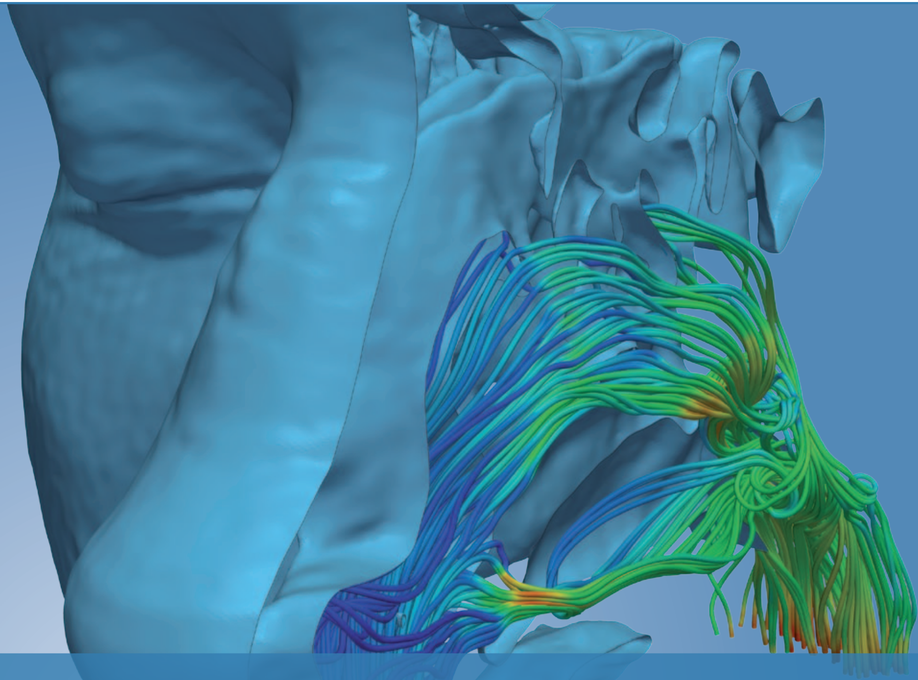
JARA Jülich Aachen Research Alliance



SLFSE (JARA-HPC), AIA (RWTH Aachen University)

SIMULATION LABORATORY
HIGHLY SCALABLE FLUIDS AND SOLIDS ENGINEERING (FSE)

AN INITIATIVE OF

RWTH AACHEN UNIVERSITY

JÜLICH FORSCHUNGSZENTRUM

SimLab FSE

Simulation Laboratory Highly Scalable Fluids and Solids Engineering (SimLab FSE)

CONTENT

3 INTRODUCTION

4-5 COOPERATIONS

6-10 RESEARCH

11 PROSPECTIVE PROJECTS / PUBLICATIONS

12 PEOPLE AND CONTACT

Motivation

Experimentally testing new designs in the field of engineering is often time consuming and expensive. Numerical simulations, in contrast, enable to easily vary model parameters and to explore a problem in all detail.

To accurately predict the physics of a realistic problem, large-scale simulations are required that pose new challenges to simulation codes and that necessitate the power of supercomputers.

