Numerical modeling, simulation and experimental analysis of fluids and fluid flows

■ Jointly with Oerlikon AM GmbH and Linde, the Chair of Aerodynamics and Fluid Mechanics investigates novel manufacturing processes and materials for additive 3D printing. The cooperation is supported by the Bavarian State Ministry for Economic Affairs, Regional Development and Energy. In addition, two new H2020-MSCA-ITN actions are being sponsored by the European Union. The 'UCOM' project investigates ultrasound cavitation and shock-tissue interaction, which aims at closing the gap between medical science and compressible fluid mechanics for fluid-mechanical destruction of cancer tissue. With 'EDEM', novel technologies for optimizing combustion processes using alternative fuels for large-ship combustion engines are developed.

In 2019, the NANOSHOCK research group published various articles in the highly-ranked journals 'Journal of Computational Physics', 'Physical Review Fluids' and 'Computers and Fluids'. Updates on the NANOSHOCK open-source code development and research results are available for the scientific community: www.nanoshock.de or hwww.aer.mw.tum.de/abteilungen/nanoshock/news.

A highlight in the field of aircraft aerodynamics in 2019 was to contribute establishing a DFG research group (FOR2895) on the topic 'Research on unsteady phenomena and interactions at high speed stall'. Our subproject will focus on 'Neuro-fuzzy based ROM methods for load calculations and analysis at high speed buffet'.

### **Aircraft and Helicopter Aerodynamics**

#### **Motivation and Objectives**

The long-term research agenda is dedicated to the continues improvement of flow simulation and analysis capabilities enhancing the efficiency of aircraft and helicopter configurations with respect to the Flightpath 2050 objectives.

Aircraft aerodynamics research is aimed at detailing flow physics understanding of leading-edge vortex interaction effects (DFG) along with turbulence model conditioning (VitAM, LuFo V-3). Analysis of Fluid-Structure-Interaction effects and

aeroelasticity is linked to elasto-flexible lifting surface characteristics (DFG) and neuro-fuzzy based reduced order models addressing buffeting and buzz (DFG). Investigations on transport aircraft wings are dedicated to wake vortex alleviation and dynamic lift enhancement (BIMOD, LuFo V-3). The research work in the field of propeller and helicopter aerodynamics is related to propeller flow analysis at strong inhomogeneous inflow conditions (HyProp, BFS), propeller optimization strategies (AURAIS, Bay. LuFo) and full fairing rotor head design optimization of the RACER configuration (FURADO, CSky2). Further, 3D-printed advanced pressure probes including novel unsteady pressure sensors are under development (ZIM). Figure 1: Flow structures on the RACER configuration based on unsteady Reynolds averaged Navier-Stokes simulations (FURADO project)

#### **Research Spotlights**

**FURADO – Improved Aerodynamics for Rotor Aircraft** Within ten years (2014-2024), the Joint Technology Initiative (JTI) Clean Sky 2 aims to make European aviation significantly 'greener' – and at the same time safer, faster and more competitive. The initiative focuses, among other target areas, on the development of the next generation of compound rotorcraft, a combination of aircraft and helicopters. The technology demonstrator 'RACER' (Rapid And Cost Efficient Rotorcraft) will be able to take off, land and hover vertically and will reach a top speed of about 410 km/h through two pusher propellers, while cruising with significantly less noise and CO<sub>2</sub> pollution than currently

available solutions. To achieve this, essential improvements in terms of weight and aerodynamic design are required. As part of the Clean Sky 2 project FURADO 'Full Fairing Rotor Head Aerodynamic Design Optimization' (www. cleansky-projects.tum.de/en/furado), conducted by the Institute of Aerodynamics and Fluid Mechanics, the optimization of the rotor head design is considered (see Figure 1). A full fairing of rotor head structural components can contribute to a significant reduction in aerodynamic drag. The aerodynamically improved geometries are obtained by means of fully automated shape optimization in conjunction with high fidelity numerical flow simulation, taking into account all relevant flow conditions as well as thermal and production aspects. A first set of geometries is delivered to the industrial partner which will be considered in the next step of the design cycle.



