

Preface

Applied research is the foundation of the Fraunhofer-Gesellschaft (FhG). The 69 Fraunhofer institutes team up with companies to transform original ideas into innovations that benefit society and strengthen both the German and the European economy. To this end, one of the key missions of a Fraunhofer institute is to bridge the gap between fundamental research, usually conducted at universities, and the requirements of industry.

The Fraunhofer Institute for Algorithms and Scientific Computing SCAI combines excellent research and application-oriented development to achieve this goal and to provide added value for our partners. SCAI develops numerical techniques, parallel algorithms, and specialized software tools to support and optimize industrial simulations. Moreover, we implement custom software solutions for production and logistics, and offer calculations on high-performance computers. Our services and products are based on state-of-the-art methods from applied mathematics and information technology. Currently, the main areas of research and development at SCAI are:

- Bioinformatics
- Fast solvers
- High performance computing
- Multiphysics
- Optimization
- Computational finance
- High performance analytics
- Meshfree multiscale methods
- Numerical data driven prediction
- Virtual material design

Within these fields of application, SCAI has developed a number of software products that focus on specific industrial requirements:

- AutoNester is a software package for automatic marker making on fabrics, leather, sheet metal, wood, or other materials. It is widely used in the garment and upholstery manufacturing industry.
- DesParO is a toolbox for the intuitive exploration, automatic analysis, and optimization of parameterized problems in production processes. It can be coupled with simulation programs or data from physical experiments.
- ModelCompare is a data analysis plug-in for finite element pre- and post-processing tools which allows for an easy comparison of similar simulation

results identifying the differences between models based on the geometry described by the mesh.

- The MpCCI software suite enables the coupling of various simulation codes to enable the speedy implementation of multiphysics applications such as fluid-structure-interaction problems. It is used in a wide range of applications from mechanical engineering, and aeroelasticity to the simulation of micro-mechanical components.
- MYNTS is a multiphysical network simulator for electrical circuits, gas and energy transport, and water distribution. It models networks as systems of differential-algebraic equations and helps users to manage, analyze, and optimize their networks.
- PackAssistant is utilized worldwide especially in the automotive industry by numerous manufacturers and suppliers to automatically compute optimal filling of transport containers with identical parts.
- The text-mining tool ProMiner supports users in the identification of genes and proteins and respective illnesses and treatments by analyzing scientific texts and libraries.
- The library SAMG provides highly efficient algorithms for the parallel solution of large linear systems of equations with sparse matrices. It is used in different industries ranging from manufacturing and automotive to oil and gas exploration.
- Tremolo-X is a massively parallel software package for molecular dynamics simulations. It is used in various projects and industrial applications in nanotechnology, materials science, biochemistry, and biophysics.

Besides the development of software tools of industrial relevance, SCAI is involved in many collaborative research projects funded by the EU and the BMBF. For instance, SCAI's bioinformatics group is coordinating AETIONOMY which is one of the flagship projects of the current Innovative Medicines Initiative; see

<https://www.scai.fraunhofer.de/en/projects.html>

for details.

The articles in this book give an overview of current research projects and selected software products of the Fraunhofer Institute for Algorithms and Scientific Computing SCAI. They show the wide range of challenges and solutions in scientific computing and its important role in applications for industry. This exciting field of applied collaborative research and development is surely attractive for scientists, practitioners, and students alike.

Sankt Augustin, Germany
April 2017

Michael Griebel
Anton Schüller
Marc Alexander Schweitzer

Scientific Computing and Algorithms in Industrial
Simulations

Projects and Products of Fraunhofer SCAI

Griebel, M.; Schüller, A.; Schweitzer, M.A. (Eds.)

2017, VIII, 376 p. 40 illus. in color., Hardcover

ISBN: 978-3-319-62457-0