Contributions

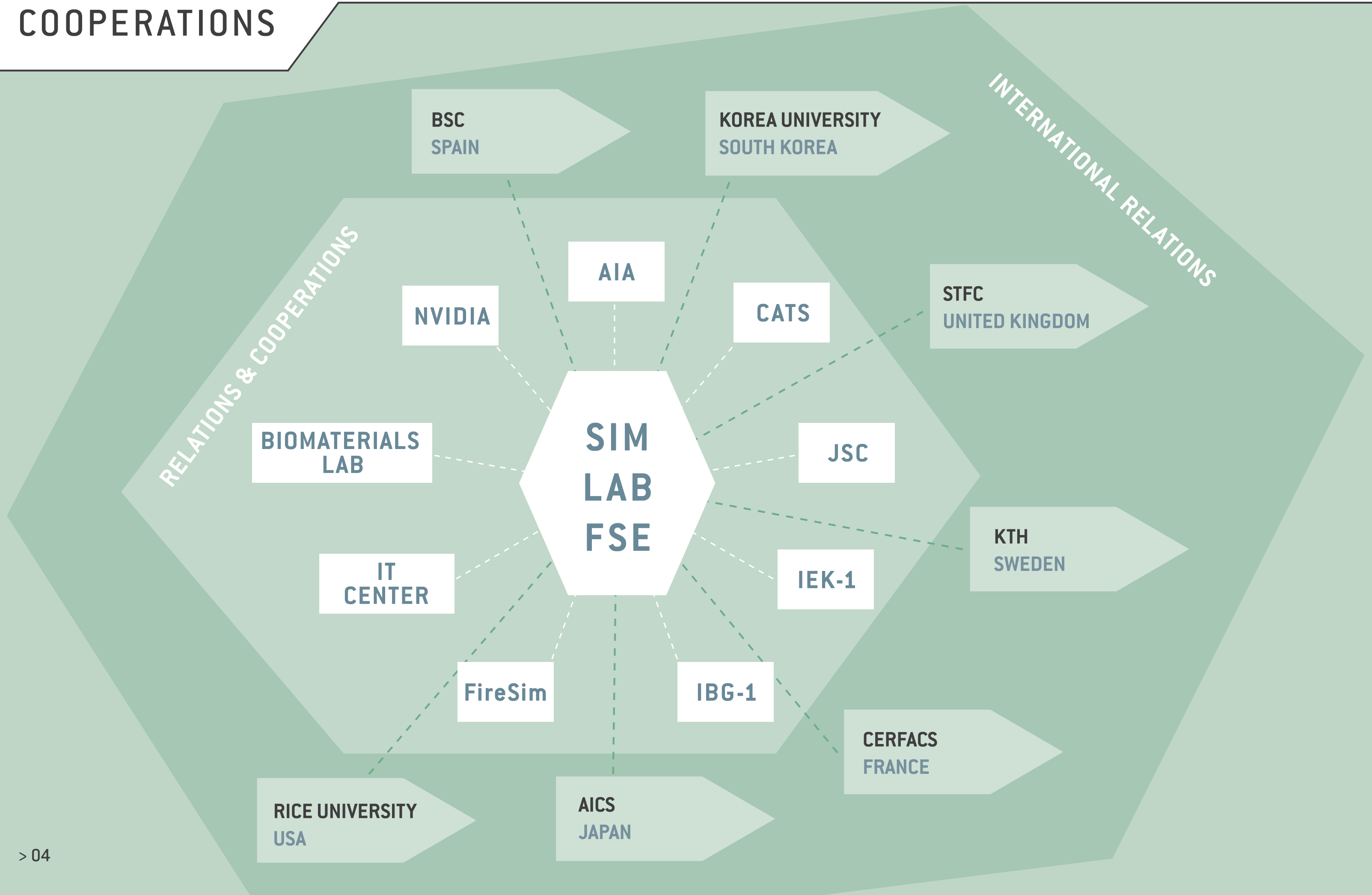
> Increasing the parallel efficiency of simulation codes and establishing an interdisciplinary interface between engineers and the HPC community. Development of highly scalable software suited for HPC systems.

> Pushing research in the fields of computational fluid dynamics, aeroacoustics, and shape optimization. Seeking solutions for questions such as: What is the origin of respiratory pathologies? How can airplane noise be reduced? How can pharmaceutical and chemical processes be optimized?

Integration into JARA-HPC

The SimLab naturally integrates into the support and research structure of JARA-HPC. It delivers efficient porting and tuning solutions for codes to run on current and future supercomputer architectures.

Synergies arising from cooperations with JARA-HPC's Cross-Sectional Groups (CSGs) are explored to find performance bottlenecks and to visualize scientific big data.



