

High Performance Computing in Science and Engineering 2024

The 27th Results and Review Workshop of the HLRS, Oct. 10 – Oct. 11, 2024
in Cooperation with the Scientific Computing Center (SCC)
of the Karlsruhe Institute of Technology (KIT), Kaiserstraße 12, 76131 Karlsruhe
at Lecture hall and foyer Room 30.10

Agenda

Thursday, October 10th, 2024

9:15 Welcome & Introduction

Prof. Dr. Martin Frank
(Director of SCC, Karlsruhe)

Prof. Dr. Thomas Ludwig
(Director of German Climate Computing Center (DKRZ), Hamburg,
Head of the Steering Committee)

Session 1: CFD

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

9:25 DNS-SHOCKPART_SCC

Numerical study of shock-wave interaction with a fully-resolved cloud of immobile particles
Swagat Kumar Nayak and Markus Uhlmann
Institut für Wasser und Umwelt, Karlsruher Institut für Technologie

9:45 FS3D_HLRS

Direct Numerical Simulations of Droplet Impact onto Heated Surfaces using the Program Free Surface 3D (FS3D)
Manish Kumar, Rishav Saha, Johanna Potyka, Kathrin Schulte, and Bernhard Weigand
Institute of Aerospace Thermodynamics (ITLR), University of Stuttgart

10:05 hpcdg_HLRS

Advancement of the Discontinuous Galerkin Solver FLEXI Towards GPU-Enabled Systems
Marcel Blind, Yannik Feldner, Daniel Kempf, Patrick Kopper, Marius Kurz, Jannik Schrempp,
Anna Schwarz, Spencer Starr, and Andrea Beck
Institute of Aerodynamics and Gas Dynamics (IAG), University of Stuttgart

10:25 TCTA-SBLI_HLRS

Numerical investigation of shock-boundary layer interaction on a highly-loaded transonic compressor cascade to compare with experimental results
Bjoern F. Klose, Edwin J. Munoz Lopez, Christian Morsbach, and Alexander Hergt
Institut für Test und Simulation für Gasturbinen, German Aerospace Center (DLR), Augsburg

10:45 Break

Session 2: CFD and Reactive Flows

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

11:05 GCS-ANPIT_HLRS

Analysis of Upstream Traveling Waves on Transonic Buffet

T. Lürkens, M. Meinke, and W. Schröder

Chair of Fluid Mechanics and Institute of Aerodynamics, RWTH Aachen University

11:25 TestSpraySynDNS_HLRS

High-Resolution Primary Atomization Simulations

for Modeling Spray Formation of a Coaxial Atomizer

Gandolfo Scialabba, Fabian Fröde and Heinz Pitsch

Institute for Combustion Technology, RWTH Aachen University

11:45 LaBoRESys_HLRS

Advancing Electrochemical Energy Storage and Conversion
through Lattice-Boltzmann Simulations

Julius Weinmiller, Benjamin Kellers, Konrad Gülicher, Thomas Jahnke,
Timo Danner, and Arnulf Latz

Institut für Technische Thermodynamik, German Aerospace Center (DLR), Stuttgart

12:05 Lunch Break

Session 3: Transport and Climate Research, Miscellaneous Topics

Chairman: Prof. Dr. Thomas Ludwig, Deutsches Klimarechenzentrum, Hamburg

13:25 ICON-ART2_SCC

Modelling of composition-climate interactions with ICON-ART

R. Ruhnke, P. Braesicke, L. Feld, P. Dietz, V. Hanft, K. Satitkovitchai,

B.-M. Sinnhuber, M. Sinnhuber, and S. Versick

Institut für Meteorologie und Klimaforschung Atmosphärische Umweltforschung,
Karlsruher Institut für Technologie

13:45 HRCM_HLRS

Providing climate information inferred from kilometer-scale modelling

Hendrik Feldmann, Marie Hundhausen, Evgenii Churiulin,

Christine Mihalyfi-Dean, and Joaquim G. Pinto

Institute of Meteorology and Climate Research Troposphere Research (IMKTRO)
Karlsruhe Institute of Technology (KIT)

14:05 CCH-SSA_SCC

Climate Change and Health in Sub-Saharan Africa: High-resolution dynamical climate -
malaria transmission modeling near Victoria Lake, Kenya

Mame Diarra Bousso Dieng and Joël Arnault

Atmospheric Environmental Research Institute of Meteorology and Climate Research
Karlsruhe Institute of Technology, KIT-Campus Alpin, Garmisch-Partenkirchen

