The IWR – Research That Bridges Traditional Disciplinary Boundaries

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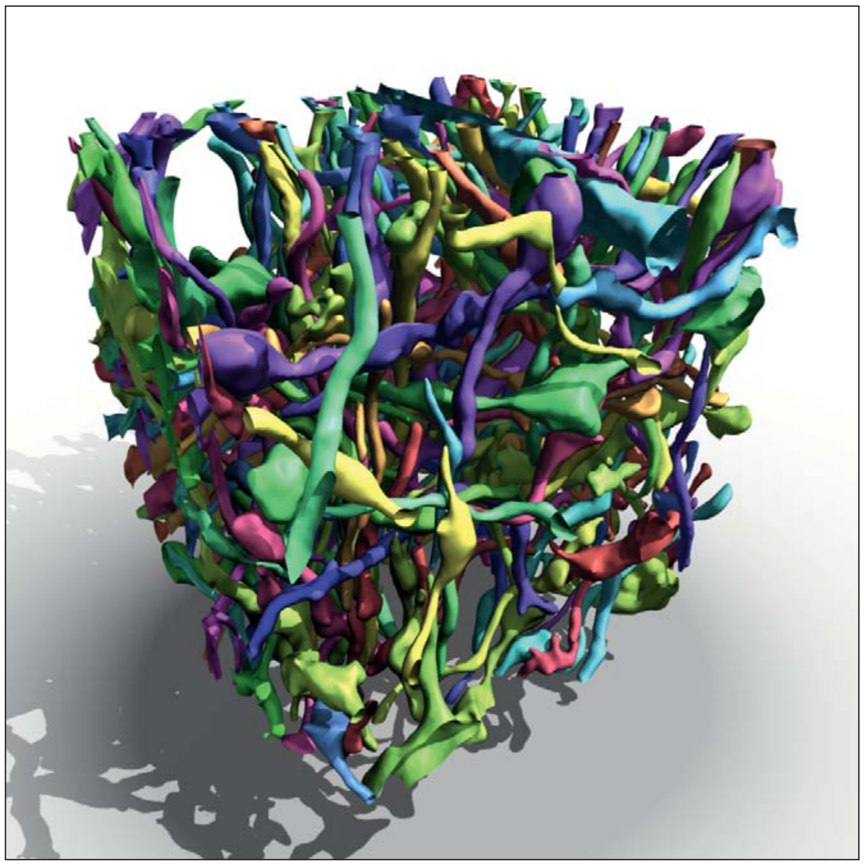
The Interdisciplinary Centre for Scientific Computing (IWR) was established in 1987. In those days, the idea of creating an interdisciplinary think tank in Heidelberg with high-power parallel computers was an ambitious, but highly attractive one. Founding director Willi Jäger, professor of mathematics, described how it came about: "In particular, the Baden-Württemberg Ministry of Science recognised how forward-looking this kind of facility would be for Heidelberg University, and with its high density of technology firms, for all of southwest Germany". "In the winter of 1985 we were intensely working through different designs – up until then there wasn't a single comparable facility in Germany." With the founding of the IWR, a decisive step was taken toward advances in science and a new, interdisciplinary science was launched, known as *scientific computing* in the USA, where it first emerged. The term *scientific computing* stands for the modelling of complex processes **#1 #2**. Together with simulation and graphic visualisation, it is the third pillar of science, an equal partner alongside theory and experimentation.

