1.3 Leibniz Research Network “Mathematical Modeling and Simulation”

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One of the hallmarks of mathematics is its universality. The same mathematical concepts and methods can be fundamental for the understanding of very different phenomena in nature, technology, economy, and many other aspects of human life. This universality also relates to modern methods of applied mathematics, which include the development of algorithms for simulation and optimization of complex problems, or the handling of large sets of data.

Fig. 1: *Member institutions of the Leibniz MMS network*

In the light of this cross-sectional and transdisciplinary character of mathematics, it was a natural step for WIAS to take the initiative for a research network on Mathematical Modeling and Simulation (MMS) around 2013, in line with the continuous efforts of the Leibniz Association to further strengthen cooperation between its institutions. The MMS network has by now 34 member institutes from all sections of the Leibniz Association. Indeed, these are not only institutes from *Section*

D: Natural Sciences, Engineering, having in some cases large departments devoted to simulation-based research with an outstanding expertise in their respective fields, but also institutes with only a small group of scientists working on MMS, where the cooperation within the network can be particularly important to open new opportunities.

A major activity within the network was the organization of an annual series of workshops, the *Leibniz MMS Days*, which so far have taken place at five different Leibniz institutions. Identifying scientific fields of common interest among the network members and putting a specific emphasis on the specialization of the hosting institute, each workshop comprised several topical sessions in various fields, such as

- computational and geophysical fluid dynamics (CFD & GFD),
- systems biology and genetics,
- statistical data analysis,
- condensed matter.

Another purpose of these meetings is to address general topics concerning basic requirements and conditions, which are of interest for researchers doing MMS, independent of their specific field. This included talks and discussions on the development and management of research software as well as questions related to the handling of research data, or scholary research communication (open science, software citation). The intensive work on the above-mentioned topics made it possible to substantially support the Mathematical Research Data Initiative (MaRDI) within the German National Research Data Infrastructure program (NFDI). The Leibniz Association has also appointed experts from the network, Georg Feulner (PIK) and Jürgen Fuhrmann (WIAS), for an ad-hoc group on research software within the framework of the priority initiative *Digital Information* of the Alliance of German Science Organisations.

Since 2018, the network has also been organizing annual summer schools for Ph.D. students whose topics were *Statistical Modeling and Data Analysis* and *Modern Programming Languages for Science and Statistics: R and Julia*. These schools took place at Oberwolfach Research Institute for Mathematics, which is also a member of the MMS network.

Fig. 2: *Participants of the MMS summer school 2019*

The role of computational and geophysical fluid dynamics in MMS

Dynamics of gases and liquids are relevant for a large number of Leibniz institutes and, hence, establish the most prominent common research topic within the MMS network. It is essential for the transport of nutrients and metabolites in animals and humans, as well as for weather forecasts and the prediction of climate change, for the quality of modern semiconductor wafers grown from crystal melts, or for the development of magnetic fields on the earth or on other celestial bodies. The basic physical laws describing the motion of fluids, the Euler and Navier–Stokes equations, form today the root of a huge, diverse, and sometimes confusing family of related mathematical models. Similarly diverse are the approaches in the research of the members of the MMS network. Some of them mainly apply commercial or non-commercial simulation tools to address specific questions from their field of research. For other research institutes, which develop their own software, scientific computing and implementation issues play a major role. Finally, WIAS as a mathematical institute performs also basic mathematical research and rigorous numerical convergence analysis, in order to get a theoretical understanding about the advantages and disadvantages of various competing simulation algorithms and to improve today's powerful simulation tools even further.

Turbulence simulation with open source CFD solvers

During the MMS Days 2017, a collaboration between WIAS, the Leibniz Institute of Agricultural Engineering and Bio-economy (ATB), and the Leibniz Institute for Tropospheric Research (TROPOS) was initiated, with the purpose of exchanging experiences in the context of turbulence modeling, and, eventually, of assessing the performance of open source CFD solvers [3].

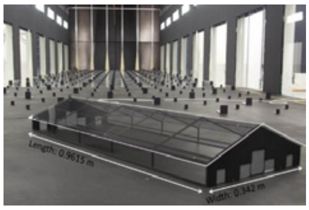

Fig. 3: Scaled barn model in the wind tunnel

The first goal was to demonstrate that these codes are able to provide reliable simulations in agricultural applications, reducing existing reservations towards the use of open source tools in this community. The second goal was to compare – in a realistic scenario – two solvers based on different meshes, discretization schemes, and turbulence models: OpenFOAM, a well-established free and open source solver and ParMooN (Parallel Mathematics and object-oriented Numerics), a finite element library developed at WIAS. The benchmark problem consisted in the simulation of the cross flow in a typical naturally ventilated barn. Experimental data were obtained via measurement campaigns in a 1:100 scaled wind tunnel model of the barn at the ATB (Figure 3). The turbulent flow was simulated solving numerically the time-dependent Navier–Stokes equations on a computational domain of 3 m length and 1 m height, including the floor and roof geometry of the wind tunnel model (see Figure 4).

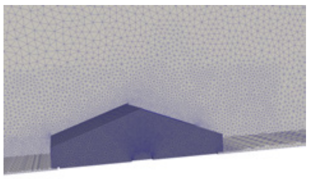

Fig. 4: Section of one spatial discretization (mesh) used in ParMooN

The results showed that both solvers achieve a good agreement with experimental data for time-averaged stream-wise and vertical-wise velocities. In particular, the air exchange was predicted with relative errors less than 5% compared to the experimental results. With respect to the turbulent quantities, good agreements at the second (downwind) half of the barn inside and especially outside the barn could be achieved. Hence, he solvers proved to be promising tools for the accurate prediction of time-dependent phenomena in an agricultural context, such as the transport of particulate matter or pathogen-laden aerosols in and around agricultural buildings.

