und Forschung

DR. JÜRGEN VARNHORN
Senatsverwaltung für Wirtschaft, Energie und Betriebe

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

THOMAS FREDERKING
Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)

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

The Board of Directors met on May 19, 2017, and December 4, 2017.

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

PROF. DR. ALFRED K. LOUIS
Universität des Saarlandes, Saarbrücken

PROF. DR. RAINER E. BURKARD
Technische Universität Graz, Austria

PROF. DR. MICHAEL DELLNITZ
Universität Paderborn

LUDGER D. SAX
Grid Optimization Europe GmbH

DR. ANNA SCHREIECK
BASF SE, Ludwigshafen

DR. REINHARD UPPENKAMP
Berlin Chemie AG, Berlin

DR. KERSTIN WAAS
Deutsche Bahn AG, Frankfurt am Main

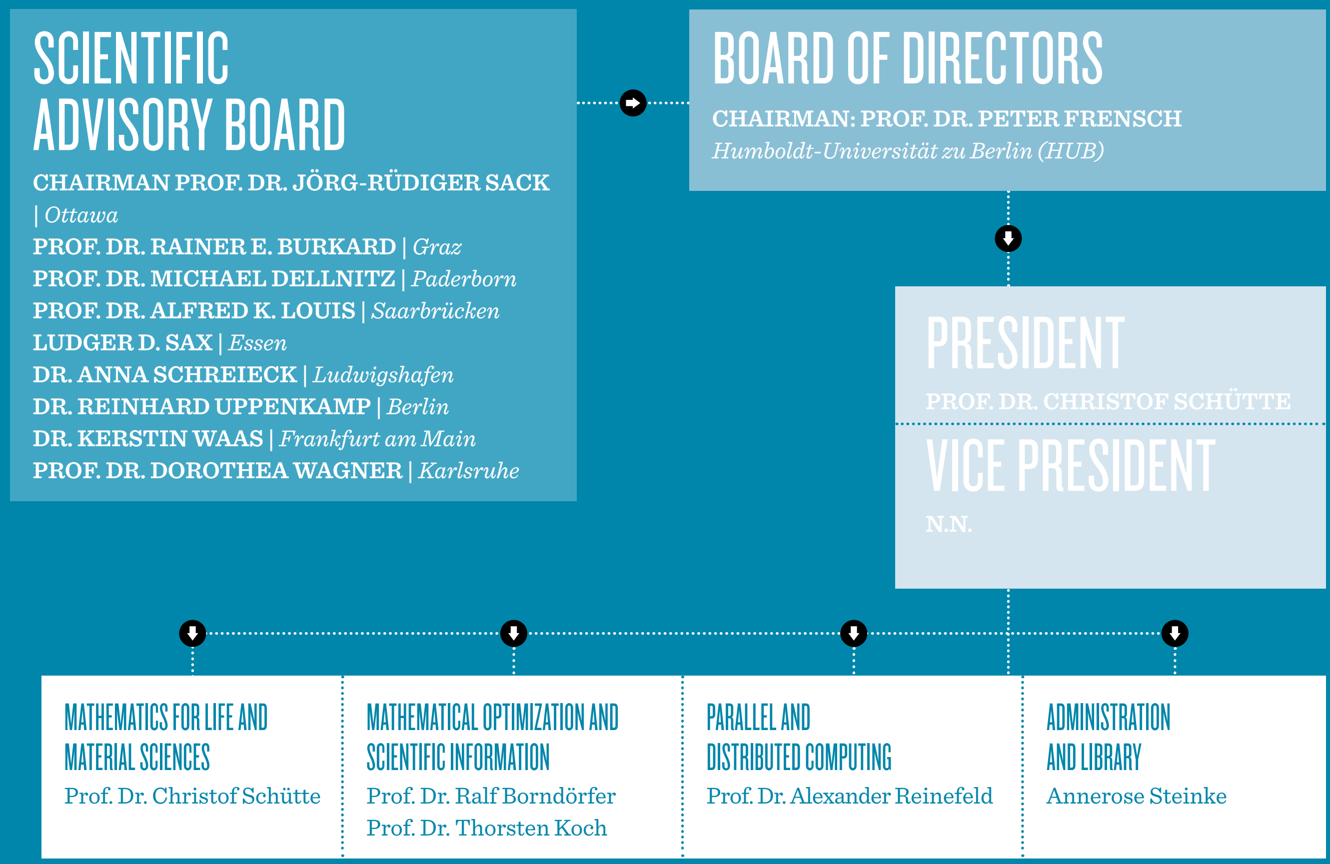
PROF. DR. DOROTHEA WAGNER
Karlsruher Institut für Technologie (KIT), Karlsruhe

The Scientific Advisory Board met on July 3 and 4, 2017, 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



ZIB STRUCTURE

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 (darker bluish color) and research service groups (lighter bluish color).

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, Since May 1, 2017 S. Burger*
- COMPUTATIONAL SYSTEMS BIOLOGY — *S. Röblitz*
- UNCERTAINTY QUANTIFICATION — *T. Sullivan*

VISUAL DATA ANALYSIS
H.-C. Hege

- VISUAL DATA ANALYSIS IN SCIENCE AND ENGINEERING — *H.-C. Hege*
- IMAGE ANALYSIS IN BIOLOGY AND MATERIAL SCIENCE — *S. Prohaska, D. Baum*
- THERAPY PLANNING — *S. Zachow*
- BIOINFORMATICS IN MEDICINE — *T. Conrad*
- MACHINE LEARNING FOR TIME SERIES — *Since June 1, 2017 H. Wu*

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

MATHEMATICAL OPTIMIZATION
R. Borndörfer, T. Koch

- MATHEMATICS OF TRANSPORTATION AND LOGISTICS — *R. Borndörfer*
- MATHEMATICAL OPTIMIZATION METHODS — *A. Gleixner*
- MATHEMATICS OF TELECOMMUNICATION — *Until June 30, 2017 R. Borndörfer*
- ENERGY NETWORK OPTIMIZATION — *J. Zittel, J. Schweiger*
- MATHEMATICS OF HEALTH CARE — *Since July 1, 2017 G. Sagnol*

SCIENTIFIC INFORMATION
T. Koch (B. Rusch)

- WEB TECHNOLOGY AND MULTIMEDIA — *W. Dalitz*
- 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*

PARALLEL AND DISTRIBUTED COMPUTING
A. Reinefeld

DISTRIBUTED ALGORITHMS
F. Schintke

- DISTRIBUTED DATA MANAGEMENT — *F. Schintke*
- SCALABLE ALGORITHMS — *T. Schütt*
- MASSIVELY PARALLEL DATA ANALYSIS — *F. Schintke*

SUPERCOMPUTING
T. Steinke

- HPC CONSULTING — *T. Steinke*
- HPC SYSTEMS — *C. Schimmel*
- ALGORITHMS FOR INNOVATIVE ARCHICTETURE — *T. Steinke*

ADMINISTRATION AND LIBRARY
A. Steinke

CORE FACILITY IT AND DATA SERVICES
C. Schäuble

- BRAIN BERLIN RESEARCH AREA INFORMATION NETWORK — *C. Schäuble*

LEGEND

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

ZIB IN NUMBERS

SEMINARS
GIVEN BY ZIB SCIENTISTS AT UNIVERSITIES

15

9

LECTURES
GIVEN BY ZIB SCIENTISTS AT UNIVERSITIES

2,004
VISITORS
LONG NIGHT OF THE SCIENCES

13,986

SCIP

OF MIP SOLVER SCIP

PROMOTION OF YOUNG SCIENTISTS:
DISSERTATIONS
MASTER'S

4 PROFESSORSHIPS OFFERED TO ZIB RESEARCHERS

136

PEER-REVIEWED PUBLICATIONS IN INTERNATIONAL SCIENTIFIC JOURNALS

230 SCIENTIFIC TALKS

65 DISTINGUISHED

165 INVITED

65 PB DATA ARCHIVE AT ZIB TOTAL CAPACITY ON 16,600 TAPES

58 OUTREACH EVENTS FOR SCHOOL CLASSES AND THE GENERAL PUBLIC

€7,896,000

€6,147,000
PROJECT-RELATED PUBLIC THIRD-PARTY FUNDS

€1,749,000
INDUSTRIAL THIRD-PARTY PROJECTS

18 AWARDS

6,150
INTERNATIONAL GUESTS AT ZIB IN 2017

99
CONFERENCES AND WORKSHOPS AT ZIB

IN JUNE 2017:
ZIB SUPERCOMPUTER IS NO.140 IN TOP500 LIST

KOMBIVERKEHR 2021 – OPTIMIZING THE LINE NETWORK OF KARLSRUHE

ZIB's research group Mathematics of Transportation and Logistics supported the design of a new line network for Karlsruhe. The optimized solution reduces costs by around 5% while travel times remain constant.

Kombiverkehr 2021 (combined traffic 2021) is currently one of the largest inner-city construction projects in Germany. It aims at increasing the overall traffic flow and the attractiveness of the city of Karlsruhe by tunneling public transport under the pedestrian zone of Karlstrasse. In this way, the tramway network is expanded, such that it becomes necessary to redesign the complete line network. As early as 2002, a line plan ("Kombi", see figure 2) was designed using the so-called "Standardisierte Bewertung" method. Kombi was supposed to be operated in 2021 after all construction works were finished. The population of Karlsruhe, however, has increased since then by around 20,000 people, such that the Kombi plan was no longer adequate. In a joint project with Verkehrsbetriebe Karlsruhe GmbH (VBK), PTV Transport Consult GmbH, and TTK Transport Technology Consult GmbH, our goal was to investigate the potentials in cost and efficiency improvements by using mathematical optimization methods, in order to find the best compromise between travel-time improvements and cost efficiency.

The mathematical basis of our line-planning optimization system is a mixed-integer linear optimization model that considers all possible line routes and passenger paths simultaneously. To favor traveling without transfers, the model is based on a novel concept of metric inequalities for direct connections, for further details see [1]. All kinds of practical and technical requirements can be included in the model, e. g. minimum cycle times for certain transportation modes, minimum frequency requirements for each station, or maximum frequency bounds on tracks. A solution of the optimization model implies a set of line routes together with frequencies of operations, such that the given passenger demand can be routed with respect to the resulting line capacities. Using bi-criteria optimization, the whole potential and the interdependencies between cost and travel-time minimization can be investigated by computing the entire Pareto front of efficient solutions.

The focus in Karlsruhe was on the redesign of the tramway network. All other transportation systems (e.g. bus and regional traffic) were considered for passenger routing as well, however, the line routes of these systems remained unchanged. The computation was done for the peak hour.

	No. tram	Cost [% Kombi]	Total travel time [T h] (incl. eight-minute transfer penalty)	Total no. transfers
Kombi	9	100.0%	131.78	124,259
C+	8	83.1%	133.82	125,302
C	7	86.8%	132.27	128,482
Final	8	95.1%	131.71	126,138
T	9	95.2%	131.42	126,130
T+	9	102.0%	130.77	122,730

Table 1: Overview of some solutions.

1 *Karlsruhe. Source: VBK/Uli Deck.*

2 *Kombi: line plan computed for the Standardisierte Bewertung.*

3 *Optimized solution.*

Potentials for travel-time improvements and cost savings were illustrated by computing different solutions addressing cost minimization, travel-time minimization, and some compromise solutions (see table 1). In several rounds of computation, evaluation, and discussion, the infrastructure, operational, service-related, etc. constraints and requirements of VBK, as well as a suitable cost model, were incorporated into both the line-planning optimizer and the accompanying micro-simulation model VISUM of PTV. In this way, realistic line plans could be computed. Assessing many alternatives (which are all Pareto optimal, i.e. realize "best possible compromises"), in the end, VBK decided on a network that yields similar travel times as the Kombi line network, but reduces costs by around 5%. This line plan is illustrated in figure 3. The Verkehrsbetriebe Karlruhe GmbH are currently evaluating the implementation of either plan for the year 2021.

ZIB'S DATA CENTER

After the presentation of ZIB's open data science infrastructure project in October 2016, the institute's core facility "IT and Data Service" (ITDS) started to rebuild and modernize the entire IT infrastructure at ZIB. From the infrastructure of the data center to virtual file systems and server environments, all IT services have been revised and reviewed since 2016. We introduced new operating and development models for IT services. ZIB's new life-cycle management system transforms the IT deployment processes from crafting to automation. The hardware basis is now strongly geared toward commodity hardware. Universal servers can be used for specific software configurations. The specifics of IT services will no longer be implemented in hardware but in software and thus at runtime of the systems.

The integration and operational density in the data center with more than 15 kW per server rack is close to the maximum cooling capacity when using in-row coolers.

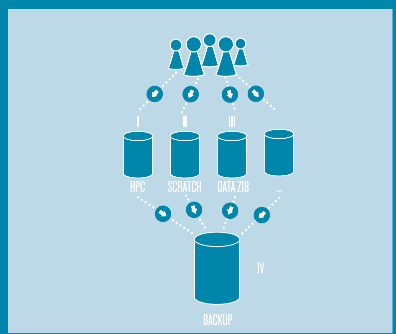
OPEN SOURCE 100 GBIT/S FIREWALLS

The Berlin Research Area Information Network (BRAIN) and ITDS are working closely together to create a 100 Gbit firewall solution based on standard hardware with open-source software components. This implements a highly flexible firewall system with horizontal scaling and building redundancy. In other words, this is a step from active/passive standby to an active/active system.

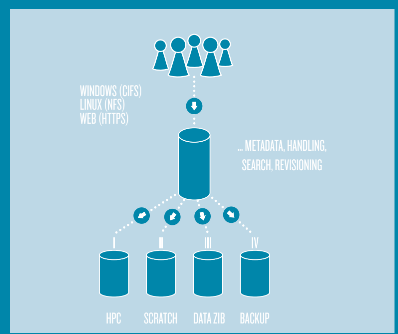
DATA MANAGEMENT

Since the beginning of 2017, the data service infrastructure has been updated: cache systems have been upgraded with the latest design SSDs, the Oracle HSM is now available in the latest version, additional protocols such as CIFS and NFS are now directly available for cooperation partners with BRAIN connection, and additional services like Nextcloud or a scalable file-system integration are possible. The connection of our largest service consumer is now available with 80 Gbit/s sustainable data rate.

NOW



FUTURE



CONVERGENCE

SCALABLE VIRTUAL FILE SYSTEM

The handling of petabytes of user data in the management for direct data access on a multiuser level is a challenge that repeatedly produces previously unresolved problems for ITDS and our users in searching, accessing, authorizing, and analyzing the data. In response, ITDS introduced a virtual file system that implements data migration, data hierarchy (HSM), metadata handling and capture, role-based management, backup and duplication, as well as versioning transparently to the user. In addition to the established access protocols, a Web interface will enable user self-service for Windows, Linux, and Mac OS X. Automation interfaces are added to build data-related applications. Before, users had to interact with many different storage and data management systems. With the introduction of the new paradigm, ITDS realized a new convergent view upon the virtual file system.

This is a shift in paradigm away from file-system management to data management. Central aspects are automatic data classification, storage inventory and classification, storage analysis, user groups and project quota, storage analysis, and storage pools that can be expanded dynamically and vendor independently.

DATA CENTER

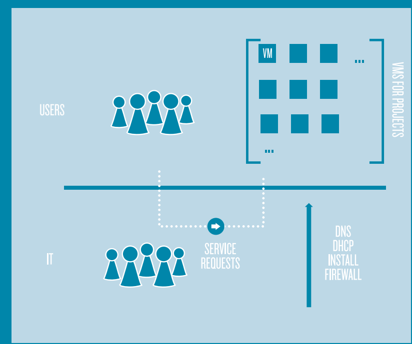
A complete renewal of ZIB's data-center operating area was started in August 2017. All server racks, the cooling, the cabling have been updated and provided with a modern and variable cooling and alignment concept combined with a hot-aisle air containment. We now operate 50 directly cooled server racks with a total capacity of 2,350 height units with a theoretical peak cooling capacity of 900 kW. In addition, redundant systems such as network and fiber channels have been strategically distributed to build a high-availability data center.

VIRTUAL INFRASTRUCTURE – TENANT MODEL

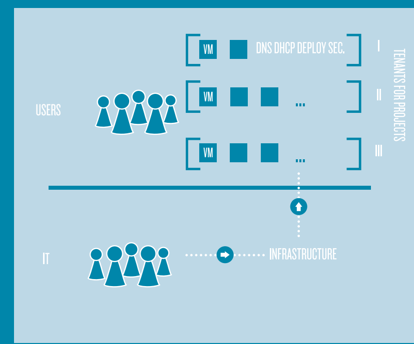
Parallel to the transformation of the data center, a new multi-tenant virtualization solution was introduced. The system now consists of 144 processors, 3.5 TB RAM, and more than 200 TB SSD memory connected with a 40 Gbit network. This allows us to combine about 200 virtual servers in a common infrastructure.

The virtual infrastructure tenant model implements a combined environment for software projects. These tenants consist of virtual servers, a firewall, IP segments, network management like DNS and DHCP, and deployment procedures for virtual machine installations.

NOW

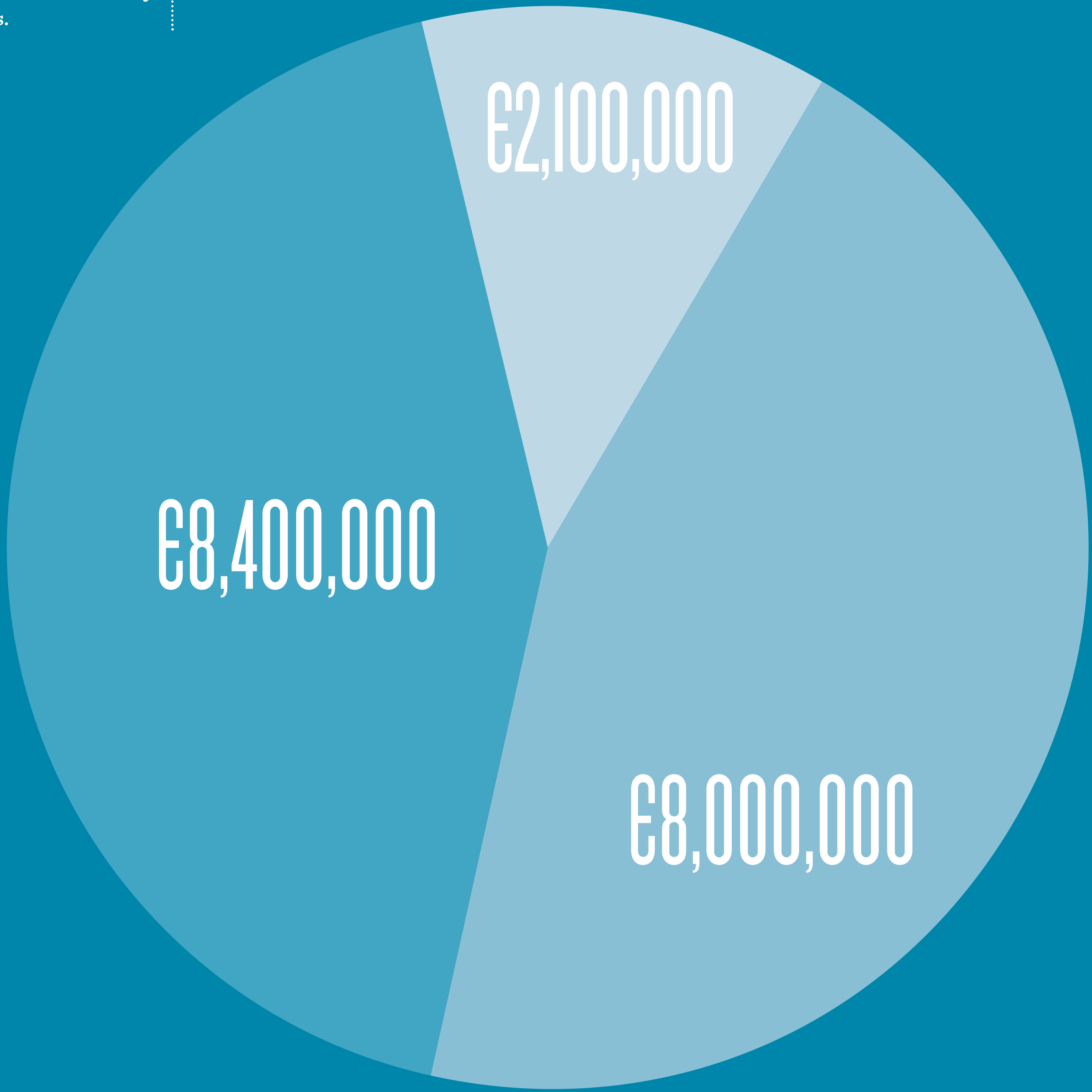


FUTURE



In 2017, the total income of ZIB comprised €18.5 million. The main part of this was made available by the Federal State of Berlin as the basic financial stock of ZIB (€8.4 million), including investments and Berlin's part of the budget of HLRN at ZIB. A similarly large part resulted from third-party funds (€8.0 million) acquired by ZIB from public funding agencies (mainly DFG and BMBF) and via industrial research projects. This was complemented by a variety of further grants like the budgets of BRAIN (State of Berlin) and KOBV (mixed funding) as well as the part of the HLRN budget made available by other German states.

ECONOMIC SITUATION IN 2017



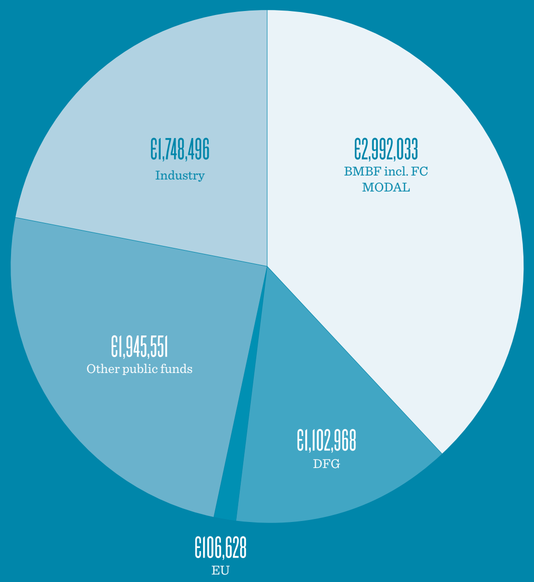
ZIB INCOME

- **45% Core budget by State of Berlin**
- **43% Third-party funds**
- **12% Further grants**

ECONOMIC SITUATION IN 2017

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

In 2017, ZIB raised third-party funding by a large number of projects. Project-related public third-party funds raised from €5.487 thousand in 2016 to €6.147 thousand in 2017, industrial third-party projects declined from €2.371 thousand to €1.749 thousand. In total, €7.896 thousand third-party funding marked a new record in ZIB's history, an increase for the sixth year in a row.