SimLab Relations and Cooperations

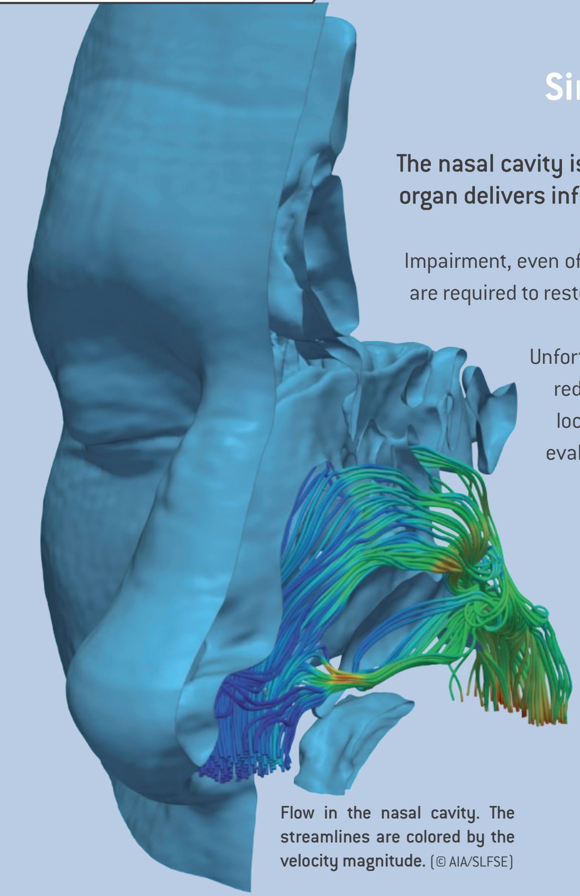
The SimLab cooperates with institutes at the RWTH Aachen University (RWTH), divisions of the Forschungszentrum Jülich (FZJ), and the University of Applied Sciences Aachen (FH Aachen):

- Chair of Fluid Mechanics and Institute of Aerodynamics (AIA), RWTH
- Chair of Computational Analysis of Technical Systems (CATS), RWTH
- Jülich Supercomputing Centre (JSC), FZJ
- IT Center, RWTH
- Biomaterials Lab, FH Aachen
- Institute of Bio- and Geosciences, Biotechnology (IBG-1), FZJ
- Institute of Energy and Climate Research, Materials Synthesis and Processing (IEK-1), FZJ
- Fire Simulation Team (FireSim), FZJ
- NVIDIA Application Lab, FZJ

International

The SimLab maintains international relations to:

- Barcelona Supercomputing Center (BSC), Spain
- Department of Mechanical Engineering, Korea University, South Korea
- Science and Technology Facility Council (STFC), Daresbury Laboratory, United Kingdom
- Department of Mechanics, KTH Royal Institute of Technology, Sweden
- Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CAERFACS), France
- Riken Advanced Institute for Computational Science (AICS), Japan
- Complex Flows of Complex Fluids, Chemical and Biomolecular Engineering, Rice University, USA



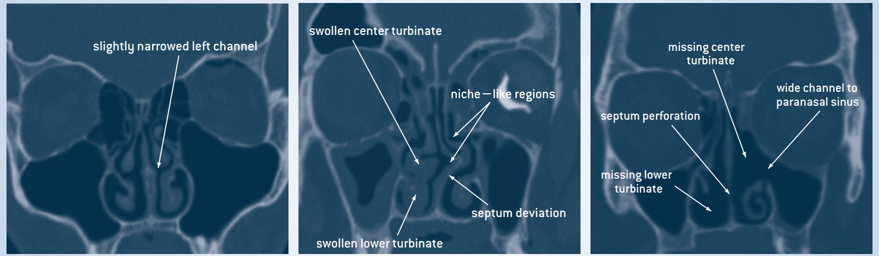
Flow in the nasal cavity. The streamlines are colored by the velocity magnitude. (© AIA/SLFSE)

Simulation of Respiratory Flow in the Human Nasal Cavity

The nasal cavity is responsible for cleaning, tempering , and humidifying the inhaled air and the olfactory organ delivers information on odors and flavors to the human brain.

Impairment, even of only some of these functions, may lead to a strong decrease of the patients' comfort so that surgeries are required to restore healthy conditions.

Unfortunately, the success rate of such surgeries is low and they often induce unwanted side effects like the reduction of the heating capability or inflammations. To derive the cause of functionality reductions and to locate potential locations for a surgery, the SimLab performs highly-resolved flow simulations enabling the evaluation of nasal cavities from a fluid mechanics point of view in a pre-surgical step.



