Report on the Hausdorff Trimester Program

Multiscale Problems: Algorithms, Numerical Analysis and Computation

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Topics

The Hausdorff Trimester Program (HTP) *Multiscale Problems: Algorithms, Numerical Analysis, Computation* concerned the numerical algorithms that underlie the computer simulation of complex processes in engineering and the sciences and, equally important, the mathematics behind them to foresee and assess their performance in practice. Among the target applications were the mechanical analysis of composite and multifunctional materials, porous media flow, wave propagation or the simulation of condensed matter.

The main characteristic of such problems is that the complex interplay of non-linear effects on various non-separable length and time scales essentially determines the overall properties. Although mathematical physics provides sound models of partial differential equations that implicitly describe these processes, the problems are intractable for an analytical solution such that their understanding and control rely on numerical simulation. From a computational point of view, however, a direct numerical treatment of such problems is often not feasible due to the fact that the resolution of all details on all relevant scales may lead to a number of degrees of freedom and computational work which exceed today's computing resources by multiple orders of magnitude.

The observation and prediction of physical phenomena from multiscale models, hence, requires insightful algorithms that adaptively select the most relevant scales based on a priori and a posteriori knowledge of the problem, effectively represent unresolved scales and quantify errors and uncertainty.

In this connection, the HTP addressed all aspects of multiscale computational partial differential equations including mesh generation, design of suitable shape functions, error analysis, adaptivity, the development and analysis of linear and non-linear solvers, software development and simulation. Amongst the particular trends were numerical (deterministic and stochastic) homogenization, model reduction techniques in the context of parameterized and inverse problems and the consistent coupling of different mathematical models across length and time scales.

Goals

On a the scientific side, the HTP aimed at the understanding and advancement of computational techniques for the efficient simulation of multiscale processes and techniques that can provide the effective properties of unresolved scales and utilize such upscaled information to efficiently attain an approximation of sufficient quality or even similar quality as a non-feasible fully resolved simulation. The HTP enhanced the development of novel multiscale methods so that the accurate, reliable and efficient computer simulation of multiscale problems becomes feasible in advanced parallel and distributed computing environments.

For this purpose, the HTP aimed to bring together experts from the scientific communities of computational multiscale modeling, computational partial differential equations and fast solvers to bridge the gap between classical theories and recent prospective trends in numerical analysis, e.g. numerical homogenization beyond scale separation, medius error analysis, low-rank matrix and tensor approximation techniques, sparse super-localization, discrete network methods, optimality of adaptive mesh-refinement, isogeometric analysis and consistent atomistic-continuum coupling.

Organization

In the framework of the HTP we organized a winter school, two thematic workshops and two seminar series that are briefly outlined below.

Winter school on Numerical Analysis of Multiscale Problems The Winter school on the *Numerical Analysis of Multiscale Problems* marked the kickoff of the HTP. With 64 participants from 14 countries the capacity of the HIM lecture was fully exhausted. The 5 lecture series given by Bjorn Engquist, Robert Lipton, Daniel Peterseim, Rob Stevenson and Barbara Wohlmuth represented the full broadness of the thematic spectrum of the program and its methodological diversity. Despite the introductory character of the lectures addressing primarily graduate students and junior researchers the lectures succeeded to be of great value also for the senior experts participating in the HTP and their integration.

Workshop on Numerical Inverse and Stochastic Homogenization The first thematic workshop on numerical homogenization had 46 participants from 12 countries. The talks addressed homogenization problems from very different angles including (stochastic) analysis (Antoine Gloria: Fluctuations in stochastic homogenization), domain decomposition (Ralf Kornhuber: *Numerical homogenization and subspace correction*), tensor calcusus (Ivan Oseledets: *QTT-FEM solvers for elliptic multiscale problems*)and many more. Dietmar Gallistl even bridged the classical theory of periodic homogenization and state-of-the-art numerical homogenization techniques. Regarding the inverse problem of homogenization there have been contributions from optimal transport (Yunan Yang: *Optimal transport and its application on seismic inversion*) and statistical inversion (Sebastian Krumscheid: *Homogenization via Statistical Inversion: Obtaining coarse-grained models from multiscale data*), to mention only a few. Some of the results of the HTP described below can certainly be traced back to questions originating from the fruitful discussions during this workshop.