ZIB THIRD-PARTY FUNDS BY SOURCE

- 1% EU
- 14% DFG
- 25% Other public funds
- 22% Industry
- 38% BMBF incl. FC MODAL

ZIB THIRD-PARTY FUNDS IN EUROS

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 the ZIB spin-off Visual Concepts GmbH)
1999 | www.visageimaging.com
Advanced visualization solutions for diagnositic imaging

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 / LBW OPTIMIZATION GMBH
2000 | www.lbw-berlin.de
Optimization and consulting in public transport
LBW Optimization GmbH was founded in 2017 and is a spinn-off of LBW GbR

LENNÉ 3D 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, and Eddystone for interactive business models

DOLOPHARM BIOSCIENCES UG
2017
A specialty pharmaceutical company focused on the clinical and commercial development of new products in pain management that meet the needs of acute and chronic care practitioners and their patients

SPIN-OFFS

NUMBER OF EMPLOYEES

In 2017, 231 people were employed at ZIB; of these, 171 positions were financed by third-party funds.

	1/1/2017			1/1/2018		
	Permanent	Temporary	TOTAL	Permanent	Temporary	TOTAL
MANAGEMENT	3	0	3	3	0	3
SCIENTISTS	15	99	114	15	100	115
SERVICE PERSONNEL	38	10	48	34	10	44
KOBV HEADQUARTERS	8	8	16	8	9	17
STUDENTS	0	55	55	0	52	52
TOTAL	64	172	236	60	171	231

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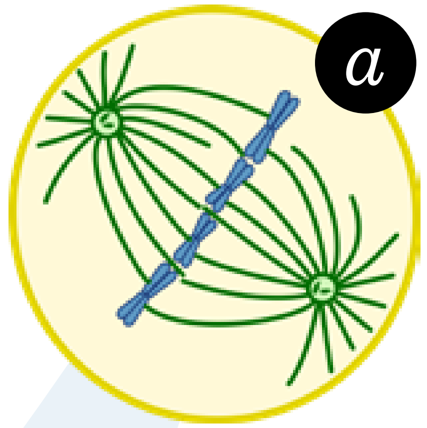
SPATIAL AND DYNAMIC STRUCTURE OF LIFE

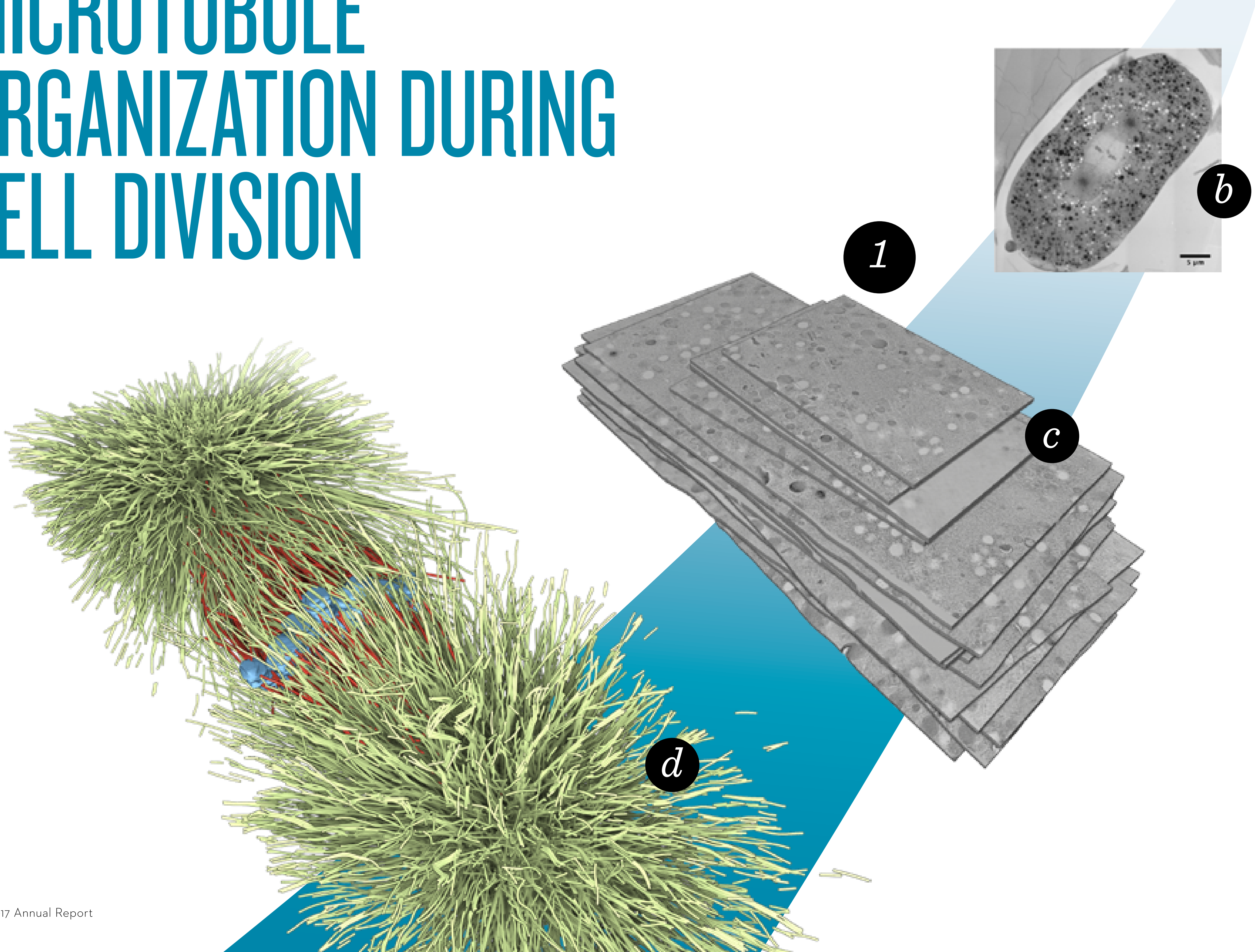
How cells organize patterns in space and time

Researchers at ZIB develop data analysis and mathematical modeling techniques and apply them in cooperation with biologists in order to gain insight into fundamental principles of biological processes, such as cell division, protein regulation, and brain formation and activity.

UNDERSTANDING MICROTUBULE ORGANIZATION DURING CELL DIVISION

1 *The mitotic spindle during the metaphase of cell division in C.elegans:* a *Schematic of the microtubule spindle (green) and the chromosomes (blue).* b *Electron-microscopy image of the full cell.* c *Complete stitched electron-tomography serial-section stack (120 GB).* d *Segmented microtubules (green, red) and chromosomes (blue).*





Microtubules are tube-like polymers that play an important role in cell division. They form the spindle, which is a microtubule assembly that segregates the chromosomes, see figure 1 (a,b). Electron tomography is the preferred technique to acquire most detailed spatial information about microtubules. The cells are prepared for electron microscopy as 300 nm thick serial sections (slices). With the application of image-processing techniques, we are able to automatically extract the microtubules within a section [1,2,3] (see figure 1). Furthermore, we have been developing reconstruction methods for joining multiple sections to create a geometric model of the entire spindle [4], see figure 1 (c,d). Our integration of automated techniques with real-time user interactions allows handling of practical challenges during day-to-day research, such as varying tomogram quality. In cooperation with TU Dresden, we visually and quantitatively analyzed entire microtubule spindles of C. elegans for the first time [5]. We identified different classes of microtubules and analyzed geometrical properties, such as length and density distributions. In particular, we investigated potential microtubule interactions based on their spatial arrangement. One major finding is that microtubules do not directly connect chromosomes and centrosomes, but form an interactive dynamic network. Currently, the full reconstruction and analysis pipeline is adapted for upcoming experiments that will study spindles in different phases of cell division, spindles in mutant organisms, meiotic spindles, and spindles of different species.

CELLULAR REACTION KINETICS

2

$$\frac{\partial P(x,t)}{\partial t} = \sum_{k=1}^{K} \left[\alpha_k(x-\nu_k)P(x-\nu_k,t) - \alpha_k(x)P(x,t) \right]$$

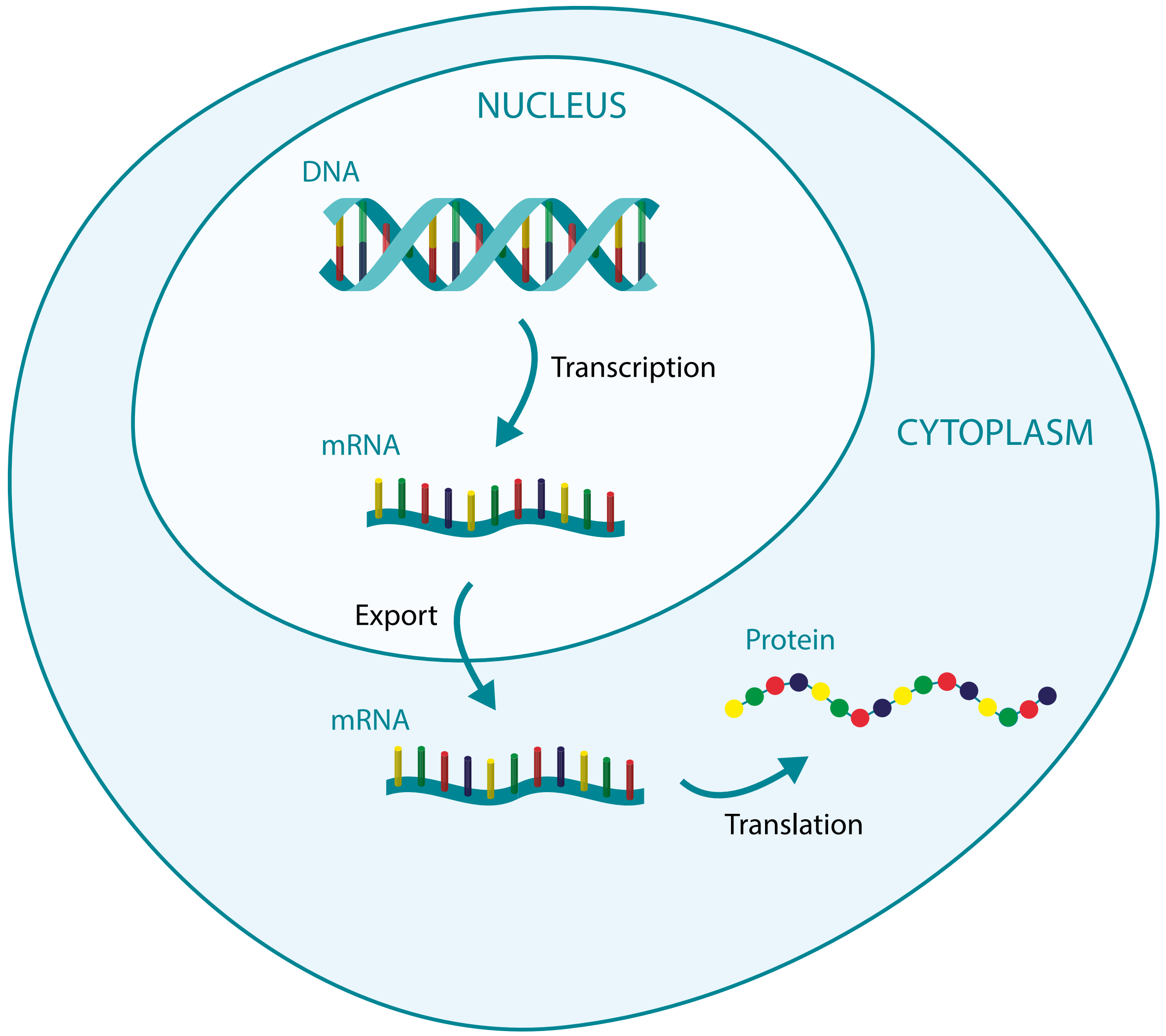
2 Chemical master equation (CME) for well-mixed stochastic reaction kinetics. It defines the temporal evolution of the probability P(x,t) to find the system at time t in a certain state x, given the reaction propensities α_k.

Accurate modeling of reaction kinetics is important to understand how biological cells work. Spatially well-mixed reaction dynamics can be modeled by the chemical master equation (CME, see formula 2), an infinite set of ordinary differential equations, which is, in general, too complex to be solved analytically. There are accurate numerical simulation schemes for solving the CME indirectly, like Gillespie's stochastic simulation algorithm [6]. For many relevant realistic settings, however, even our high-performance computers fail to create reliable statistics within an acceptable amount of time. This is the motivation to reduce the model complexity by considering approximative mathematical formulations of the cellular dynamics. Especially multiscale reaction systems, which often appear in real-world applications, are in the focus of our investigations because they require new combinations of existing approximation methods.

An example for a cellular reaction process that involves cascades of particle numbers is the process of gene expression, which is relevant for all known life. See figure 2 for an illustration. The information encoded in a gene is used for the synthesis of functional gene products, the proteins, which typically arise in bursts with much higher abundance than all other involved reactive species. In collaboration with the DFG research center CRC 1114 "Scaling cascades in complex systems," we applied new hybrid methods to efficiently simulate the gene expression process and showed that, in contrast to classical uniform approximation methods, advanced hybrid schemes are able to reproduce the characteristic patterns of the cellular dynamics [7].

But what can we do if the central well-mixed assumption underlying the CME is broken and some spatial resolution is needed to capture the dynamics? Based on mathematical theory, we have been developing suitable extended models, like the spatiotemporal CME [8], to include the necessary spatial information, with the level of detail adapted to the reactive system under consideration. A eukaryotic cell, for example, naturally decomposes into several compartments (e.g. the nucleus and parts of the cytoplasm (see figure 3), which both have a central meaning for the process of gene expression. By making use of this natural cellular structure, we obtain models that are computationally practical and at the same time close to the reality of a biological cell. Spatiotemporal hybrid models form the basis for the simulation of cellular reaction kinetics in all relevant details; their use in massive simulation environments, however, still poses significant challenges that will be the motivation for further research in this direction at ZIB.

3 Gene expression in a eukaryotic cell. In the nucleus, the DNA is transcribed into messenger RNA (mRNA), which is then exported to the cytoplasm and translated into proteins. Such cellular reaction kinetics can appropriately be characterized by the spatiotemporal chemical master equation [8].



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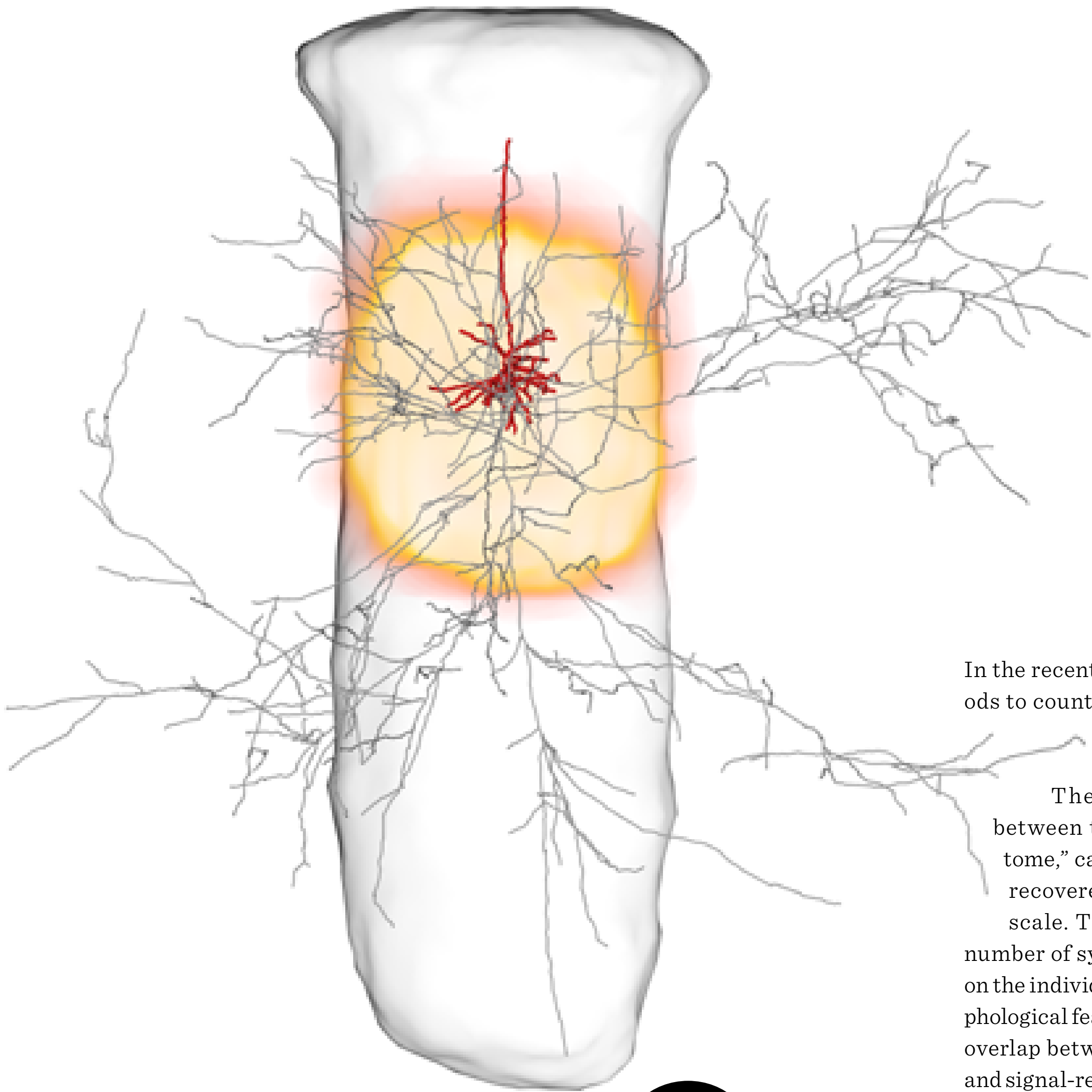
3-D BRAIN MODELING TO UNDERSTAND SENSORY INFORMATION PROCESSING

How does the brain process information from our senses, and how does this ultimately lead to specific behavior? To investigate this question, we, together with our collaborators at CAESAR Bonn, created an anatomically realistic model of the part of the rat brain that processes information from the whisker hairs on the animal's snout. The model consists of a large network of interconnected neurons.



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4 Single "spiny pyramid" neuron in a cortical column (transparent cylinder) in the rat brain, with its dendrites (red) and axons (gray). Synapse density (yellow) indicates where neurons of this type receive information through synaptic contacts. Data: M. Oberlaender (CAESAR Bonn).

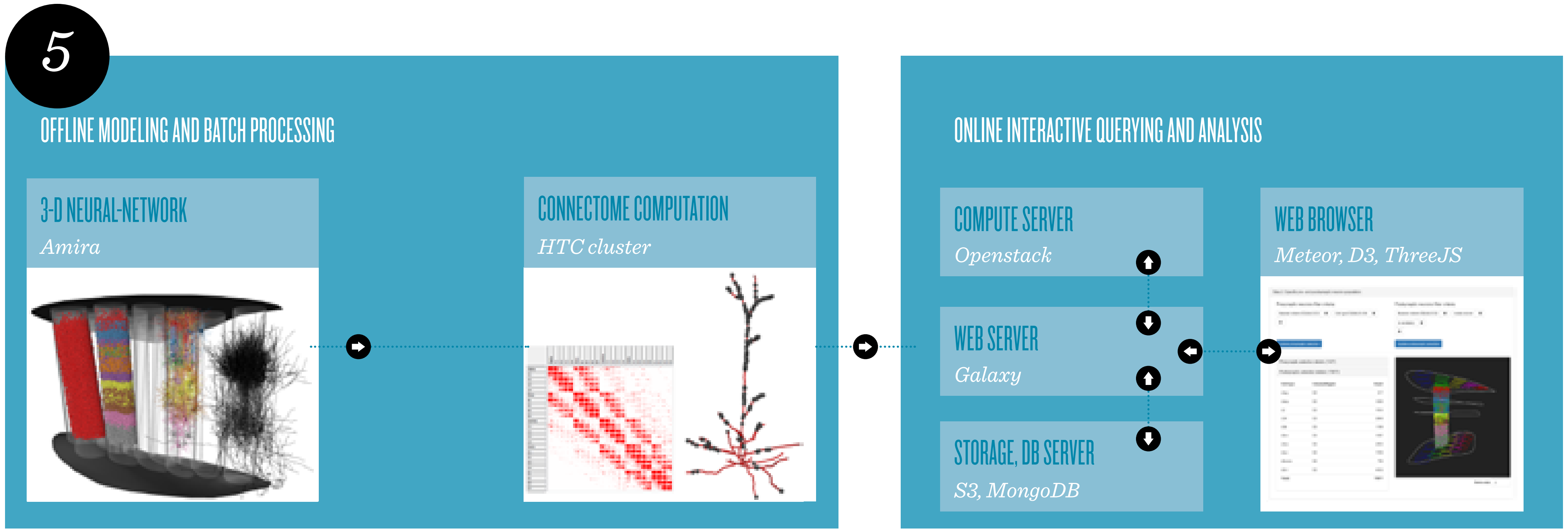
5 Modeling and analysis pipeline, consisting of an offline and an online part. The 3-D neural-network model is created using the Amira visualization software. The large connectome dataset is precomputed on a batch cluster. A Web application, intended for the research community and implemented using state-of-the-art Web frameworks and cloud technologies, provides a query interface to extract and analyze on the fly specific subsets of the large dataset.

In the recent past, we developed methods to count the number of neurons in the network from 3-D microscope images [9]. The synaptic connectivity between them, called the "connectome," cannot, however, be directly recovered from image data at this scale. Therefore, we estimate the number of synapses and their location on the individual neurons based on morphological features, in particular spatial overlap between signal-sending axons and signal-receiving dendrites (figure 5) [10]. This predicted connectivity turned out to match available measurements well.

Based on this realistic model, neuron simulations can be performed, which may provide insight into the function of each neuron type in the network [11]. Also, mathematical models, for example, describing population dynamics [12], can be tested using this model, and may lead to a better understanding of biological mechanisms involved.

Currently, we are developing a Web application to make this model publicly available to the research community. Neuroscientists can perform in-silico experiments by interactively defining queries that extract specific information from this large dataset on the fly (figure 5).

Within the Priority Programme "Computational Connectomics" of the DFG (German Research Foundation) starting 2018, we aim to use a data-driven Bayesian approach to investigate more in depth what anatomical properties underlie synapse formation in order to make even more accurate predictions of network connectivity.



