

International Graduiertenkolleg 710

**Complex Processes:
Modeling, Simulation and Optimization**

Final Report
(2001 – 2009)

Heidelberg, August 05, 2010

Interdisziplinäres Zentrum für Wissenschaftliches Rechnen (IWR)
Universität Heidelberg
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Table of Contents

1. General Information	1
2. Overall Scientific and Structural Results	3
3. Qualification, Supervision and Cooperation.....	6
3.1 Qualification and supervision.....	6
3.2 Reorganization of the doctorate and related courses of studies	10
3.3 Research students and qualifying students.....	10
3.4 Gender equality	11
3.5 Cooperation	11

Appendix

I Lists of Members	A1
1a: Doctoral students of the GK: funded by DFG grants	A2
1b: Associated doctoral students of the GK: funded by other grants	A6
1c: Doctoral students at the international partner institution in Warsaw	A8
1d: Postdoctoral members of the GK: funded by DFG grants	A9
1e: Associated postdoctoral members of the GK: funded by other grants	A10
1f: Qualifying students	A11
1g: Research students.....	A12
IIa Individual Reports – Doctoral Students	A14
IIb Individual Reports – Postdoctoral Members	A166
III List of Publications	A210

1. General Information

- German title: "Komplexe Prozesse: Modellierung, Simulation und Optimierung"
- English title: "Complex Processes: Modeling, Simulation and Optimization"
- Duration: 01.01.2001 - 31.12.2009
- Chairman: Prof. Dr. Dr. h.c. Hans Georg Bock (University of Heidelberg)
- Chairman: Prof. Dr. Marek Niezgodka (University of Warsaw)

- Participating researchers including period of time of their participation in alphabetical order:

Heidelberg researchers

Prof. Dr. Peter Bastian	01.01.2004 - 31.12.2010
Prof. Dr. Dr. h.c. Hans Georg Bock	01.01.2001 - 31.12.2010
Prof. Dr. Dr. h.c. Lorenz Cederbaum	01.01.2001 - 31.12.2010
Prof. Dr. Rainer Dahlhaus	01.01.2001 - 30.06.2005 and 01.07.2008 - 31.12.2010
Prof. Dr. Eva Gutheil	01.01.2001 - 31.12.2010
Prof. Dr. Dr. h.c. mult. Willi Jäger	01.01.2001 - 31.12.2010
Prof. Dr. Jörg Langowski	01.07.2005 - 31.12.2010
Prof. Dr. Enno Mammen	01.01.2001 - 31.12.2003
Prof. Dr. Dr. h.c. Rolf Rannacher	01.01.2001 - 31.12.2010
Prof. Dr. Gerhard Reinelt	01.01.2001 - 31.12.2010
Prof. Dr. Kurt Roth	01.01.2001 - 30.06.2005
Prof. Dr. Jeremy Smith	01.01.2001 - 31.12.2010
Prof. Dr. Angela Stevens	01.04.2007 - 31.12.2010
Prof. Dr. Werner M. Tscharnuter	01.01.2001 - 31.12.2003
Prof. Dr. Dr. h.c. Jürgen Warnatz	01.01.2001 - 22.12.2007 (deceased)
Prof. Dr. Rainer Wehrse	01.01.2001 - 30.06.2005
Prof. Dr. Gabriel Wittum	01.01.2001 - 30.09.2008
Prof. Dr. Jürgen Wolfrum	01.01.2001 - 31.12.2010

Warsaw researchers

Prof. Dr. Jan Antosiewicz	01.01.2004 - 30.06.2005
Prof. Dr. Jerzy Baldyga	01.01.2004 - 31.12.2010
Prof. Dr. Helena Dodziuk	01.07.2005 - 31.12.2010
Prof. Dr. Jerzy Gorecki	01.01.2004 - 31.12.2010
Prof. Dr. Leon Gradon	01.01.2004 - 31.12.2010
Prof. Dr. Krzysztof Kurzydowski	01.01.2004 - 30.06.2005
Prof. Dr. Marcin Leonowicz	01.01.2004 - 30.06.2005
Prof. Dr. Bogdan Lesyng	01.01.2004 - 31.12.2010
Prof. Dr. Marek Nawalany	01.01.2004 - 30.06.2005

Prof. Dr. Marek Niezgodka	01.01.2004 - 31.12.2010
Prof. Dr. Lucjan Piela	01.07.2005 - 31.12.2010
Prof. Dr. Tadeusz Rychter	01.07.2005 - 31.10.2005 (deceased)
Prof. Dr. Stanislaw Sieniutycz	01.01.2004 - 30.06.2005
Prof. Dr. Ewa Sikora	01.07.2005 - 31.12.2010
Prof. Dr. Jacek Waniewski	01.07.2005 - 31.12.2010
Prof. Dr. Wojciech Wislicki	01.01.2004 - 31.12.2010
Prof. Dr. Stanislaw Wronski	01.01.2004 - 30.06.2005
Prof. Dr. Maciej Zylicz	01.01.2005 - 31.12.2010

- Research fields and specialisations of the Heidelberg researchers:

Mathematics and Computer Science

- Continuous Optimization
- Applied Analysis
- Numerical Mathematics
- Parallel Computing
- Discrete Optimization
- Multiscale Modeling

Biology

- Biocomputing
- Computational Molecular Biology

Chemistry

- Multi-Scale Reaction-Transport Processes
- Molecular Quantum Dynamics
- Multiphase Flows and Combustion
- Catalytic Reaction Processes

Physics and Astronomy

- Environmental Physics
- Porous Media Flows
- Theoretical Astrophysics
- Radiative Transport

- Research fields and specialisations of the Warsaw researchers:

Mathematics

- Applied Analysis

Physics

- Biophysics
- Biocomputing
- Theoretical Physics
- Statistical Thermodynamics
- Environmental Physics

Biology

- Cell Biology
- Biomedical Engineering

Chemistry

- Chemical Reaction Engineering
- Chemical Kinetics
- Quantum Chemistry
- Physical Chemistry
- Chemical and Process Engineering

Material Science and Engineering

- Material Science

2. Overall Scientific and Structural Results

2.1 A short history of the International Research Training Group (GRK 710)

The International Research Training Group GRK 710 "Complex Processes: Modeling, Simulation and Optimization" was a novel type of research training programme because it integrated an international doctoral programme, with interdisciplinary collaborative research projects between the partner institutions IWR at Heidelberg and ICM at Warsaw as well as a local doctoral programme to promote interdisciplinary collaborative projects between research groups of IWR.

It started originally as a *Graduiertenkolleg* of IWR on January 1, 2001. Right from the start there were plans to augment it into an international doctoral programme, despite the fact that neither complementary funding programmes on the Polish side nor even bilateral agreements on a political level existed. However, using third party funding of ICM and additional generous funding by the DFG, a collaborative doctoral programme could be started, and eventually GRK 710 was transformed into an international research training group from January 1, 2004. Its basis were 12 research groups at IWR and 12 at ICM.

2.2 The partner institutes

The two partner institutes and their research groups contributed both joint and complementary expertise in various areas relevant for the research programme, which provided an optimal starting point to create synergies within a joint doctoral programme. Both institutions had strong groups in applied analysis and mathematical modeling of complex nonlinear processes, in the molecular biosciences and physical and biological chemistry, and in high performance computing. IWR could contribute strong expertise in numerical differential equations and algorithmic optimization, whereas ICM contributed strong complementary expertise in computer graphics and visualization, chemical engineering and material science.

2.3 Research aims and structural aims

Over the past decades modeling, simulation and optimization of scientific processes have developed into a "third pillar of science" bridging the traditional approaches of theory and experiment. In order to meet the demand from the growing complexity of processes and problems under investigation, the overall research goals were

- the development of new and innovative methods for modeling, simulation and optimization of complex processes,
- driven by the challenges provided by selected scientific application areas, particularly physical and biological chemistry, molecular biology, and chemical engineering

Key methodological areas to tackle complexity were homogenization and model reduction, multi-level algorithms, goal-oriented adaptivity, all-at-once approaches in optimization, and parallel algorithms.

Clearly the promotion of new mathematical and computational methodology to advance the development of computational science and engineering requires interdisciplinary collaboration, not only between mathematics, computer science and natural sciences, but also between their subdisciplines.

The structural aims pursued by establishing an interdisciplinary and international doctoral programme may be summarized as follows.

- To develop best practice methods that cope with the challenges provided by the interdisciplinarity of the projects, which pose high requirements from both the doctoral students and their supervisors and mentors.
- To develop feasible structures and procedures that allow to develop an international doctoral programme at two very distant locations where the doctoral students nevertheless form a coherent group.

- To introduce the necessary structural changes into the respective university environments and to promote the formation of structured doctoral programmes in analogy to the DFG Graduiertenkollegs in Poland.
- To ensure early scientific independence of our doctoral students and an early integration into the international scientific community, and to provide an ideal training ground to achieve these aims.
- Finally, an ambitious aim was if possible to form a reference model for others how to establish such interdisciplinary and international ventures.

2.4 Results

Most of these aims have been very successfully achieved and some even overachieved beyond our expectations.

The International Research Training Group (IRTG) established a successful structured doctoral programme for its interdisciplinary research goals in modeling, simulation and optimization of complex processes in science and engineering. All doctoral theses were strictly interdisciplinary. Dedicated measures to cope with the high demands this poses on students were the supervising scheme with two supervisors from two relevant fields of expertise at ICM and IWR, plus two mentors from their groups, and a specially tailored programme of short courses that covered the necessary range from the introductory and tutorial level to the international top level research was established.

The special form of the short course programme plus additional topical small conferences and workshops relevant for the students' work (27 in the years 2004 to 2009 alone) as well as mutual research stays at the research group of the partner institute, fostered coherence in the group of students and helped realized a corporate identity, which was definitely supported by numerous social events.