14:25 MMHBF2_HLRS

Molecular Simulations: A Thermodynamic Study of Bulk and Interface Behavior

Simon Homes, Isabel Nitzke, Denis Saric, Gabriela Guevara-Carrion, and Jadran Vrabec

Fachgebiet Thermodynamik, Technische Universität Berlin

14:45 Break

Session 4: Materials Science and Computer Science

Chairman: Prof. Dr. Birgit Strodel, Forschungszentrum Jülich

- 15:05** [Def-2-Dim_HLRS](#)
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, T. Barnowsky,
F. Davies, M. Jain, P. Santra, and A. V. Krasheninnikov
Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf
- 15:25** [Confsolv2_SCC](#)
Confinement effects on fluid mixtures
Marc Högler and Niels Hansen
Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart
- 15:45** [basictoolbox_SCC](#)
Scalable Discrete Algorithms for Big Data Applications
Lukas Hübner, Florian Kurpicz, Peter Sanders, Matthias Schimek,
Dominik Schreiber, Daniel Seemaier, and Tim Niklas Uhl
Institute of Theoretical Informatics - Algorithm Engineering, Karlsruhe Institute of Technology
- 16:05** [GCS-MDDC_HLRS](#)
Saving Energy in Molecular Fluid Dynamics by using Molecular-Continuum Simulations
Ruben Horn, Amartya Das Sharma, and Philipp Neumann
Chair for High Performance Computing, Helmut Schmidt University Hamburg
- 16:25** **Break**
- 16:40** **Poster Session**
- CFD ---
- [DNSPImpJets_HLRS poster as pdf](#)
Reynolds analogy in smooth-wall turbulent impinging jets
Francesco Secchi
Institut für Strömungsmechanik (ISTM), Karlsruhe Institute of Technology
- [GCS-lesdg_HLRS poster as pdf](#)
Recent Progress of Wall-Modeled Large Eddy Simulation
in the Discontinuous Galerkin Solver FLEXI
Marcel Blind, Yannik Feldner, Jannik Schrempp, and Andrea Beck
Institute of Aerodynamics and Gas Dynamics, University of Stuttgart
- [GCS-Sopf_HLRS poster as pdf](#)
Prediction of Propeller-Airfoil Interaction Noise
Zhe Yang, Matthias Meinke, and Wolfgang Schroeder
Chair of Fluid Mechanics and Institute of Aerodynamics, RWTH Aachen University
- [hpcmphas_HLRS poster as pdf](#)
Recent Results in the Construction of High-Order Numerical Methods
for Compressible Multiphase and Multispecies Flows
Daniel Appel, Steven Jöns, Jens Keim, Pascal Mossier, Philipp Oestringer,
Amalía Travnicek, and Andrea Beck
Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

[SootDNS_HLRS poster as pdf](#)

DNS study on soot oxidation and break-through in non-premixed turbulent jet flames
Gandolfo Scialabba, Michael Gauding, and Heinz Pitsch
Institut für Technische Verbrennung, RWTH Aachen University

[TuCoWi_HLRS poster as pdf](#)

Turbulent Drag Reduction on a Transonic Airfoil with a Shockwave Blades
Davide Gatti, Niccolo' Berizzi, Sergio Pirozzoli, and Maurizio Quadrio
Institute of Fluid Mechanics, Karlsruhe Institute of Technology

--- Reactive Flows ---

[MULTIPHASE_HLRS poster as pdf](#)

Super-resolution of turbulent velocity and scalar fields using different scalar distributions
Ali Shamooni and Oliver T. Stein, and Andreas Kronenburg
Institut für Technische Verbrennung (ITV), Universität Stuttgart

--- Transport and Climate Research ---

[CLIFOOD2_HLRS poster as pdf](#)

Advanced Weather Forecasts for Ethiopia by Optimized Initialization and Perturbation
with Satellite Data
Tamene Mekonnen Adgeh, Thomas Schwitalla, and Kirsten Warrach-Sagi
Institute of Physics and Meteorology, University of Hohenheim

[WRFSCALE_HLRS poster as pdf](#)

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

--- Miscellaneous Topics ---

[IMPD_HLRS poster as pdf](#)

High Performance Computing for DSMC Simulations
of Low Knudsen Number Transitional Flows
M. Pfeiffer , J. Beyer , F. Garmirian, F. Hild , S. Lauterbach , C. Marianowski,
T. Ott, R. Tietz , and S. Fasoulas
Institute of Space Systems, University of Stuttgart

--- Materials Research ---

[H-Embrittlement_HLRS poster as pdf](#)

Understanding the Yield Stress Anomaly in Ni₃Al via Atomistic Simulations
Xiang Xu, Xi Zhang, and Blazej Grabowski
Institute for Materials Science, University of Stuttgart