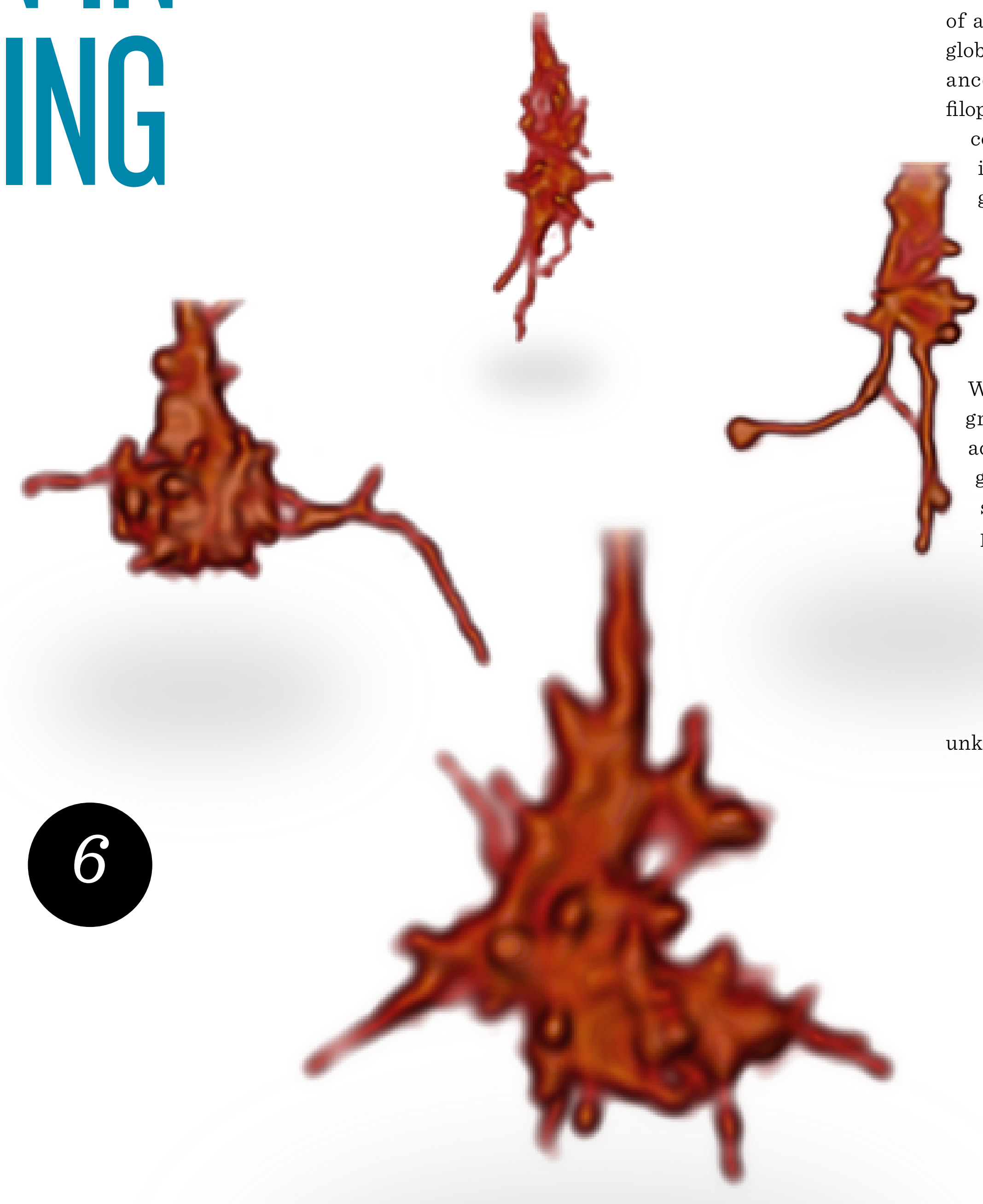
STOCHASTICITY DRIVING PATTERN FORMATION IN BRAIN WIRING

Neurons form specific patterns in a very robust and reliable way during brain development. How axons and dendrites find the appropriate synaptic partners has been studied for decades. But the question is posed today with a new twist.

6 *Four examples of growth cones with extending filopodia of varying number and shape, displayed as volume renderings for individual time points from in-vivo microscopy image time series. Data courtesy R. Hiesinger.*

7 *Statistics of filopodia dynamics extracted from 4-D microscopy data. Length, a characteristic quantity, appears to be correlated with filopodia lifetime, and differs between mutants (green) and wild type (blue) for growth cones during synaptogenesis. Data courtesy of R. Hiesinger.*

8 *25 axons in a spatially periodic setting growing to a robust and quasi-regular space-filling but contact-avoiding pattern.*



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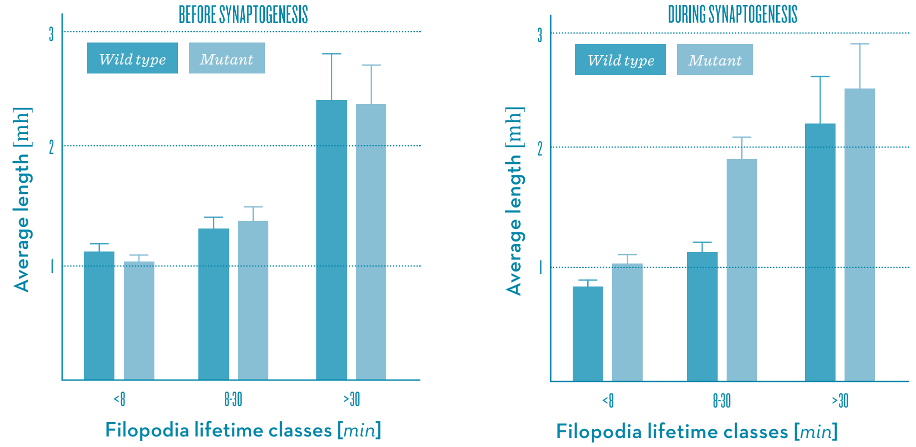


AXON GUIDANCE REVISITED

For the last 70 years, the dominant model of axon guidance has been based on global concentration gradients of guidance molecules. During axon growth, filopodia, small extrusions of the growth cone, sprout in different directions, as is visible in microscopy images. The general assumption has been that the filopodia sample the surroundings for chemical gradients of guidance molecules, allowing them to find the right direction despite the stochasticity of molecule sensing.

With new microscopy technology, the group of R. Hiesinger (FU) is able to acquire in-vivo 4-D movies of axons growing in drosophila brains, which shed new light on the brain wiring process. The filopodia dynamics feature a much richer structure than would be necessary for stochastic gradient sampling (figure 6). Currently, the role of these complex dynamics for brain wiring is essentially unknown.

LOOKING FOR SIMPLICITY

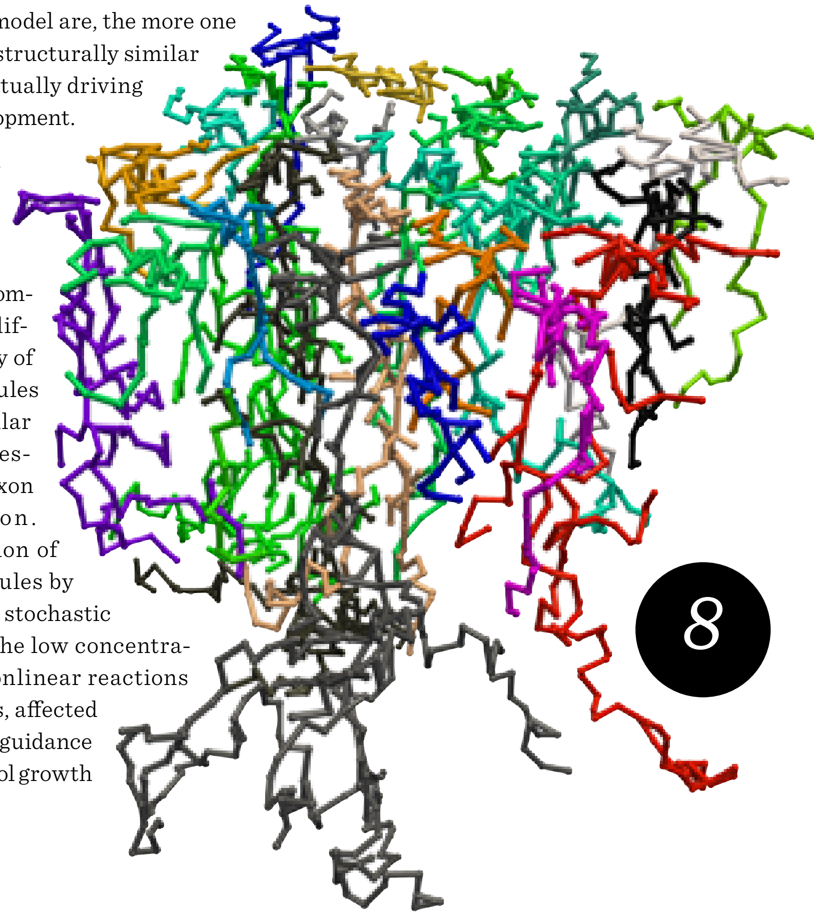
The genome is too small for encoding the brain wiring explicitly. Thus, the pattern must emerge from rather simple regulatory mechanisms encoded in the genome [13]. One compelling hypothesis is that these developmental rules do not only tolerate randomness in the axons' environment, but use stochasticity as a driving force and to achieve robustness.

In a joint Matheon project with M. von Kleist (FU), we aim at identifying mechanistic models that are both physically plausible and able to reproduce observed wiring patterns and the statistics of filopodia dynamics (figure 7). The simpler and more general the mechanisms forming such a model are, the more one can expect that structurally similar processes are actually driving the neural development.

As a first candidate, we consider a model comprising three essential components. First, diffusion and decay of guidance molecules in the extracellular space seem necessary for inter-axon communication. Second, reception of guidance molecules by the filopodia is a stochastic process due to the low concentration. Finally, nonlinear reactions within the axons, affected by the sensing of guidance molecules, control growth and retraction of filopodia as well as release of guidance molecules [14].

For simulating such models, solvers for deterministic partial differential equations describing diffusion, reaction, and transport processes need to be coupled to a stochastic simulation algorithm [6] capturing the random events of guidance molecule reception and filopodia growth.

One of the simplest models of this type, containing just a single type of guidance molecule, can already create robust and quasi-regular space-filling axon structures that avoid self-contact as well as neighbor contact (figure 8).



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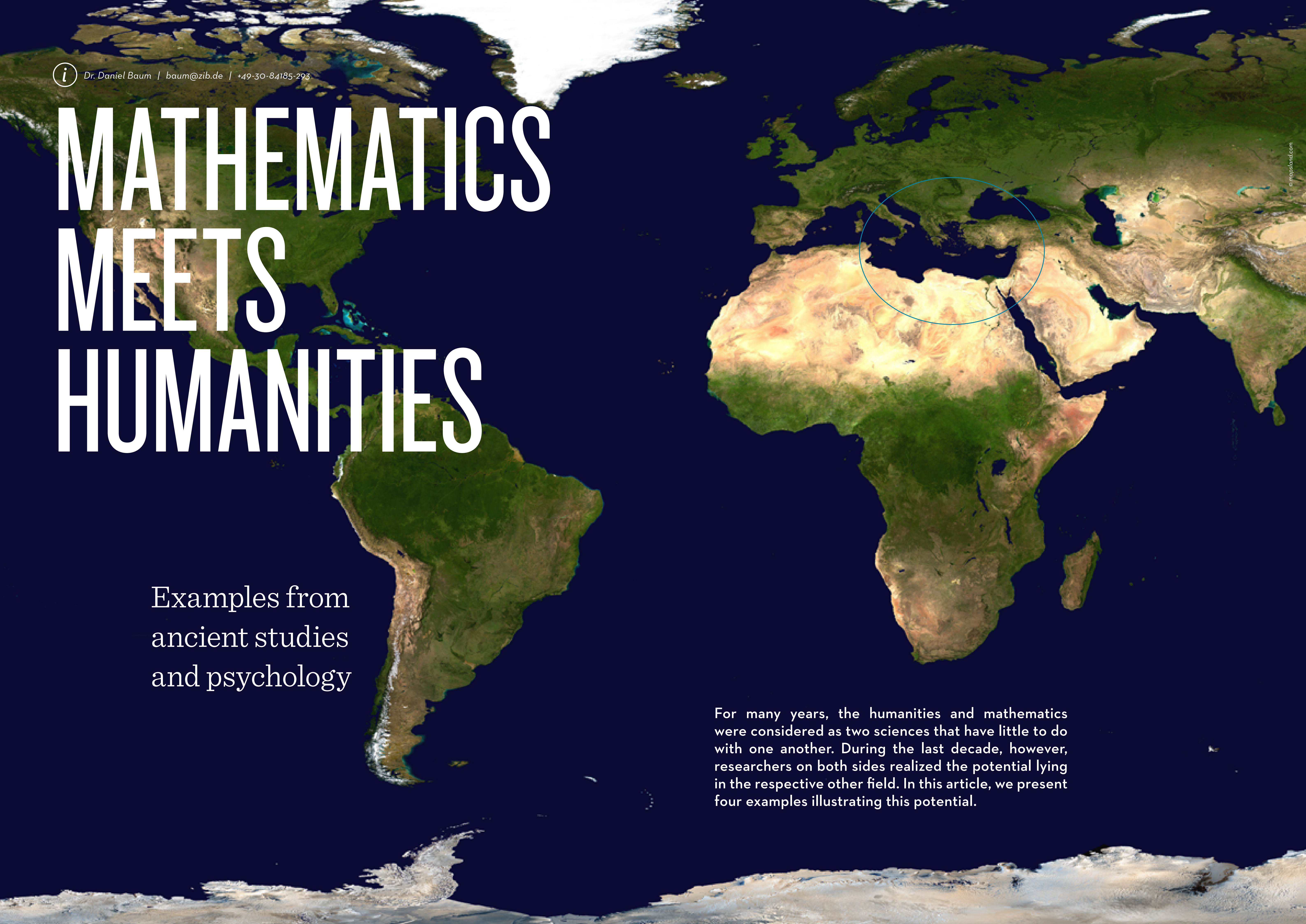
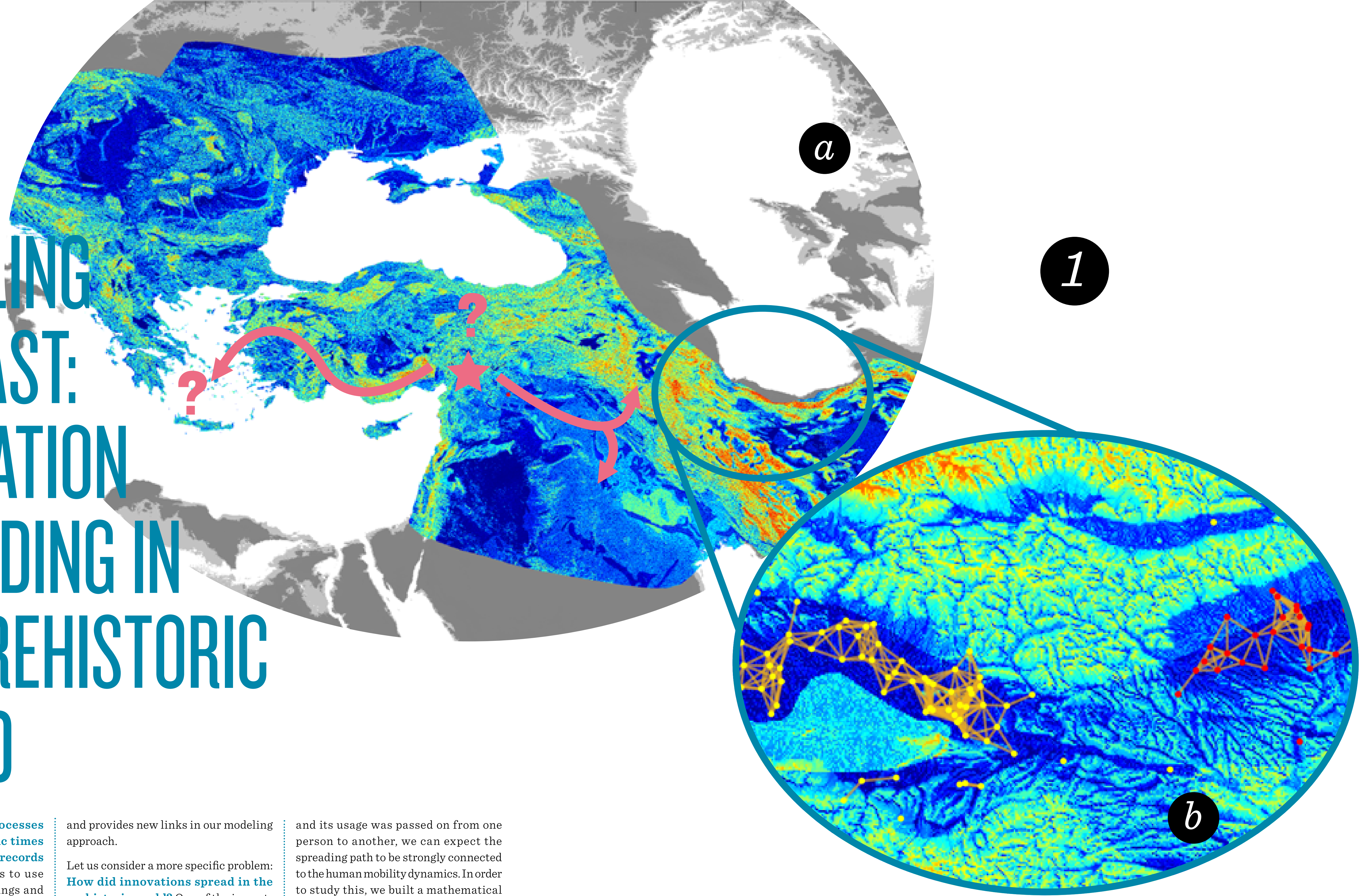
MATHEMATICS MEETS HUMANITIES

Examples from ancient studies and psychology



For many years, the humanities and mathematics were considered as two sciences that have little to do with one another. During the last decade, however, researchers on both sides realized the potential lying in the respective other field. In this article, we present four examples illustrating this potential.

MODELING THE PAST: INNOVATION SPREADING IN THE PREHISTORIC WORLD

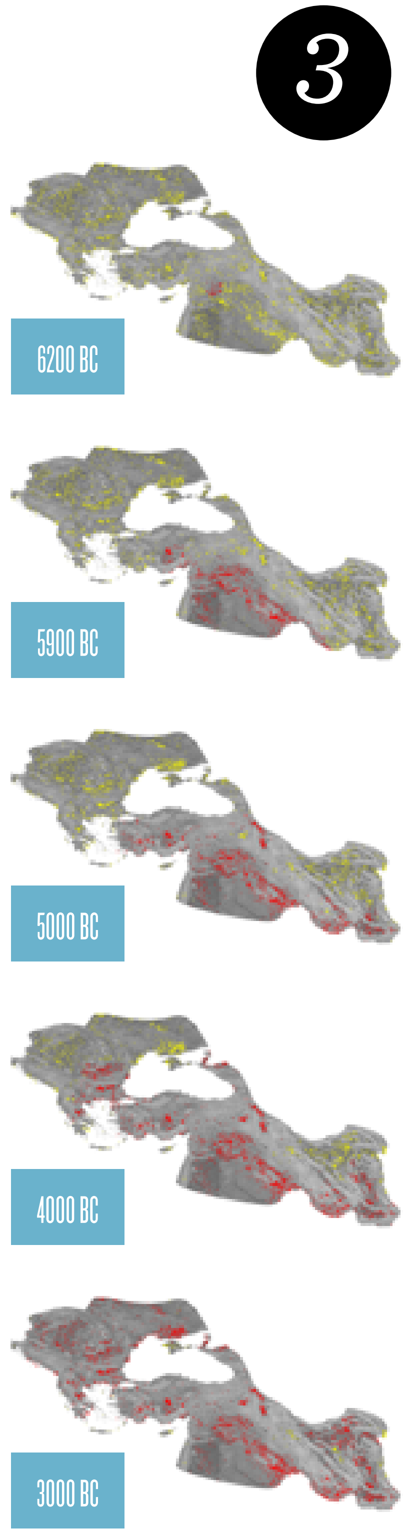


1 Geographical area of our interest for wooly sheep spreading. a Suitability landscape constructed from environmental data; the assumed origin of the woolly sheep is around Tell Sabi Abyad (star). b Agents move in the suitability landscape and adopters (red) of the innovation can pass on the innovation to neighboring non-adopters (yellow) with a certain probability.

How can we understand processes that happened in prehistoric times when there were no written records of events? One possibility is to use available archaeological findings and build a good mathematical model that we can study. However, most of the existing archaeological data is sparse and uncertain; lots of information is unknown and there is no procedure to repeat the history and obtain new data. To deal with these problems, we work closely with researchers from the humanities, whose expertise enhances our studies and provides new links in our modeling approach.

Let us consider a more specific problem: **How did innovations spread in the prehistoric world?** One of the impactful innovations that spread from the Near East to Europe between 6200 and 3000 BC, was the wool-bearing sheep. The change from herding hairy sheep to woolly sheep was an essential driving force for the later textile production. But the exact spreading path is unknown. Since the knowledge of an innovation and its usage was passed on from one person to another, we can expect the spreading path to be strongly connected to the human mobility dynamics. In order to study this, we built a mathematical model that allows us to simulate both human migration and innovation spreading. These simulations can be used to analyze dynamical properties of the two processes, explore how they are coupled, and discover the important factors that could have affected this innovation spreading.

Through a fruitful collaboration with experts from the Cluster of Excellence TOPOI, we gained access to the archaeological and environmental data. We used this data to build a suitability landscape that indicates how suitable a particular region was for herding woolly sheep in the respective period (see figure 1a). Then, we constructed an agent-based model (ABM) in order to simulate possible spreading scenarios. An ABM consists of a set of rules describing the behavior of agents and their interaction patterns with each other and the environment. In our model, an agent represents a group of people in the ancient world. Agents move in the suitability landscape by following the so-called dynamical equation, according to which they move freely but with a bias toward regions that are attractive for herding woolly sheep. At the same time, agents can interact socially with other agents in their vicinity and pass on the innovation with a certain probability. By applying this abstract model to the example of the woolly sheep (figure 2), we can generate time series for the spreading process (see figure 3)[1]. This opens up new research questions like: What are the best parameters of our model? How did the innovation spread between different geographical regions? With our research, we try to answer such questions and, thus, help understand processes in prehistoric times.



INFO BOX

This research is done in collaboration with Brigitta Schütt (Freie Universität Berlin, FB Geowissenschaften and TOPOI, Berlin, Germany), Wolfram Schier (Freie Universität Berlin, FB Geschichts- und Kulturwissenschaften and TOPOI, Berlin, Germany), Daniel Fürstenau (Freie Universität Berlin, FB Wirtschaftswissenschaft and Einstein Center Digital Future, Berlin, Germany), and their coworkers. It has been partially funded by the Cluster of Excellence TOPOI – The Formation and Transformation of Space and Knowledge in Ancient Civilizations and ECMath (Einstein Center for Mathematics Berlin).

Snapshots of one realization of the wool-bearing sheep innovation spreading in the prehistoric world.

ACCESSING HIDDEN TEXTS IN EGYPTIAN PAPYRI

One of the best sources of information about our cultural origin is provided by written texts.

For example, excavations in Elephantine, a small island in the Nile in Egypt, brought to light large quantities of papyri, telling us 4,000 years of cultural history of various religious, ethnic, and linguistic groups that lived there [2,3]. The papyri are typically rolled or folded (see figure 4). However, for papyri that are too fragile to be physically unfolded or unrolled, the writings are inaccessible.

Our aim is to make such papyri readable. For this, we acquire a 3-D tomographic image of it, reconstruct the papyrus geometrically on the computer, virtually unfold and unroll it, and finally visualize the writing on it [4]. A prerequisite is that the tomographic method depicts the writing with a sufficiently high contrast. For documents written with ferrous ink, this is the case when using X-ray-based tomography.

For virtual unrolling, we depict cross sections in high detail, allowing the user to define manually closed polylines that approximate the contours (figure 6, left); using interpolation and extrapolation, similar contours are computed in other planes (figure 6, right). Ensuring that the number of points in each polyline is equal, a quadrangular 2-D mesh is implicitly defined, representing a surface; this surface is flattened such that differences in the distances between neighbored contour points are minimized (figure 5).