All in all 67 doctoral students at Heidelberg (8 at Warsaw) and a total of 16 postdocs belonged to the International Research Training Group. Until today we have 39 completed doctoral theses, 14 doctoral students are still working within the IRTG, ten continue their research on positions in the participating research groups, four left the IRTG prematurely to continue their studies at other places. Their scientific results were very successful and led to numerous innovations and breakthroughs some of which even found their way into industrial practice and patent applications. We just mention the Interatomic Coulombic Decay investigations where model-based simulation allow prediction of effects that could only later be experimentally verified, the development of the Dual-Weighted Residual adaptivity methods which cut down the effort by orders of magnitude as do the new methods for Optimum Experimental Design that deliver orders of magnitude higher amounts of information. An additional significant proof of success are the four of the doctoral students and postdocs, which are already university professors or lecturers, and two more expecting corresponding offers, as well as the four which are now junior research group leaders with their own funding.

2.5 Impact on structural and institutional changes

We summarize here some of the most important structural changes that were strongly dependent on the activities of the international research training programme.

- An agreement between the Universities of Warsaw and Heidelberg for joint doctoral degrees has been established.
- The structured interdisciplinary doctoral programme for the development of mathematical and computational methods for the challenges of emerging areas in computational science and engineering has served as an important nucleus to establish the new Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences in the framework of the German Excellence Initiative. It pursues similar aims on a broader basis of disciplines and methodological areas for 150 doctoral students from seven faculties at Heidelberg.
- In order to alleviate the tight bonds of traditional disciplinary exams, a new adequate form of interdisciplinary doctoral exams was introduced in Heidelberg. Originally promoted by this IRTG

this new form is planned to be adopted throughout the University of Heidelberg in its framework of regulations, e.g. to allow collaborations between humanities and science. Also, the mentoring scheme introduced by the IRTG has been adopted by several other graduate programmes. The interdisciplinary research programme and the structures of the IRTG have also found followers in similar initiatives for IRTG or Graduate Schools outside Heidelberg and even outside Germany.

- In Poland the activities of the IRTG have influenced the introduction of the "International PhD Projects Programme" (MPD) by the Fundacja na rzecz Nauki Polskiej (FNP), the president of which is Maciej Zylicz, a member of our IRTG. Practically this has already led to a new international doctoral programme on the Polish side for 15 doctoral projects funded by the FNP, "Mathematical Methods in Natural Sciences" chaired by Piotr Gwiazda. This new programme, four principal investigators of which are IWR members, is not bilateral, but includes German, French and Czech institutions.
- IWR also pursues plans for a new IRTG together with the Necas Center at Prague and the ICM at Warsaw. Presently however, we are still struggling to find a way for complementary financing of our Czech partners.

2.6 Future trends

What are the scientific visions for the next decade? Modeling, simulation and optimization of complex processes has now reached a certain maturity that has already significantly transformed the research in a number of areas in science and engineering, and of development in the industry.

We see it now opening up new territories in research, e.g., in the social sciences, the cognitive sciences, in medicine and public health, and even in the humanities where methods of scientific computing have already started to play a significant role in the historical and cultural sciences such as archeology and conservation. All these areas provide new challenges and require new and different mathematical and computational techniques.

Also in the more traditional areas of application, we see that the complexity of both processes and problem formulations continues to grow. This puts even higher demands on the quality and detail of mathematical models and on the adaptivity of solution algorithms, but also on the mathematical problems that need to be solved.

The advent of novel and precise techniques for model validation and the emerging possibilities for precisely calibrated detailed models by dedicated optimally designed experiments are beginning to again transform computational science and engineering. Modeling and simulation are no longer restricted to trial and error on a computer experiment to gain scientific insight. Rather, the expectations from a quantitatively correct and detailed virtual model world are much higher. Inverse problems methodology and optimization based simulation methods are required that actually allow to find solutions in a complex model world that obey or optimize certain performance criteria subject to numerous restrictions. More and more, modeling, simulation and optimization will grow into an enabling technology that allows strategic approaches ("rational design") to the solution of scientific and engineering problems.

3. Qualification, Supervision, and Cooperation

3.1 Qualification and supervision

Due to the strictly interdisciplinary nature of the Graduiertenkolleg's (GK) projects, the accompanying study programme had to comply with two boundary conditions:

- The doctoral students in the GK came from different scientific backgrounds, and they were not necessarily already well trained in interdisciplinary research.
- The interdisciplinary nature of the dissertation projects required profound knowledge in various methodological aspects of modeling, simulation and optimization, in the development of scientific software, often combined with parallel computing, and strength in at least one application area.

The GK made every effort in order to reduce the potential difficulties in the beginning of the students' research work that resulted from the interdisciplinarity of their projects, and to avoid unnecessary loss of productive time.

On the one hand, particular care was taken in the selection of the doctoral students, their doctoral projects and work programme, and also their supervisors. These efforts were complemented on the other hand by

- a compact study programme to ensure basic common knowledge of the state-of-the-art as well as special courses and trainings tailored to meet the specific demands of the doctoral projects,
- an intensive individual support of the doctoral students by two supervisors and two mentors from the two collaborating research groups,
- an effective embedding of the doctoral projects into an active scientific environment in both research groups.

Courses

The study programme of the GK was planned jointly by doctoral students, postdocs and supervisors. To facilitate the participation of students and supervisors of the partner institution, the joint study programme consisted of short courses and workshops. The language of the courses was mainly English.