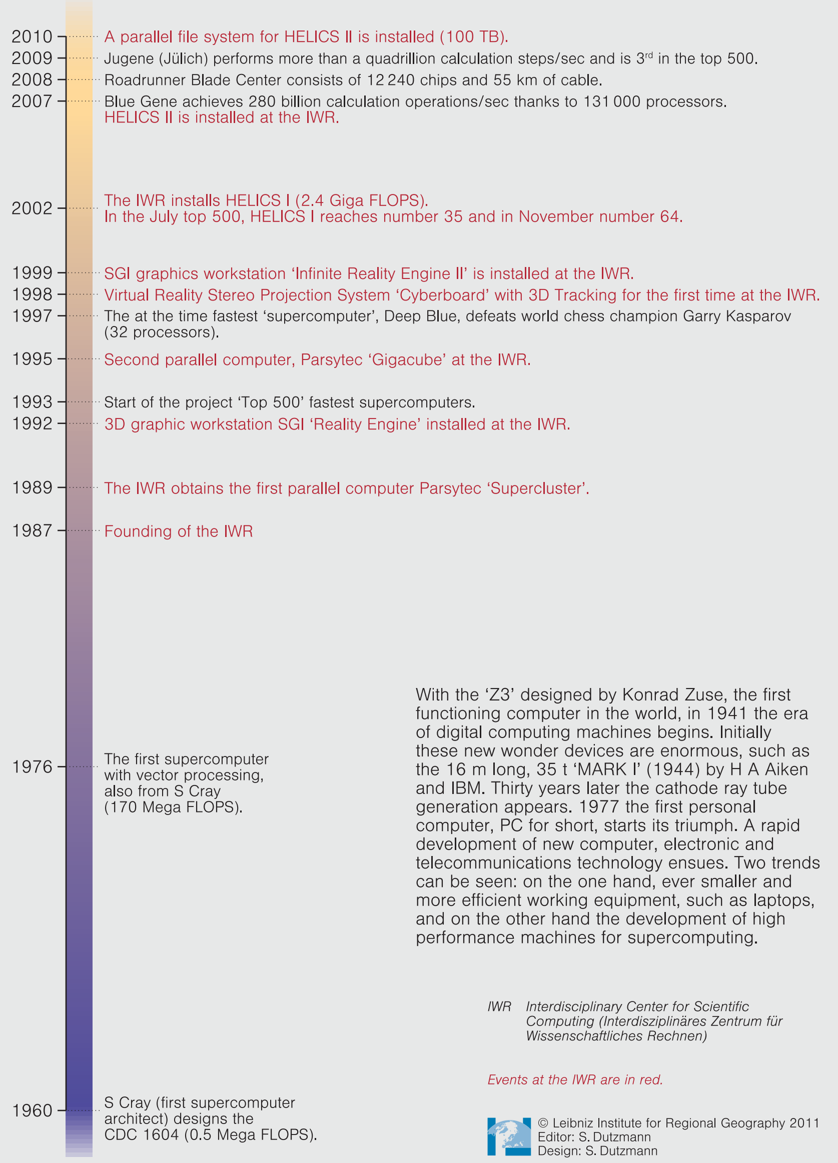
Secret world of algorithms

Starting with just over a dozen scientists, this first such institution in Germany began to formulate algorithms and mathematical models for highly complex problems. The first computer system was purchased in 1989 at a cost 1.5 million deutschmarks, a mere fraction of what comparable powerful computers with a slightly less intelligent network structure cost at the time. The new institution took on the systematic development of new types of solution



With its intensively linked nerve cells, the human brain is among the most complex structures on earth. Although the way individual nerve cells function has been well analysed, a thorough understanding of human thought and memory is still in its infancy. Newly developed microscopes allow three-dimensional photographs of large areas of the brain to be taken at a previously unknown resolution and, together with proper image analysis, reveal major pieces of a "circuit diagram".