For virtual unfolding, each step of the physical folding process is virtually undone.

After a series of steps, the unfolded papyrus becomes topologically equivalent to a role, which is then unrolled, as described before. In each step, we provide the user with an overview of the current state using volume rendering (see figure 7, left); furthermore, we display cross sections in high detail in which the user can interactively draw polylines. For the actual unfolding, Moving Least Squares deformation is applied based on these polylines to unfold the package as rigidly as possible. After all folds have virtually been undone, we unroll the roll as described previously. In a final step, an equalization is performed that largely eliminates all distortions that accumulated during the whole procedure. Then the writing is visualized using contrast-enhancing techniques (figure 7, right).

Only some papyri are described with ferrous ink; for the majority, soot ink was used. For this case, alternative tomographic procedures are currently being investigated, in the hope of finding one that offers sufficient contrast.

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a

b

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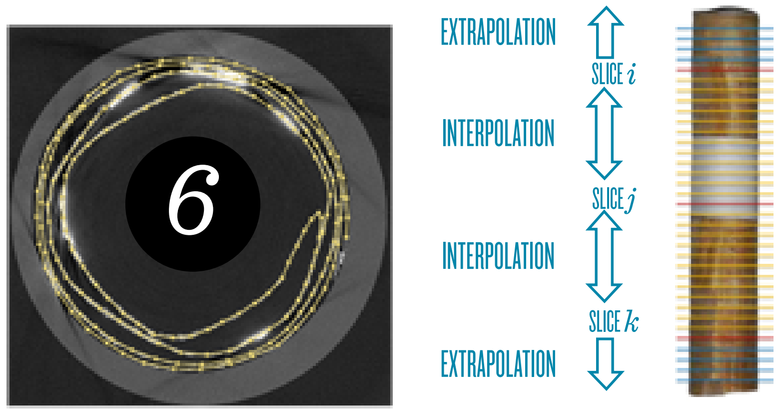

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4 Left: Photograph of sealed legal texts. Right: Physically unfolded package. (ÄMP Berlin, SMB)

5 a Volume rendering of CT scan of rolled mock-up papyrus. b Virtually unfolded mock-up from CT scan seen on the left.

6 Virtual unrolling of a papyrus roll. Right: Red contours are interactively set; yellow and blue contours are computed by inter- and extrapolation. Left: Depiction of a cross section.

7 Left: Computer-tomographic (CT) scan of folded mock-up papyrus. Right: Virtually unfolded papyrus from CT scan seen on the left.

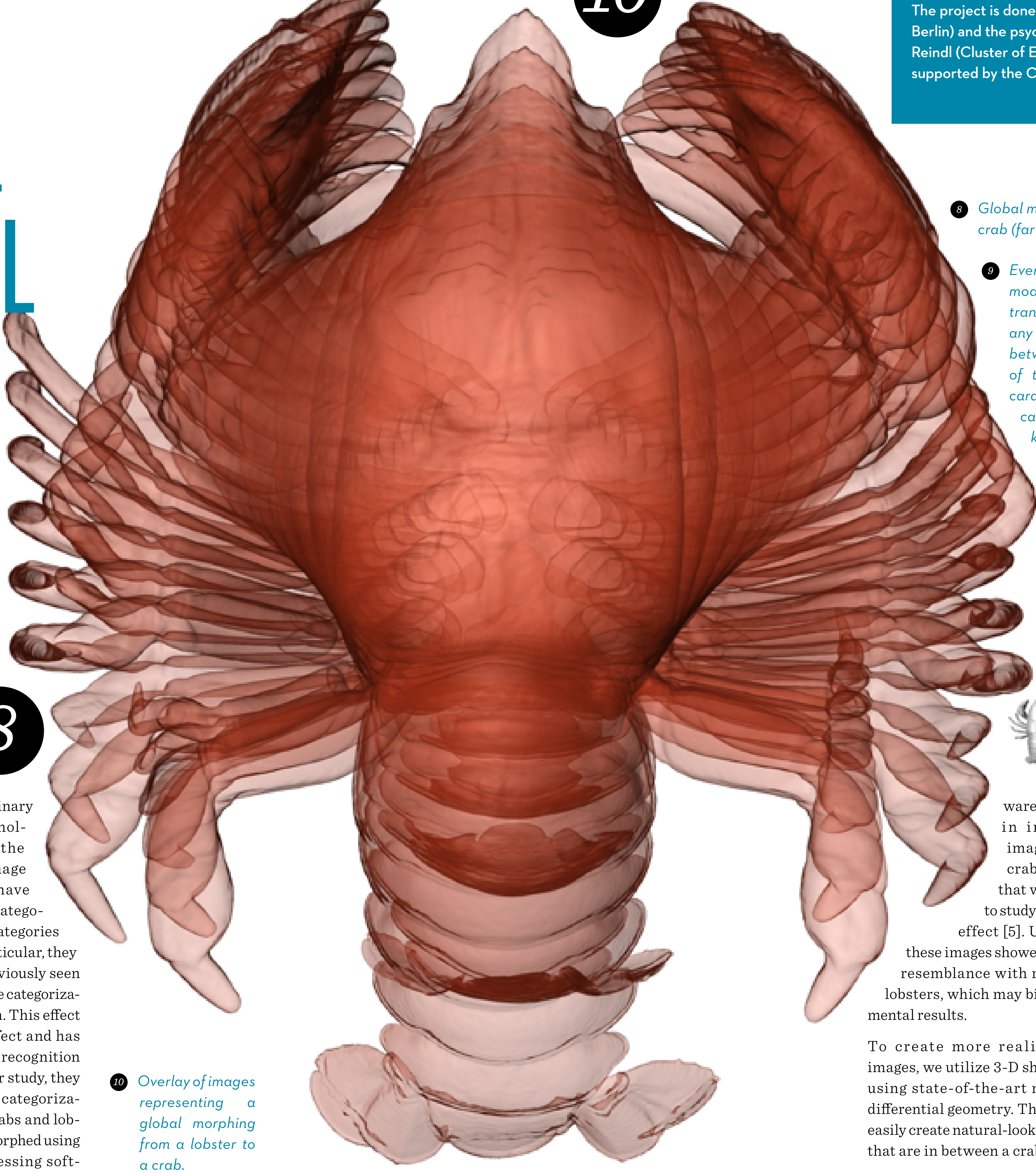
INFO BOX

This project was carried out in collaboration with the archaeologist Verena M. Lepper (Ägyptisches Museum und Papyrussammlung (ÄMP) – Staatliche Museen zu Berlin (SMB) – Stiftung Preußischer Kulturbesitz), the physicists Heinz-Eberhard Mahnke (Freie Universität Berlin, FB Physik and TOPOI, Berlin, Germany) and Ingo Manke (Helmholtz-Zentrum Berlin), and their coworkers. It was financially supported by the Starting Grant ELEPHANTINE of the European Research Council (ERC), the Beauftragte der Bundesregierung für Kultur und Medien (BKM), the Cluster of Excellence TOPOI (The Formation and Transformation of Space and Knowledge in Ancient Civilizations) of the Deutsche Forschungsgemeinschaft (DFG).

3-D MESH MORPHING FOR PSYCHOLOGICAL EXPERIMENTS

INFO BOX

The project is done in collaboration with the biologist Gerhard Scholtz (HU Berlin) and the psychologists Torsten Schubert (University Halle) and Antonia Reindl (Cluster of Excellence Image Knowledge Gestaltung). It is financially supported by the Cluster of Excellence "Image Knowledge Gestaltung".



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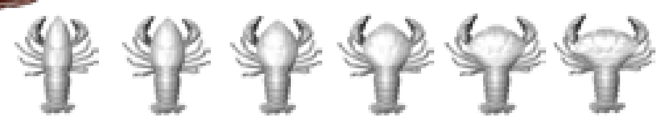

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8 Global morphing from a lobster (far left) to a crab (far right).

9 Even though only the carapace is modified, the images show a smooth transition of the whole object without any noticeable artifacts at the joints between the carapace and other parts of the body. Local morphing of the carapace from a lobster (far left) to the carapace of a crab (far right) while keeping all other parts fixed as in the lobster.

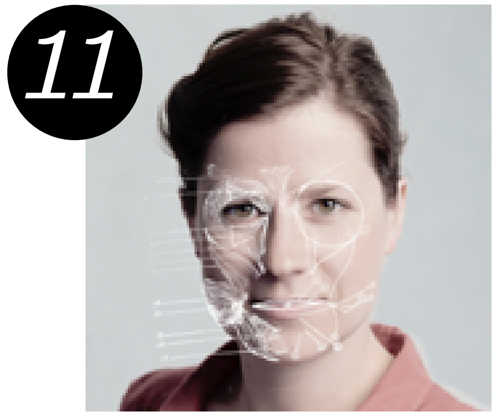
Understanding how object recognition and categorization is performed by the human brain is a topic that has been studied in psychology for many years. As a result, it is widely believed that for this task our brain builds up a mental representation of objects. Studies have shown that such mental representations are not fixed but remain flexible and are subject to continuous short- and long-term adaptation. The majority of such studies have so far concentrated on human faces, the recognition of which plays a very essential role in our daily life. Hence, it is not clear how these findings generalize to the recognition and categorization of other objects.

Therefore, in an interdisciplinary project, perceptual psychologists and biologists in the Cluster of Excellence "Image Knowledge Gestaltung" have been investigating object categorization on the biological categories of crabs and lobsters. In particular, they are investigating how a previously seen input stimulus influences the categorization decision of a test person. This effect is known as adaptation effect and has been shown to exist for the recognition of human faces [6]. For their study, they produced images in which categorization-relevant features of crabs and lobsters were systematically morphed using standard 2-D image-processing software. This resulted in intermediate images between a crab and a lobster that were then used to study the adaptation effect [5]. Unfortunately, these images showed a rather poor resemblance with real crabs and lobsters, which may bias the experimental results.

10 Overlay of images representing a global morphing from a lobster to a crab.

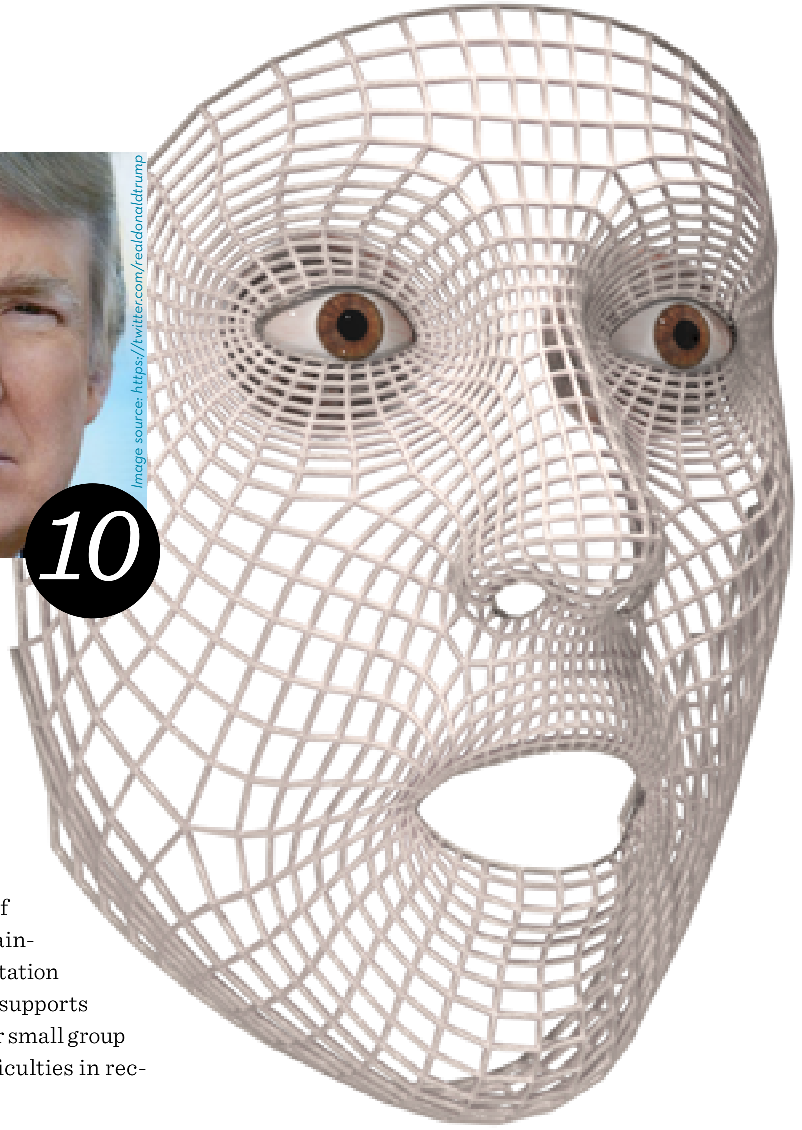
To create more realistic-looking images, we utilize 3-D shape morphing using state-of-the-art methods from differential geometry. This allows us to easily create natural-looking 3-D shapes that are in between a crab and a lobster (see figure 8). Controlled psychological experiments, however, require local mesh morphing that transforms one part (e.g. the carapace) of the animal at a time. To achieve this goal, we developed an approach that combines two previously proposed methods for mesh morphing to obtain a natural-looking transformation of selected parts of the mesh, while keeping the rest of the mesh as stable as possible (see figure 9). From the interpolated representations, standardized images were created that much better resemble real crabs and lobsters even though artificial. Currently, new psychological experiments are being carried out using these new images, thus greatly improving the experimental conditions.

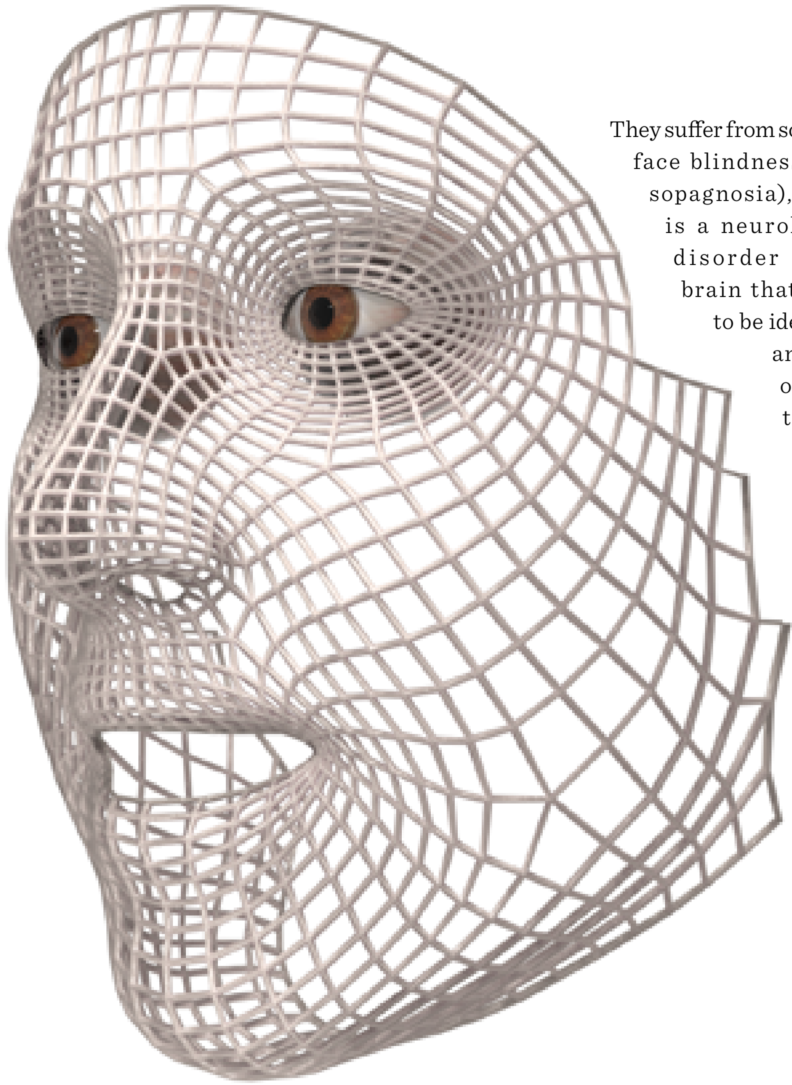
FACIAL MORPHOLOGY AND ITS APPLICATIONS



Our face has an immense significance for interpersonal communication. Sympathy and antipathy for others often depend on our first impression. Already within milliseconds, stereotypes may have been triggered by an opponent's face. The perception of facial expressions determines our interpretation of statements (see figure 10). Similarly, we always use facial expressions – consciously or unconsciously – to emphasize what we say. Therefore, the face and its perception have been the subject of art and science for centuries and are still intensively researched.

People with congenital or acquired facial malformations, or palsy due to nerve damage, are often stigmatized. An aim of facial plastic surgery is to correct such dysplasia in view of a normal or natural facial anatomy. To plan and perform surgical modifications of faces in such a way that both desired aesthetic visual appearance and expressions are considered is still a challenge.





A small percentage of the population suffers from an autism-spectrum disorder. Those people often have difficulties in interpreting facial expressions. It is difficult for them to imagine what other people think or feel, which causes impairments of social interaction. The training of expression interpretation and production therefore supports their social skills. Another small group of the population has difficulties in recognizing familiar faces. They suffer from so-called face blindness (prosopagnosia), which is a neurological disorder of the brain that needs to be identified and thoroughly tested for any treatment.

Together with our collaborators from anthropology, we have studied regular facial development in male and female children. Nonlinear growth trajectories were determined for the use in the early diagnosis of syndromes. Similarly, typical aging effects like facial sagging have been investigated morphometrically. For the analysis and synthesis of facial expressions (computational facial morphology), we have established a 3-D morphable model that is able to synthesize various individual nuances beyond typical expression categories [6]. Their significance for expression perception is being investigated in a broad user study as part of the Mimik-Explorer shown at the German Hygiene Museum in Dresden.

In collaboration with psychologists, we are developing novel experiments for the investigation of self-representation based on virtual-reality techniques. Our goal is to gain understanding of the role of facial identity in (virtual) communication. For the planning of facial surgery, our work allows the assessment of expressions before and after treatments [7]. For example, in facial palsy, a detailed planning of facial nerve reanimation along with an objective follow-up evaluation method can be established.

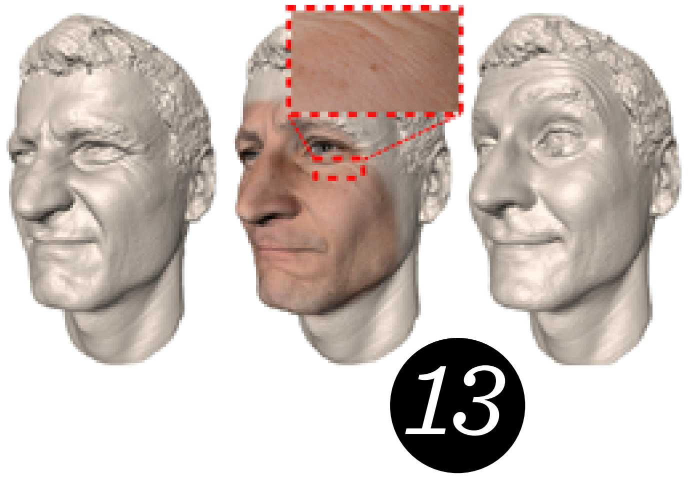
INFO BOX

With applications in anthropology, medicine, psychology, and affective computing in mind, we target questions like: (a) How do facial proportions vary in a normal or healthy range, (b) what kinds of growth and aging trajectories can be observed during childhood or in elderly people, (c) are there characteristic patterns for facial expressions giving rise to an objective classification scheme, and (d) is it possible to employ such a scheme to artificially synthesize plausible expressions? These are all driving questions in research that motivate an in-depth analysis of the almost endless diversity of real faces.

10 We have probably all encountered the experience of drawing conclusions from interpreting other people's facial expressions. Disputes up to serious conflicts may have arisen from a (mis)interpretation of facial expressions. Hence, facial expressions and their deliberate use are intensively trained, not only in acting but also for successful negotiations (e.g. in business and politics).

11 Expressions are formed by the actions of facial muscles. In our research, we are studying the resulting effects on the facial surface.

DIGITAL FACIAL MORPHOLOGY

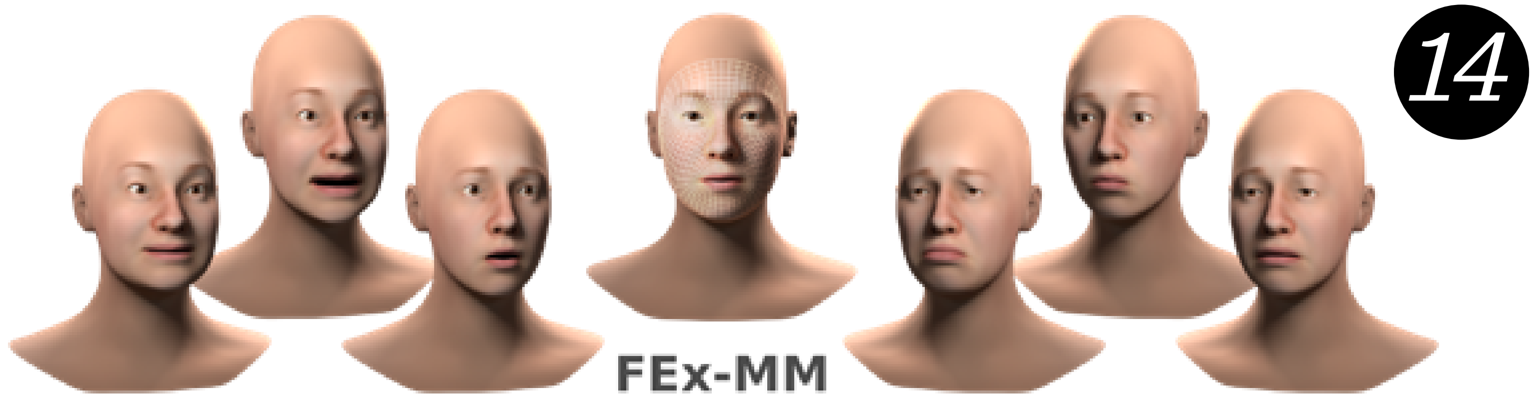


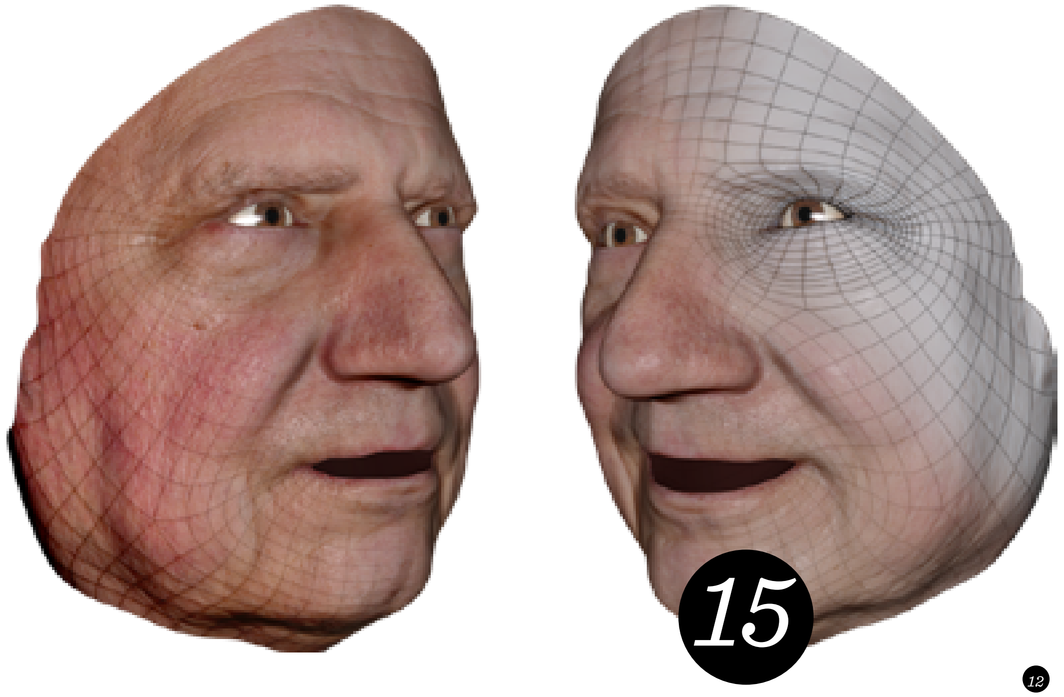
COMPUTATIONAL ANALYSIS OF FACIAL MORPHOLOGY AND EXPRESSIONS

Computational facial morphology offers the opportunity to apply mathematical methods for the analysis of facial shape and proportions as well as skin appearance and expression. Based on image and geometry processing, statistics, and machine learning, the relation of facial morphology to attributes like sex, age, culture, and so forth, can be studied. Similarly, characteristic patterns describing the change in shape and appearance due to expressions can be precisely extracted and quantified from a representative set of facial performances. Our research comprises (1) the development of new techniques for the acquisition of high-resolution 3-D faces, (2) their integration into a large-scale database, and, using this, (3) establishing a foundation of morphological analysis as well as applications in psychology and medicine.