Figure 2: Large transport aircraft near field wake vortex structures visualized in several cross flow planes obtained by stereoscopic particle image velocimetry (BIMOD project)

### BIMOD – Dynamic Lift Enhancement and Wake Vortex Manipulation

Modern transport aircraft featuring advanced dropped hinged flaps generally offer the architecture in which periodical oscillations of the flaps are possible when an adapted actuator concept is applied. On the one hand, this capability can be used for a periodic alteration of the spanwise lift distribution and with it the wake vortex centroid positions in order to accelerate exponential growth of natural wake vortex instabilities to foster wake vortex decay. On the other hand, periodic oscillations of flaps allow for higher deflection angles thus increasing maximum lift due to the dynamic lift effect compared to classical high lift conditions with constant flap deflection angles. The effects are studied by conducting complementary experimental and numerical simulations. Figure 2 shows the respective wind tunnel model. Motivation of the former concept is a potential reduction of separation distances during approach, whereas the latter concept might contribute to reducing



Figure 3: Wind tunnel model of a generic wing planform morphing configuration featuring an elasto-flexible lifting surface mounted in test section of wind tunnel A (MEMWing project)

airplane weight or enabling alternative approach trajectories. The research project is carried out together with the RWTH Aachen, Institute of Aerospace Systems and Institute of Structural Mechanics and Lightweight Design.

#### MEMWing – Unsteady Aerodynamics of Adaptive Elasto-flexible Membrane Wing

Revolutionary concepts for unmanned aerial vehicles are aimed at mission scenarios that include both proportions of efficient loiter flight and high maneuverability flight. This requires aircraft which can optimally adapt their aerodynamic properties to the respective application conditions. This project is therefore concerned with new, technically feasible solutions for such versatile aircraft, based on an adaptive wing configuration with an adjustable aero-elastic flexible wing. The considered model consists of a beam structure with joints for varying aspect ratio, sweep and local incidence and a flexible lifting surface (see Figure 3). Due to the anisotropic structural design, the deformation of the wing under aerodynamic loads leads to a passive flow control. A fundamental understanding of these mechanisms and the aerodynamic properties is gained by means of detailed wind tunnel model experiments and numerical simulations. The current project is dedicated to linking the aerodynamic characteristics to specific target variables and to exploiting the concept with respect to overall unsteady aerodynamic problems resulting from stall behavior and gust impact. The basic concept of the

massive form adaption as well as the use of a flexible lifting surface and its technical implementation combines fundamentally new approaches.

#### Key results

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### DNS of Passive-Scalar Transport in Turbulent Channel Flow using the LBM on Parallel GPU Architectures



Passive-scalar heat transfer of a fully developed turbulent channel flow. Cooled top wall (blue) and heated bottom wall (red)

The construction of complex technical systems requires sustainable numerical methods to allow for simulations with coupled fluid mechanical and thermal characteristics. Often the numerical simulations are performed using conventional numerical methods based on the spatial and temporal discretization of the continuity, Navier-Stokes and the energy equations. Such methods highly depend on the quality of the mesh, which generation could be tedious and time-consuming especially for problems with complex geometry. An alternative approach which copes with the deficiencies mentioned above is the Lattice Boltzmann Method (LBM). Derived from its kinematic nature, the main advantages of the LBM are its intrinsic parallelism and the capability to simulate complex geometries with suitable accuracy.

We have designed a GPU implementation of the thermal double-distribution LBM with Boussinesq approximation that guarantees optimal utilization of the GPU resources and minimizes the amount of global memory accesses to ensure an optimal performance. The parallel implementation of the thermal LBM is validated with a natural convection benchmark solution proposed by De Vahl Davis (Table 1.). The framework successfully captures the characteristics of the velocity and the temperature fields.