Modeling, simulation, and optimization of geothermal energy production

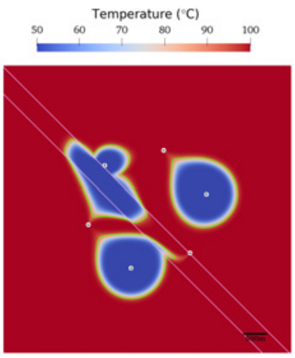

Fig. 5: *Temperature field in a hexagonal multi-well configuration with a thin damage region with lower permeability*

Geothermal energy, i.e., the energy stored as heat in the subsurface, constitutes a renewable resource that can be sustainably recovered using diverse concepts, such as district heating in urban environments. Geothermal plants operate through multiple *wells*, from which hot water is extracted (production wells) and colder water is injected (injection wells). The collaboration between WIAS and the Leibniz Institute for Applied Geophysics (LIAG), initiated during the MMS Days 2018, aimed at applying advanced finite element methods for porous media flows, combined with an open source optimization framework (NLopt), for the modeling, simulation, and optimization of the geothermal energy production.

The considered problem consisted in optimizing the installation – given a particular topological structure – in order to maximize the extracted energy and delaying the so-called *thermal breakthrough*, i.e., the time when the cold water front reaches the production well. In [4], we simulated the energy production process considering a Brinkman problem for the groundwater flow in a saturated aquifer and an advection-diffusion model for the temperature distribution. We investigated numerically the optimal positioning and spacing of multi-well arrays in the form of a lattice and a hexagonal structure, considering structural heterogeneities as well as varying reservoir temperatures. In particular, the results demonstrated that the proposed numerical framework is able to efficiently handle generic geometrical and geological configurations, and can be thus flexibly used in the context of multi-variable optimization problems.

Novel well-balanced schemes for the compressible Navier–Stokes equations

The annual "MMS Mini Workshop on CFD & GFD" triggered a collaboration between the Leibniz-Institute of Atmospheric Physics (IAP) and WIAS. Typical challenges of flow simulations are certain kinds of *extreme force balances* that can develop during the time evolution of the fluid motion. Many kinds of different physical forces determine the fluid motion simultaneously, e.g., the pressure gradient, the inertial force, the friction force, the Coriolis force, or the centrifugal force. But often only a few forces are dominant at a certain point in time. The starting point for the collaboration was substantial progress at WIAS on the question how to handle certain extreme force balances like *hydrostatics, geostrophic flows, high Reynolds number flows* in incompressible flows, i.e., in liquids [1], providing a novel approach how to implement a basic mathematical law, namely "gradient fields are irrotational", in the simulation algorithms. Since in meteorology, such extreme force balances in the atmosphere play a similar role, the question arised whether the WIAS results could be extended from incompressible to the mathematically much more challenging compressible flows, i.e., from liquids to gases. As a result, a novel kind of so-called *well-balanced schemes for compressible flows* was constructed that are able to handle certain kinds of extreme force balances in low Mach number and stratified flows, which are typical for meteorological applications [2]. Furthermore, the notion of a *gradient-robust scheme* was introduced.

A network dynamics model for the auditory cortex

Another cooperation within the MMS network was established between the Leibniz Institute for Neurobiology (LIN) in Magdeburg and WIAS. The subject of research here is a dynamical network model for the auditory cortex in the brain, which was developed at LIN together with colleagues from the Lancaster University, UK. This model is based on a detailed knowledge of anatomical and physiological structures (see Figure 6) and should contribute to a deeper understanding of the experimental findings in the *Non-Invasive Brain Imaging* lab at LIN.

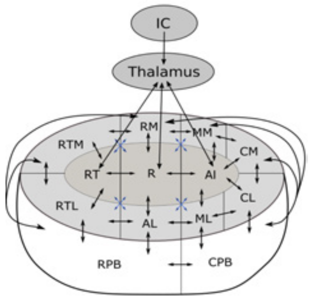

Fig. 6: *Network structure in the auditory cortex: connectivity between different core, belt, and parabelt regions*

The purpose of the ongoing cooperation is a mathematical analysis of the dynamics of this model using advanced tools from dynamical network theory. In particular, we are using multiple time-scale methods to analyze the adaptation to multiple external stimuli. In this way, the adaptation of the cortical response to repetitive stimulation could be understood as a result of the short-term synaptic depression that was included in the model by a dynamical adaptation of the connectivity weights with a recovery on a slow time scale, see Figure 7. Moreover, a hierarchical network approach was used to describe the connectivity structure on different levels of complexity and, in this way, to understand the role of the physiological complexity on a functional level.

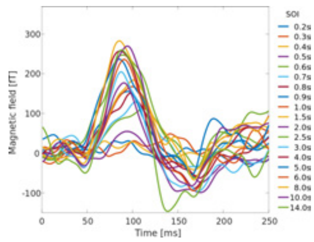

Fig. 7: *Simulated response of the auditory cortex for repetitive stimulation at different rates*

Conclusions and outlook

With the increasing importance of interdisciplinary research and cooperation, the Leibniz MMS network establishes a unique tool to strengthen the role of mathematical research within the Leibniz Association and to raise synergies among the member institutes. For WIAS it provides the opportunity to identify new important fields for its own research and to initiate collaborations with the prospect of launching joint, third-party funded projects.

References

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