The study programme was based on a cycle of fundamental short courses in the methodological areas, repeated roughly every three semesters. These courses provided our students with a broad knowledge of state-of-the-art methods in modeling, simulation and optimization. It complemented their know-how in their special areas and served as a common knowledge and communication platform. The cycle time of three semesters took into account that our doctoral students were not selected in cohorts, but were accepted in a more or less continual fashion.

The following chart outlines the principal scheme of these fundamental short courses:

WS 04/05	SS 05	WS 05/06
Discrete Optimization (Reinelt, Oswald, Sager (IWR) et al.)	Parallel Programming (Bastian (IWR) et al.)	Multiscale Analysis (Niezgodka (ICM), Jäger, Friedmann (IWR) et al.)
Dynamic Process Optimization (Bock, Diehl, Mombaur (IWR) et al.)	Modeling, Simulation and Control in Chemical and Process Engineering (Baldyga, Gradon, Waniewski (ICM) - Bock, Diehl, Schlöder, Wittum (IWR))	Numerical Methods for PDE (Rannacher (IWR) et al.)
Modeling with Differential Equations (Braack, Lebedz (IWR) et al.)		Scientific Visualization and Computer Graphics (Nowinski (ICM), Krömker (IWR) et al.)

They were usually organized as "schools" or "tutorial workshops" of 2 to 5 days and included introductory and tutorial training units, practical training in the application of scientific software, but

also lectures presenting recent research results. The lecturers and the organizers of the practical exercises came from the research groups at IWR and ICM – often the doctoral students themselves –, or were invited in the framework of our international guest programme.

Our doctoral students, of course, also had the opportunity to participate in further special lectures connected to the topics of their research projects from the teaching of their supervisors' groups, the general course programme of IWR, or the university's faculties.

Training of software skills

All doctoral students were involved in more or less extensive software development work. The fundamental short courses mentioned above often involved components of practical training with software packages at IWR or ICM and made use of the computer pools, e.g., at IWR. According to the actual demand of the dissertation projects or the interests of the doctoral students, more intensive individual trainings with the software systems being developed or employed in the research groups of the principal investigators at IWR were available, such as

- Numerical solution of PDE, with DEAL-II, GASCOIGNE (Rannacher, Kanschat, Braack et al.) and UG, DUNE (Bastian, Wittum et al.)
- Numerical solution of ODE and DAE with ODESIM, DAESIM, MBSSIM, and parameter estimation, optimal control, optimum experimental design with PARFIT, MUSCOD, VPLAN/OPTX (Bock, Schlöder et al.)
- Simulation of chemical reaction systems with HOMREA, DIFRUN, DETCHEM-Channel (Warnatz, Gutheil, Lebiez et al.)
- Simulation of molecular dynamics with CHARMM (Smith, Fischer et al.)
- Discrete optimization with ABACUS, PORTA (Reinelt, Oswald et al.)

Correspondingly, the research groups at ICM offered the following trainings:

- Simulation of molecular dynamics with ACCELRYSS and TRIPOS software (Lesyng, Rudnicki, Piechota et al.)
- Material science modelling and simulation with ACCELRYSS (Materials Studio) (Rudnicki, Piechota et al.)
- Scientific data visualization with AVS software (Nowinski et al.)
- Computational fluid dynamics with FLUENT software (Trykozko et al.).

Training of "extra-curricular" skills

The study programme also included units for the training of extra-curricular skills and knowledge. Depending on the demand by the doctoral students, periodically specific courses have been offered on such topics, such as

- Presentation techniques (rhetoric), constructive debating, etc.,
- Project planning and project management.

To meet the demand by our foreign as well as German doctoral students, we have offered English and Polish language courses to make it easier for our students to spend longer periods in Warsaw. It is important to note that the GK considered another category of "extra-curricular" qualifications to be of high relevance, namely the education and training of our doctoral students in important skills required from top young scientists seeking a career in academia as university professors and researchers, or in the research and development departments of industry. This includes abilities like the writing of grant proposals, the organization of conferences and workshops, developing strategies for publications and for the integration into the international scientific community, or the active engagement in academic administration.

Small conferences and workshops

Periodically, the GK organized small scientific conferences or workshops on topics of general or more specific interest in the framework of its research programme, where also leading researchers from outside Heidelberg or Warsaw were invited.

For the last funding period the following scientific conferences were organized:

2005:

- "Mathematical Techniques for Multiscale Analysis" (organizers: Hartmann, Marciniak-Czochra, Ptashnyk)
- "Understanding and Control of Complex Chemical Processes" (organizers: Gutheil, Gorecki)
- "COUCH – Conference on Optimization under Uncertainties" (organizers: Bock, Kostina, Albersmeyer)
- "Methods of Molecular Simulation" (organizers: Imhof, Noe, Krachtus)
- "COMREF 2005 – Computational Methods for Multidimensional Flows" (organizers: Braack, Rannacher)
- Winter School "Modeling and Simulation of Complex Processes" (organizers: Lebedz, Braack)

2006:

- "Methods of Molecular Simulation" (organizers: Noe, Imhof, Voltz)
- "International Conference on High Performance Scientific Computing" (organizers: Bock, Phu, An, Dien, Grötschel, Hoai, Jäger, Minh, Niezgodka, Osborne, Phuong, Putlitz, Rannacher, Reinelt, Richter, Thai)

2007:

- "Scientific Computing and the Cultural Heritage" (organizers: Bock, Jäger, Winckler)
- "Methods of Molecular Simulation" (organizers: Imhof, Voltz, Prinz)
- "13th Czech-French-German Conference on Optimization" (organizers: Bock, Diehl, Reinelt, Mombaur, Sager, Schlöder)
- "DayVis – Days in Visualization" (organizers: Winckler, Schlöder)
- "From the Structure of Brain Neuronal Networks to Network Activity" (organizers: Matthäus, Elsässer)

2008:

- "Methods of Molecular Simulations" (organizers: Imhof, Langowski, Prinz)
- "Conference on Modeling, Simulation and Optimization of Complex Processes" (organizers: Braack, Jäger, Kanschat, Kostina, Phu, Reinelt, Schlöder)

2009:

- "MMS 2009 Methods of Molecular Simulations" (organizers: Imhof, Cournia, Koppole, Prinz, Smith)
- "Modellgestützte Parameterschätzung: Theorie und Anwendungen" (organizers: Bock, Carraro, Jäger, Körkel, Rannacher, Schlöder)
- Spring School "Multiscale Methods and Modelling in Biophysics and Systems Biology" (organizers: Heermann, Yixue, Lei)

In addition, a number of complementary scientific meetings were held at ICM and organized mainly by our Warsaw partners. In particular this includes:

2005:

- 5th Fall Workshop "Complex Processes: Modelling, Simulation and Optimisation" (organizers: Bock, Niezgodka, Rannacher, Trykozko, Szymanowska)
- "Modeling, Simulation and Control in Chemical Engineering" (organizers: Gradon, Bock, Diehl, Kühl)

2006:

- "Prague–Heidelberg Workshop on Nonlinear Analysis" (organizers: Feistauer, Dolejsi, Felcman, Knobloch, Rokyta, John, Stara, Malek)
- "Dynamic Developments over Complex Networks" (organizers: Niezgodka, Trykozko, Cytowski)

2007:

- "Visualization and Image Processing" (organizers: Niezgodka, Nowinski, Borucki)
- Spring Workshop "Complex Processes: Modelling, Simulation and Optimisation" (organizers: Bock, Niezgodka, Trykozko)

2008:

- "Data Driven Modelling and Optimization" (organizers: Niezgodka, Trykozko, Szymanska, Lopuszynski)
- "Mathematical Modelling of Cellular Biosystems" (organizers: Marciniak-Czochra, Szymanska, Trykozko, Doktorski)

2009:

- "Mathematical Modelling of Cellular Biosystems II" (organizers: Marciniak-Czochra, Niezgodka, Trykozko)

Obligations of the doctoral students

In order not to delay the duration of the doctoral process, the participation of our students in the study programme did not exceed 6 to 8 hours per week. Accordingly, the doctoral students participated in two courses of the study programme per semester in their first year, and in one course per semester in their second year. The third year was essentially reserved to the writing of the dissertation and the preparation for the oral examination.

Apart from the study programme, three periodical events were mandatory for the doctoral students:

(1) The Seminar of the GK

In general, the Seminar of the GK took place every week during the teaching period and in larger intervals outside. In the Seminar, the doctoral students reported about recent results of and future plans for their research as well as themes of topical interest. Each doctoral student was expected to give a presentation at least once a year. The Seminar was also the place to discuss current problems of general interest, and for the planning of events and courses, and had stimulated a number of additional cross-disciplinary research projects among the doctoral students.

(2) The Annual Colloquium of the GK

Once a year there was a two- or three-day colloquium of all doctoral students, postdocs and the advisors in Heidelberg to which also our Polish partners were invited. During this event, all doctoral students and postdocs reported about the progress of their research. On the one hand, the colloquium served as an additional element of progress control for the individual projects as well as the GK as a whole. On the other hand, the meeting provided additional opportunities for students and supervisors to identify new areas of interdisciplinary research, and also contributed to the social relations within the GK.

(3) The Joint ICM/IWR Workshops "Complex Processes: Modeling, Simulation, and Optimization"

These were annual meetings of the doctoral students, postdocs, supervisors and mentors from Heidelberg and Warsaw. Each of them had about 40 participants. The workshops were mandatory for all doctoral students involved in joint Heidelberg/Warsaw projects. They were also very interesting for those GK members planning a joint Heidelberg-Warsaw project, because of its scientific excellence, and of course also because of the social events involved. The joint workshops were of utmost importance for the progress and development of the GK as well as its local components at IWR and ICM.

The GK took strict care that its students were involved in teaching obligations at their home faculties only as far as this was paid for and the salary did not exceed the allowed EUR 3000 per year.

Supervision

Two supervisors with different scientific background were assigned to each doctoral student. Hence the students were connected with two relatively large research groups with on average 15 doctoral students and postdocs each.