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

[3DLP-Master_HLRS poster as pdf](#)

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

[PhoMatX_HLRS poster as pdf](#)

Energy transfer in tetracene-sensitized silicon solar cell
from massively parallel ab-initio simulations

M. Krenz, A. Bocchini, I.A. Ruiz Alvarado, K.L. Franzke, T. Biktagirov,
U. Gerstmann, and W.G. Schmidt

Theoretische Materialphysik, Universität Paderborn

[SPECSY_HLRS poster as pdf](#)

Spectroelectrochemistry for water splitting and CO₂ reduction

Holger Euchner, Jongmin Kim, and Matthias M. May

Institut für Physikalische und Theoretische Chemie, Universität Tübingen

[Terminat_SCC poster as pdf](#)

Anharmonic correction to adsorption free energy of O-species on Pt(111) surface
from thermodynamic integration using MLFF-MD simulations

Thanh-Nam Huynh and Dmitry I. Sharapa

Institut für Katalysforschung und -technologie, Karlsruher Institut für Technologie (KIT)

--- Physics ---

[BNSMIC_HLRS poster as pdf](#)

Binary neutron star mergers: the bulk viscosity effect, long-term simulation
and the gravitational wave emitted

Michail Chabanov, Jin-liang Jiang, Harry Ho-Yin Ng, Luciano Rezzolla, Samuel Tootle,
and Konrad Topolski

Institut für Theoretische Physik, Goethe University Frankfurt am Main

[MHD_HLRS poster as pdf](#)

Non-linear magnetohydrodynamic simulations of magnetic confinement fusion plasmas

I. Holod, M. Hoelzl, A. Cathey, W. Tang, and H. Bergstroem

Numerical Methods in Plasma Physics, Max Planck Institute for Plasma Physics, Garching

[simhydro_SCC poster as pdf](#)

Ab Initio Simulation of Hydrogen at Extreme Conditions

Tobias Dornheim and Jan Vorberger

Helmholtz-Zentrum Dresden-Rossendorf

18:15 Break

18:30 Social Event: Dinner at the “Dürer-Saal des Gastdozentenhauses” of KIT

Friday, October 11th, 2024

Session 5: Molecules, Interfaces, and Solids

Chairman: Prof. Dr. Lars Pastewka, Universität Freiburg

9:15 [automat1_HLRS](#)

Data-Driven Design of 2D Non-van derWaals Materials and 2D Heterostructures

Tom Barnowsky, Anastasiia Nihei, Mani Lokamani, and Rico Friedrich

Theoretical Chemistry, Technische Universität Dresden

9:35 [FCSS_HLRS](#)

Effect of Mg doping on the LiNbO₃ ferroelectric phase transition

Mike N. Pionteck, Felix Bernhardt, Kevin Eberheim, Christa Fink, Alexander Kapp,

Florian A. Pfeiffer, Nils A. Schäfer, Leonard M. Verhoff, Ferdinand Ziese, and Simone Sanna

Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

9:55 [Dynathor_HLRS](#)

Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase
in a Phospholipid Bilayer

Jonathan Teuffel, Sophia Ber, Stefan Richter, Goutam Mukherjee,

Bosco Sungho Han, and Rebecca C. Wade

Molecular and Cellular Modeling Group, Heidelberg Institute for Theoretical Studies (HITS)

10:15 **Break**

Session 6: Physics

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

10:40 [WGTSPseudo2d_HLRS](#)

Simulations of the KATRIN Windowless Gaseous Tritium Source

Felix Spanier, Christian Sendlinger, and Josi Schulze

Institut für Theoretische Astrophysik, Universität Heidelberg

11:00 [stabwf_HLRS](#)

QCD simulations with stabilized Wilson fermions, towards the physical pion mass
at a fine lattice spacing

Rocco Francesco Basta, Francesca Cuteri, Anthony Francis, Patrick Fritzsich, Giovanni Pederiva,

Antonio Rago, Andrea Shindler, Andre Walker-Loud, and Savvas Zafeiropoulos

Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main

11:20 [GCS-nearcrit_HLRS](#)

Standard model's predictions on near-critical behaviour to be seen in collider experiment

Szabolcs Borsanyi, Zoltan Fodor, Jana N. Gunther, Sandor D. Katz, Paolo Parotto,

Attila Pasztor, David Pesznyak, Kalman K. Szabo, and Chik Him Wong

Department of Physics, University of Wuppertal

11:40 **Lunch Break**

13:00 **Awarding of [Golden Spikes of HLRS](#)**

13:20 **End**