

Agenda

25th Results and Review Workshop of the HLRS

Tuesday, October 4th, 2022

9:00 Welcome

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

9:05 Opening

Prof. Dr. Wolfgang E. Nagel, Universität Dresden
(Former Chair of the Steering Committee of HLRS)

Session 1: CFD

Chairman: Prof. Dr.-Ing. Ewald Krämer, Universität Stuttgart

9:15 FS3D

Towards DNS of Droplet-Jet Collisions of Immiscible Liquids with FS3D
Johanna Potyka, Jonathan Stober, Jonathan Wurst, Matthias Ibach, Jonas Steigerwald,
Bernhard Weigand, and Kathrin Schulte
Insitut für Thermodynamik der Luft- und Raumfahrt, Universität Stuttgart

9:35 DNSFREE

Direct numerical simulation of turbulent shallow flows with deformable free-surface
Aman G. Kidanemariam, Markus Uhlmann, and Ivan Marusic
Institute for Hydromechanics, Karlsruhe Institute of Technology

9:55 mixgauss

Turbulent Mixed Convection over Structured Surfaces
Kay Schäfer, Juan Pedro Mellado, Bettina Frohnäpfel
Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology (KIT)

10:15 TuCoWi

Annual Report of the project TuCoWi (44212) - turbulent flow Control over a transonic wing
Maurizio Quadrio, Alessandro Chiarini, Jacopo Banchetti, Davide Gatti, Antonio Memmolo,
and Sergio Pirozzoli
Institute of Fluid Mechanics (ISTM), Karlsruhe Institute of Technology (KIT)

10:35 Break

10:55 CPE

Advances in Computational Process Engineering using Lattice Boltzmann Methods
on High Performance Computers for Solving Fluid Flow Problems
Adrian Kummerländer, Fedor Bukreev, Simon F. R. Berg, Marcio Dorn, and Mathias J. Krause
Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology

11:15 DGDES

Applications of a Discontinuous Galerkin Chimera Method on 3D Flow Problems
Fabian Genuit, Manuel Keßler, and Ewald Krämer
Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

11:35 **GCS-lesdg**

Performance Improvements for Large Scale Simulations Using the Discontinuous Galerkin Framework FLEXI

Marcel Blind, Patrick Kopper, Daniel Kempf, Marius Kurz, Anna Schwarz, Andrea Beck, and Claus-Dieter Munz

Institute of Aerodynamics and Gas Dynamics (IAG), University of Stuttgart

11:55 **Lunch Break**

Session 2: Reactive Flows, Transport and Climate Research

Chairman:

13:10 **2PHASE**

Simulation und Modellierung von Zweiphasenströmungen - 2PHASE (Abschlussbericht)

A. Kronenburg

Institut für Technische Verbrennung, Universität Stuttgart

13:30 **LaBoRESys**

Lattice Boltzmann Simulation of Flow, Transport, and Reactions in Battery Components

Martin P. Lautenschläger

Institut für Technische Thermodynamik, Computergestützte Elektrochemie, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Ulm

13:50 **CCH-SSA**

Climate Change and Health in Sub-Saharan Africa: High resolution dynamical climate - malaria transmission modelling

Diarra Dieng, Joël Arnault, Benjamin Ferch, and Harald Kunstmann

Atmospheric Environmental Research Institute of Meteorology and Climate Research, Karlsruhe Institute of Technology (KIT/IMK-IFU)

14:10 **MCRPH-WCB**

The role of microphysical processes for warm conveyor belt ascent

Annika Oertel, Corinna Hoose, Christian M. Grams, and Annette K. Miltenberger

Institute of Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute of Technology

14:30 **trainABL**

Closing the gap of scales for turbulence-resolving simulations in meteorology

Cedrick Ansorge, Jonathan Kostelecky, and Steven van der Linden

Institut für Geophysik und Meteorologie, Universität zu Köln

14:50 **Break**

Session 3: Miscellaneous Topics, Computer Science and Bioinformatics

Chairman:

15:10 **CRYALB**

Simulations of crystal growth using lattice Boltzmann formulation

Q.Tan, S.A.Hosseini, and D.Thévenin

Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg

15:30 **MMHBF2**

High-performance computing as a key to new insights into thermodynamics

Simon Homes, Ivan Antolovic, Robin Fingerhut, Gabriela Guevara-Carrion,

Matthias Heinen, Isabel Nitzke, Denis Saric, and Jadran Vrabec

Thermodynamik und Thermische Verfahrenstechnik, Technische Universität Berlin

15:50 **GCS-MDDC**

Fault Tolerant Molecular-Continuum Flow Simulation

Vahid Jafari, Piet Jarmatz, Helene Wittenberg, Amartya Das Sharma, Louis Viot, Felix Maurer, Niklas Wittmer, and Philipp Neumann