1 Milestones in the history of the IWR and supercomputers 1960-2010

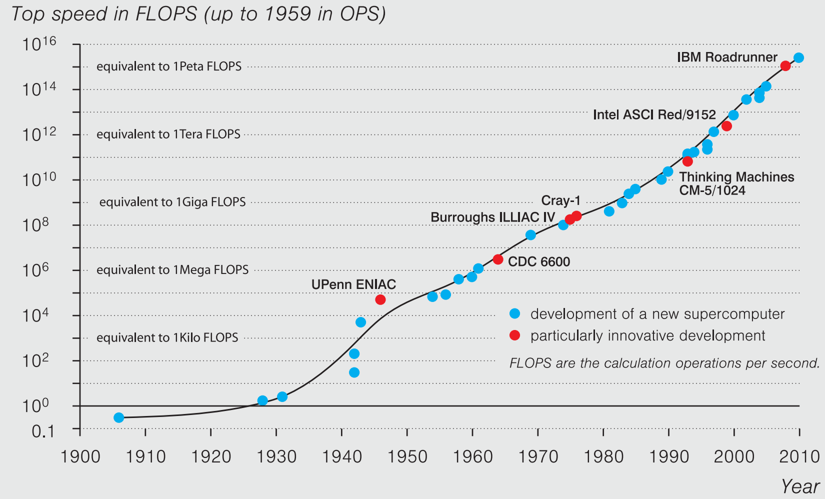


With the 'Z3' designed by Konrad Zuse, the first functioning computer in the world, in 1941 the era of digital computing machines begins. Initially these new wonder devices are enormous, such as the 16 m long, 35 t 'MARK I' (1944) by H A Aiken and IBM. Thirty years later the cathode ray tube generation appears. 1977 the first personal computer, PC for short, starts its triumph. A rapid development of new computer, electronic and telecommunications technology ensues. Two trends can be seen: on the one hand, ever smaller and more efficient working equipment, such as laptops, and on the other hand the development of high performance machines for supercomputing.

IWR Interdisciplinary Center for Scientific Computing (Interdisziplinäres Zentrum für Wissenschaftliches Rechnen)

Events at the IWR are in red.

2 Processing speed of Computers 1906-2010



Supercomputers are characterised by the fact that their performances are always in the upper range of achievable performances. In 2010 this is around 1760 Peta FLOPS - i.e. 1760 quadrillion (10^{15}) calculation operations per second.

methods and making previously non-understood phenomena "computable" – an innovative and future-oriented step.

In the early days of the IWR, technical and scientific phenomena were of primary interest. Questions such as "What combustion processes take place in a motor?", "How do pollutants disperse in the ocean?" or "How does a protein fold?" were coherently formulated mathematically by physicists, chemists and engineers and then simulated in the computer. Like then, the IWR is continually exploring new frontiers in its day-to-day research: Its co-operations have extended its reach into the social sciences, humanities, economics and the life sciences.

How do I formulate my problem mathematically?

For many disciplines outside of mathematics, the possibilities of scientific computing represent a quantum leap in terms of methods. In the spirit of "There is nothing more practical than a good theory", the co-operation at the IWR unleashed a veritable flood of knowledge for many scientific disciplines.

In the 1990s, environmental physicist Bernd Jähne received a professorship at the IWR and began to systematically expand the field of image processing. The success of the *Image Sequence Analysis to Investigate Dynamic Processes* research group of the German Research Foundation (DFG) illustrates just how significant this added knowledge was. It developed image processing methods for analysing transmission, exchange and growth processes that opened up a number of new areas of application. The scientists gained a detailed understanding of what processes occur in the cell nucleus and how pollutants disperse in the troposphere. Industry's keen interest in image processing was reflected in the establishment of an endowed professorship by BOSCH, assumed by chemist Fred A. Hamprecht (research focus: *Multidimensional Image Processing*), who at 27 was the youngest professor at the university at the time.