CAMERA FACIALIS – 3-D FACIAL PERFORMANCE CAPTURE

Human face perception is particularly sensitive to the subtlest details. For the acquisition of high-resolution facial details including small wrinkles resulting from micro expressions, the 3-D portrait studio Camera Facialis (see figure 12) has been established at ZIB [8]. In contrast to expensive and laborious commercial setups common in entertainment productions and media art, Camera Facialis has been built on top of affordable optical devices and commodity hardware to enable ultrafast, high-fidelity measurements for a very detailed capture of facial performances in a large-scale manner (see figure 14).





ZIB 3-D FACE DATABASE

Photometric reconstruction of 3-D faces is usually a tedious manual process even for expert users. To establish a comprehensive large-scale 3-D face database, we have developed a fully automated reconstruction pipeline for high-throughput data acquisition. This has been achieved by consequent integration of statistical shape templates. Detailed 3-D facial scans result from specifically optimized algorithms [9]. That way, several thousand faces have already been integrated into the 3-D face database, which is continuously extended for digital facial morphology.

DIGITAL 3-D FACIAL MORPHOLOGY

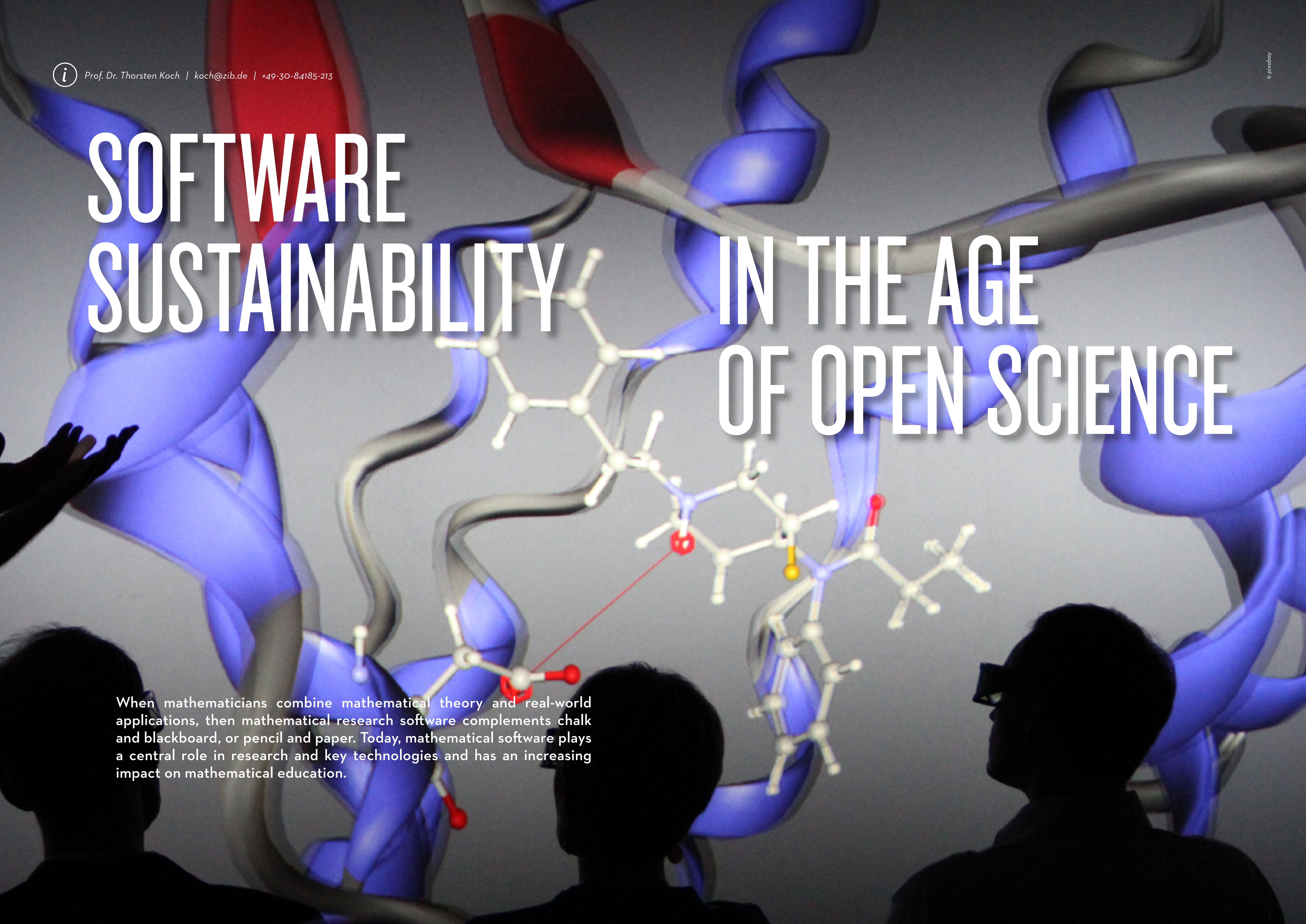
The statistical analysis of shape and appearance requires a well-defined mathematical framework. Descriptors are needed to transform a face into a typically high-dimensional space, where similarities or distances, correlations, or clusters can be analyzed. At ZIB, we are developing correspondence-based descriptors that take the Riemannian structure of shape spaces into account [10]. We enable the analysis of facial features up to the level of wrinkles and skin pores by establishing accurate dense correspondence with our techniques (see figure 15) [6].

12 The 3-D portrait studio Camera Facialis uses multiview photogrammetry to capture high-resolution 3-D facial performances.

13 Expression scans from the ZIB 3-D Face Database with photographic texture containing high-resolution skin details.

14 Nuances of facial expressions synthesized using expression patterns determined by statistical shape analysis.

15 In the Camera Facialis, 3-D face scans in dense correspondence to an animatable surface mesh are acquired. On top of a neutral face scan (left), arbitrary expression patterns extracted from the ZIB face database can be transferred, for instance, the smile expression shown on the right.



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SOFTWARE SUSTAINABILITY IN THE AGE OF OPEN SCIENCE

When mathematicians combine mathematical theory and real-world applications, then mathematical research software complements chalk and blackboard, or pencil and paper. Today, mathematical software plays a central role in research and key technologies and has an increasing impact on mathematical education.

Since its creation more than 30 years ago, ZIB has promoted this combination as a significant extension of scientific work. This has resulted in many software packages, some of which are of outstanding importance to the scientific community. Prominent examples today include SCIP in the area of optimization, KASKADE for numerical mathematics, and AMIRA for scientific visualization and data analysis. An overview of software developed at ZIB can be found here: http://www.zib.de/software.

Software Sustainability is a new working area that has been gaining momentum in the past few years. With the continuing shift toward data-centric science, the software utilized to produce the scientific output is increasingly regarded as an equally important "product of science" itself.

A general understanding is evolving that not only a publication, but also the documented and available datasets should get scientific credit. Moreover, there is a growing consensus in the research-data-management community that research software could be considered as datasets (i.e. research data). Publication and reuse of software is necessary to ensure validity, reproducibility, and to drive further discoveries. Since a common research-data-management practice fosters publication along the principles of Open Access, software should also be made publicly available, ideally corresponding to the FAIR principles of research-data management: data should be Findable, Accessible, Interoperable, and Reusable.

To transfer these principles to the management of research software is a true challenge, especially because software is characterized by an exceptional variety of dependencies on other entities (hardware, OS, algorithms, etc.), which renders it very difficult to define an encapsulated status as a datum. In addition, software is a living entity that evolves over time. The concept of Software Sustainability involves development, deployment, maintenance, and publication efforts, with the aim to ensure the ongoing functionality of research software. The incorporation of Software Sustainability methods at ZIB is part of increasing efforts to conduct research in accordance with open-science principles.

SOFTWARE SUSTAINABILITY AT ZIB

In order to establish sustainable software development practices, a variety of infrastructure and organizational measures have to be addressed. The following approaches, services, and project results form the basis and starting point for these measures. In recent years there have been several activities to promote research-data management. One of the essential first steps was the formation of a focus group supporting the handling of research data, composed of researchers from different divisions and departments at ZIB. This group has started to identify common needs across all departments and divisions. It acts as a contact point concerning all questions related to research-data management, including the generation of data-management plans. Its most important action item is publication of research data and research software. A twofold strategy is being pursued to increase the visibility of produced software. In addition to the project page (i.e., the product page of the research software, which is maintained by the respective research group), all released versions of a software are intended to be published as research data with the institutional repository OPUS (https://opus4.kobv.de/opus4-zib/home). In this context, the Kooperativer Bibliotheksverbund Berlin-Brandenburg (KOBV), part of ZIB since 1997, provides support for OPUS.

OPUS is utilized to present landing pages (called front doors in OPUS) for specific software with an additional set of metadata and a download link. The software packages will reside on a dedicated download server. OPUS itself is an open-source product of ZIB, published under a GNU General Public License. Current work on OPUS involves other important features with regard to open-science principles: automatic DOI minting and ORCID implementation.

Another aspect of the long-term availability of research software is being addressed by the experimental application of digital preservation techniques. The OAIS-compliant digital preservation system EWIG at ZIB, which is composed of freely available open-source components, is used as a research-software source-code archive, accompanied by extensive metadata. To date, the incorporation of digital preservation strategies within the context of software sustainability has not been straightforward. There is a gap to be closed between software archiving and maintenance approaches on the one hand, and long-term aspects of digital curation of software on the other.

A further step to achieve software sustainability at ZIB involves the use of the swMATH portal that analyzes mathematical publications for software citations. The aim is to identify the connection of research software and scientific articles that present results based on the use of this software.

1 *Figure 1: Search interface of ZIB OPUS institutional repository*

SWMATH – AN OPEN-ACCESS DATABASE FOR MATHEMATICAL SOFTWARE

swMATH

How does one find software for a specific mathematical problem? Is there already a solution or an implementation? What is the mathematical background? Who are the authors? What hardware do you need? Is there any documentation? Is it free for educational use or do you need a license? Moreover, it is also a real problem to cite software when writing a scientific paper. Where to find the software? Which version was used? Is it accessible? Can you reproduce the results?

The project swMATH (www.swmath.org) is an attempt to develop and establish an information service for mathematical software and mathematical research data. It started as a project of Mathematisches Forschungsinstitut Oberwolfach (MFO) and FIZ Karlsruhe, and is presently continued as a project of the Research Campus MODAL at ZIB. swMATH provides information about mathematical software and its mathematical background. It will improve the visibility of software and strengthen the role of software within mathematics. swMATH is focused on software, but also benchmarks, data collections, and manuals are listed.

CENTRAL IDEA: PUBLICATION-BASED APPROACH

The most informative and relevant secondary source for information about mathematical software is the corresponding scientific literature. Therefore, the most complete bibliographic database of mathematical literature, zbMATH (the former Zentralblatt MATH), is used as a basis to extract information about mathematical software. The fact that zbMATH covers almost all mathematical journals with a focus on mathematical software is of crucial importance.

zbMATH provides a review or a summary, characteristic key phrases, the references lists, and classification of the mathematical subjects and application areas of mathematical publications. Also, information about the authors, the sources, and the language of the publication are presented. Today, the database zbMATH stores the bibliographic data of nearly four million peer-reviewed mathematical publications with an increase of 10,000 items per month. In general, this approach ensures quality control.

ANALYZING ZBMATH

The manual maintenance of Web databases is an effort that is both expensive and time-consuming. Therefore, the use of machine-based methods for the data analysis and content generation has been a significant aspect in the design of the swMATH service from its beginning. Heuristic methods have been developed for identification and to analyze software information in zbMATH entries. The information regarding publications citing a software is aggregated and provides a profile of the software and its context involving use cases, mathematical background, acceptance, life cycle, related software, and a list of publications citing the software. The publication-based approach is the basic step in the swMATH workflow and provides general information about mathematical software. But details, such as source code, versions, the technical environment, license information, documentation, manuals, or installation guides, as well as links to related benchmarks or data collections, are missing. This kind of information can be found on

WEB-BASED APPROACH

the websites related to the software, in repositories, or on portals, which provide information about and access to software for a special subject. Therefore, some concepts for capturing and analyzing further information about software from websites, software repositories, and Internet archives have been developed. In principle, we are faced with the same tasks as in the publication-based approach: identification of the relevant information and analyzing and structuring the information about a software. But instead of publications, we have to extract it from information on the Web.

The swMATH pages represent an online portal to retrieve information regarding mathematical software: they provide general information about the software, namely the profile of a software derived from the publication-based approach and links to other relevant Web resources that contain more detailed information. Each swMATH page has a unique identifier, which can be used for the citation of a software.

FINDING SOFTWARE IN SWMATH

swMATH offers several ways to find software. Based on the referenced publications, swMATH analyzes the abstracts and the MSC classification for each software entry. This allows software to be searched by key word (e.g. “integer programming”) or by browsing through the MSC classification scheme (e.g. “90C10”). Additionally, swMATH classifies all entries by types, for example, programming languages, benchmarks, data collections, or Web services. Last but not least, you also have access to documentation and manuals wherever it is accessible.

An important side effect of analyzing research papers is the discovery of related software: if software S1 is referred by paper P1 and paper P2 refers not only to software S1, but also software S2, we conclude that S1 is related to S2. This helps to identify more than one possible software solution for solving a given problem.

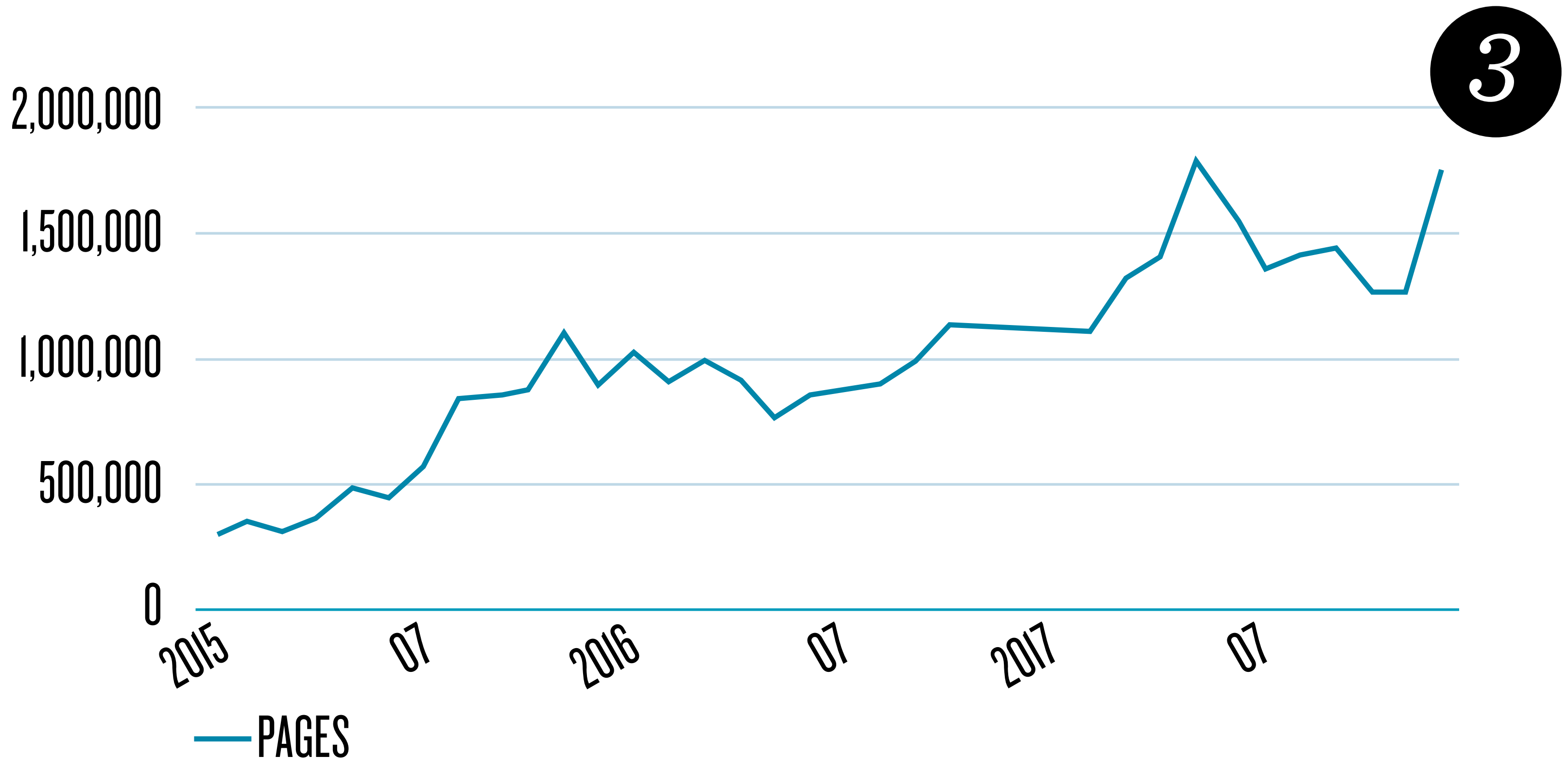
HOW TO CITE SOFTWARE?

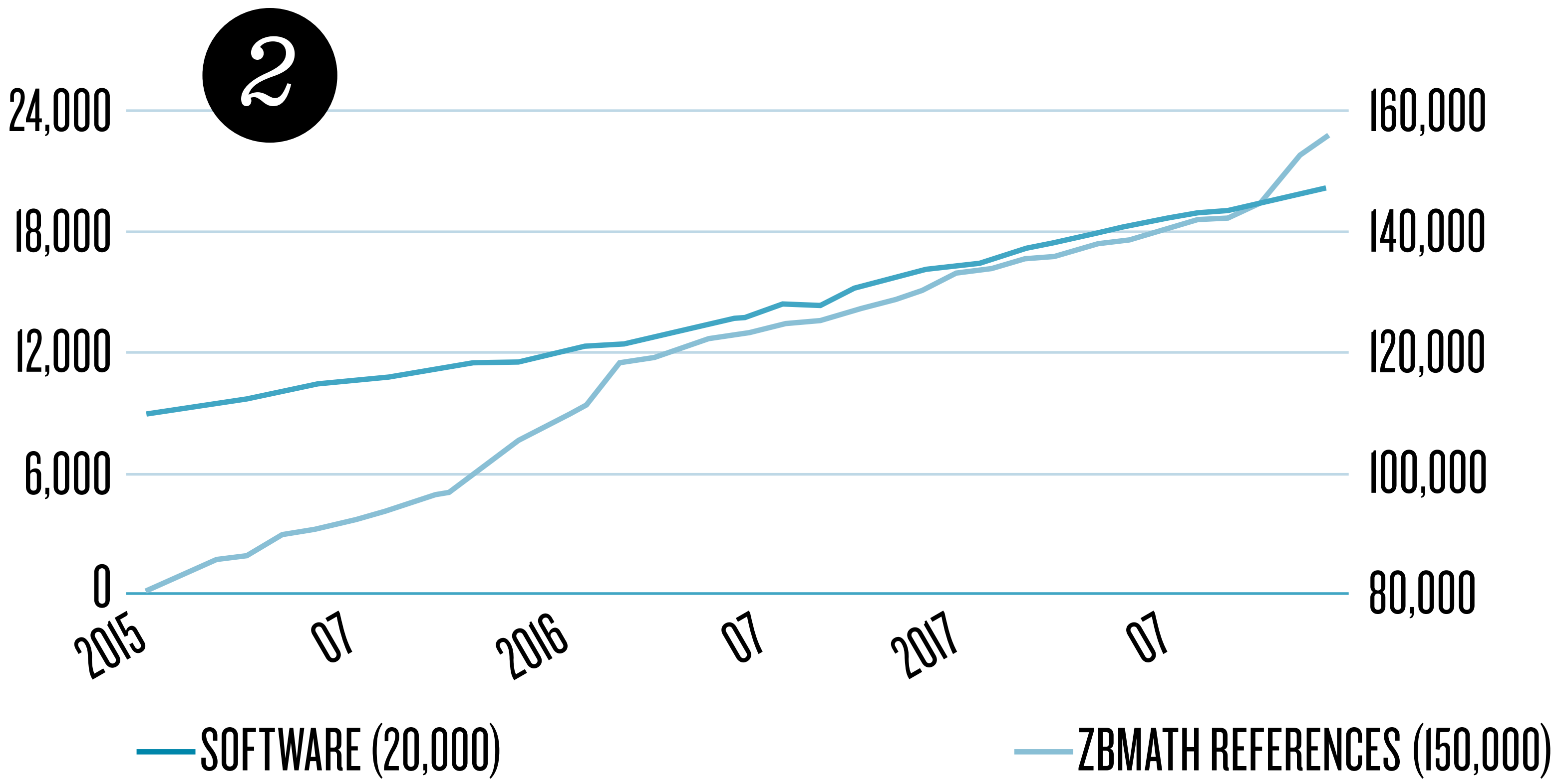
When analyzing zbMATH articles, you will find different citation styles for software. Software companies, repositories, and publishers give different recommendations for citing software or research data. swMATH will close this gap. In cooperation with related communities, e.g. the Software Citation Working Group of the FORCE11 Initiative, we are working on standards for citing software and research data.