Most of the time, the students had their workplace in one of the groups. However, in order to foster the interdisciplinary collaboration, the students took their workplace for several months in the research group of the other supervisor instead. They participated in the group's meetings and seminars and were thus integrated into versatile international scientific collaborations. To our experience, the direct exchange of know-how with other doctoral students and postdocs about methods, algorithms and software was indispensable for the progress of research projects in scientific computing. Heidelberg doctoral students involved in Warsaw-Heidelberg research projects had to spend at least 6 months in Warsaw (and vice versa).

Additionally, two mentors from both research groups were assigned to each doctoral student. Mentors could be postdocs or experienced doctoral students. Based on earlier very positive experience, the mentor concept was introduced as a constitutive element in the GK and appears to be successful. The doctoral students benefited from having two young researchers as additional advisors. On the other hand, the mentors had the opportunity to gain practical experience in promoting junior scientists, which helped them to form their own junior research groups.

Performance Control

Several instruments helped to monitor the research progress and served as measures for performance control of which self control was one of the most important components:

- extensive guidance, advice and support by two professors and two mentors,
- progress reports and presentations in the seminars of both research groups,
- at least one presentation per year in the Seminar of the GK,
- mandatory presentation in the Annual Colloquium of the GK, and presentations in the joint ICM-IWR Workshops,
- written progress report after each year including work programme for the next year,
- additionally, outline of a dissertation after the second year.

The progress reports and the assessments by the two supervisors also provided the basis for the decision about an extension of the fellowships.

One of the most important means of self control for researchers is the assessment of the quality of their results provided by presentations at conferences and by submitting papers to a journal review.

3.2 Reorganization of the doctorate and related courses of studies

The GK influenced the design or reorganization of the following courses of studies:

- diploma study course “Mathematik mit Ausrichtung Wissenschaftliches Rechnen” and master study course “Scientific Computing”: One major subject here are methods of applied mathematics and applied computer sciences. Essential parts of the study programme deal with modeling, simulation and optimization of complex processes.
- Bachelor and master study course “Anwendungsorientierte Informatik”: The focus here is on applied computer sciences and software engineering, especially in the area of computer based simulation and optimization of complex processes. Both study courses allowed for a seamless transition to doctoral studies within the GK.

Furthermore, the doctorate was reorganized in order to enable interdisciplinary doctorates. In this case, the examining board consists of four examiners representing at least three different subjects. It is explicitly allowed to include people from outside the University of Heidelberg. This was especially important for dissertation projects that were strongly related to engineering like many of the joint research projects together with our colleagues from Warsaw.

3.3 Research students and qualifying students

Research students were excellent graduate students that performed independent scientific work usually directly related to a dissertation project of a doctoral student or a research topic of one of the postdocs. Typical tasks for research students arose naturally from the interdisciplinary character of the research projects within the GK. In general, these projects were located at the intersection of the development of novel computational methods and challenging applications. This resulted in a multitude of independent scientific problems that could be tackled by qualified graduate students. In this way, research students were given an early constructive introduction into the topics and methods of the interdisciplinary research of the GK, whereas the supplementary research performed by the research students helped the doctoral students concentrate on the central topics of their projects.

Qualifying students were students in a one-year phase of a “Qualifikationsstudium” that, usually after an oral examination, entitled them to be accepted as a doctoral student at a faculty of the University of Heidelberg. We accepted those students in the GK under exactly the same conditions as the doctoral students. The only difference to doctoral students was that they followed a study and training programme during this year – based on the GK’s programme – which was individually tailored to the

required qualification upgrade as well as their doctoral project. These qualification fellowships were particularly helpful for excellent foreign applicants for a doctoral fellowship that, however, did not have a sufficiently broad education yet for an interdisciplinary research topic in modeling, simulation and optimization of complex processes. In our experience, often the background of the applicants in computational mathematics and software development needed improvement.

3.4 Gender equality

Within the GK and IWR, special measures are taken to promote gender equality. The Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences (HGS MathComp) draws inspiration from the experiences made in the GK. There, the following measures are taken in order to substantially increase the number of excellent female scientists:

- Full-time child care: Improving and enlarging the University child care facility and providing full-time child care (from age two months to 12 years). The University reserves a minimum of five places in its day nursery for the HGS. To support conference participation of parents with children, individual funds are provided for persons, for example grandparents, to take care of the children.
- Short-term care: For short notice (and short-term) care requirements, a “just in time” or “back-up” care initiative is implemented.
- Olympia-Morata program: This University of Heidelberg program is directed at young female scientists working towards their “Habilitation” (postdoctoral qualification) and provides 50 per cent of the salary for 2 years if the other 50 percent is secured through another source.
- Young scientists in the HGS with children are, if necessary, equipped with appropriate working facilities at home, at the cost of the HGS, and should flexible working hours as far as possible.
- Meetings of the HGS’s governing bodies are scheduled, whenever possible, at times which are convenient for members with children.

3.5 Cooperation

International contacts and visits abroad

The students and postdocs of the GK were strongly encouraged to build up and maintain close scientific relations to researchers in the international community. In the GK they found excellent conditions to do so.