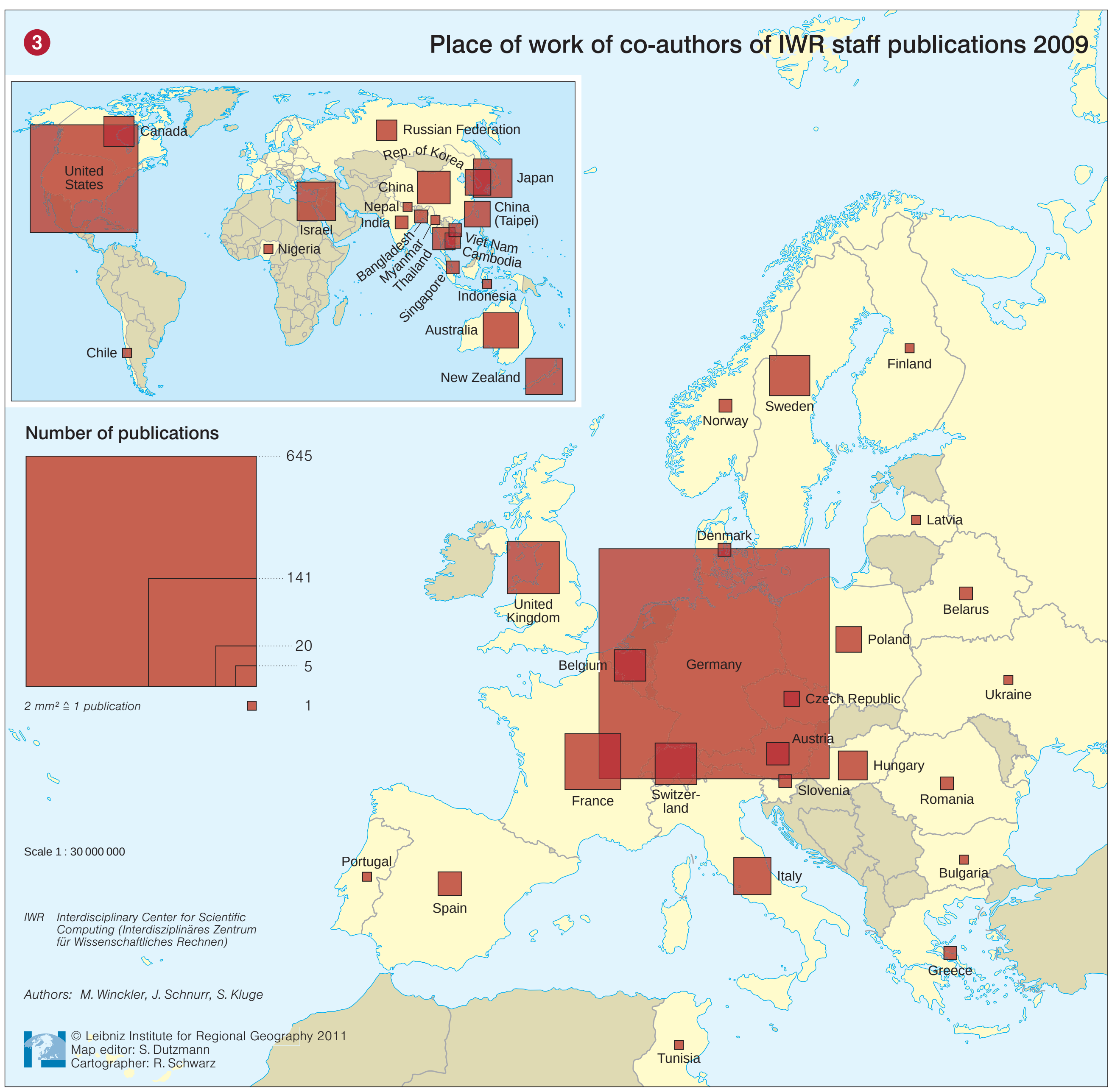
On 1 January 2008, a new arm of the IWR was born, the *Heidelberg Collaboratory for Image Processing* (HCI), based on its success within the Excellence Initiative. This innovative *Industry on Campus* project partnered BOSCH, Heidelberg Printing Machines, and the medium-sized firms Heidelberg Engineering, Silicon Software (Mannheim) and PCO AG (Kelheim). In April 2010 another International Research Training Group was formed at the IWR, the *Spatio/Temporal Graphical Models and Applications in Image Analysis* group. It brings together the fields of image processing and mathematics, conducts its work at the HCI and is integrated into the *Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences* (HGS MathComp).

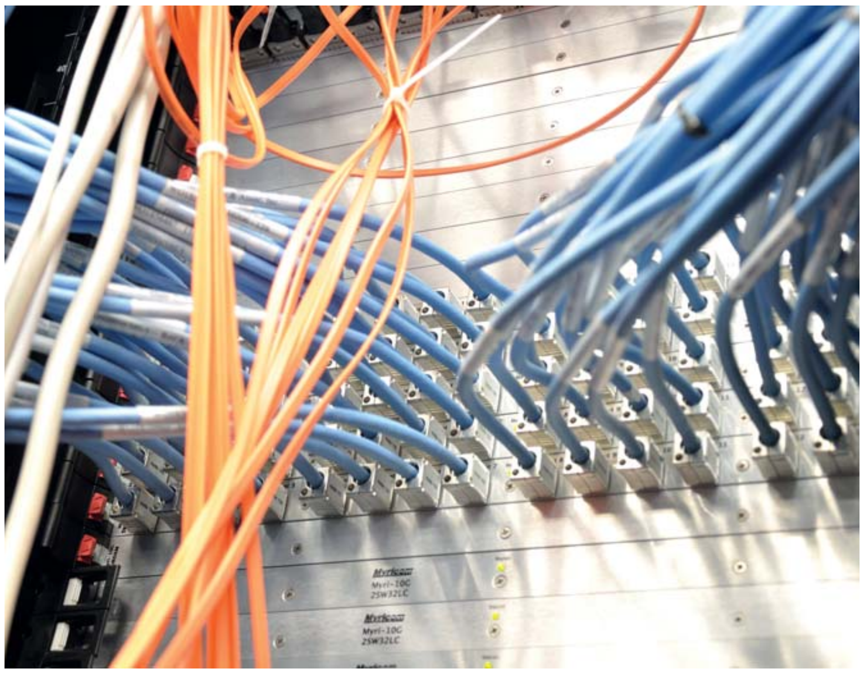
Of paramount importance to IWR researchers is their independence. "Our desire is to develop new theories for problems through practical experience, not simply through the application of existing knowledge. We in no way see ourselves as an extended workbench of the business world. We are in search of fundamentally new methods that companies can then take and turn into technical process methods themselves", explains Jähne.