VISIBILITY OF AUTHORS

Careers in the scientific community are based on the visibility of papers published in peer-reviewed journals. But what about the contributions of software developers? Do they get any credit for writing software while helping to find solutions to a mathematical problem? Software developers play a different role to the authors of publications. swMATH lists the authors of a software and builds a citation graph presenting the annual numbers of publications citing the software. This also characterizes the development stage and reflects the distribution and acceptance of the software. A large number of publications indicate that the software has been widely used and can be considered as an indicator for the quality of the software.

If you take, for example, the SCIP Optimization Suite, you find more than 250 bibliographical entries in zbMATH that cite the software. The software packages with most citations are MATLAB (8,000 references), CPLEX, MAPLE, MATHEMATICA, and R, each with more than 4,000 references.





STATE OF THE ART AND CHALLENGES

Currently (i.e. December 2017), swMATH contains information about more than 20,000 software entries with nearly 270,000 software references in publications. swMATH is an innovative service for mathematical software citations and has unique features. The swMATH service is largely based on the automatic processing of information and requires little effort for maintenance. Usage statistics reveal increasing interest in the service.

Software information is challenging because it is highly dynamic and standards for software information, e.g. for software citations and metadata schemes, have been missing until now. The swMATH project working group will participate in the development of standards and will work on both new concept algorithms for a more complete recording of mathematical software and on improved content analysis of the information about a software.

2 Figure 2: swMATH figures for software and zbMATH references 2015–2017

3 Figure 3: Usage statistics for swmath.org 2015–2017 (Apache log file, Webalizer pages, no robots).

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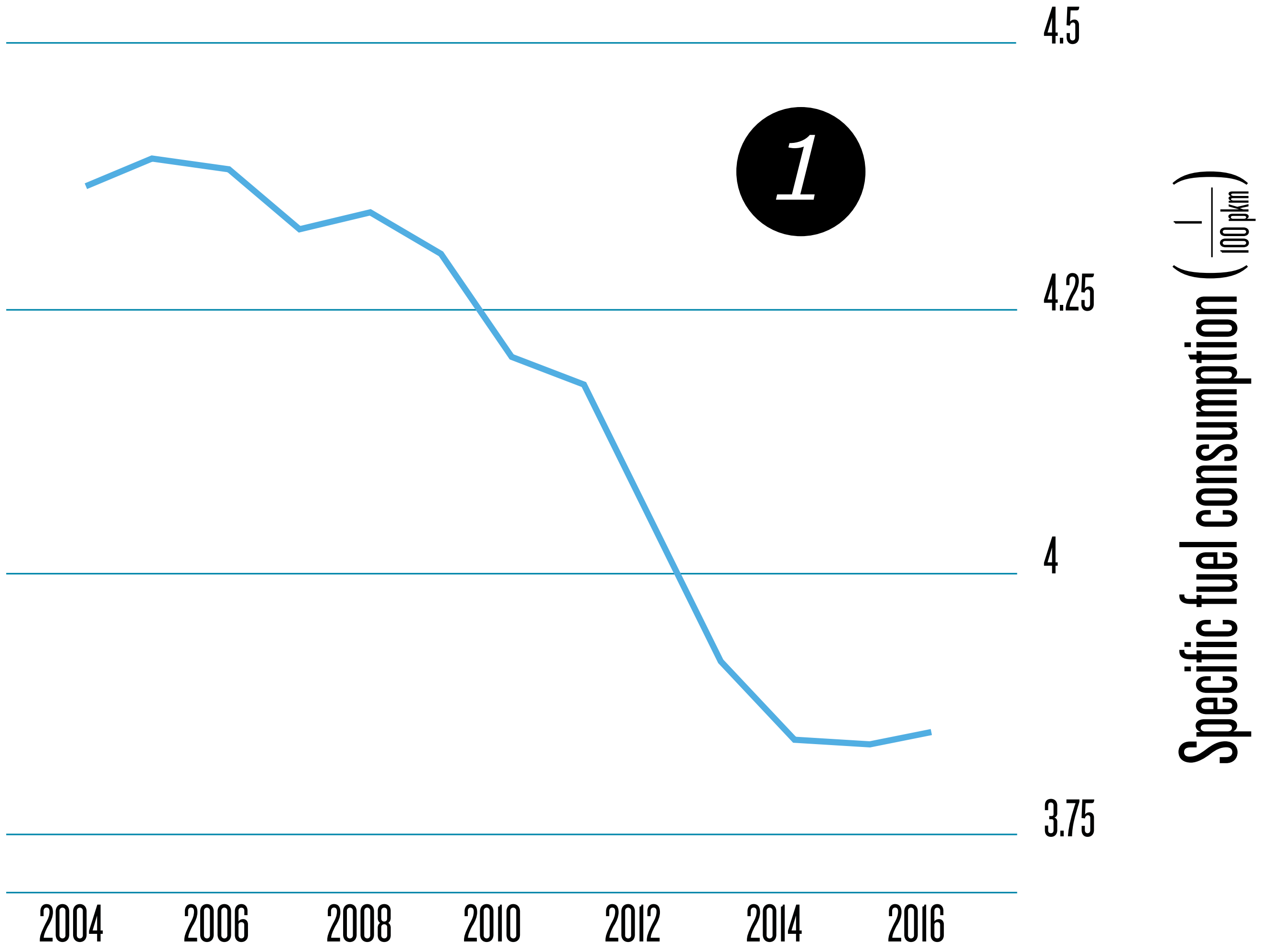
20,000 FEET ABOVE THE GROUND

New navigation systems for aircraft save fuel and time



1 *Specific fuel consumption for the Lufthansa fleet (source: [4])*

Cheap air transport has become a matter of course since the 1980s. It allows us to see the world and visit remote countries on vacations, as well as to attend multiple business meetings per week around the country or continent, and to still sit down for dinner with the family at home in the evening. Because of these amenities, the market for passenger transportation has been and will be a growing one.

According to a recent forecast by the International Air Transport Association (IATA) [1], the current number of four billion air travelers per annum will double by 2036. As air connectivity of countries is assumed to be a stimulus for growth and prosperity [2], such prognoses are good news. However, the increase in air-traffic volume also presents challenges: the infrastructure needs to be constantly adapted to handle ever-larger numbers of passengers, the safety of passengers and crews needs to be ensured, and emissions of CO_2 and other pollutants should be minimized.

The past decades have witnessed a significant improvement regarding the environmental impact. For example, in figure 1, we can see how the Lufthansa Group managed to reduce the fuel consumption of their fleet to 3.85 l per passenger and per 100 km during 2017. The most obvious factor contributing to this is technical progress of aircraft, and particularly engines [3]. However, as aircraft are often used for around 25 years, fleet renewal is a long-term task for an airline. Therefore, short-term measures, such as minimizing fuel consumption through efficient trajectory planning, are equally important. Here is where ZIB comes into play.

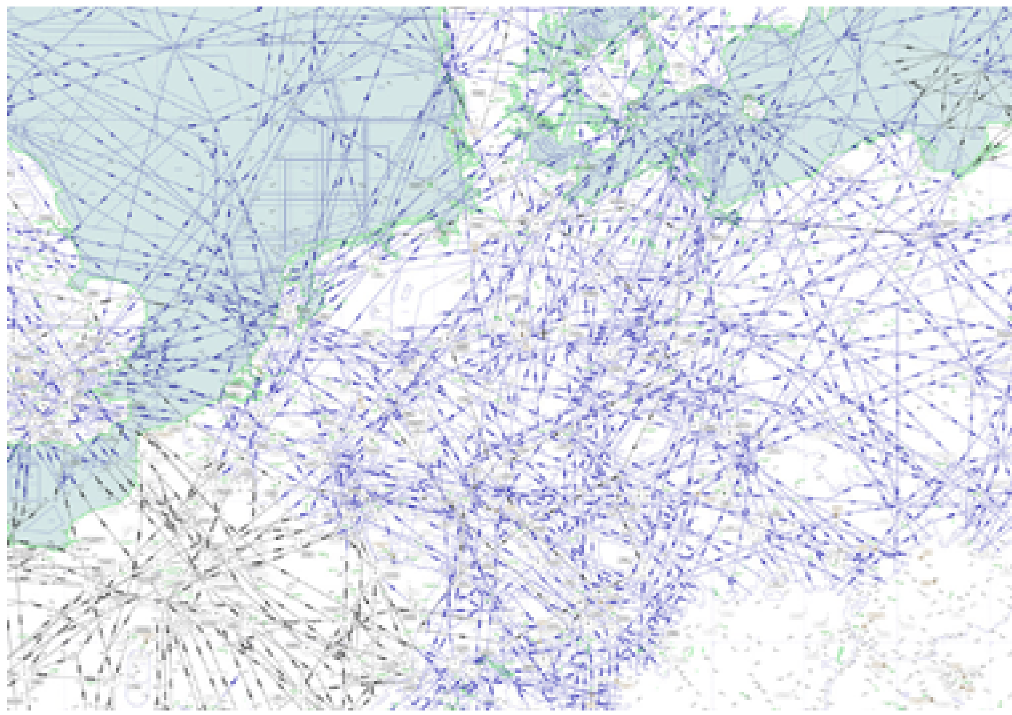
Together with Lufthansa Systems GmbH & Co. KG, a leading provider of IT solutions to the airline industry, the Optimization department at ZIB is working on the development of VOLAR, a brand-new system for flight-trajectory optimization, which will ultimately become the core optimizer of Lufthansa Systems' flight-planning software Lido/Flight. Similar to a car navigation system, many airlines use Lido/Flight to compute the most efficient routes for their aircraft. Unlike in car navigation, however, a plane cannot stop in midair if something goes wrong. The weather plays a much more important role. And fueling is really critical. Too much is not good, as every liter of kerosene must be lifted into the air, requiring even more fuel. Too little, however, is even worse. Balancing safety and efficiency is therefore a delicate task, which must be addressed with advanced mathematical methods. This is also the way to deal with all the constraints of flight planning.

Aircraft are not allowed to fly along the shortest curve between any two airports. Instead, they must adhere to airways, which are invisible roads in the sky spanning the entire planet. The set of all such airways and their intersections define the airway network. In mathematics, such a construct is called a graph. The set is not only defined on one altitude, but on several layers stacked on top of each other. These layers, roughly 300 m apart, correspond to the possible altitudes on which aircraft are allowed to cruise.

A representation of the airway network over Germany can be seen in figure 2.

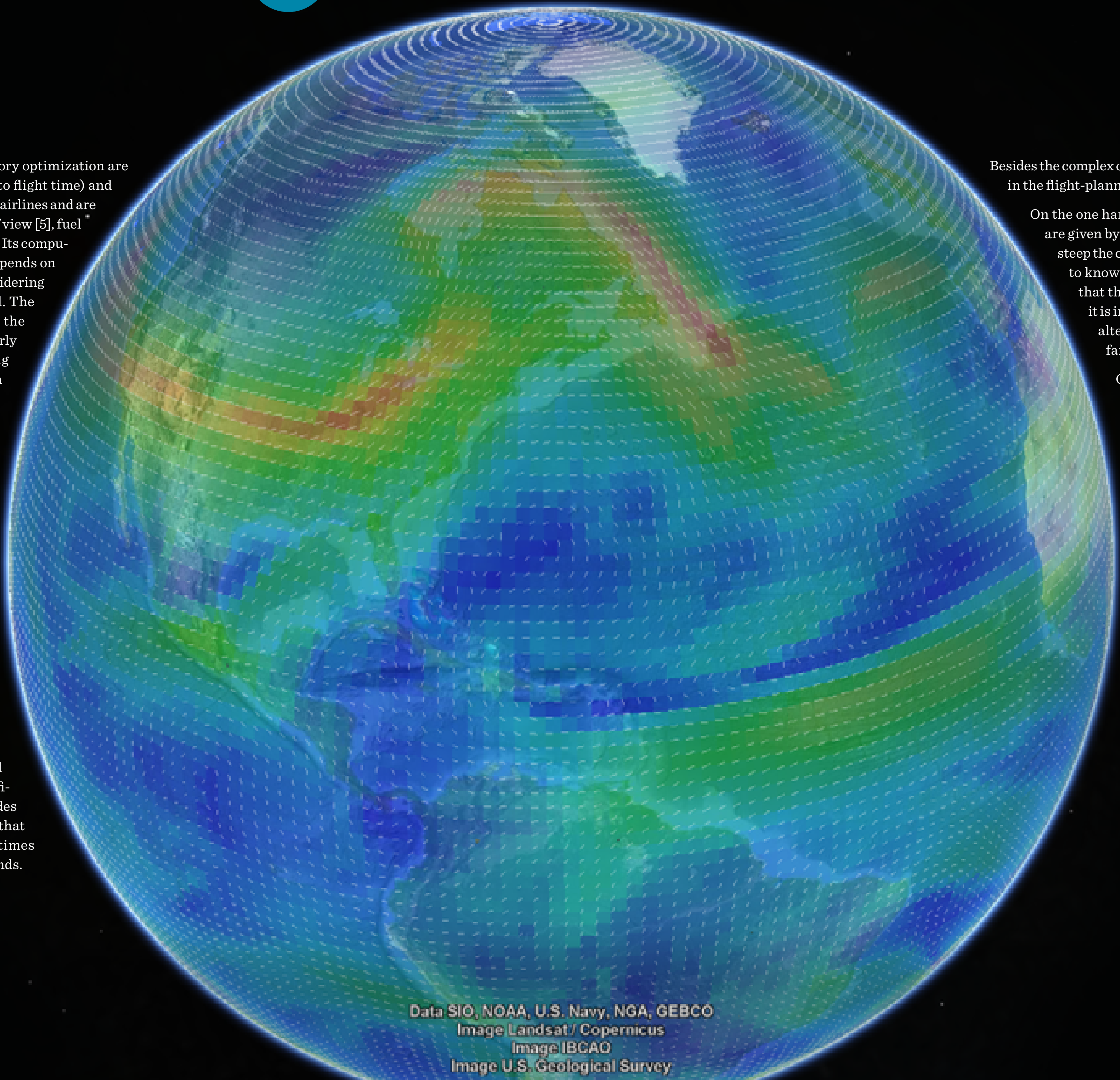
After fixing a pair of airports as the departure and the destination nodes in this graph, the main objective of flight planning is to find a minimum cost path – a chain of airways – connecting them. The problem of computing a minimum cost/shortest path between two nodes on a graph is well studied and also very relevant in real-world applications. Pedestrians in the city try to walk along paths with minimum distance. Car navigation systems seek to find the shortest path to a destination by minimizing the total travel time, which may vary depending on traffic. The flight-planning problem is similar in nature, but it has a much more complex cost function.

2



2 *Airway network over Germany (source: skyvector.com).*

3



3 High-altitude wind over the American continent on a specific day. Blue is still air, strong wind is represented in red. (Representation: Google Earth)

The relevant cost components for flight-trajectory optimization are fuel consumption (which is usually correlated to flight time) and overflight fees. While the latter play a big role for airlines and are very interesting from the mathematical point of view [5], fuel consumption is by far the most important factor. Its computation is not straightforward, since it heavily depends on the weather. This can be best understood by considering jet streams, which are currents of strong wind. The best-known example is the jet stream around the North Pole, which blows east and is particularly relevant for aviation over the Atlantic. Flying along jet streams significantly decreases both flight time and fuel consumption. Similarly, flying in the opposite direction should be avoided, which is why flights from Europe to North America often make a detour over Greenland. The jet stream is clearly visible over North America in figure 3.

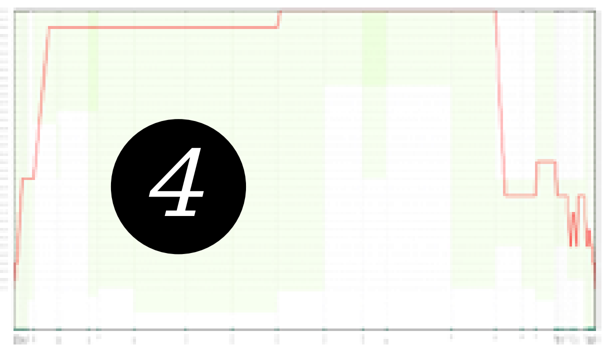
In a sense, wind on airways is similar to traffic jams on roads, since it can reduce or increase an airway's effective length, or even block it. Considering such time-dependent factors during optimization is always a major challenge, as a lot of data has to be processed. For instance, weather data is needed not only on the horizontal level, but also on the vertical level and on a time horizon of more than 24 hours.

Furthermore, fuel consumption at any given time is dependent on the aircraft's weight (which itself depends on the current fuel amount) and altitude. In general, lighter aircraft are more efficient than heavier ones, and flying at high altitudes is better than at low altitudes. However, given that the wind is stronger at high altitudes, it sometimes makes sense to fly lower to avoid strong headwinds.

Besides the complex cost function, there are many other challenges to consider in the flight-planning problem. A good example is the diverse constraints.

On the one hand, there are so-called aerodynamic constraints. These are given by the flight dynamics, which determine, for example, how steep the climb or descent angle can be. For instance, it is important to know exactly at what moment to initiate the final descent, so that the destination airport can be reached comfortably. Also, it is important to always have enough fuel onboard to reach an alternate airport in case of an emergency, such as an engine failure.

On the other hand, there are less obvious operative constraints, which regulate how the airspace may be used. These constraints have objectives such as avoiding congestion, ensuring safety, and enforcing regional legislation (such as night-flying restrictions to reduce noise). These constraints are managed by air-navigation service providers around the world (e.g. EUROCONTROL in Europe, through the monthly Route Availability Document publication). Such a restriction can, for example, forbid the usage of Belgian airways for flights departing from Luxembourg on weekdays after 10 p.m. In this case, it is easy to imagine why this restriction is published: aircraft would fly at low altitudes over the Belgian airspace, hence causing too much noise at night. As of January 2018, the European Route Availability Document consists of over 13,000 restrictions. Considering all of them during the search for an optimal flight trajectory increases the problem's complexity considerably, since they make it NP-hard.



4 *The vertical profile of a flight computed between Frankfurt and Minneapolis. The final segment follows a "zigzag" pattern, efficient with respect to fuel consumption but probably uncomfortable for the passengers.*

5 *Adam Schienle at the award ceremony of the GFFT.*

6 *Two routes from Taipei to New York: the red one was precomputed, the green one was computed by VOLAR.*

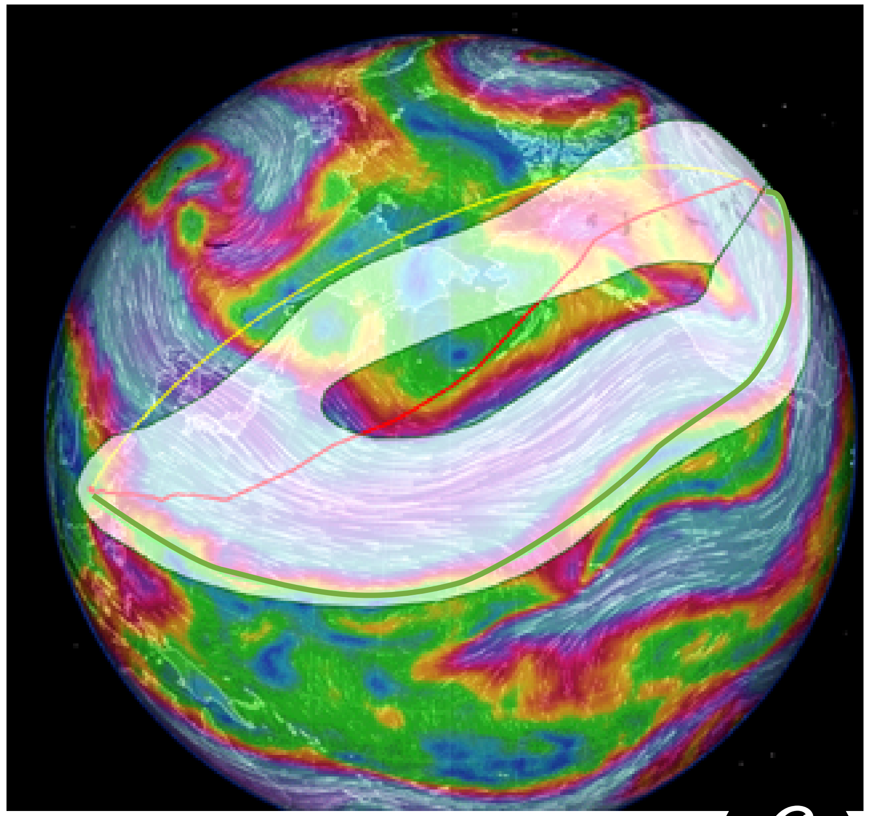
Another example of human-made constraints are comfort constraints, which are not easy to model but intuitively are clear. In particular, the most fuel-efficient route sometimes results in a pattern that pilots are unlikely to follow, such as in figure 4.

Currently, the VOLAR software developed at ZIB is capable of computing optimal trajectories that consider weather, aircraft performance, overflight fees, and traffic restrictions. It is based on original research that has been well received in the operations-research community. As an example, Adam Schienle's master's thesis [6], which focuses on minimizing flight time under consideration of wind, won awards both at the OR conference in Berlin and the Gemeinnützige Gesellschaft zur Förderung des Forschungstransfers e.V., both in 2017. Furthermore, the research paper [7] won the prestigious Best Paper Award at the international Algorithmic Approaches for Transportation Modeling, Optimization, and Systems workshop (ATMOS 2017). The scope of these works is as follows.

Since both a short runtime and low memory usage are essential in real-world flight planning, it is necessary to restrict the search space of our algorithms. Roughly speaking, this means that if we want to fly from Berlin to Tenerife, there is little sense in looking for a flight trajectory overflying Russia. This was in part achieved after introducing the Super-Optimal Wind, which is based on a simple observation: aircraft travel faster when being pushed along by tailwinds (wind from the back), and when there is as little crosswind (wind from the side) as possible. Hence, we can calculate the "best" wind conditions we may expect for a given weather forecast. This allows the search space to be reduced drastically. Furthermore, it also ensures that the optimal route is not cut off by this reduction. This is done by adapting the well-known A* algorithm.

The efficiency of this method can be demonstrated at the following striking example. On April 25, 2017, at 3:00 a.m. UTC, a flight leaving Taipei Taoyuan Airport was scheduled to go to New York John F. Kennedy International Airport.

On that day, there was an unusually strong jet stream above the Northern Pacific. While for airlines it is common to fly routes that lie close to a geodesic between the departure and destination airports, on this day, flying a big detour to take advantage of the unusual jet stream paid off. Figure 4 shows this phenomenon. The yellow line represents the great circle connection between Taipei and New York. The red line shows a common flight route between both cities and the green one was computed by VOLAR, taking advantage of the jet stream described above. The shaded area (in gray) in figure 6 shows the search space inspected by VOLAR (i.e, the regions in which the optimal route is looked for). To do so, VOLAR uses the Super-Optimal Wind. It is remarkable that the red route is not even considered by our algorithm, since it lies partially outside of the shaded area – it is simply not a potential candidate for the optimal trajectory. Indeed, as the table in figure 6 shows, the green route saves 5,665 kg of fuel and 5,335 USD compared to the red one, even though it is significantly longer.



