

# Agenda

## 26<sup>th</sup> Results and Review Workshop of the HLRS

Thursday, October 12<sup>th</sup>, 2023

**9:00 Welcome**

Prof. Dr.-Ing. Dr. h.c. Dr. h.c. Hon. Prof. E.h. Michael M. Resch  
(Director of HLRS)

**Session 1: CFD**

Chairman: Prof. Dr.-Ing. Andrea Beck, Universität Stuttgart

**9:05 parDtOOMeetsCanada**

Optimization of a non-standard pump from galvanic industry with the island model  
Ines Waldsteiner, Alexander Tismer, and Stefan Riedelbauch  
Institut für Strömungsmechanik und Hydraulische Strömungsmaschinen (IHS),  
Universität Stuttgart

**9:25 hpcmphas**

A High-Order Framework for Compressible Droplet Dynamics  
Daniel Appel, Steven Jöns, Jens Keim, Pascal Mossier, Andrea Beck, and Claus-Dieter Munz  
Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

**9:45 FS3D**

DNS of the Early Phase of Oblique Droplet Impact on Thin Films with FS3D  
Jonathan Stober, Johanna Potyka, Matthias Ibach, Bernhard Weigand, and Kathrin Schulte  
Institute of Aerospace Thermodynamics, University of Stuttgart

**10:05 GCS-Lamt**

Computational aspects for DNS of compressible turbulent boundary layers  
on up to full machine size  
Tobias Gibis, Jason Appelbaum, and Christoph Wenzel  
Institute of Aerodynamics and Gas Dynamics (IAG), University of Stuttgart

**10:25 Break**

**10:40 PoroDNS**

Modeling of Coupled Turbulent Channel-Porous Media Flow through  
a Deep Autoencoder-Echo State Network Framework  
Xu Chu, Sandeep Pandey, Yanchao Liu, and Bernhard Weigand  
Cluster of Excellence SimTech, University of Stuttgart

**11:00 DNSPImpJets**

Direct numerical simulation of turbulent impinging jets heat transfer  
Francesco Secchi  
Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology

**11:20 TuCoWi**

Accurate and Efficient Direct Numerical Simulation of Drag Reduction via Riblets  
Davide Gatti and Maurizio Quadrio  
Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology

**11:40** **GCS-Sopf**

CFD-driven Surrogate-based Optimization

Fabian Hübenthal, Xiao Shao, Matthias Meinke, and Wolfgang Schröder

Institute of Aerodynamics, RWTH Aachen University

**12:00** **Lunch Break**

**Session 2: CFD, Reactive Flows, Miscellaneous Topics, Transport and Climate Research**

Chairman: Prof. Dr. Volker Wulfmeyer, Universität Hohenheim

**13:15** **SootDNS**

Soot oxidation in a turbulent temporally evolving non-premixed air/ethylene jet

Gandolfo Scialabba, Lukas Berger, and Heinz Pitsch

Institut für Technische Verbrennung, RWTH Aachen

**13:35** **scrcomb**

IDDES of a LOX/CH<sub>4</sub> Model Rocket Combustion Chamber at Real Gas Conditions

Timo Seitz, Ansgar Lechtenberg, Jan Martin, Justin S. Hardi, and Peter Gerlinger

Institut für Verbrennungstechnik, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Stuttgart

**13:55** **DUEHAWK2021**

HPC in Fluid-Mechanics - Materials Synthesis and Hydrogen Combustion

Seung-Jin Baik, Luis Cifuentes, Jonas Eigemann, Linus Engelmann, Dominik Meller,

Patrick Wollny, Robert Externbrink, and Andreas M. Kempf

Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen

**14:15** **CRYALB**

Thermal effects connected to crystallization dynamics: a lattice Boltzmann study

Q. Tan, S.A. Hosseini, and D. Thévenin

Laboratory of Fluid Dynamics and Technical Flow, Otto von Guericke University Magdeburg

**14:35** **trainABL**

Direct Representation of Roughness in the Atmospheric Boundary Layer

Cedrick Ansorge and Jonathan Kostelecky

Institut für Meteorologie, Freie Universität Berlin

**14:55** **Break**

**Session 3: Computer Science, Bioinformatics and Materials Science**

Chairman: Prof. Dr. Lars Pastewka, Universität Freiburg

**15:15** **EXAHD**

The Sparse Grid Combination Technique for Higher-Dimensional Simulations at Extreme Scales

Theresa Pollinger, Marcel Breyer, and Dirk Pflüger

Institut für Parallele und Verteilte Systeme, Universität Stuttgart

**15:35** **GCS-MDDC**

Extensions to the MaMiCo Software Stack for Flexible, Massively Parallel

Molecular-Continuum Flow Simulation

Louis Viot, Amartya Das Sharma, and Philipp Neumann

Chair for High Performance Computing, Helmut-Schmidt-Universität Hamburg

**15:55** [GCS-ReSTFAS](#)

Regulation of substrate transport in the early stages of fatty acid synthesis  
Helmut Grubmüller and Florian Leidner  
Max-Planck-Institut für Multidisziplinäre Naturwissenschaften,  
Max-Planck Gesellschaft, Göttingen

