Berlin Mathematics Research Center
MATH+

Descriptions of Application Areas, Emerging Fields and Transfer Units

Application Areas (AA)

AA 1 "Life Sciences" (Klipp, Noé, Schütte)

In recent years, there has been a revolution in the capability to measure and observe the processes of life on many temporal and spatial scales. Simultaneously, our ability to perform extensive simulations of molecular, cellular, and tissue-scale processes has substantially improved and will continue to do so. Despite the impressive progress that has been made, fundamental challenges exist that are not systematically solved, in particular, the timescale barrier and the accuracy barrier: The timescale barrier results from the fact, that many processes occur on timescales that are not accessible to direct numerical simulation on the level of required resolution, even on dedicated supercomputers. When trying to circumvent this problem by means of models with reduced resolution, it is very difficult to achieve the required level of accuracy (accuracy barrier).

AA1 is focused on developing next generation tools for spatiotemporal modeling and simulation across the molecular and cellular scales by means of new data-driven multiscale modeling methods that permit the simulation of realistic molecular and cellular processes and overcome the timescale and accuracy barriers of existing approaches. Projects in AA1 target seamless integration of new mathematical approaches with incorporation of experimental data, massive simulation, and/or large-scale data analysis.

AA 2 "Materials, Light, Devices" (Kornhuber, Mielke, Müller)

The modeling and simulation of advanced materials, which includes solids and fluids, provides the key to future generations of modern devices relying on physical effects on the micro, nano or quantum scale. Examples include organic LED displays, single-photon emitters, tunable nanopores, or lithium-ion batteries.

Truly predictive mathematical models typically involve coupled hierarchies of multiple scales and physical regimes. Efficient and reliable numerical simulations are typically based on sound thermodynamical models in combination with structure preservation in subsequent model reduction and discretization. The increasing availability of experimental and process data arising from modern measurement and storage opportunities allows for complementing physics-based descriptions based on partial differential equations by novel data-driven modeling techniques. This opens the door to a new predictive quality of numerical simulations in a multitude of applications.

The current projects cover the following topics: hybrid electrothermal modeling for OLEDs, excitons in polymer chains, quantum-classical modeling for quantum-dot lasers, data-driven approximation of electronic band structures for nanodevices, electrocatalytic effects in solvents and their boundary layers, nonlinear behavior in suspension flows.

AA 3 "Networks" (Joswig, Skutella)

Next generation networks with their abundance of real-time data represent a prime example of how increasing digitization raises the technological and social need of progressing mathematization. The wealth of interconnections between formerly mostly independent entities is creating new and complex network structures and fundamentally changing the way in which existing networks (such as, e.g., traffic, logistics, telecommunication, energy, biological, and social networks) can be analyzed, designed and operated, what users expect, and how they behave and interact.

Research in AA3 addresses these challenges and develops the necessary mathematical foundations and efficient algorithmic techniques for dealing with next generation networks that are large and complex, changing and evolving over time, and can often not be observed directly or in their entirety. This requires, in particular, innovation in discrete applied mathematics, efficient algorithms, and related fields.

AA 4 "Energy and Markets" (Mehrmann, Reiß, Tischendorf)

A secure efficient and sustainable energy supply is a key priority for society. The operating environments for energy systems have changed drastically over the past decade and have created a need for fundamental revisions to classical practices in almost all energy sectors. The associated challenges stem from a multitude of different energy sources, including fossil fuels and different types of renewable energies, or energy carriers, such as gas/oil or power networks, different storage devices, including batteries and water reservoirs, and a multitude of energy conversion options, such as power-to-gas or gas-to-heat.

AA4 forms a framework of interdisciplinary teams of mathematicians, scientists, engineers, and economists to develop new mathematical methods for modeling, simulation, optimization, risk analysis and real-time decision-making under uncertainty in energy production/distribution under market conditions. The research topics include energy-based modeling via hierarchies of port-Hamiltonian partial differential algebraic equations, stochastic modeling of intraday electricity markets, equilibria for energy markets under energy transport constraints, rough analysis and deep networks for optimal control in energy markets, analysis and simulation of stochastic partial differential algebraic equations, optimization with implicit probabilistic constraints and a numerical treatment of Maxwell's equations for isolated optical sources and scatterers in periodic environments to optimize solar fuel devices.

Emerging Fields (EF)

EF 1 "Extracting Dynamical Laws from Complex Data" (Eisert, Kutyniok, Müller)

This Emerging Field aims to develop novel methods, through combining machine learning and mathematical process simulation, which are able to derive effective dynamical laws from data. As a result, we anticipate to obtain models which generate understanding and physical insights, and can be simulated efficiently, resulting in unprecedented speed-ups compared to the often intractable classical direct simulation methods such as for the time-dependent Schrödinger equation in quantum processes.