6

CASE STUDY: TAPEI – NEW YORK

Boeing B777-300ER, April 25, 2017, great circle distance = 12,565 km

	Using typical search space reduction	Using dynamic search space reduction	GAIN
Distance flown (km)	13,385	14,635	-1,250
Flight time (hours)	14:40	13:55	0:45
Fuel burn (kg)	95,524	89,859	5,665 = 17.8 t CO_2
Overflight fees (USD)	2,291	1,139	1,152
Total costs (USD)*	76,453	71,118	5,335

*based on: fuel price 500 USD/ton, flight time costs: 1,800 USD/hour

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SCALABILITY AND CONCURRENCY

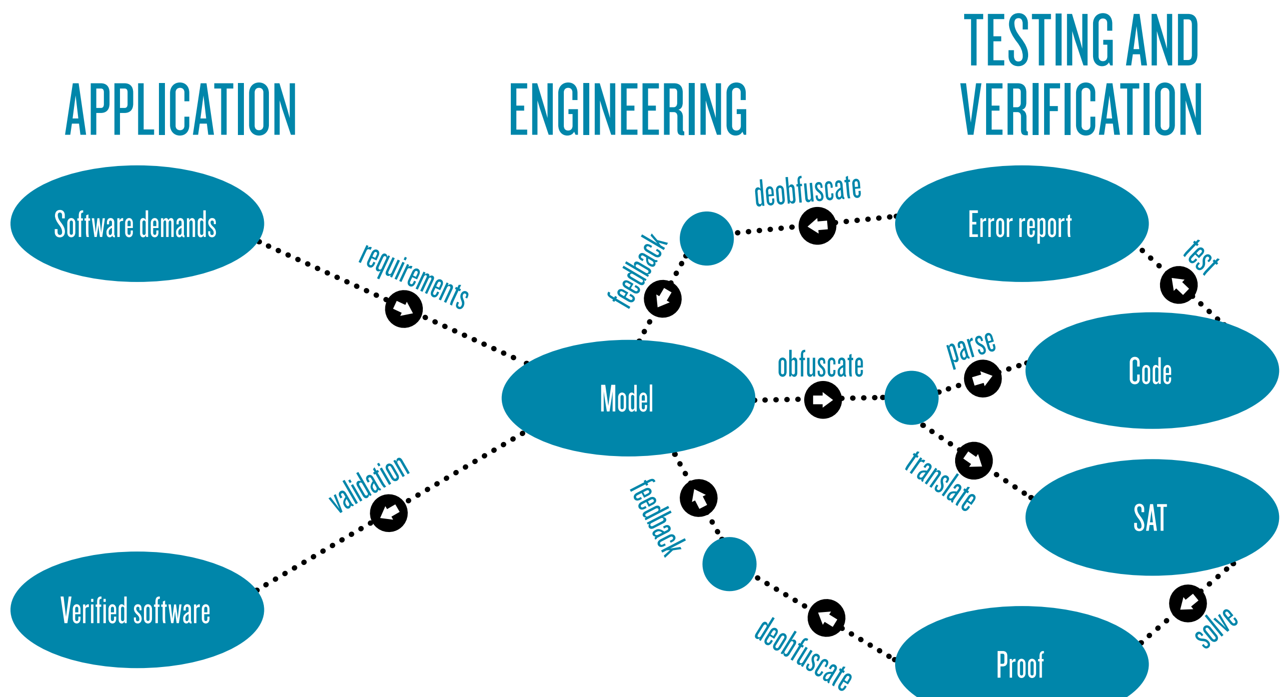
Challenges from Two Interdisciplinary Research Projects

How to chop and distribute hundreds of continuous high-bandwidth data streams efficiently in a network so that, for each time frame, the sensor data is collected in a particular analysis node? How to exploit modern network capabilities, like remote direct memory access, to improve the scalability of SAT solving on supercomputers? How to effectively test shared-memory parallel programs for concurrency bugs due to data races? These are three exemplary research questions we are currently tackling in two interdisciplinary research projects in the fields of high-energy physics and the automotive industry.

HIGHLY PARALLEL SOFTWARE VERIFICATION

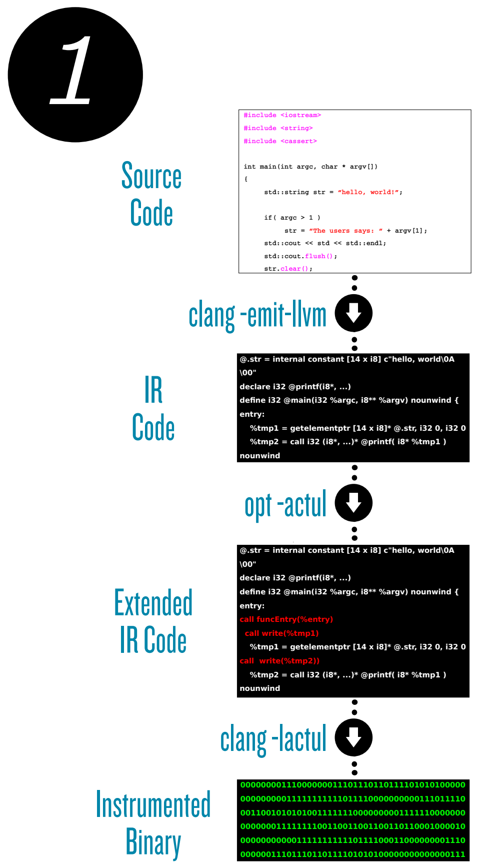
Embedded software in modern cars enables new opportunities regarding the passengers' safety and comfort, but it simultaneously presents great challenges for the automotive industry. The software has to guarantee high security standards. Unfortunately, the complexity of the verification and testing grows exponentially with the size of the software. Hence, parallel methods are needed. In the BMBF project Highly Parallel Software Verification (HPSV), partners from the automotive industry work together with researchers from Christian-Albrechts-Universität Kiel and ZIB. We are developing a high-performance software infrastructure to accelerate the verification and testing process, tackle more complex problems, and also make the deployment of new and more complex features possible.

In the software-engineering process, statechart models are created according to predefined requirements. The model formally describes the behavior of the software and can be directly parsed into source code or translated into SAT formulas. Combined with formal requirements, the correctness of the model can be verified. Two alternative model representations are used to expose potential faults in the modeling process: critical concurrency issues can be found in the source code and SAT formulas can be used to prove that the predefined requirements are satisfied by the model. Both methods are completely automated and thereby give the engineers precise feedback with concurrency error reports and detailed proof pointing out where inconsistencies may remain in the model. To allow testing and verification as a service model in this highly competitive field, the models are obfuscated during the testing and verification process. The resulting feedback is then deobfuscated to make it interpretable in the automotive industry.



AUTOMATIC TESTING OF CONCURRENT PROGRAMS

Concurrent applications are particularly hard to debug. Since multiple threads access the same memory locations, data races can lead to unintended program behavior and requirement violations. Data races may occur with multiple unordered accesses to the same memory location by two or more threads, where at least one modifies the memory state. We developed Actul, a compile-time tool that detects data races. It checks data races for their harmfulness (i.e. whether they may cause a program violation).

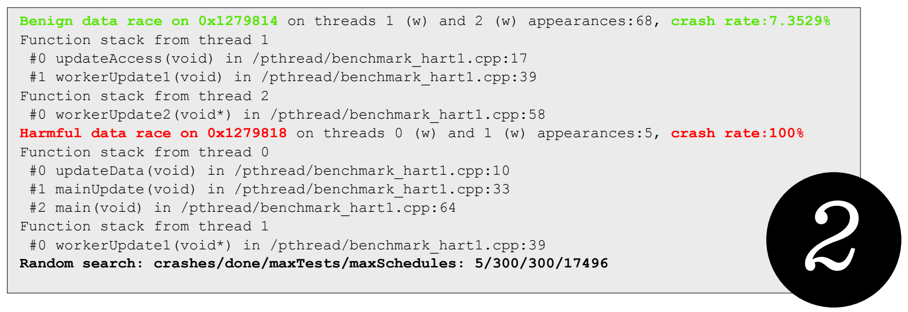


COMPILE-TIME INSTRUMENTATION

Actul is based on the LLVM compiler infrastructure. Source code is translated into the intermediate representation language (IR) of LLVM. Then each memory- and concurrency-relevant instruction in the IR code is modified to allow Actul to monitor all memory accesses and to control the thread execution order. Thus, the OS scheduler is overwritten by a user-level, deterministic scheduler, which records and replays executions and can reorder events in a subsequent execution. The instrumented IR code is compiled and linked against the Actul runtime library, which provides the functionalities of the scheduler and the test environment. Executing the resulting binary starts the testing, where Actul automatically starts and analyzes multiple test cases in parallel.

CLASSIFYING DATA RACES

Data-race detectors often report false positives (i.e. potential data races that never happen in practice because of user-defined synchronizations or implicit orderings in the program workflow). Actul excludes false positives by replaying data races in additional test runs, with a different access order. For further analysis, the reorderable data races are permuted with other such data-races. Based on these test runs, each data-race access order is correlated with appearing program violations. Therefore, harmful data races can be identified as a root cause of a violation without the need to check each false positive or benign data race manually, as typically would be necessary with other tools.



```
Benign data race on 0x1279814 on threads 1 (w) and 2 (w) appearances:68, crash rate:7.3529%
Function stack from thread 1
 #0 updateAccess(void) in /pthread/benchmark_hart1.cpp:17
 #1 workerUpdate1(void) in /pthread/benchmark_hart1.cpp:39
Function stack from thread 2
 #0 workerUpdate2(void*) in /pthread/benchmark_hart1.cpp:58
Harmful data race on 0x1279818 on threads 0 (w) and 1 (w) appearances:5, crash rate:100%
Function stack from thread 0
 #0 updateData(void) in /pthread/benchmark_hart1.cpp:10
 #1 mainUpdate(void) in /pthread/benchmark_hart1.cpp:33
 #2 main(void) in /pthread/benchmark_hart1.cpp:64
Function stack from thread 1
 #0 workerUpdate1(void*) in /pthread/benchmark_hart1.cpp:39
Random search: crashes/done/maxTests/maxSchedules: 5/300/300/17496
```


1 Instrumentation workflow of Actul using the LLVM compiler infrastructure and the Clang compiler.

2 Example error report of Actul's concurrency analysis for one benign and one harmful data race.

3

FASTER DEBUGGING PROCESS

BENCHMARK	HARMFUL DATA RACES	SERIAL RUNTIME	PARALLEL RUNTIME	THREADSANITIZER FOUND DATA RACES	THREADSANITIZER RUNTIME
DynMatMul2	0	245.2s	53.7s	5	0.9s
ping_pong	0	4.7s	0.8s	3	0.05s
queue_bad	1	1.0s	0.6s	0	0.01s
stringbuffer	1	2.1s	1.7s	0	1.2s
TaskQueue3	1	8.2s	4.8s	2	0.5s

SCALING WITH UNSTRUCTURED ASYNCHRONOUS COMMUNICATION

SAT SOLVING IN CONTEXT OF MODEL VALIDATION

The Boolean satisfiability problem (SAT) consists of literals and clauses. In our context, different literals describe different states of components of a model (e.g. the current speed of a car). A clause describes a group of these components that are connected with each other (e.g. the interaction between the regulation yield by a cruise control and the actual speed of the car). All clauses represent the whole model with all connections representing the requirements of the system (e.g. at some point, the speed should match the specification of the cruise control).

Finding SAT solutions is NP complete. The search space of a valid assignment is reduced with the conflict-driven-clause-learning approach (cdcl). While checking different assignments, either a valid assignment of all literals is found or we get a contradiction with this assignment leading to a reduction of the search space by introducing new clauses. These clauses are the key to finding a solution to the problem. With such assignments, we can either globally prove the correctness of the model or its unsatisfiability, which indicates system defects. These system defects can then be reported back to correct the system (e.g. the maximum speed is less than the specification of the cruise control and cannot be reached).

3 *Runtime analysis of Actul and LLVM-ThreadSanitizer on an Intel Xeon Phi 7250 CPU: 68 cores, 1.4 GHz. The harmful data race found by Actul are the only harmful races in the benchmark. The parallel runtime is generated by running independent tests in parallel on one node.*

4 *Offering data (MPI_Compare_and_swap) with situational receiving (MPI_Get) and finishing data transfer (MPI_Accumulate) via RMA.*

5 *Accumulated runtime characteristic correlated with the accumulated amount of exchanged clauses for different combinations of clause types for two different problem classes of problems from the SAT competition 2013.*

SCALING SAT

Each solver learns its own clauses to reduce its search space. Exchanging these clauses will help other solvers to improve. While scaling up, the exchange of too many clauses is not necessarily beneficial because a huge amount of possible clauses can reduce the effectiveness of each solver due to handling too much data. Therefore, we need an effective and flexible way to exchange clauses based on an offer–select scheme.

RDMA COMMUNICATION APPROACH

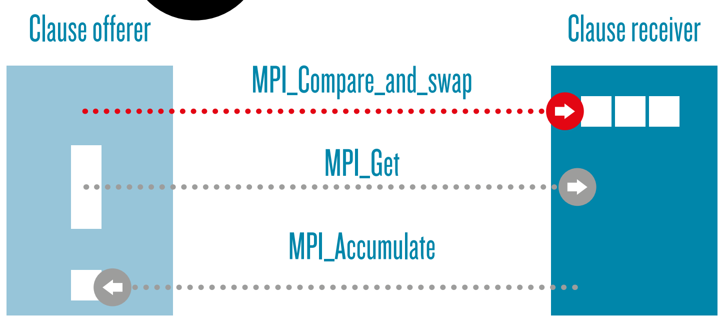
Remote direct memory access (RDMA) offers an efficient way to asynchronously distribute packages of learned clauses to a set of solvers. First, each solver offers such a package to other solvers, including a scoring value. Each solver selects a limited number of these packages based on the scoring value, retrieves them, and informs the offerers when done.

RDMA allows us to establish this unstructured, asynchronous communication pattern. Depending on the system size, network capabilities, and state of the problem-solving process, we can adjust the number of offers that each solver distributes and the number of offers each solver then actually takes.

CLAUSE SELECTION VIA SCORING SCHEME

Clauses have different characteristic values (e.g. literal block distance (LBD)) indicating under what circumstances the clause is generated. Thus, we can distinguish between different types of clauses. A scoring scheme can now rate the packages of clauses depending on the scoring of a package. The decision of fetching or declining a package depends on this score comparing it to all other scores of potential packages. So, we can select the best subset of packages for fetching to reduce the amount of clauses exchanged.

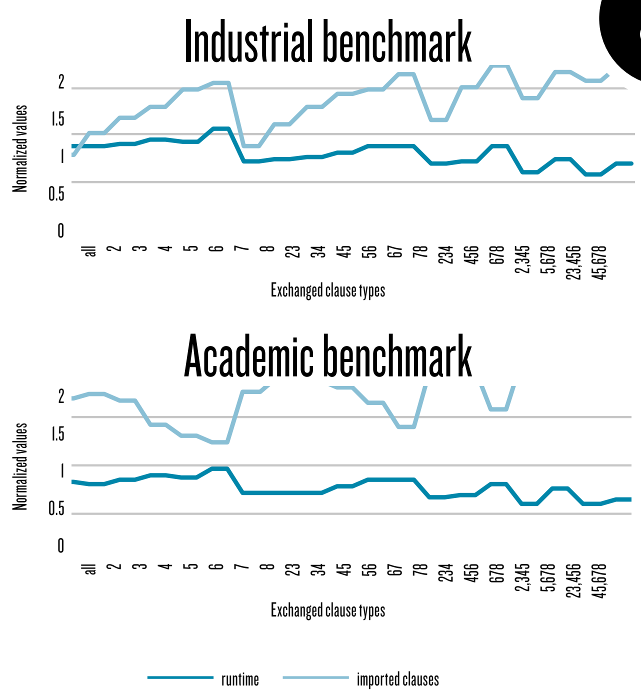
4



RESULTS AND FUTURE WORK

The type of clauses greatly influences the overall solution time. When scaling the problem to parallel systems, only those clauses that help reducing the runtime should be distributed among the processes. We will further study the effect of different heuristic clause distributions on the overall runtime.

5



SCALING HIGH-BANDWIDTH DATA STREAMS

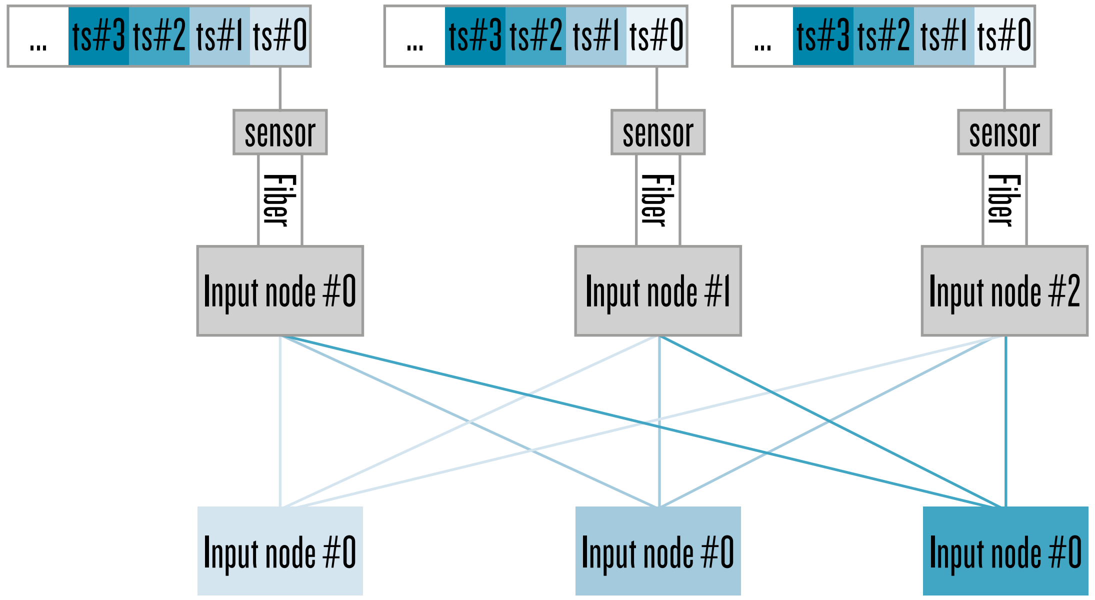
COMPRESSED-BARYONIC-MATTER EXPERIMENT

The compressed-baryonic-matter (CBM) experiment at the Facility for Antiproton and Ion Research (FAIR) in Darmstadt aims to explore the quantum-chromodynamics (QCD) phase diagram in the region of high baryon densities using high-energy nucleus–nucleus collisions. Many sensors surround the experiment to collect data during beam time. The overall data rate from the sensors is expected to exceed 1 TB/s (1,000,000,000,000 bytes per second).

The CBM data streams from about 600 input channels have to be spread and grouped to form views of time intervals. The grouped data is analyzed to detect and discover different phenomena.

Approximately 600 nodes will be used to spread and group data streams. This is done by the First-Level Event Selector (FLES), a high-performance compute cluster. The software to build time slices for the analysis, called FLESnet, must be scalable, highly available, and fault-tolerant.

FLESNET ARCHITECTURE



The high-level design of FLESnet consists of two kinds of processes (called nodes in the following): input and compute nodes. Input nodes receive data from the sensor links via a custom FPGA-based input interface and chop the stream into time intervals, called micro time slices, before distributing them for time-slice building. Compute nodes receive micro time slices of a corresponding time interval from all input nodes to form complete time slices before analyzing them further.

Each compute node reserves one buffer in its memory for each input node. Input nodes use remote direct memory access (RDMA) to write their contribution directly to the compute nodes' memory and inform them accordingly. Before overwriting the same memory address in the buffer, input nodes wait for an acknowledgement from the compute node that the time slice was processed and the buffer is free for reuse.

FLESNET CHALLENGES

FLESnet faces several challenges in its design:

Portability: FLESnet was implemented using the API of InfiniBand Verbs and relied on connection-oriented communication. To also exploit other modern interconnects, we ported FLESnet to the open-source framework OpenFabrics Interface (OFI) Libfabric. This widens the spectrum of clusters FLESnet can run on and keeps future decisions on the actual computer and networking hardware flexible.

Synchronization: Although each input node can fill its buffer space at each compute node, buffer space cannot be reused until contributions from all input nodes are received to complete the time slice and the analysis is finished. Therefore, a single lazy node or slow connection would cause input nodes to be out of synchronization and slow down the entire cluster.

Scalability: Due to the limited buffer space, each compute node should receive the contributions from all input nodes for a particular time slice in a small time frame. As a result, input nodes should send their data coordinated to not overload individual network links or become blocked due to full buffers at compute nodes. On the other hand, FLESnet's aggregate bandwidth should scale linearly with the number of nodes.

Monitoring, scheduling, and fault tolerance: FLESnet has to avoid network congestion, node failures, and load imbalances on heterogeneous hardware. It must be able to tolerate node and link failures because the beam time is costly and each physics experiment is unique and cannot be repeated.

DISTRIBUTED DETERMINISTIC SCHEDULER

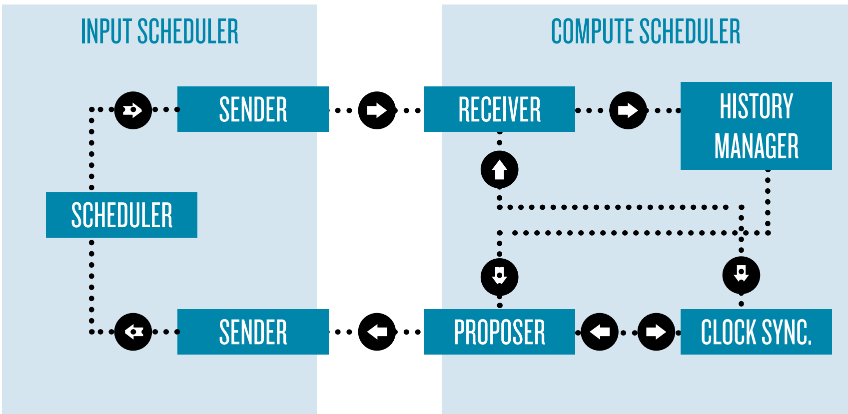
To address the outlined challenges, FLESnet is supposed to transmit data in high throughput and low latency. It should minimize the time gap between the first and last delivered contributions of each time slice to compute nodes. FLESnet should not congest a single node or link at a time or leave other nodes or links idle. Our distributed deterministic scheduler (DDS) synchronizes the input nodes to send their contributions within a particular time interval. Furthermore, it attempts to eliminate the end-point congestion at compute nodes. To do so, DDS proposes a start time and duration for each interval of time slice distribution that input nodes should follow. DDS consists of two schedulers, one at the input nodes and another at the compute nodes.

COMPUTE SCHEDULER

The compute scheduler stores the history of the transmitted intervals and proposes the needed information for the upcoming intervals. It consists of four modules: receiver, history manager, proposer, and clock synchronizer. The receiver module collects the actual starting times and durations from input schedulers. After that, it sends them to the history-manager module to calculate statistics and storage. The proposer module calculates the expected starting time and duration of up coming intervals based on the statistics from the history manager and sends it to input schedulers. The clock-synchronizer module considers different clock drifts between different machines for higher accuracy.

