In the previous chapters, topics such as fluid mechanics, structural mechanics, aerodynamics, thermodynamics, chemistry, combustion, and so forth have been addressed. In the following, another degree of interdisciplinary research is emphasized. The articles clearly show the link between applied mathematics, fundamental physics, computer science, and the ability to develop certain models such that a closed mathematical description can be achieved which can be solved by massively parallel algorithms on up-to-date high performance computers. In other words, it is the collaboration of several scientific fields which defines the area of numerical simulations and determines the progress in fundamental and applied research. The subsequent papers will confirm simulations to be used to corroborate physical models and to develop new theories.

In the contribution of the Goethe Center for Scientific Computing of the Goethe University Frankfurt mathematical modeling is considered to enhance the understanding of permeation processes in the skin. For the epidermis, a morphology model consisting of agglomerated tetrakaidecahedra was proposed. A tetrakaidecahedron (TKD) is a polygon with 14 faces providing a dense spatial packing. This property has been discovered by Lord Kelvin studying foam cells. Based on TKD shaped cells a geometry model for the stratum corneum (SC), i.e., the outermost layer of the epidermis was introduced. This region is believed to be responsible for the barrier property of the skin. Nowadays, computing interactions in large networks of cells became feasible. To fully resolve the highly differing scales between corneocytes and the surrounding lipid layer, very fine grids are required. Considering the complex TKD based geometric model and the unstructured nature of the associated grids, massively parallel computers are required. In the article

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of the Goethe University Frankfurt the parallel meshing involved in preparing distributed grid hierarchies for the application of massively parallel multigrid solvers on TKD based grids is discussed.

Seismic applications of full waveform investigation are discussed by the Geo-
physical Institute of the Karlsruhe Institute of Technology. Since natural resources are precious, the number of underground constructions increases. It is important to map earth’s geological structures accurately by collecting seismic data and transforming them into subsurface images. Therefore, full waveform inversion (FWI) that accounts for the full information content of seismic recordings is developed. FWI retrieves multiparameter models of the subsurface by solving the full wave equation. It allows to map structures on sub-wavelength scales. Thus, FWI helps to improve both petrophysical interpretation and geotechnical characterization of the subsurface. The focus of this study is on the implementation of the time-domain FWI and its application to seismic field-data problems. It comprises two- and three-dimensional modeling of viscoelastic wavefields and exploits straightforward and efficient parallelization by domain decomposition and source parallelization leading to a significant speedup on parallel computers.

The contribution on the impact of pores on microstructure conduction is from the Institute of Applied Materials, Karlsruhe Institut of Technology and the Institute of Materials and Processes, Hochschule Karlsruhe Technik und Wirtschaft. Several of the most important problems in the research of materials science deal with ceramic materials. Besides ceramics, many materials with unique electrical, chemical, mechanical and optical properties can be found. However, in most cases, processing ceramics and fabricating ceramic parts involve powder techniques and, in particular, sintering to form a functional microstructure. During sintering, a body of compacted powder redistributes its volume to fill inner cavities or pores. This process is driven by minimizing the surface energy and involves diffusion of material and simultaneous migration of interfaces. According to a qualitative model, the sintering process can be divided in three stages. In the initial stage, particles are in contact with each other forming a grain boundary and a sintering neck. In the intermediate stage, the surface energy drives the coalescent network of particles to local shape changes and enhanced shrinking. In the final stage of sintering, the remaining porosity is decreased to 10% and grain growth starts to occur in addition to shrinkage and diffusion. This grain growth decreases the driving force for further sintering and is undesirable for most applications, but hard to avoid. In this contribution, a model to treat pore coalescence and to describe more complex pore interactions is introduced.

The interior dynamics of the terrestrial planets is considered in the contribution of the Institute of Planetary Research of the German Aerospace Center and the University of Applied Sciences in Berlin. Numerous data from various space missions over the past decades have revealed that all other terrestrial bodies apart from the Earth operate in the so-called stagnant lid regime. While the surface of the Earth is broken into seven major plates, the surface of all other terrestrial bodies is covered by an immobile layer. These two different convection styles have important implications for the interior evolution and result in different evolutionary paths for
the volcanic outgassing and the core cooling. The atmosphere and the magnetic field are fundamental in maintaining habitable conditions at the surface by regulating the temperatures to allow for liquid water and shielding against solar radiations. In order to constrain the conditions necessary for habitability it is important to understand the thermo-chemical evolution of the interior of the Earth and other terrestrial bodies. To this end, numerical simulations of planetary interiors have become one of the most important tools to tackle complex fluid dynamics problems. In this study recent improvements and results using the mantle convection code Gaia will be presented.

The contribution by Mario Heene, Alfredo Parra Hinojosa, Michael Obersteiner, and Dirk Pflüger presents results from the EXAHD project. EXAHD is one of the sixteen cross-disciplinary consortia in DFG’s Priority Programme 1648 “SPPEXA—Software for Exascale Computing”. The overall research topic of EXAHD is to demonstrate that higher dimensional simulation problems—here the 5D gyrokinetic equations in plasma physics—can be successfully, efficiently, and scalably tackled via minimal-invasive extensions to existing software (here GENE) with the help of the sparse grid combination technique. The concrete topic of the paper presented here, however, has a different flavor. It explores the elegant fault-tolerance features the combination technique offers through its multi-level characteristics. This means an algorithmic or application-driven fault tolerance that can do without checkpointing or process replication—which will be an asset in exascale times.