Building interdisciplinary bridges at Ruperto Carola

The IWR is a central institution of the university and reports directly to the rectorate. Its members are attached to the IWR and their own institute on a parity basis and are nominated by the rectorate. They form the Extended Board of Directors. IWR members teach at their respective institutes. The graduands and doctoral candidates can also avail themselves of the technical facilities of the IWR if needed. Eleven "core professors" are located directly at the

Thanks to modelling, scientists have a completely new view of their objects of investigation. Like here – in the 3D visualisation of a blood vessel – use of a high-performance computer and the development of special algorithms opens up a whole range of new methodical approaches to scientific disciplines. In this regard, the IWR is indispensible to the interdisciplinary bridges being built at Ruperto Carola.





Getting scientific problems onto the computer is crucial. But simply using a high-performance computer is not enough. Even more important is developing programmes that can model the phenomenon under study with precision. This requires intensive interdisciplinary exchange among the scientists.

IWR, with offices there. There are currently about 40 research groups at the IWR; they publish their results worldwide **#3**.

In 1992 the International Research Training Group *Modelling and Scientific Computing in Mathematics and Life Sciences* (term until 1999) began its work, followed in 1993 by the special research area *Reactive Currents, Diffusion and Transmission* (active until 2004). In 2000 the International Research Training Group *Complex Processes: Modelling, Simulation, and Optimisation* was founded, which in co-operation with the Warsaw *Interdisciplinary Centre for Mathematical and Computational Modelling* (ICM) advised young scientists through the completion of its term in 2009. In 2004 the *Centre for Modelling and Simulation in the Biosciences* (BIOMS) took up its work at the IWR. Other research institutes involved in the BIOMS include the German Cancer Center (DKFZ), the European Molecular Biology Laboratory (EMBL), the Heidelberg Institute for Theoretical Studies (HITS), the Max Planck Institute for Medical Research (MPImF) and the Centre for Molecular Biology of Heidelberg University (ZMBH). The BIOMS is particularly focused on supporting the biological sciences through scientific computing. This enables the graphic understanding of biological processes down to the cellular and molecular level. The IWR currently works from two locations: the larger piece of the organisation – where the high tech computer systems are housed – is at Im Neuenheimer Feld 368; the HCI and other research groups carry out their work at Speyerer Straße 6.

In the field of scientific computing, the IWR has the largest structured doctoral programme in the world. It prepares top young researchers for their scientific career and makes a lasting contribution to Heidelberg University's international renown.

Scientific computing permeates our society

"Right now an entire range of completely new areas of research are opening up to us. Particularly in our collaboration with the cultural sciences, we're breaking completely new ground in terms of method," states Hans-Georg Bock, IWR Managing Director. "Today we can plainly see the extent to which mathematical modelling of physical laws and the optimisation of production processes have permeated our environment – our entire society – in all areas." Comparable quantum leaps, such as those achieved in the biosciences in recent years through model-supported simulation, are now spilling over into an entire range of other fields of research.