#### Table 1. Average Nusselt number at the hot wall

Ra	Present Study	Benchmark	Error (%)
10 <sup>3</sup>	1.1174	1.118	0.05
<b>10</b> <sup>4</sup>	2.2482	2.243	-0.23
10 <sup>5</sup>	4.5291	4.519	-0.22
10 <sup>6</sup>	8.8127	8.8	-0.14

To test the capabilities of the parallel LBM we perform a Direct Numerical Simulation (DNS) of a passive-scalar heat transfer in a turbulent channel flow at Re<sub>1</sub> = 180. All length and time scales are resolved, making the simulation extremely computationally expensive with a cost scaling as Re<sup>3</sup>. The size of the simulation domain is adjusted to ensure that the turbulence fluctuations are uncorrelated for the considered Re<sub>1</sub>. The streamwise and spanwise directions are 4 $\pi$ H and 2 $\pi$ H, respectively, and the height of the domain is 2 $\pi$ H. The simulations are performed on a uniform mesh with  $\Delta x^{+} = \Delta y^{+} = \Delta z^{+} = 2$  and total number of nodes N<sub>x</sub> × N<sub>y</sub> × N<sub>2</sub> = 1132 x 568 x 180 = 115 735 680.

The centerline Mach number is  $Ma_c = 0.05$  with  $u_c = 17$  m/s for air at 15°C and 1 atm. The total physical simulation time is  $t_{total} = 3.6 \times 10^6 \Delta t = 0.187$ s with  $\Delta t = 5.17 \times 10^{-8}$ s. The simulation run for 21 hours total wall time on a NVIDIA DGX-1 with 8 NVIDIA Tesla V100 with approximately 5500 MNUPS. This value includes mesh generation and regular outputs of section cuts and domain-averaged wall shear stress for monitoring. The maximum computational performance is about 6500 MNUPS when only one final output is carried out.

The obtained results for the mean velocity profile ( $<u^+>$ ) and the Reynolds stresses are in excellent agreement with

the reference data. The temperature field statistics agree reasonably well with the reference data; however, further simulations have to be performed to ensure the robustness of the LBM framework.

#### Publications

- Pachalieva A., Niedermeier, C. A., and Indinger, T., 'Numerical Simulation of Coupled Aero-Thermodynamic Systems Based on the Lattice-Boltzmann Method', 2018 JSAE Annual Congress (Spring), 23–25 May 2018, Pacifico Yokohama, Japan.
- Pachalieva, A., Niedermeier, C. A., and Indinger, T. (2019). Massively Parallel GPU Implementation of the Lattice-Boltzmann Method for the Simulation of Coupled Aero-Thermodynamic Systems. International Journal of Automotive Engineering, 10(1), 125–132.



Turbulence flow statistics. Excellent agreement with reference data for the flow field and reasonable agreement for the temperature field at two different Prandtl numbers

### Species-clustered Splitting Scheme for the Integration of Large-scale Chemical Kinetics using Detailed Mechanisms



Species distribution in the diffusion space with first three diffusion coordinates of species for n-hexadecane mechanism

#### **Motivation and Objectives**

Gasoline, diesel and jet fuels, particularly those derived from petroleum sources, are composed of hundreds of components. As the number of hydrocarbon species grows, so does the dimensionality of the kinetic mechanism to model hydrocarbon oxidation. For example, the detailed mechanism for methyl decanoate, a biomass fuel surrogate, consists of 3036 species and 8555 reactions. For the accurate prediction of combustion processes such as ignition, extinction and flame propagation, the efficient solution of large-scale detailed chemical kinetics is key, though limited by the current computing power.

#### **Solution Approach**

We have developed a species-clustered integrator for chemical kinetics with large detailed mechanisms based on operator-splitting. The ordinary differential equation (ODE) system of large-scale chemical kinetics is split into clusters of species using graph partition methods. The theoretically expected speedup in computational efficiency is reproduced by numerical experiments on three zero-dimensional (0D) auto-ignition problems, considering detailed hydrocarbon/air combustion mechanisms at varying scales, from 53 species with 325 reactions of methane to 2115 species with 8157 reactions of n-hexadecane.

