

## **Key Technologies**

The area of Key Technologies is dedicated to mathematical models that play an important role in the systems unc consideration. Besides physical, chemical or biological models from first principles, data driven models from machi learning and artificial intelligence are becoming more and more important. Furthermore, new theoretical methods is model-based mathematical optimisation, complexity reduction, experimental design and control are also developed a implemented in the CDS.

**Mathematical models** of the systems under consideration play an important role. They allow expert knowledge to be harness and provide the basis for simulation, analyses, optimisation and control. For many of the systems and processes unc consideration, differential equations have proven to be a suitable modelling tool. However, modelling also includes constraints a objective functions. Our vision here is to pursue digital twins for the dynamic systems under investigation, which include varic models of different levels of detail. Depending on what is to be investigated, suitable models can now be used - for examp complexity-reduced convex equilibrium models as an underestimate for non-convex transient differential equation models optimisation algorithms for calculating lower bounds.

In the **discretisation of mathematical models**, e.g. with finite element methods, the**mostly infinite-dimensional problems approximated by finite-dimensional systems that can be mapped on the computer.** This often leads to very large systems equations or optimisation problems whose solution must be approximated with simulation tools. The requirements of t application regularly push the problem complexity beyond the threshold of what can be realised on modern computer systems. I develop and implement parallelisable high-performance tools based on efficient solution methods. For dimensiona reduction, error-controlled adaptive controls are designed which optimally adapt the discretisation to the model under investigati and control all error components that occur. Here, derivative-based techniques come into play, which also play an important role optimisation in the form of adjoint equations. To use modern hardware (e.g. accelerator cards or manycore CPUs), classi-discretisation techniques are combined with machine learning concepts in hybrid approaches.



We develop structure-exploiting first-discretize-then-optimize methods for the optimisation of dynamical systems. The are iterative, derivative-based, deterministic and suitable to be efficiently extended to handle integers and uncertaintie Optimisation is also an enabling technology for the following key technologies.

The regulation and control of complex systems is often challenging. In addition to theoretical analyses regarding stability a controllability, we develop **efficient methods of nonlinear model predictive control (NMPC)** which can be coupled with sta and parameter estimations. **Methods of online experimental design or dual control** are also developed and put to use. Efficient methods based on matrix and tensor calculus are also developed in the CDS.

Data can be used to discriminate between different hypothesis models, to estimate model parameters, and to train neu networks. The question of which data to generate or use in order to obtain high statistical power is called experimen design. Maximising the available information is a particularly structured optimisation problem that poseschallenges to t statistical modelling of the optimisation problem and to the methods used, especially when complex dynamic processes a considered.

The CDS makes contributions to > Magdeburg's Al research (https://ki.ovgu.de/index.php?show=forschung). These are characteris by application-driven interdisciplinary research and development of new approaches in dynamic contexts This includ both the development of new machine learning (ML) models and algorithms as well as innovative, application-specific concepts their use. We pursue the vision of a high acceptance of the developed approaches by working with efficient, explainable and sa models and methods. We develop hybrid models that combine the advantages of expert knowledge from first-principles w flexibility of data-driven surrogate models. Special methodological focus is on i) a systems-theoretical view and the development hybrid models, ii) efficient algorithms for the simulation and optimisation of hybrid models, iii) the analysis and optimisation (semi)-autonomous complex systems in real time, and iv) mathematically sound and complexity-reducing model and meth



Complexity is a property that makes it difficult to find an appropriate mathematical description of a real process, to recognise t fundamental structures and properties of mathematical objects, or to solve a given mathematical problem algorithmica efficiently. **Complexity reduction** refers to all approaches that solve these difficulties in a systematic way and help to achieve t aforementioned goals. For many tasks, approximation and dimensionality reduction are the tools of choice, but we see complex reduction much more generally and, for example, also make purposeful use of embeddings in higher-dimensional spaces.

To drive and round off the application-driven development of models and methods, we develop **efficient algorithms** a implement them in software packages that are used in the application areas of the CDS. Examples are contributions to t software packages

casadi > https://web.casadi.org/ (https://web.casadi.org/)

gascoigne > https://www.gascoigne.de/ (https://gascoigne.math.uni-magdeburg.de/)

pymor > https://pymor.org/ (https://pymor.org/)

pycombina > https://github.com/adbuerger/pycombina (https://github.com/adbuerger/pycombina)

scip > https://www.scipopt.org/ (https://www.scipopt.org/)

and many project-specific implementations.



## Research

- Energy Conversion
  Chemical Production
  Active Substances
  Key Technologies