Long gone cultures awake anew

Through new analysis methods in character recognition on cuneiform script and papyrus fragments or the reconstruction of fallen monuments, historians, archaeologists, and art historians have an undreamt of capability to augment their traditional sources of research. On the computer, illegible text can be reconstructed and deciphered, destroyed temples and palaces raised

❶ The HGS MathComp – a magnet for young researchers

A key priority of the IWR is the optimal education of its doctoral candidates. Many scientists who earned their doctoral degree at the IWR have gone on to become well-respected university professors. The high percentage of young women researchers is extraordinarily high – and has been since the very beginning. As a seat of learning for the natural sciences and mathematics, the IWR seeks to achieve the ideal in terms of *gender equality* in Germany. The *Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences* (HGS MathComp) was founded on 1 November 2007 within the framework of the Excellence Initiative. Their sights are set high. As the world's largest structured doctoral programme in the field of scientific computing with an interdisciplinary bent, the school stands for the promotion of creativity and interdisciplinary methods. The experience that the young scientists gain in interdisciplinary research projects, such as measuring ancient temple complexes or interpreting climate models, is unique. Once they complete their doctoral degrees, many go on to do pioneering work themselves. In a short time, the IWR has established itself on the international stage as an excellent centre of learning.

2 IWR on the leading edge of research – *pioneering projects*

Scientific computing is a key technology in solving complex problems in science, technology, business and society. Its foundations are

Mathematical models and their analysis;

Numerical procedures for their calculation;

Methods for analysing and processing data;

Procedures and software for simulating and optimising systems;

The use of the latest computer systems and methods in information processing.

One trademark of scientific computing is that its results and tools can be used successfully in very different fields. This is possible because the mathematical concepts and methods used capture the essential characteristics of the systems under observation. For over twenty years, the IWR has made substantial contributions to the understanding of complex physical and chemical processes, such as combustion processes or reactive currents and transmission in the environment and astrophysics. It has assumed a leading role in the quantitative description of biological systems, especially in the Center for Modelling and Simulation in the Biosciences (BIOMS) and the BIOQUANT network.

Pioneering projects at the IWR, which explore new realms of scientific computing, deal with innovative fields in the

Environmental sciences: Quantitative determination of system data for transmission and reactions of chemical substances in the atmosphere from remote sensing data;

Material sciences and biosciences: Determination of chemical and physical properties of large molecules and molecular systems based on quantum mechanical calculations, processes at boundary layers and at the nano-scale level;

Medicine and the public health sector: Currents and transmission in the circulatory system and respiratory system, origination and course of infarcts, dynamics of stem cell populations, dynamics of movement and the movement apparatus, progression of epidemic diseases and the development of resistant pathogens;

Finance and economics: Modelling, simulation and optimisation of the dynamics of prices and sales of goods, particularly products from the fields of energy, petrochemistry and transportation;

Neurosciences, psychology and psychotherapy: Modelling and simulation of physiological processes in the brain and analysis of the relationship between the dynamics of cognitive, mental and psychical processes and conditions, diagnostics and treatment of disease, converting research results into intelligent, autonomous systems;

Cultural sciences: Collection and processing of materials and objects using computer-assisted methods and instruments, especially of historical monuments and finds (especially temple complexes in Angkor, > image), of text and image data (of documents in cuneiform script and of inscriptions), measures for the restoration, maintenance and optimal documentation of cultural heritage sites.

Pioneering projects develop new methods for:

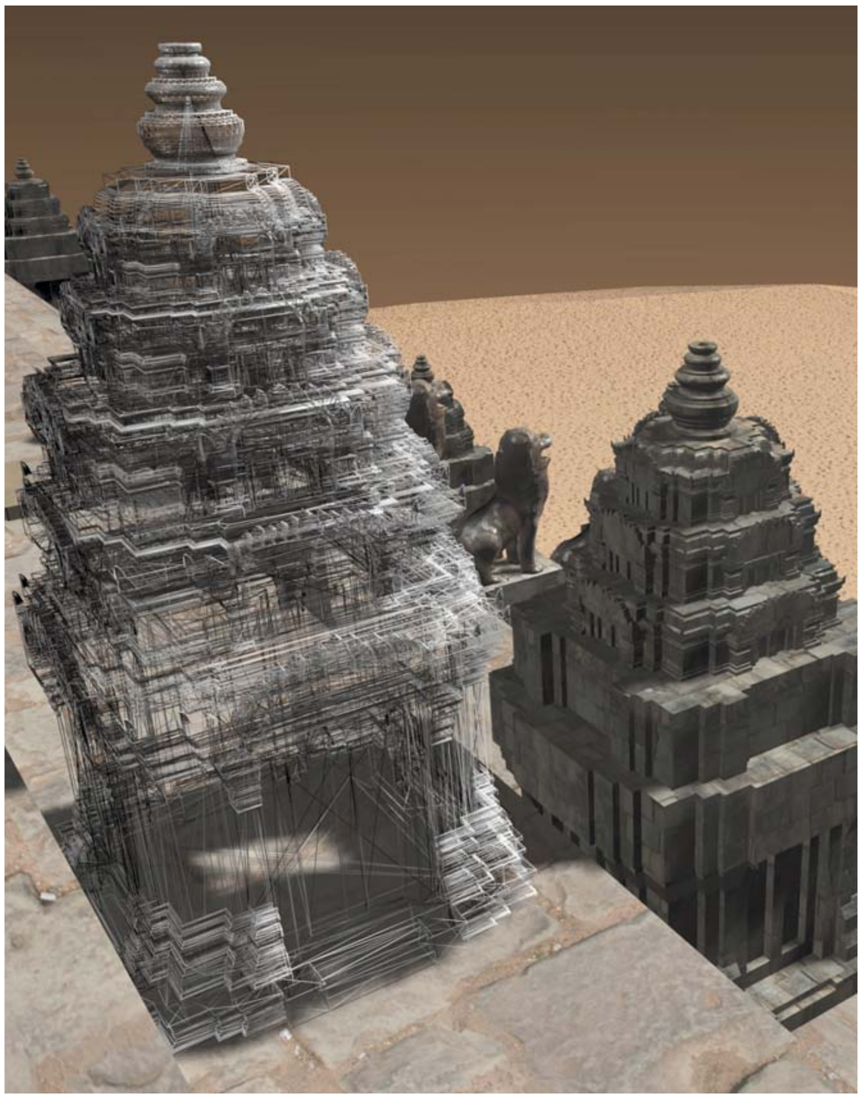
Complex systems of processes on different scales: from genes and cellular processes to the behaviour of organs and organisms; from the dynamics of atoms and molecules to the behaviour of materials;

Analysis and calculation of processes in complex networks, development of tools to characterise structures and their dynamics in chemical, biological, social and economic networks;

Model-based and object-oriented image processing: processing of data using models for the underlying processes, such as currents and transmission in the atmosphere or in the circulatory systems of organs; recognition of structures and objects in image data;

Optimal determination of process parameters, developed using a radiation transmission test case;

Efficient software adapted to the specific requirements of the different areas of application and computer structures.



In the computer, cultures of times long past arise again in their former grandeur. The *pioneering projects* of the IWR are setting trends the world over, especially in its collaborations with the cultural sciences. The interdisciplinary research methods currently under development represent a quantum leap for many subject areas.

again in their former grandeur, broken clay tablets reassembled to relinquish their long forgotten secrets. The modelling of ancient temples in Cambodia (> image), supported by the Daimler and Benz Foundation, met with strong public favour. The new *Computational Humanities* field of research is not only gaining attention internationally, but IWR scientists are being sought out as trailblazers and expert advisors on comparable research projects all over the world.

"It is with good reason we attach great importance to our *pioneering projects*" **§2**, Bock explains. "In collaboration with the experts, today we are building the arsenal of methods that will inform their scientific endeavours in five or ten years. Whether in medicine, the humanities or cultural sciences, there's a real sense of transformation and ardent enthusiasm for the new tools we're co-developing." Far-reaching strides have also been made in the material sciences as well as *industrial optimisation*, inducing BASF to finance a junior group devoted to basic research in mathematics.

Top young researchers at the IWR – a bridge to the future

With respect to the advancement of young researchers, the IWR's firm eye on the future makes it a veritable Mecca for young international scientists (> image). Over the last several years, the IWR has systematically built up a research environment with training programmes that offers them optimal preparation for careers as top international scientists. In the field of scientific computing, the IWR is a unique magnet for doctoral students – currently 140 at HGS MathComp **§1** alone – and postdoctoral researchers from all over the globe. A significant number of former doctoral candidates at the IWR have meanwhile been appointed to professorships; many others are captains of industry. As top researchers of tomorrow, many will retain close ties with Ruperto Carola as their training ground, thereby making a lasting contribution to the university's international renown.