#### **Key Results**

- A species-clustered splitting scheme for the integration of large-scale chemical kinetics using detailed mechanisms. J. H. Wang, S. C. Pan, X.Y. Hu N. A. Adams, Combustion and Flame 205 (2019) 41–54
- A split random time-stepping method for stiff and nonstiff detonation capturing. J. H. Wang, S. C. Pan, X.Y. Hu N. A. Adams, Combustion and Flame 204 (2019) 397–413
- A partial characteristic decomposition for multi-species Euler equations. J. H. Wang, S. C. Pan, X.Y. Hu N. A. Adams, Computers and Fluids 181 (2019) 364–382

### Machine Learning Group – AER

#### Motivation

Fluid flows are challenging due to their inherent nonlinearity, the occurrence of complex multi-scale phenomena and data scarcity. Therefore, the application of machine learning algorithms in the field of fluid dynamics has been more reserved compared to other fields in which machine learning is more prominent. Nevertheless, machine learning poses unique opportunities for the fluid mechanics community. The amount of data of fluid flows from experiments and simulations has been growing continuously and machine learning provides a plethora of techniques to extract information about the system at hand. Detailed knowledge about the underlying flow physics facilitates augmenting classical machine learning methodologies with first principles.

We are solving the inverse problem of inferring the flow field from the deformation of the interface in multi-phase flows. Shown are the steady state pressure (left) and velocity (right) fields of a drop sheared in a Couette flow.

Emphasis is placed on the better evaluation of data from simulations and measurements as well as on the design of numerical methods. We apply Gaussian processes to investigate process parameters of classical two-phase flows (e.g. bubble collapse, rising bubble). Physically informed Neural Networks give us a unique possibility to infer unknown quantities of interest from known data (e.g. sparse measurements). Additionally, machine learning is used to enhance classical numerical methods (e.g. ENO/ WENO) in order to devise adaptive data-driven algorithms.

#### **Solution Approach**

Currently, we pursue several different strategies of incorporating machine learning into the field of fluid mechanics.

### Free-stream Preserving Linear-upwind and WENO Schemes on Curvilinear Grids

#### **Motivation and Objectives**

In computational fluid dynamics (CFD), it is well known that finite-difference schemes are more computational efficient compared with the same order accurate finite-volume schemes. Therefore, many linear, nonlinear and hybrid high-order finite-different schemes have been developed. However, despite the above-mentioned advantages, these high-order schemes are problematic when they are applied to curvilinear grids due to the lack of geometric conservation law (GCL). The grid Jacobian and metrics calculated in curvilinear coordinates can introduce large errors, degrade accuracy or cause numerical instability even when the flow is uniform, i.e. free-stream preserving problem.

#### **Solution Approach**

We propose a method for general linear-upwind and WENO schemes preserving free-stream on stationary curvilinear grids. Following Lax-Friedrichs splitting, this method rewrites the numerical flux into a central term, which







(d) WENO-CUFP

30 equally spaced density contours from 0.25 to 6.00 of wind tunnel with a step problem. The results are obtained by the traditional WENO scheme (a) and several schemes with the free-streaming method applied. achieves free-stream preserving by using a symmetrical conservative metric method, and a numerical dissipative term with a local difference form of conservative variables for neighboring grid-point pairs. In order to achieve free-stream preservation for the latter term, the local differences are modified to share the same Jacobian and metric terms evaluated by high order schemes. In addition, this method allows a simple hybridization switching between linear-upwind and WENO schemes for improving computational efficiency and reducing numerical dissipation.

#### **Key Results**

- Free-stream preserving linear-upwind and WENO schemes on curvilinear grids. Y. J. Zhu and X. Y. Hu, Journal of Computational Physics 399 (2019) 108907.
- A targeted ENO scheme as implicit model for turbulent and genuine sub-grid scales. L. Fu, X. Y. Hu and N. A. Adams. Commun. Comput. Phys. 26 (2019) 311–345.

