Report on the Hausdorff Trimester Program

Analysis and Numerics for High Dimensional Problems

May - August 2011

Organizers:
Michael Griebel (INS, Universität Bonn, FRG),
Wolfgang Hackbusch (MPI for Mathematics in the Sciences, Leipzig, FRG),
Markus Hegland (ANU, Canberra, Australia),
Christoph Schwab (SAM, ETH Zürich, Switzerland)

Topics

The HIM Workshop was devoted to the following themes.

- Foundation, modelling and complexity of high-dimensional problems
- Geometric multi-scale analysis and high-dimensional analysis
- Statistical learning theory, data analysis and data mining
- Stochastic approaches, path integral formulations and their approximations, rough paths theory
- Renormalisation theory and multi-scale modelling methods
- Numerical approximations in high dimensions (sparse grids, Kronecker products, $\mathcal{H}$-matrices, exponential approaches, adaptive approximation, dimension reduction)
- Application areas in physics and the natural sciences (Schrödinger and Dirac equations, Langevin, master and Fokker-Planck equations, differential equations with stochastic parameters and stochastic partial differential equations)

Goals

Partial differential equations related to high-dimensional parameter spaces are a major challenge and of increasing importance in the sciences and in engineering. For such problems, the so-called "curse of dimension" prevents an efficient treatment by standard numerical discretisation for most of the problems. The resulting enormous computational challenges cannot be met merely by larger computers, but require fundamentally new mathematical and algorithmic ideas. These can only be envisioned by an interdisciplinary attempt which involves modelling, analysis, stochastics and numerics.

While several topics of high-dimensional problems are in a certain sense well understood from a mathematical perspective, a large number of technical issues are rather open and mathematical issues, and related algorithms and applications are still relatively undeveloped. The objective of the proposed semester program was to bring together internationally leading experts from analysis, stochastics and numerics to survey the current state of the art, to present the different approaches, to possibly further investigate common problem formulations, and to initiate research directions for analysis, development and implementation of innovative methods and algorithms for the numerical solution of high-dimensional problems and partial differential equations. Particular attention was directed at promising application fields of science and engineering and, particularly, at high-dimensional data analysis. In recent years, in part as response to the increasing appearance of high-dimensional PDEs in applications, dimension-reduction techniques for modeling by lower-dimensional surrogates, (such as, for example, DFT in electron structure calculations), numerical path integral approximation and numerical techniques which circumvent the curse of dimensionality have been addressed independently in different fields.

The 2011 HIM trimester programme allowed, for the first time, to place these hitherto rather incoherent developments in a broader perspective and opened several perspectives for dealing with high-dimensional PDEs from a combined point of view, involving modelling, analysis, stochastics and numerics.

Organization

The activities included five topical workshops and two summer-schools in addition to several seminars. Moreover, the 4th Workshop on High-dimensio-

nal Approximation (HDA) was held during the trimester in Bonn.

The goal of the first workshop was to strengthen the research on the mathematical understanding and analysis of sparse grid discretisation. Particular focus was given to aspects arising from applications. It was organised by Hans-Joachim Bungartz (TU Munich), Jochen Garcke (Bonn), Michael Griebel, and Markus Hegland. More than 40 researchers from four different continents attended the workshop in Bonn, Germany, from May 16 to 20. Speakers included Jochen Garcke, Christoph Reisinger (Oxford), Rob Stevenson (Amsterdam), Hermann G. Matthies (Braunschweig), Helmut Harbrecht (Basel), Ralf Hiptmair (ETH Zürich), Wolfgang Hackbusch (MPI Leipzig), Heinz-Jürgen Flad (TU Berlin), Dung Dinh (Hanoi), Thomas Gerstner (Frankfurt) in addition to many postdoctoral fellows and PhD students. The presentations were evenly distributed between mathematicians and computational scientists and applications included control theory and signal processing, quantum chemistry, plasma physics, option pricing, economics and statistics. Selected presentations were published in Springer's Lecture Notes in Computational Science and Engineerings. The exchange at the workshop was so inspiring especially for the early career researchers and PhD students that it was decided to make this the first in a series of workshops. The second workshop on sparse grids was held at the Institute for Advanced Study of the TU Munich from July 2 to 6, 2012. The format of this workshop was identical to the original HIM workshop and included 32 talks.