Workshop on Non-local Material Models and Concurrent Multiscale Methods The second workshop on non-local material models and concurrent multiscale methods essentially marked the closing event of the HTP. There were 38 participants from 11 countries. This workshop addressed the interdisciplinary aspects of the HTP with scientific contributions from engineers, e.g. Jiun-Shyan Chen (*Fracture to damage multiscale mechanics and modeling of brittle materials*) and Wing Kam Liu (*Self-consistent clustering analysis for data-driven design of multiscale material systems*). Among many interesting talks on peridynamics, fracture models and multiscale methods the workshop also comprised first results of the HTP (by Guanglian Li and Mira Schedensack).

Trimester & Junior Seminar We established a regular research seminar at the Hausdorff Institute with lectures of 21 senior scientists and selected younger participants. The lectures covered all topics of the program from *Universal scalable robust solvers from computational information games* by H. Owhadi (Caltech), *Convergence of discrete exterior calculus* by G. Tsogterel to the *Mathematics of liquid crystals* by John Ball.

In addition to the Trimester seminar, D. Gallistl established a Junior seminar where PhD students and young PostDocs get the chance to report on there research in a smaller audience. This turned out to be a nice forum for informal discussions and fostered interactions between the younger participants that led to fruitful collaborations (e.g. Gedicke and Brown or Gallistl and Verfürth).

Results

The participants of the HTP have been quite productive. Until today, 37 preprints have originated from the program and 3 preprints are in preparation. Substantial parts of several PhD and habilitation thesis have also been written during the HTP.

The scientific success of the program is clearly reflected by these results ranging from the theory of finite elements for computational partial differential equations [13, 12, 28, 4] to multiscale applications in material sciences [37], geophysics [42], ecology [30] and condensed matter physics [1]. Among the core results are new methods for numerical wave propagation propagation heterogeneous media and their numerical analysis [25, 40, 26, 34, 38, 27], a priori and a posteriori estimates in (numerical) stochastic homogenization and uncertainty quantification [19, 18, 24, 17, 15, 29], numerical treatment of multiphysics problems [2, 31] and optimal control problems [9], the development and analysis of non-local fracture models [32, 33, 16], non-divergence form partial differential equations [35, 36, 21], novel convergence results in elastoplastic evolution [14], computational techniques for interface problems [5, 39] as well as numerical analysis in the context of singular flows [7] and nonlinear eigenvalue problems [6],

Even more striking then these numerous diverse results is the initiation of connections between some of these seemingly diverse results that would probably not have been happened without the HTP. Examples are the connection of numerical homogenization and fractional calculus [11, 10], the bridge between numerical and periodic homogenization [23], the application of tensor calculus in space-time Galerkin methods [8], the impact of domain decompostion in the theory on the decay of Green's functions and eigenfunction localization in the theory partial differential equations [3], optimal transport and multiscale analysis [42], finite element exterior calculus and numerical homogenization [22] to study negative refraction phenomena of electromagnetic waves. It is exactly such unexpected connections that make the program a success story.

Apart from the preprints mentioned above, the impact of the program on younger participants is clearly shown by the fact that 3 Master students finished their theses and started PhD projects on topics originating from the HTP (Roland Maier, Dora Varga and Denis Düsseldorf). Moreover, Barbara Verfürth wrote significant parts of her PhD thesis [41] during her stay and Dietmar Gallistl finished essential parts of his habilitation thesis [20]. Two more habilitations with contributions from the HTP are in preparation (Mira Schedensack and Josche Gedicke).

During the HTP, two of the organizers initiated a follow-up workshop on Computational Multiscale Method at Oberwolfach which will be held in summer 2019. We further hope that there will be the possibility of a workshop at the Hausdorff Institute in 2020/21.

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