First of all, they could and did exploit the institutionalized relations with the University of Warsaw within the GK, which offered them one or two short term visits at ICM per semester as part of the study programme, as well as longer stays if this complied with their research work. In addition, we were building up close institutional ties to other research institutions with a similar research scope, beginning with the Charles University in Prague and the University of Milan.

Next, the Visiting Professor Programme and the organization of courses and workshops as well as conferences with the participation of internationally renowned speakers gave our students an excellent opportunity to bring the most influential scientists in their own field to their home turf in Heidelberg, and it gave the visitors ample time to become acquainted with the student’s latest research results.

It was at least of equal importance that without exception all research groups of the GK were actively integrated into the international scientific community, and closely linked with other international leading research groups. It was therefore common practice to send advanced graduate or doctoral students to research visits at groups abroad if this was compliant with the progress of their research. Hence the support of such activities of the GK by the DFG was strongly appreciated.

The GK also encouraged doctoral students to actively participate in international conferences and supported this financially within its budgetary frame, if a paper was presented or a poster had been accepted. Since the subjects of the research groups within the GK covered a wide area, also the approval of the student’s plans by the supervisors was necessary, to make sure the efforts were well invested.

Last but not least, it should be mentioned that ICM and IWR were actively involved in supporting scientists and academic institutions in developing countries through collaboration and exchange. We encouraged our doctoral students to participate in such activities, to contribute to the progress in their research field, but also to gain cross-cultural experiences that might benefit them some day.

As an example, we encouraged them to seize the opportunities given by our close scientific collaboration with the Vietnamese Academy of Science and Technology, such as our annual joint workshops on topics of Scientific Computing, and the triennial International Conference "High Performance Scientific Computing – Modeling, Simulation and Optimization of Complex Processes".

Integration of visiting researchers into the study programme (visiting professor programme)

In order to fulfill its aims the study programme of the GK incorporated the latest international research in modeling, simulation and optimization of complex processes, which made the Visiting Professor Programme of the GK extremely important. It allowed inviting internationally renowned scientists for individual lectures, lecture series and short courses.

In addition, our guests had intensive collaborations with our doctoral students on problems arising from their dissertation projects. Some served as additional advisors in the close sense and as reviewers of the theses or members of the oral examination committee. Our Visiting Professors complemented the scientific expertise within the GK and made a significant contribution to the scientific supervision of the doctoral students.

Apart from the resources for the Visiting Professor Programme, complemented by IWR funds, also our partner institution ICM disposed of several funding sources that enabled stays of visiting researchers. Among those were EU funds from the FP5 for the Centre of Excellence for Multi-Scale Biomolecular Modelling, Bioinformatics and Applications (MAMBA) at ICM, as well as other financial resources from research projects with industry.

The following overview of scientists having participated in the Visiting Professor Programme is separated into short visits (less than one week) and longer stays:

2001:

less than one week	at least one week
R. Lefebvre, Paris G. Feichtinger, Wien F. Remacle, Liège	S. Marron, Chapel Hill R. Longman, New York D. Frantzeskakis, Athen H. Phu, Hanoi

2002:

less than one week	at least one week
F. Potra, Maryland S. Siripant, Chulalong Korn A. Mikelic, Lyon A. Piatnitski, Moskau M. Niezgodka, Warschau S. Wronski, Warschau N. Balashevich, Minsk	M. Osborne, Canberra R. Longman, New York S. Wronski, Warschau

2003:

less than one week	at least one week
M. Niezgodka, Warschau C. lung, Montpellier M. Powell, Cambridge J. Sanday, World Monument Fund (Nepal) F. Richter, Paris B. Lesyng, Warschau A. Woclaw, Gliwice K. Nowinski, Warschau J. Gorecki, Warschau P. Grangeat, Grenoble	J. Reginato, Rio Cuarto H. Phu, Hanoi J. Mizerski, Warschau A. Trykozko, Warschau O. Kostyukova, Minsk

T. Sorokina, Athens (Georgia)	
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2004:

less than one week	at least one week
M. Niezgodka, Warschau M. Zylicz, Warschau H. Zhu, Shanghai T. Miura, Oxford P. Toint, Namur A. Trykozko, Warschau J. Haslinger, Prag M. Bendsö, Kopenhagen M. Berggren, Uppsala P. Weglenski, Warschau M. Feistauer, Prag M. Dembo, Boston A. Mogilner, Davis J. Radomski, Warschau J. Rychter, Warschau H. Dodziuk, Warschau J. Gorecki, Warschau L. Magni, Pavia D. Frantzeskakis, Athen	S. Siripant, Chulalong Korn M. Hegland, Canberra M. Osborne, Canberra O. Kostyukova, Minsk R. Longman, New York U. Ascher, Univ. of British Columbia