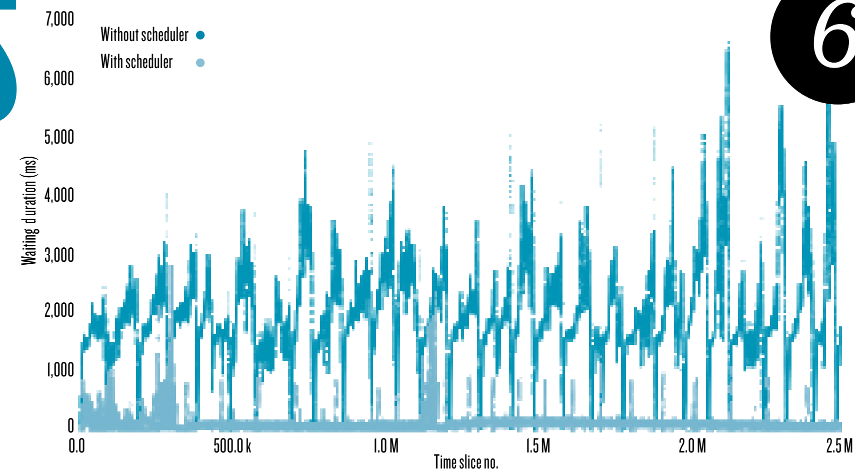
INPUT SCHEDULER

The input scheduler receives the proposed starting time and duration of an interval, and then schedules the transmission accordingly. It consists of three modules: sender, receiver, and scheduler. The sender module updates the transmitted messages to compute nodes and includes the actual starting time and duration of the completed interval. The receiver module receives the proposed interval information from the compute scheduler. The scheduler module schedules the transmission according to the receiver information from the receiver module. It informs the sender module once a complete interval is transmitted.



RESULTS

6

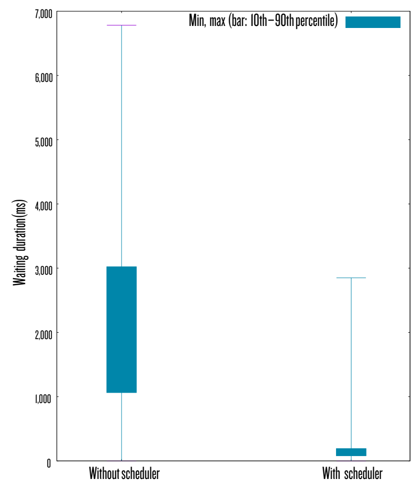


SYNCHRONIZATION OVERHEAD

DDS minimizes the duration needed for a compute node to receive a complete time slice. Figure 6 depicts the time gap between the first and last arrival of 2.5 million time slices with/without our scheduler on 192 nodes, 96 input nodes, and 96 compute nodes. This figure shows how the DDS helped in minimizing the duration needed to receive a complete time slice.

Figure 7 depicts the variance with and without the scheduler compared with the minimum and maximum waiting duration of each. It shows that 90% of the needed waiting duration is exceptionally small when DDS is used.

7



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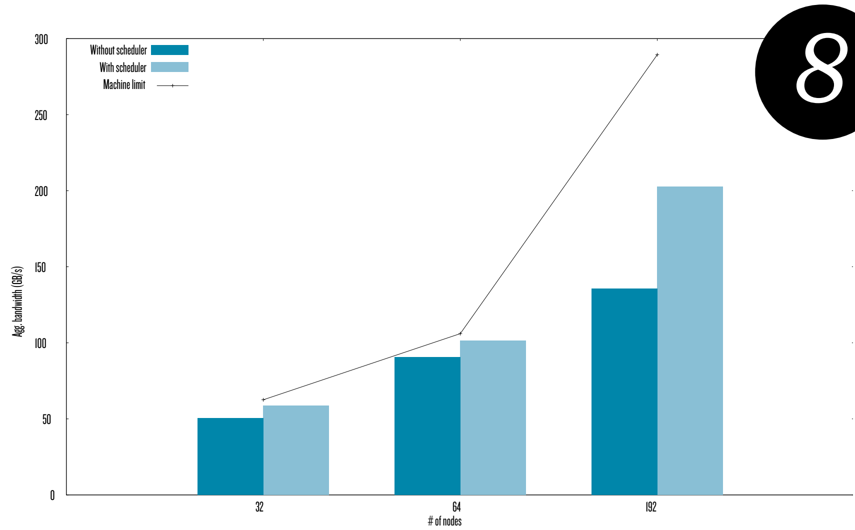

SCALABILITY

DDS also enhanced the performance of FLESnet. Figure 8 shows how the aggregated bandwidth is enhanced using DDS compared with no scheduler.

FUTURE WORK

We plan to further enhance the scheduler to achieve an aggregated bandwidth as close as possible to the machine limit. Furthermore, we aim to design and implement a fault-tolerance mechanism so that FLESnet can tolerate faults in nodes and the underlying network.

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DUSTING OFF COMETARY SURFACES

Photo: ESA/Rosetta/NavCam

Modeling gas and dust around comet Churyumov-Gerasimenko

The European Space Agency Rosetta mission to comet 67P/Churyumov-Gerasimenko (67P/C-G) sent back millions of observations during its journey around the sun.

ZIB contributed to the scientific analysis of the space mission by modeling the gas and dust environment around the comet on the HLRN supercomputer.

COMETS: VISITORS FROM OUTER SPACE AND ANCIENT TIMES

A spectacular and beautiful show of a bright comet with long tail and large coma is a rare experience for observers from earth. Most comets pass at a safe distance from earth around the sun on highly elongated orbits and are active only during a couple of months at closest approach to the sun (the perihelion). Periodic comets, designated with the suffix P in astronomical literature, are faithful visitors and have been regularly observed starting with comet 1P/Halley (orbital period 75 years).

What makes comets so interesting, apart from the spectacular appearance of the glowing tail that emerges through outgassing and ionization in the near-solar parts of the comet's path?

Comets are messengers from the early stages of the solar system's formation billions of years ago and provide important clues about the early formation of complex molecules. Furthermore, collisions of comets with earth over millions of years provided our planet with organic materials and water.

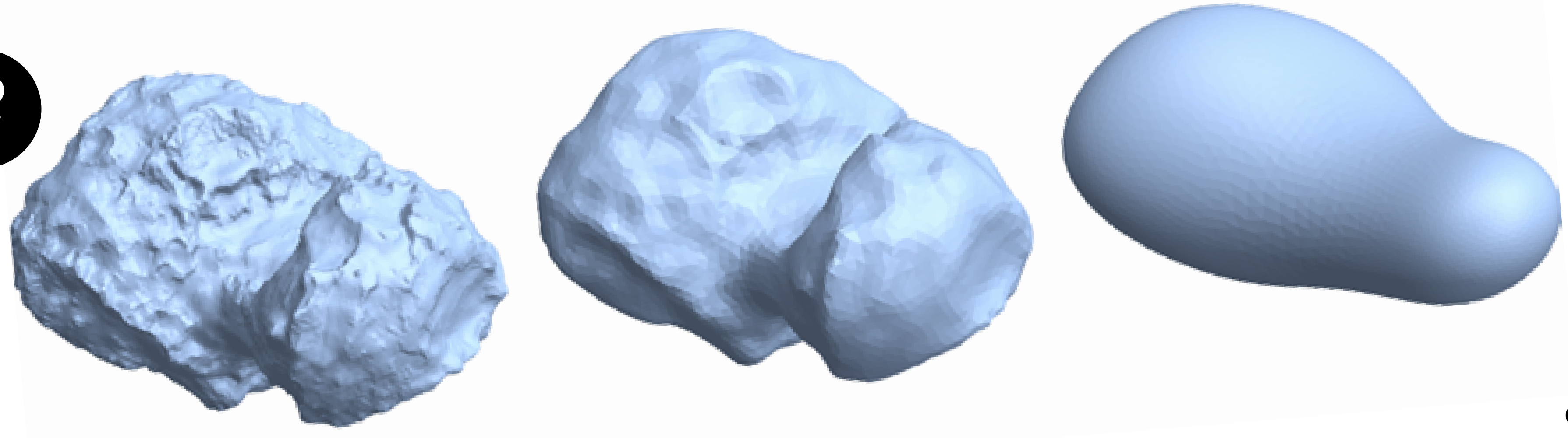
Earthbound telescopes have no chances to resolve the kilometer-sized nucleus, surrounded by a tenuous gas atmosphere (figure 2); this can be revealed only by satellites making a long journey through space to get very close to the comet. Mass spectrometers, developed for the Rosetta mission at the University of Bern, allow Prof. Kathrin Altwegg's (University of Bern) team to obtain a detailed inventory of molecular abundances and isotopic ratios.

ROSETTA'S LONG JOURNEY TO COMET 67P/CHURYUMOV-GERASIMENKO

The comet 67P/C-G has been expelled by Jupiter from the cold, outer regions of our solar system and is presently losing about 1/2000 of its total mass on each of its 6.4-year round-trips.

Rosetta followed the path of 67P/C-G from close distance (20–200 km) to find out how water and dust are distributed on the comet and which factors drive the development of the dust and gas tail and inner atmosphere (coma). Astronomers have a difficult task predicting the activity of a specific comet and to link the often million-kilometer-long tail to specific physical processes at the surface of the only few-kilometer-sized nuclei.

2

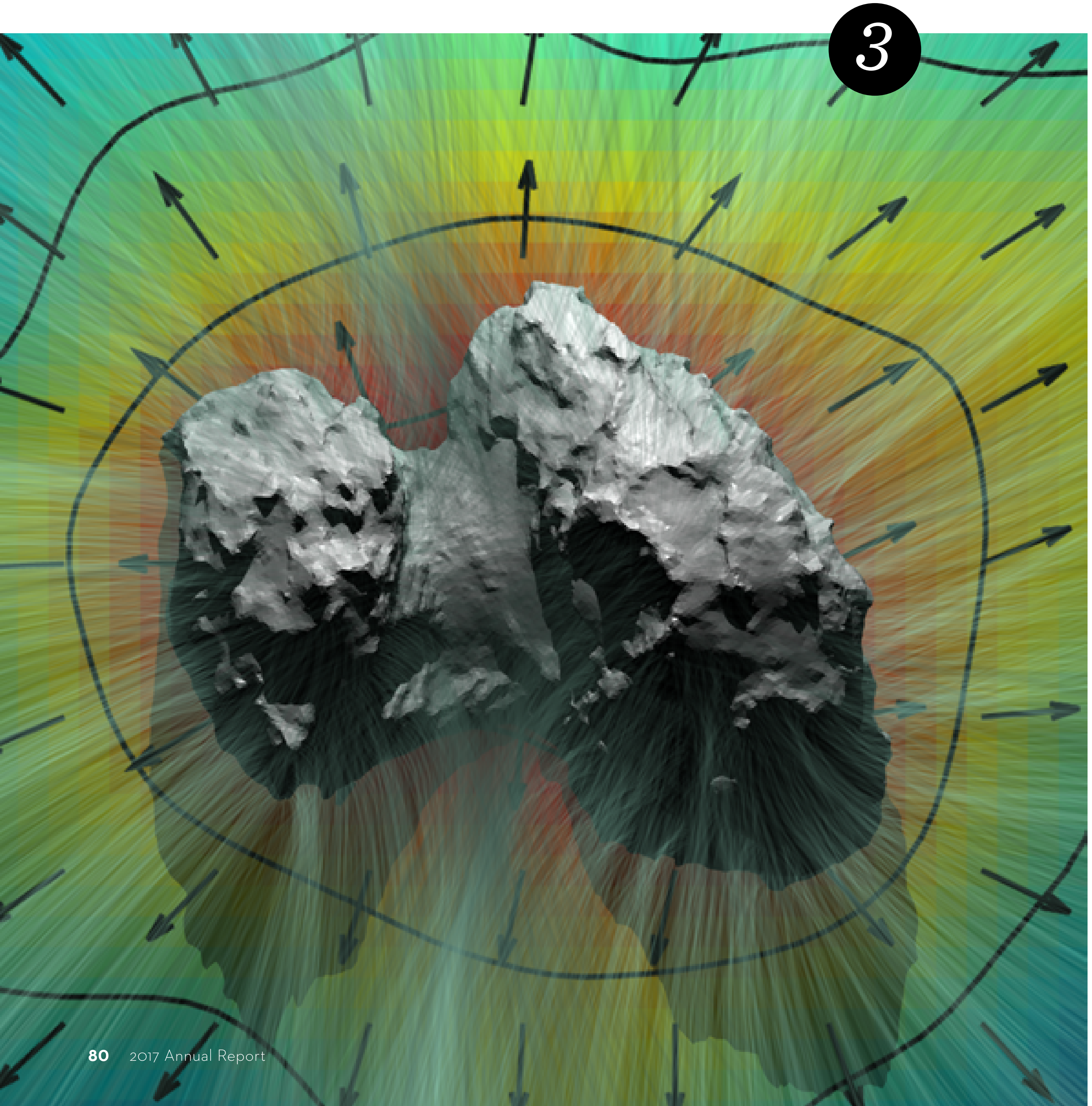


2 The nucleus of 67P/Churyumov-Gerasimenko: a space potato sized 4 km x 3.5 km x 3.5 km, consisting of dust (carbon-rich compounds and silicates) and ice. The complex shape of the rotating nucleus requires high-resolution mesh-based models for the dust and gas emission across the surface [1]. Simplified shape models help to pin down the sources of gas and dust emitted from the surface.

PREDICTING THE TAILS OF COMETS

At ZIB, we developed a detailed dust and gas forecast for 67P/C-G that has been compared with the downlinked images. Of particular interest are agglomerations of dust in space, imaged as brighter strikes around the nucleus and referred to as "jets." Before Rosetta's encounter, it was hypothesized that the dust jets are caused by isolated patches of activity on the surface (pointing to a large heterogeneity of the surface composition).

To analyze this in detail requires the development and implementation of models for simulating millions of dust particles around the rotating nucleus, taking into account the acceleration of dust grains by the evaporating gas and the gravitational pull of the odd-shaped nucleus. An effective parallelization is required, which allows us to simulate different scenarios. One unexpected outcome of the simulations performed at the HLRN supercomputer facility hosted at ZIB is that it is possible to predict the near-surface dust distribution of 67P/C-G with high accuracy just based on the shape of the nucleus.



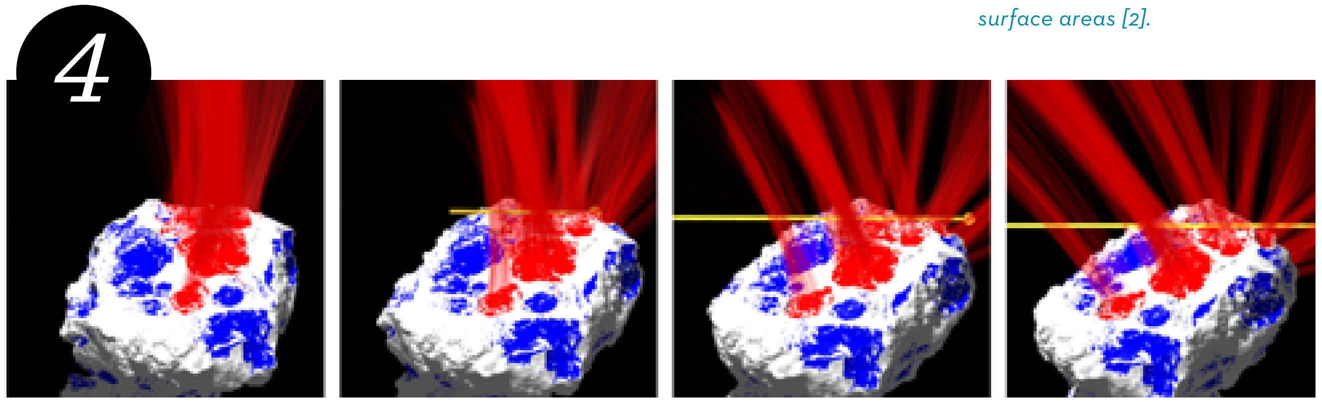
THE SHAPE OF THE NUCLEUS AND THE OBSERVER PERSPECTIVE

In a collaboration between the Supercomputing and Visual Data Analysis departments at ZIB, we used the Amira software to deform a mesh representation of the nucleus to study how the curvature of the surface affects the dust release. The best match between the model and Rosetta's observation is obtained if we consider globally uniform dust emission from the entire sunlit nucleus, instead from localized patches. This suggests a rather homogeneous composition of the surface of 67P/C-G. Higher dust levels are stemming from concave areas on the surface, which act as a lense, leading to a convergence of dust trajectories several kilometers above the surface (figure 3).

How can our findings be reconciled with the rapidly changing appearance of "jets" around 67P/C-G seen in many images? The 3-D visualization of the modeled dust cloud reveals that the imaged dust concentrations are highly sensitive to the perspective of the observer (Rosetta's camera). Higher intensities in the images ("jets") are caused by multiple concave areas aligned along the line of sight (figure 4). Our simulations take into account the 12-hour rotation of the nucleus, which lead to the curved appearance of dust jets further away from the nucleus: any observer standing on the cometary surface would get firsthand confirmation of the Coriolis effect.

3 Simulation of dust trajectories from the sunlit and shaded surface. Dust is accelerated within the gas field (arrows) and is lifted off the surface. The rotation of the comet during the travel time of the dust results in curved trajectories due to the Coriolis force [1].

4 Image analysis of the brightest point in the Rosetta image taken on April 12, 2015, 12:12, decomposed into all contributing dust sources along the line of sight (yellow line) from Rosetta's perspective. The bright jet seen from Rosetta's perspective originates from multiple sources and, in addition, from background contributions from all sunlit surface areas [2].



THE GAS ATMOSPHERE

Bright, short-living outbreaks resulting in very bright localized dust jets, have also been observed in the weeks around perihelion (August 12, 2015). In collaboration with the Rosina/COPS team at the University of Bern, data points from the cometary pressure sensor instrument onboard Rosetta allowed us to reconstruct the most likely gas sources linked to the observed outbreaks. As it turns out, the dust outbreaks are not happening at random locations, but are highly correlated with carbon-dioxide-rich areas (figure 5). This is interesting because for the total gas emission on 67P/C-G, the water emission tops the carbon-dioxide release.

PREPARING THE NEXT RENDEZVOUS WITH 67P/C-G

For the first time, Rosetta and simultaneous telescopic observations provide a unified picture of the evolution of the surface and the coma of a comet. A follow-up mission to comet 67P/C-G at its next visit to the inner solar system has been proposed and might lead to an unexpected reunion with Rosetta and its lander Philae. If the theoretical models pan out, next time we might be able to predict what the images of the dust tail and coma of 67P/C-G will look like.

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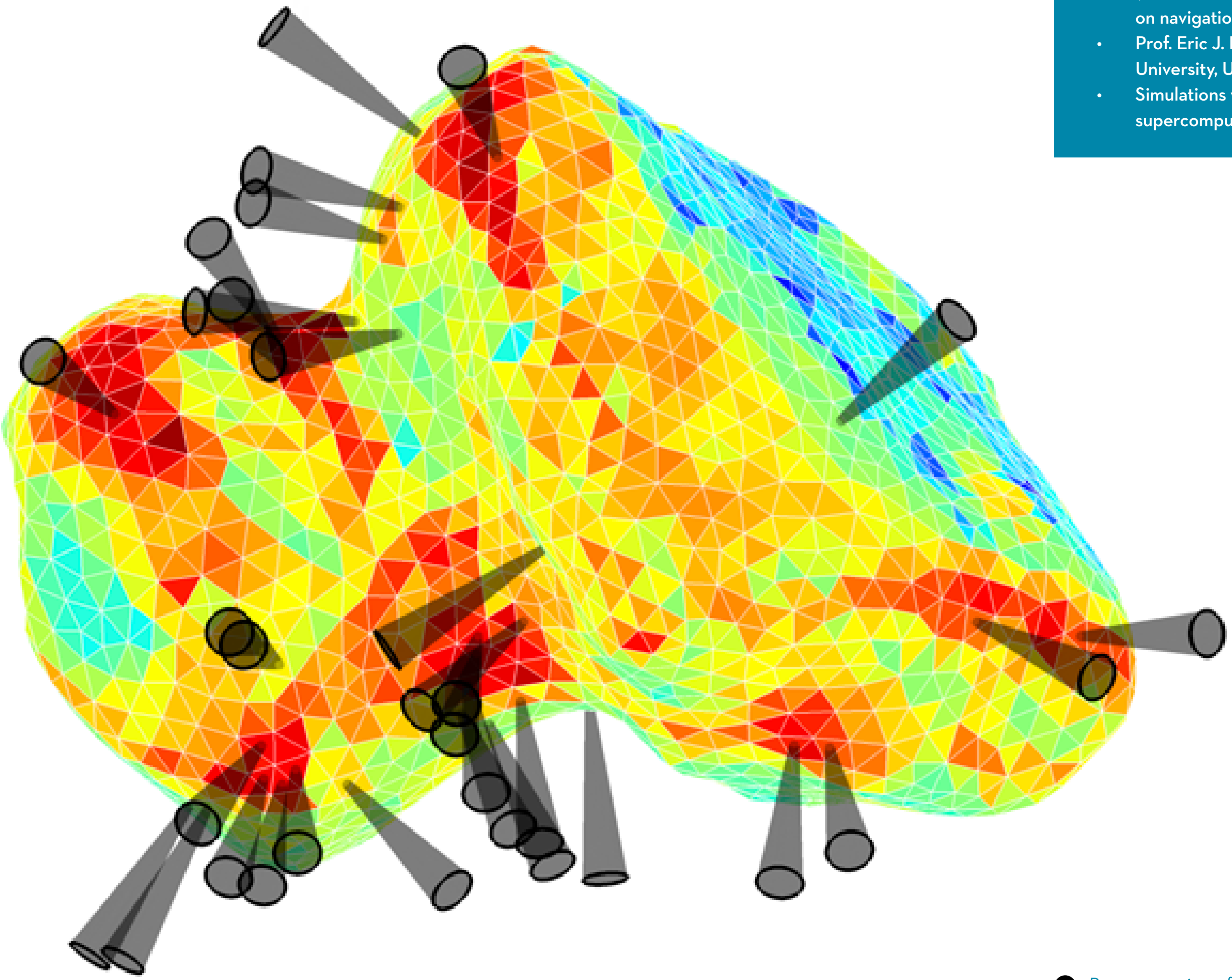

COLLABORATIONS AND FUNDING:

- Prof. Kathrin Altwegg, University of Bern, Switzerland, responsible for the Rosina: Rosetta Orbiter Spectrometer for Ion and Neutral Analysis instrument onboard Rosetta and the COmetary Pressure Sensor (COPS)
- Dr. Martin Rubin, University of Bern, Switzerland
- Mattias Malmer, Stockholm, Sweden (reconstruction of the shape of the nucleus based on navigation camera images)
- Prof. Eric J. Heller, Department of Physics, Harvard University, USA
- Simulations were performed on the HLRN supercomputing facilities at ZIB

5 *Reconstruction of carbon-dioxide sources on the surface of 67P/C-G and locations of observed dust outbreaks [3], [4].*

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