CT images of three different nasal cavities. Left: patient with slightly swollen turbinates; center: patient with a septum deviation and impaired respiratory capabilities; right: patient after a surgery. (© AIA/SLFSE)

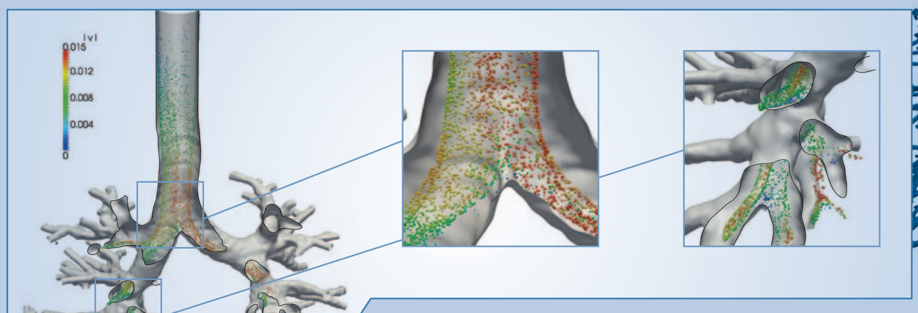
Contact: Andreas Lintermann, lintermann@jara.rwth-aachen.de

Particle Simulation in the Whole Respiratory Tract

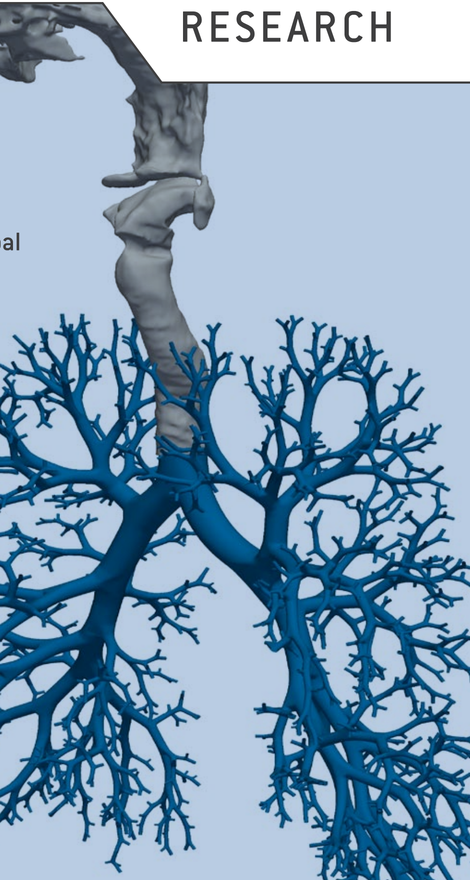
Nowadays, urban environments are polluted by fine dust particles consisting of Diesel aerosols, coal particles, wood dust, or volcanic ashes, to name just a few.

These particles have a size in the range of 2-10μm and consequently they follow the flow down the airway to the bronchioles of the lung where they deposit. Their deposition may cause severe damage and can lead to coughing, bronchitis, and even lung cancer.

To understand the transportation and deposition behavior of such particles, the SimLab performs coupled flow/particle simulations in the whole respiratory tract. The scientists are able to evaluate the filtering function of the nasal cavity, the influence of accelerated air in the larynx, and the dependence of the deposition on the particle size and mass.



Particle simulation in the human lung. The particles are colored by their velocity magnitude. The aerosols distribute into the different branches of the airway and deposit in fine lung generations. (© AIA/SLFSE)



Geometry of the whole respiratory tract down to the 12th bifurcation generation of the human lung. (© AIA/SLFSE)