### NANOSHOCK – Manufacturing Shock Interactions for Innovative Nanoscale Processes

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 667483)

#### **Motivation and Objectives**

We want to investigate the potential of shockwaves for in-situ control of fluid processes with surgical precision. Shockwaves are discontinuities in the macroscopic fluid state that can lead to extreme temperatures, pressures and concentrations of energy. Applications of such shock interactions range from kidney-stone lithotripsy and drug delivery, to advanced aircraft design. With the use of properly focused shockwaves on tissue material, e.g. lesions with unprecedented surgical precision can be generated. Alternatively, improving combustion by enhanced mixing of fuels, shockwave interactions can help to further destabilize and atomize spray droplets. Our overall objective is to understand and predict the formation and control of shocks in complex environments, such as living organisms, using computational methods.



Shock-bubble interaction at an Air-Helium interface: 3D volumetric rendering of the vorticity and translucent representation of the bubble surface

#### **Solution Approach**

We develop best-in-class numerical methods with unprecedented accuracy and stability, and implement them in our simulation framework ALPACA [2] (available to the public on request, see http://nanoshock.org for more information). ALPACA allows us to investigate the highly complex dynamics of shock-driven multiphase flows. A high computational efficiency is required to capture the nonlinear character of such problems and to resolve



Shock-bubble interaction at a Water-Air interface: Velocity field inside the bubble. Classical schemes suffer from numerical instabilities (left). Modified schemes cure those instabilities (right).

the wide range of involved temporal and spatial scales. Therefore, we develop temporal and spatial adaptation techniques [4] and employ MPI-parallelization to benefit from modern supercomputers. Newly developed numerical schemes cure drawbacks of the discretization of shock-driven problems [1]. Recent highly-resolved three dimensional simulations give insight into the formation of interface instabilities, which play an important role in biomedical applications [3,5].

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### Shear-flow Phenomena in Compressible Two-phase Flows – Shedding Mechanisms and Droplet Break-up

#### **Motivation and Objectives**

#### Shocks and Re-entrant Jets in Cavitating Flows

Cavitating flows may exhibit an intrinsic instability called 'shedding' [1-2]. The shedding process causes highly transient flow features that may generate noise, vibration, loss of performance and erosive damage to hydraulic machineries [5]. We perform wall-resolved Large Eddy Simulations using in-house computational fluid dynamics codes [1]. In the following, two types of re-entrant jet dynamics are investigated based on the example of a nozzle flow within a square duct. Figure 1 shows typical patterns of shear flow cavitation arising from the inlet edge of the square duct. Grey iso-surfaces indicate water-vapor two-phase patterns and blue iso-surfaces highlight reverse motion of the liquid. Depending on the operating conditions, the classical 're-entrant flow' or the 'condensation shock' appear and lead to recompression of the vapor as well as to Rayleigh-Taylor and Kelvin-Helmholtz instabilities.



Figure 1: Shear flow cavitation patterns (grey iso-surfaces) and reversed liquid motion (blue iso-surfaces) featuring jet-like and shock-like recompression scenarios

#### Shock-induced Break-up of Non-Newtonian Liquid Droplets

The break-up of liquid droplets in a gaseous ambient is a key element of atomization processes. The present work experimentally studies the breakup of single viscoelastic droplets subject to shock-induced gas flow [3]. Millimeter-sized droplets, made from aqueous polymer solutions of carboxymethylcellulose (CMC) and polyacrylamide (PAM), are examined. Both non-Newtonian liquids share similar shear viscosities while the latter shows a stronger extensional viscosity. Droplets are injected discretely into the test section of the shock tube at the AER where shock waves generate a high-speed air flow. The droplet



Figure 2: A shock-induced air flow breaks up a drop of water (left), CMC (center) and PA (right)

deformation is visualized by a focused shadowgraph system and recorded as consecutive images with a Shimadzu HPV-X ultra-high-speed camera. Figure 2 shows the differences of the breakup process between the two non-Newtonian viscoelastic liquids and the Newtonian counterpart, water.

#### **Solution Approach**

We develop and improve mathematical models and highly efficient numerical approaches for simulation of compressible multi-phase flows, especially physically consistent LES (Large Eddy Simulation) codes. The codes are capable of high performance computations on supercomputers, such as SuperMUC at the Leibniz-Rechenzentrum München. In addition to computational fluid mechanics approaches, experimental investigations are performed at AER. The shock tube at the institute is equipped with a droplet generator in order to investigate shock-induced droplet break-up processes. State-of-the art high speed cameras/sensors allow for high quality data acquisition. In addition to droplet break-up mechanisms, we investigate shock-induced multi-bubble collapses of gas bubbles in a slightly non-Newtonian gelatin [4].