The second workshop organised by Jochen Garcke from May 30 to June 3 brought together researchers interested in manifold learning and dimension reduction. The 40 participants included researchers from machine learning, numerical mathematics, linear algebra, topology, geometry, and statistics. Some of the key topics featured were the applications of manifold learning to real world problems, theoretical limitations of current algorithms, connections between the different algorithms, dimensionality estimation and the efficient realization of manifold learning algorithms. Presentations were given, among others, by John Lee (Louvain), Neil Lawrence (Manchester), Dan Kushnir (Yale), Rodrigo Iza Teran (Fraunhofer Bonn), Matthias Hein (Saarbrücken), Alexander Gorban (Leicester), Michael Kirby (Colorado State), Felix Krahmer (Göttingen), Zhenyue Zhang (Zhejiang), Xavier Pennec (INRIA).

The third workshop was held from June 20 - 24, 2011. Its focus was on the theoretical aspects of high-dimensional problems and information-based complexity. The goal was to get a better understanding of problems of

higher dimensions from the view of geometric analysis, functional analysis, stochastics and complexity theory. Here, the concentration of measure phenomenon, ultrametric spaces, dimension embedding and reduction, learning theory or information based complexity are well studied, but these different areas developed independently without much interaction. The third workshop brought together researchers interested in the areas of geometric and functional analysis, information based complexity and multiscale analysis. It was co-organised with the senior participants Vladimir Pestow (Ottawa), Ian Sloan (UNSW Sydney), and Henryk Wozniakowski (Columbia, NY and Warsaw). Presentations were given by Vladimir Pestov, Peter Binev (South Carolina), Alexander Gorban (Leicester), Thomas Kühn (Leipzig), Michael Gnewuch (Kiel), Aicke Hinrichs (Jena), Josef Dick (UNSW Sydney), Erich Novak (Jena), Greg Wasilkowski (Kentucky), Leszek Plaskota (Warsaw), Henryk Wozniakowski, Erzsebet Merenyi (Rice), and Holger Rauhut (Bonn). There was a lively exchange between the groups from information-based complexity, pure mathematics and approximation theory.

The fourth workshop was organised by Lars Grasedyck and Wolfgang Hackbusch. Its subject was on tensor approximation in high dimensions. The topics included multilinear algebra, numerical analysis for tensor approximations, efficient arithmetics in data-sparse tensor formats with special emphasis on the Schrödinger equation and on PDEs with stochastic/many parameters and applications of tensor approximations in biology, chemistry, physics and engineering. Speakers included Hans de Sterck (Waterloo), Lars Grasedyck (Aachen), Rob Stevenson (Amsterdam), Reinhold Schneider (Berlin), Lek-Heng Lim (Chicago), Ivan Oseledets (Russian Academy of Sciences), Thomas Huckle (Munich), and Boris Khoromski (Leipzig). The workshop was held in the first week of August and was supported by a summer-school on Hierarchical Tensor Approximation and on $\mathcal{H}$-matrices.

The fifth workshop was organised by Christoph Schwab from August 8 to 12, 2011. Its focus was on high-dimensional aspects of stochastic PDEs. Here, principal algorithmic directions were presented and the mathematical foundations for these novel solution methods were discussed. In particular, it addressed the mathematical formulation and regularity of PDEs with random inputs, sparsity in tensorized discretization schemes and various implementational aspects. Furthermore, the relations to recently emerging concepts around adaptive low rank techniques in multilinear algebra matrix computations were of particular interest. Presentations were given, among others, by Stephan Dalke (Marburg), Siddhartha Mishra (Zürich), Mikhail Lifshits (St.

Petersburg), Viet Ha Hoang (Nanyang), Stig Larsson (Chalmers), Helmuth Harbrecht (Basel), Olivier Le Maitre (LIMSI-CNRS) and Fabio Nobile (Milano).

Furthermore, a Trimester Seminar was organized which included 3 presentations (total of 5 hours). These provided an in-depth discussion of tensors and their connections to sparse grids. The presentations were given by Wolfgang Hackbusch (2 seminars) and Reinhold Schneider (TU Berlin).

Results

Scientific results of the trimester program are documented in the 21 publications on the webpage. Furthermore, one of the organisers finished a comprehensive monograph on 'Tensor Spaces and Numerical Tensor Calculus' during the trimester (published by Springer). New collaborations were started at the trimester across subdisciplinary boundaries and resulted in papers by Chernov and Schwab, Hegland and Wasilkowski, Dinh and Ullrich, Lifshits and Wozniakowski. Selected results of the first workshop have appeared in Springers Lecture Notes in Computational Science and Engineering [Sparse Grids and Applications, edited by J. Garcke and M. Griebel, LNCSE 88, Springer 2013].