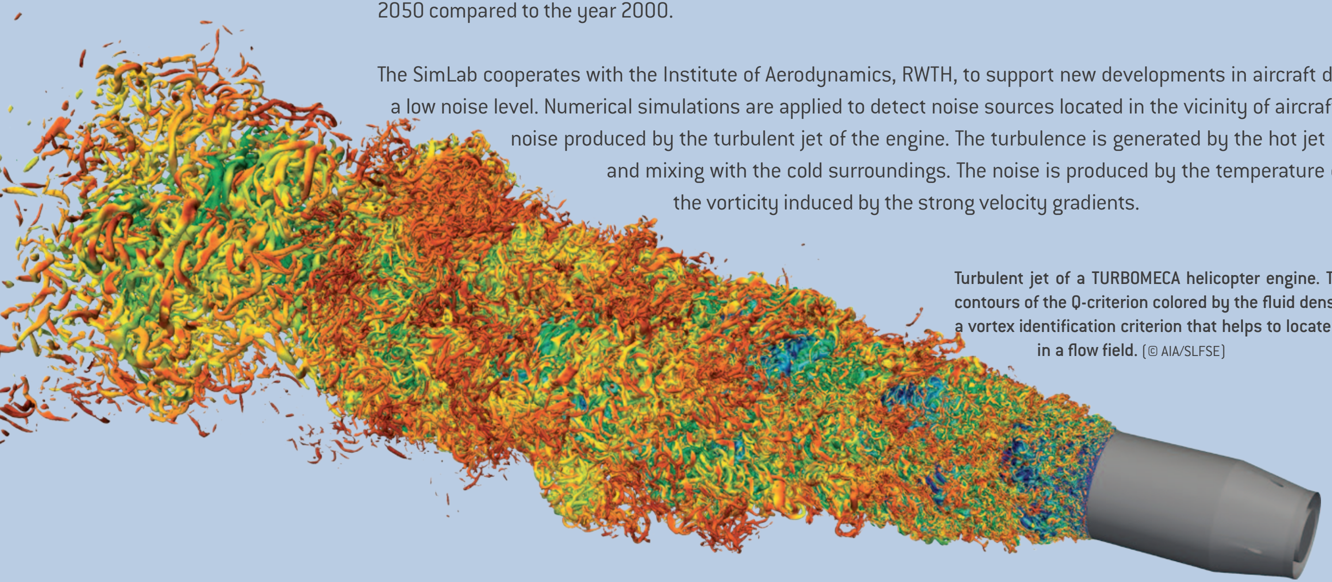
Contact: Andreas Lintermann, lintermann@jara.rwth-aachen.de

Noise Prediction of Aircraft Engines

Residents living in close vicinity of airports are regularly annoyed by the noise emitted by starting and landing planes.

To push the developments towards designing low-noise aircraft, the Advisory Council of Aeronautical Research in Europe (ACARE) released an agenda named "Flightpath 2050". This agenda aims at reducing the noise emission of aircrafts by 65% in the year 2050 compared to the year 2000.

The SimLab cooperates with the Institute of Aerodynamics, RWTH, to support new developments in aircraft design that exhibit a low noise level. Numerical simulations are applied to detect noise sources located in the vicinity of aircraft engines, i.e., the noise produced by the turbulent jet of the engine. The turbulence is generated by the hot jet exiting the nozzle and mixing with the cold surroundings. The noise is produced by the temperature difference and by the vorticity induced by the strong velocity gradients.



Turbulent jet of a TURBOMECA helicopter engine. The image shows the contours of the Q-criterion colored by the fluid density. The Q-criterion is a vortex identification criterion that helps to locate turbulent structures in a flow field. [© AIA/SLFSE]

