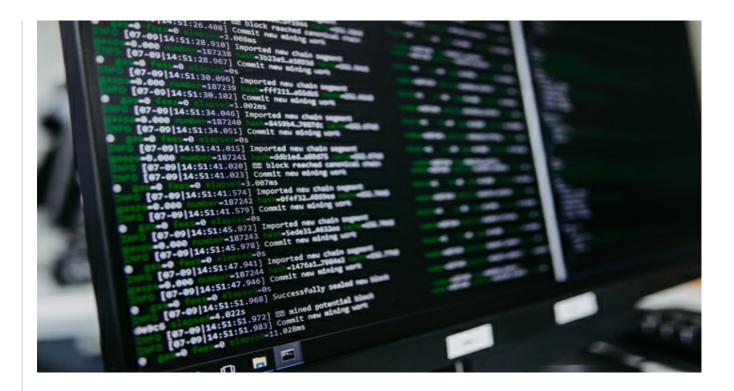## Key Technologies

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

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

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

development.

Complexity is a property that makes it difficult to find an appropriate mathematical description of a real process, to recognise the fundamental structures and properties of mathematical objects, or to solve a given mathematical problem algorithmically efficiently. **Complexity reduction** refers to all approaches that solve these difficulties in a systematic way and help to achieve the aforementioned goals. For many tasks, approximation and dimensionality reduction are the tools of choice, but we see complexity 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** and implement them in software packages that are used in the application areas of the CDS. Examples are contributions to the software packages

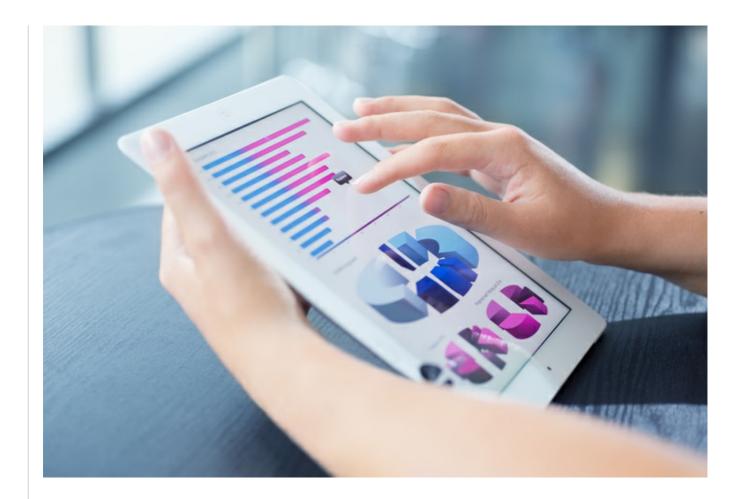casadi › https://web.casadi.org/ (https://web.casadi.org/)

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