This program faces several challenges. First, current machine learning methods are often black-box approaches, which are not sufficient for scientific simulation and measurement data. And, second, current machine learning methods study mostly static, stationary, and complete data, however scientific data is often dynamic, nonstationary, incomplete, multimodal, and multiscale.

Consequently, the projects within this Emerging Field focus either on the development of a theory for machine learning, in particular, deep learning, or approach this problem complex from the application side. Moreover, the projects are typically characterized by a high degree of interdisciplinarity as well as by utilizing a combination of numerous mathematical areas.

EF 2 "Digital Shapes" (Bobenko, Hege)

The shape of material objects plays an important role in a variety of research and application areas. Shapes can be constructed or computed, e.g., in engineering and architecture, or they can be empirically given, e.g., in medicine, materials science and archaeology. Shape is a key factor in understanding complex phenomena, gaining knowledge and optimizing industrial processes. For computerized processing, shapes generally need to be discretized.

A major challenge in the digital age is to deal with the increasing amount of data, for example in large-scale clinical studies. This requires the development of robust, efficient, and automatic analysis and processing tools. Such tools must be based on flexible and geometrically consistent descriptions of complex and realistic geometries.

EF2 deals with the mathematics behind this: What are smooth discrete shapes, how can shapes be reconstructed, interpolated, compared and characterized? Specific questions we are concerned with are the definition and theory of smooth discrete surfaces, the theories and algorithms for generating particularly regular volume triangulations, for characterizing cellular microstructures topologically and geometrically, and for reconstructing and analyzing parameter-dependent shapes.

EF 3 "Model-based Imaging" (Hintermüller, Spokoiny)

Motivated by applications in magnetic resonance imaging (related to fingerprinting and multimodality), electron and X-ray microscopy, as well as the identification of particle properties from macroscopic data, the research in EF3 has its focus on the following main directions: (i) Integrated physics-based imaging (IPI) including model learning based reconstruction; (ii) Information extraction from multimodal data; (iii) Advanced variational methods and solver design for problems with huge-scale data.

One of the main perspective goals of EF 3 is to extend the notion of integrated physics-based imaging to other modalities such as X-ray microscopy, where the state system will be related to Maxwell's equations, or electron-holography, where phase-information, leading to a notoriously complicated retrieval problem, becomes relevant. Another major challenge which will come into the focus of EF 3 is the quantification of uncertainties for clustering problems and of geometric information in imaging, such as segmentations or other topological structures.

In general, success in these themes requires major advances in modeling, analysis, hierarchical or non-smooth optimization, statistics-based learning and high-performance computations. The long-term vision of EF 3 is to establish an internationally recognized Berlin-wide platform for quantitative image processing and imaging, where innovation in the applied sciences and device engineering are driven by new mathematical developments.

EF 4 "Particles and Agents" (Friz, König)

This Emerging Field focusses on modeling and analysis of spatial complex systems involving a large number of small, interacting entities that have a smaller or larger scope of possibilities to take influence on the system. In Physics, these entities are often just particles and show little more features than their location in space and one additional property like a mass. Also in Physics, but more in the Social Sciences, there are also a lot of situations in which these entities are much more structured and have highly involved possibilities, they might even be models for human beings that can experience their neighborhood and make own decisions, in which case we call them agents.

The main focus in EF4 is on developing and analyzing models in situations that have not yet been consistently modeled by mathematics. A "non mainstream" modeling is intended. Often the biggest difficulty is to take into account the "human factor" in a convincing manner such that mathematical tools can be applied to a rigorous analysis, e.g., of agent-based models and simulations.

The ultimate goal is the detection of macroscopic phenomena like phase transitions, transitions between metastable regimes, and tipping, that emerge from microscopic rules.

Emerging Field 5 "Concepts of Change in Historical Processes" (Fless, Klein)

A central challenge in the study of historical civilizations is the construction of plausible, evidence-based narratives describing complex processes of change that affected and shaped past societies. Archaeological evidence bears substantial intrinsic complexity: it is often fragmentary and has been subject to prior transformations, displacements, and preservation processes. Owing to the inherent difficulties of inferring such spatio-temporal processes from the data, their interpretation constitutes a prime subject for advanced mathematical modeling and formalized reasoning.

In response, EF 5 aims to (i) develop an ontology for processes of change in ancient societies and to cast its key scientific concepts, such as "resilience," "tipping points," and "migration waves" in mathematical terms; to (ii) advance model development for historical change processes, such as the spreading of innovations in ancient cultures, and analyze these models in the light of the developed concepts of change; and to (iii) explore relevant research data with advanced techniques of data analysis, and devise methods for integrating the data into the models under development.

Transfer Unit

The goal of the MATH+ Transfer Unit (TrU) is the translation of research results into industry and society, mainly through the development of prototypes or demonstrators based on basic research in other MATH+ research units. TrU projects do not aim at off-the-shelf development but are defined via a basic research question that fits to the overall agenda of MATH+. Each project requires a cooperation contract regarding an equal public-private partnership.