Contact: Michael Schlottke-Lakemper, schlottke-lakemper@jara.rwth-aachen.de

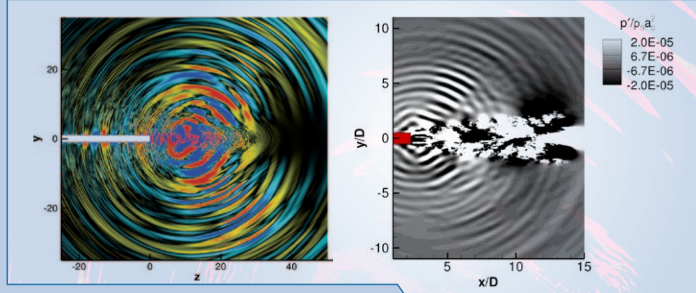
RESEARCH

Shape Optimization of Chevron Nozzles

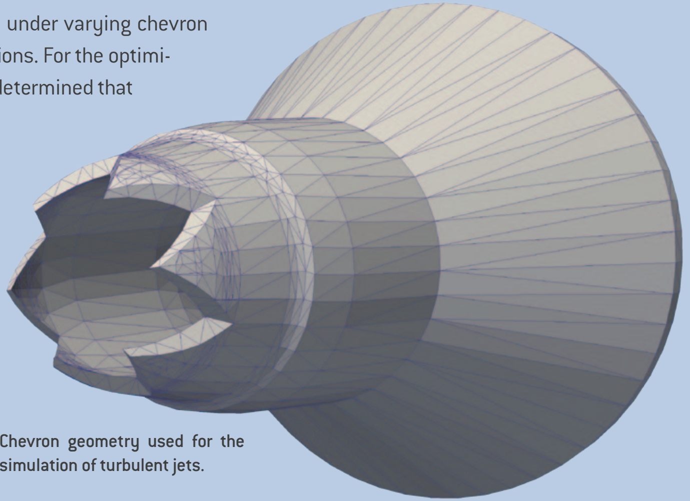
The researchers of the SimLab aim to find the optimal shape for so called chevrons, which are crown-like attachments mounted to the engines of aircraft.

These chevrons modify the turbulence intensity of the engine jet by influencing the mixing of the cold and hot jet layers in such a way that the emitted noise is reduced. However, this mechanism also decreases the thrust and makes the engine less efficient. To determine a reasonable trade-off between the noise production and the loss of thrust, optimization algorithms are used to adapt the shape of the chevrons.

The simulation of this problem involves solving the flow field and the aeroacoustics under varying chevron geometries and evaluating the noise and thrust produced by the different configurations. For the optimization, the parameter space is varied so that for the solution space a gradient can be determined that leads to a global optimum, i.e., to a low-noise and high-thrust chevron shape.



Acoustic pressure fields of turbulent jets. (c AIA/SLFSE)



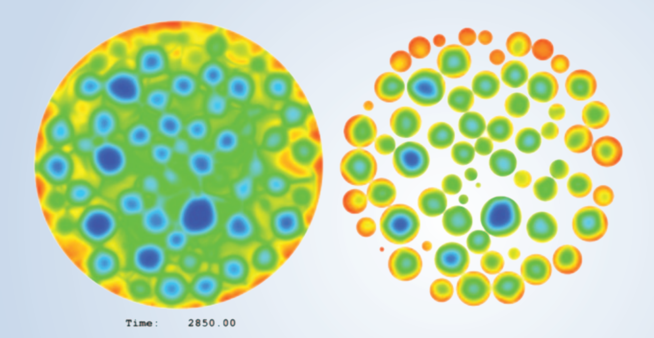
Chevron geometry used for the simulation of turbulent jets.

Contact: Manuel Kosel, kosel@jara.rwth-aachen.de

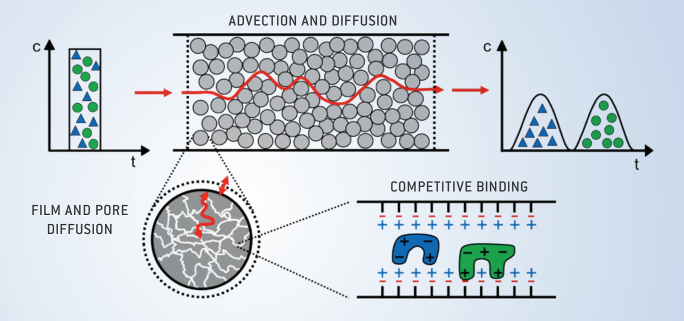
Packed-Bed Chromatography Simulations

Packed-Bed chromatography is one of the most important unit operations for isolating and purifying highly-valued product molecules in chemical and pharmaceutical applications.

The packing of the reactive polydisperse particles within the chromatography column and the shape of the column wall have a major influence on the efficiency of this method. The SimLab jointly develops new highly scalable methods for predicting the efficiency of large-scale columns as they are used in industrial applications with the Chair of Computational Analysis of Technical Systems, RWTH, and the the Institute of Bio- and Geoscience, FZJ. Therefore, the problem is subdivided into a fluid domain governed by advection and diffusion, and a diffusion-reaction domain modeling the binding and release process inside the porous particles.