**16:15** [pace3d](#)

Phase-field simulation of sintering processes  
Marco Seiz, Henrik Hierl, Michael Kellner, and Britta Nestler  
Institute of Applied Materials, Karlsruhe Institute of Technology

**16:35** **Break**

**16:45** **Poster Session**

--- CFD ---

[hpcdg poster as pdf](#)

Towards Exascale CFD Simulations Using the Discontinuous Galerkin Solver FLEXI  
Marcel Blind, Min Gao, Daniel Kempf, Patrick Kopper, Marius Kurz, Anna Schwarz,  
and Andrea Beck  
Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

[HybridKT poster as pdf](#)

Highly Resolved Hybrid RANS-LES Simulations of Different Operating Points  
of a Model Kaplan Turbine  
S. Jossberger  
Institute of Fluid Mechanics and Hydraulic Machinery, University of Stuttgart

[Hyperbol poster as pdf](#)

CFD of transient operations of a pump turbine  
Marco Zorn and Stefan Riedelbauch  
Institute of Fluid Mechanics and Hydraulic Machinery, University of Stuttgart

[PbusRobe poster as pdf](#)

Numerical simulation of coating processes using high-speed rotary bells  
Bo Shen, Nico Guettler, Qiaoyan Ye, and Oliver Tiedje  
FhG-IPA, Fraunhofer-Institut für Produktionstechnik und Automatisierung IPA, Stuttgart

[TENwinds poster as pdf](#)

Trailing Edge Noise of Wind Turbine Blades  
Kathrin Stahl, Jana Gericke, Harald Klimach, and Sabine Roller  
Institut für Softwaremethoden zur Produktvirtualisierung,  
Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Dresden

[UnsteadyTurbo poster as pdf](#)

HPC-simulations of unsteady turbomachinery flows  
Nikola Kovachev, Simon Hummel, and Christopher Fuhrer  
Institute of Thermal Turbomachinery and Machinery Laboratory, University of Stuttgart

[WEALoads poster as pdf](#)

Unsteady Blade Root Aerodynamics of a 2MW Wind Turbine Equipped with Vortex Generators  
Ferdinand Seel, Filippo Gajo, Louis Gagnon, Thorsten Lutz, and Ewald Krämer  
Institut für Aerodynamik und Gasdynamik, Universität Stuttgart

--- Reactive Flows ---

[MULTIPHASE poster as pdf](#)

Advancement of Sparse Particle Method for High-Performance Computing  
Jan Wilhelm Gärtner, Oliver T. Stein, and Andreas Kronenburg  
Simulation of Reacting Thermo-Fluid Systems, Engler-Bunte-Institut,  
Karlsruhe Institute of Technology

--- Transport and Climate Research ---

[HRCM poster as pdf](#)

High-resolution climate change information for extremes and land use change  
Hendrik Feldmann, Marie Hundhausen, Regina Kohlhepp, Marcus Breil, Armenia Franco-Diaz,  
and Joaquim G. Pinto  
Institute for Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute of Technology

[WRFSCALE poster as pdf](#)

WRF simulations to investigate processes across scales  
Hans-Stefan Bauer, Oliver Branch, and Benjamin Körner  
Institute of Physics and Meteorology, University of Hohenheim

--- Miscellaneous Topics ---

[MMHBF2 poster as pdf](#)

Unveiling thermodynamic properties and interfacial phenomena in pure fluids and mixtures  
Simon Homes, Isabel Nitzke, Denis Saric, and Jadran Vrabec  
Institut für Prozess- und Verfahrenstechnik, Fachgebiet Thermodynamik,  
Technische Universität Berlin

--- Materials Research ---

[Def-2-Dim poster as pdf](#)

Production of defects in two-dimensional materials under ion and electron irradiation:  
insights from advanced first-principles calculations  
S. Kretschmer, M. Ghorbani-Asl, R. Friedrich, X. Zhang, T. Barnowsky, F. Davies, M. Jain,  
P. Santra, and A. V. Krasheninnikov  
Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

[H-Embrittlement poster as pdf](#)

Drag of dislocations by cross-slip?  
Xiang Xu, Xi Zhang, Siegfried Schmauder, and Blazej Grabowski  
Institute of Materials Science, University of Stuttgart

--- Molecules, Interfaces, and Solids ---

[SPECSY poster as pdf](#)

Spectro-Electrochemistry for water splitting and CO<sub>2</sub> reduction  
Holger Euchner, Jongmin Kim, and Matthias M. May  
Institut für Physikalische und Theoretische Chemie, Universität Tübingen

[FCSS poster as pdf](#)