Our research is funded by the European Union (project 'UCOM' and project 'EDEM'), the European Space Agency, the German Research Foundation (DFG), and by partners from the automotive industry.

#### **Key Results**

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# Smoothed Particle Hydrodynamics Simulation of Melt Pool Dynamics in Selective Laser Melting



Smoothed particle hydrodynamics simulation of the melting pool dynamics in selective laser melting. Above is a cross-sectional depiction of the melting pool, where the melt is colorized by its temperature.

#### **Motivation and Objectives**

Selective Laser Melting (SLM) is one of the main driving technologies in Additive Manufacturing (AM): Metallic powder material is successively melted layer by layer using laser beam irradiation to build parts with highly complex geometries. In addition, SLM allows the combination of various materials and shielding gases to achieve tailormade material properties. These key properties make the SLM process especially attractive for aerospace and automotive applications, where highly loaded parts with lightweight and complex design are required. However, predictive simulations of the SLM process are challenging due to its multiphysical nature involving complex melt pool dynamics with phase-change phenomena. The objective of this project is to advance the frontiers in understanding the SLM process by latest computational methods. We develop a predictive SPH-based simulation framework to investigate SLM in a virtual lab.

#### **Solution Approach**

A novel simulation framework is developed for the detailed investigation of the SLM process. A building block is the meshless Smoothed Particle Hydrodynamics (SPH) method, which, as opposed to grid-based methods such as the Finite-Volume (FV) and Finite-Element (FE) method, handles multiphase problems with complex topological changes with ease in a conservative fashion. One of the key challenges regarding the simulation of the SLM process is the in-depth description of the melt pool dynamics, which is both challenging from a physical and computational perspective. Within our SPH framework, we pursue a unified description of the melting pool dynamics by resolving all relevant physical mechanisms including surface tension effects, convection currents [1] and phase-change phenomena. An efficient hybrid CPU/GPU parallelization strategy is utilized to benefit from modern computer architectures and to allow for highly resolved simulations. By combining novel numerical methods with high-performance computing, our framework aims at improving the state-of-the-art for predicitive SLM simulations and, ultimately, manufacturing technologies.

#### References

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#### **Research Foci**

- Numerical fluid and flow modeling and simulation
- Complex fluids
- Turbulent and transitional flows
- Aerodynamics of aircraft and automobiles
- Environmental aerodynamics

#### Competences

- Multi-physics code and particle-based model development
- DrivAer car geometry
- Experimental aerodynamics

#### Infrastructure

- 3 low-speed wind tunnels and moving belt system
- 2 shock tubes

#### Courses

- Grundlagen der Fluidmechanik I
- Fluidmechanik II
- Computational Solid and Fluid Dynamics
- Aerodynamik des Flugzeugs I
- Aerodynamik des Flugzeugs II
- Grenzschichttheorie
- Angewandte CFD
- Gasdynamik
- Turbulente Strömungen
- Aerodynamik bodengebundener Fahrzeuge
- Aerodynamik der Bauwerke
- Aerodynamik von Hochleistungsfahrzeugen
- Instationäre Aerodynamik I
- Physik der Fluide
- Numerische Methoden f
  ür Erhaltungsgleichungen
- Aerodynamik der Raumfahrzeuge Wiedereintrittsaerodynamik
- Particle-Simulation Methods for Fluid Dynamics
- Biofluid Mechanics
- Grundlagen der experimentellen Strömungsmechanik
- An Introduction to Microfluidic Simulations
- Instationäre Aerodynamik II
- Strömungsphysik und Modellgesetze
- Praktikum Aerodynamik des Flugzeugs
- Praktikum Simulation turbulenter Strömungen auf HPC-Systemen
- Praktikum Experimentelle Strömungsmechanik