Concentration profiles in slices of the polydisperse packing in the chromatography column. (© IBG-1/CATS/SLFSE)



The governing processes in packed-bed chromatography columns; fluid flow in a porous medium (advection and diffusion), and adsorption. (© IBG-1/CATS/SLFSE)

Contact: Metin Cakircali, cakircali@jara.rwth-aachen.de

Future Research

The current research and developments pursued in the SimLab allow for further investigations in the fields of respiratory flow, aeroacoustics, and in industrial manufacturing processes. The SimLab will extend the available implementations to tackle additional prospective research topics:

- Simulation of the fluid-structure interaction in the obstructive sleep apnea syndrome (OSAS)
- Optimization of surgery methods for the increase of respiratory efficiency and reduction of the probability of airway collapses in the OSAS by application of shape optimization algorithms
- Analysis of the aeroacoustic damping of highway noise barriers influenced by local wind conditions and their influence on urban environments
- Simulation of the alignment involved in the formation of the tubes in the manufacturing process of nanotubes
- Parallel in-situ visualization of large-scale simulation datasets in cooperation with the JARA-HPC CSG "Immersive Visualization"

Publications

Lintermann, A., Meinke, M., & Schröder, W. (2012). Investigations of Nasal Cavity Flows based on a Lattice-Boltzmann Method. High Performance Computing on Vector Systems 2011, 143–158. Springer Berlin Heidelberg.

Lintermann, A., Meinke, M., & Schröder, W. (2013). Fluid mechanics based classification of the respiratory efficiency of several nasal cavities. Computers in Biology and Medicine, 43(11), 1833–1852.

Lintermann, A., Schlimpert, S., Grimmen, J.H., Günther, C., Meinke, M., & Schröder, W. (2014). Massively parallel grid generation on HPC systems. Computer Methods in Applied Mechanics and Engineering, 277, 131–153.

Schlottke, M., Meinke, M., & Schröder, W. (2014). A hybrid discontinuous Galerkin-finite volume method for computational aeroacoustics. In 19. DGLR-Fachsymposium der STAB. München: Springer Berlin.

Püttmann, A., Nicolai, M., Behr, M., & von Lieres, E. (2014). Stabilized space-time finite elements for high-definition simulation of packed bed chromatography. Finite Elements in Analysis and Design, 86, 1–11.

Schlottke, M., Cheng, H.-J., Lintermann, A., Meinke, M., & Schröder, W. (2015). A direct-hybrid hierarchical Cartesian mesh method for computational aeroacoustics. In AIAA Aviation. Dallas, Texas, USA.

Cetin, M.O., Koh, S.R., Meinke, M., & Schröder, W. (2015). Aeroacoustic Analysis of a Helicopter Engine Jet Including a Realistic Nozzle Geometry. In AIAA Aviation. Dallas, Texas, USA.

JARA Jülich Aachen Research Alliance

PEOPLE

SIMLAB HIGHLY SCALABLE FLUIDS AND SOLIDS ENGINEERING, JARA-HPC, RWTH AACHEN UNIVERSITY

Metin Cakircali, M.Sc.
Manuel Kosel, Dipl.-Ing.
Michael Schlottke-Lakemper, Dipl.-Ing., M.Sc.
Andreas Lintermann, Dr.-Ing. Dipl.-Inform.

STEERING BOARD

Wolfgang Schröder, Univ.-Prof. Dr.-Ing.
Chair of Fluid Mechanics and
Institute of Aerodynamics, RWTH Aachen University

Marek Behr, Univ.-Prof. ,Ph.D.
Chair of Computational Analysis
of Technical Systems, RWTH Aachen University

Paul Gibbon, Prof. Dr.
Jülich Supercomputing Centre,
Forschungszentrum Jülich

CONTACT

Andreas Lintermann

lintermann@jara.rwth-aachen.de
www.jara.org

AN INITIATIVE OF

RWTH AACHEN UNIVERSITY

JÜLICH FORSCHUNGSZENTRUM