First principles investigation of the LiNbO<sub>3</sub> and LiTaO<sub>3</sub> lattice dynamics under uniaxial stress  
Mike N. Pionteck, Felix Bernhardt, Kevin Eberheim, Christa Fink, Florian A. Pfeiffer,  
Nils A. Schäfer, Leonard M. Verhoff, Ferdinand Ziese, and Simone Sanna  
Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

[LASMD poster as pdf](#)

Novel non-thermal Ablation Mechanics in the Laser Ablation of Silicon  
Dominic Klein, Simon Kümmel, and Johannes Roth  
Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

--- Physics ---

[BNSMIC poster as pdf](#)

Microphysical aspects of binary neutron star mergers  
Michail Chabanov, Christian Ecker, Carlo Musolino, Luciano Rezzolla, Samuel Tootle,  
and Konrad Topolski  
Institute for Theoretical Physics, Goethe University Frankfurt am Main

[GCS-wprecision poster as pdf](#)

Lattice QCD with high precision  
Zoltan Fodor, Fabian Frech, Christian Holbling, and Balint Toth  
Department of Physics, University of Wuppertal

[stabwf poster as pdf](#)

QCD simulations with stabilised Wilson fermions, towards the physical pion mass  
at a fine lattice spacing  
Francesca Cuteri, Rocco Francesco Basta, Anthony Francis, Patrick Fritzschn, Giovanni Pederiva,  
Antonio Rago, Andrea Shindler, Andre Walker-Loud, and Savvas Zafeiropoulos  
Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main

[TDEglobalsimulation poster as pdf](#)

Global Relativistic Magneto-hydrodynamics Simulations of the Long-term Evolution  
of Tidal Debris in Tidal Disruption Events of Stars  
Taeho Ryu, Ruggero Valli, Rob Farmer, Ruediger Pakmor, Rosalba Perna, Selma de Mink,  
Volker Springel, Julian Krolik, and Tsvi Piran  
Max-Planck-Institut für Astrophysik, Max-Planck-Gesellschaft, Garching

**18:00 Break**

**19:00 Social Event: Dinner at the "Internationales Begegnungszentrum" of the University of Stuttgart**

**Friday, October 13<sup>th</sup>, 2023**

**Session 4: Molecules, Interfaces, and Solids**

Chairman: Prof. Dr. Lars Pastewka, Universität Freiburg

**9:15 DEFTD**

Large-scale ab initio modeling of hydrogen production on stepped surfaces  
of SrTiO<sub>3</sub> perovskite nanoparticles  
Maksim Sokolov, Yuri A. Mastrikov, Eugene A. Kotomin, and Joachim Maier  
Max Planck Institute for Solid State Research, Max Planck Society, Stuttgart

**9:35 3DLP-Master**

Molecular Dynamics Simulation of Laser-based Powder Bed Fusion  
Kevin Vietz, Jonas Schmid, and Johannes Roth  
Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

**9:55 PhoMatX**

Understanding AlInP(001) surfaces from massively parallel ab-initio simulations  
I.A. Ruiz Alvarado, L.J. Glahn, M. Krenz, A. Bocchini, K.L. Franzke, U. Gerstmann,  
and W.G. Schmidt  
Department Physik, Universität Paderborn

**10:15 Break**

**Session 5: Physics**

Chairman: Prof. Dr. Andreas Frommer, Bergische Universität Wuppertal

**10:35 GCS-HQCD**

Hadronic contributions to the anomalous magnetic moment of the muon from Lattice QCD  
G. von Hippel, S. Kuberski, H.B. Meyer, D. Mohler, S. Paul, and H. Wittig  
Helmholtz Institute Mainz, Johannes Gutenberg University Mainz

**10:55 RinQCD4PANDA**

Hadron scattering and resonances for PANDA physics  
J. Bulava, B. Hoerz, R. J. Hudspith, M. F. M. Lutz, D. Mohler, and C. Morningstar  
Institut für Kernphysik, Technische Universität Darmstadt

**11:15 microBNS**

44163 microBNS yearly report 2023  
Maximilian Jacobi, Federico Guercilena, and Almudena Arcones  
Institut für Kernphysik, Technische Universität Darmstadt

**11:35 GWanalysis**

Simulating Binary Neutron Star Mergers  
Tim Dietrich, Bernd Brügmann, Edoardo Giangrandi, Henrique Leonhard Gieg,  
Nina Kunert, Ivan Markin, Vsevolod Nedora, Anna Neuweiler, Henrik Rose,  
Peter Tsun Ho Pang, Federico Schianchi, Ashwin Shirke, and Maximiliano Ujevic  
Institute for Physics and Astrophysics - Theoretical Astrophysics, University of Potsdam

**11:55 Lunch Break**

**13:10 Awarding of [Golden Spikes of HLRS](#)**

**13:30 End**

**13:40 Guided Tour - Computer Room and Visualisation (Virtual Reality, Cave)**

anytime [HLRS - Hawk - Virtual Tour](#)

anytime [HLRS - Virtual Reality](#)