2005:

less than one week	at least one week
A. Trykozko, Warschau M. Niezgodka, Warschau J. Baldyga, Warschau L. Gradon, Warschau L. Piela, Warschau B. Lesyng, Warschau W. Wislicki, Warschau M. Zylicz, Warschau P. Weglenski, Warschau K. Frackowiak, Warschau F. Chernousko, Moskau U. Peskin, Haifa V. Veliov, Wien T. Ohtsuka, Osaka G. Worth, Birmingham B. Amadei, Colorado W. Gu, New York B. Oostenbrink, Amsterdam A. Shapiro, Atlanta A. Ben-Tal, Haifa C. Floudas, Princeton A. Mikelic, Lyon D. Golvatyy, Akron A. Swierczwekska, Warschau P. Gwiazda, Warschau M. van der Loo, Nijmegen D. Frantzeskakis, Athen J. Malek, Prag M. Rokyta, Prag V. Dolejsi, Prag	J. Gorecki, Warschau L. Biegler, Carnegie Mellon R. Longman, New York H. Phu, Hanoi G. Fagas, Cork A. Piatnitski, Narvik

2006:

less than one week	at least one week
M. Niezgodka, Warschau	M. Bossi, Pavia

<p>F. Rendl, Klagenfurt S. Kameswaran, Carnegie Mellon M. Thera, Limoges S. Tsou, Oxford L. Andersson, Linköping L. Abrahamsson, Uppsala S. Andrews, Berkeley J. Baldyga, Warschau J. Vandewalle, Leuven J. Trylska, Warschau J. Kästner, Warrington D. Wales, Bishops Stotford J. Majewski, Warschau W. Wislicki, Warschau A. Trykozko, Warschau</p>	<p>C. Albanesi, Pavia S. Siripant, Chulalong Korn G. Fagas, Cork V. H. Tran, Ho Chi Minh City T. A. Phan, Hanoi V. Zavala, Carnegie Mellon Y. Kawajiri, Carnegie Mellon</p>
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2007:

less than one week	at least one week
<p>S. Jbabdi, Oxford T. Tran, Hanoi J. J. Velasquez, Madrid J. Asenjo, Santiago de Chile C. Etchebest, Paris P. Auffinger, Straßburg M. Viloca, Barcelona R. Russell, Burnaby H. Thieme, Arizona State M. Filocha, Warschau G. Kanschat, Texas A&M P. Pardalos, Univ. of Florida J. Ramsay, Montreal R. Finn, Stanford F. Pietrucci, Triest A. Foni, Genf M. Fornassier, Wien V. Milisic, Grenoble S. Nescasova, Prag B. Lesyng, Warschau L. Vicente, Coimbra R. Griesse, Linz C. Scherer, Delft M. Valasek, Prag M. Grünwald, Wien</p>	<p>A. Piatnitski, Narvik A. Skubachevskii, Moskau A. Ito, Warschau V. H. Tran, Ho Chi Minh City N. M. Tran, Ho Chi Minh City R. Suon, Phnom Penh H. Phu, Hanoi T. Roubicek, Prag S. Bunna, Phnom Penh P. T. An, Hanoi M. Ptashnyk, Oxford S. Phasy, Vientiane R. Fletcher, Dundee P. Maréchal, Toulouse G. Carlier, Paris E. Trélat, Orléans D. Preiss, Coventry Z. Strakos, Birmingham</p>

2008:

less than one week	at least one week
M. Niezgodka, Warschau	T. T. Nguyen, Hanoi
B. Lesyng, Warschau	V. V. P. Le, Hanoi
J. Majewski, Warschau	A. Skubachevski, Moskau
K. Bajer, Warschau	G.-Q. Chen, Evanston
M.-F. Carlier, Gif-sur-Yvette	H. Phu, Hanoi
J. Gorecki, Warschau	C. Westbrook, Livermore
F. Multon, Rennes	K.-K. Kang, Suwon
R. Dibble, Berkeley	J. Velaszquez, Madrid
R. Kee, Colorado	M. Saunders, Stanford
D. Lauvergnat, Paris	A. Trykozko, Warschau
F. Chernousko, Moskau	A. Smith, St. Andrews
M. Feistauer, Prag	C. Choquet, Marseille
F. Brezzi, Pavia	G. Kanschat, Texas A&M
I. Bischofs-Pfeifer, Berkeley	H. J. Ferreau, Leuven
S. Macchietto, London	R. Longman, New York
A. Bardow, Delft	O. Kostyukova, Minsk
Y. Velkov, Stockholm	O. Krichevski, Beer-Sheva

2009:

less than one week	at least one week
M. Niezgodka, Warschau	K.-K. Kang, Suwon
A. Trykozko, Warschau	A. Tadjer, Sofia
B. Lesyng, Warschau	H. Phu, Hanoi
J. Majewski, Warschau	R. Longman, New York
K. Bajer, Warschau	O. Kostyukova, Minsk
O. Christiansen, Aarhus	G. Kostin, Moskau
E. Salje, Cambridge	A. Stokes, St. Andrews
M. Herrero, Madrid	
G. Kanschat, Texas A&M	
B. Murdukhovich, Wayne State	
U. Ascher, Univ. of British Columbia	
J. Velaszquez, Madrid	
E. Ovcharov, Edinburgh	
G. Kneller, Paris	
F. Merzel, Ljubljana	
P. Bolhuis, Amsterdam	
M. Field, Grenoble	
B. Rutherford, Saclay	
N. Doltsinis, London	
J. Villa i Freixa, Barcelona	

Appendix I:
Lists of Members