Chair for High Performance Computing, Helmut-Schmidt-Universität /
Universität der Bundeswehr Hamburg

16:10 **Tarantella**

Scalable Deep Learning with Tarantella: Performance Analysis

Alexandra Carpen-Amarie

Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Kaiserslautern

16:30 **EnzymAgglo**

Data-Driven Multiscale Modeling of Self-Assembly and Hierarchical Structural Formation in Biological Macro-Molecular Systems

Philipp Nicolas Depta, Maksym Dosta, and Stefan Heinrich

Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology

16:50 **Break**

17:00 **Poster Session**

--- CFD ---

CO2Absorber [poster as pdf](#)

Modeling the Gas Liquid Interface of Falling Film Reactors in Fully Developed Flow Regime

K.V. Muthukumar, M. Okrashevski, N. Bürkle, D.M. Aguirre Bermudez, M. Haber, R. Koch, H.-J. Bauer, and C. Ates

Institut für Thermische Strömungsmaschinen, Karlsruhe Institute of Technology (KIT)

GCS-Lamt [poster as pdf](#)

Favorable-Pressure-Gradient Influence on Supersonic Film Cooling with Turbulent Main Flow

Johannes M. F. Peter, Tobias Gibis, and Markus J. Kloker

Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

PorodNS [poster as pdf](#)

An investigation of information flux between turbulent boundary layer and porous medium

Xu Chu, Wenkang Wang, and Bernhard Weigand

Cluster of Excellence SimTech, University of Stuttgart

SCBOPT [poster as pdf](#)

On the Effects of Wing-Gust Interactions and Wing Flap Deflections on the HTP Aerodynamics

Junaid Ullah, Marco Hillebrand, Maximilian Ehrle, Thorsten Lutz, Wolfgang Heinze, and Jochen Wild

Institute of Aerodynamics and Gas Dynamics, University of Stuttgart

unrgh2 [poster as pdf](#)

Study of data-driven prediction of roughness skin friction

Jiasheng Yang, Alexander Stroh, and Pourya Forooghi

Institute of Fluid Mechanics, Karlsruhe Institute of Technology

--- Reactive Flows ---

[MULTIPHASE poster as pdf](#)

Flame structure analysis and flamelet modeling of turbulent pulverized solid fuel combustion with flue gas recirculation

Ali Shamooni, Oliver T. Stein, Andreas Kronenburg, Xu Wen, Hendrik Nicolai, Christian Hasse, and Andreas M. Kempf

Institute for Combustion Technology, University of Stuttgart

--- Transport and Climate Research ---

[HRCM poster as pdf](#)

Impact of land-use change and user-tailored climate change information from a high-resolution climate simulation ensemble

Hendrik Feldmann, Marie Hundhausen, Regina Kohlhepp, and Marcus Breil

Institute for Meteorology and Climate Research (IMK-TRO), Karlsruhe Institute of Technology

[WRFSCALE poster as pdf](#)

WRF simulations to investigate processes across scales (WRFSCALE)

Hans-Stefan Bauer and Oliver Branch

Institute of Physics and Meteorology, University of Hohenheim

--- Miscellaneous Topics ---

[ShapeOptCompMat poster as pdf](#)

Geometric Constrained Scalable Algorithm for PDE-Constrained Shape Optimization

Jose Pinzon, Martin Siebenborn, and Andreas Vogel

Department of Mathematics, Hamburg University

--- Computer Science ---

[exaFSA poster as pdf](#)

Improving the Performance and Scalability of Partitioned Multi-Physics Simulation

Amin Totounferoush and Miriam Schulte

Institute for Parallel and Distributed Systems (IPVS), University of Stuttgart

--- Bioinformatics ---

[EnzSim poster as pdf](#)

Parameter study of solvent systems by molecular dynamics simulations (Project: EnzSim)

Matthias Gültig, Jan Range, Benjamin Schmitz, and Jürgen Pleiss

Institut für Biochemie und Technische Biochemie, Universität Stuttgart

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

[GaPSi poster as pdf](#)

Organic functionalization on solid surfaces

Badal Mondal, Raza Ullah Khan, Florian Kreuter, Patrick Maue, Sudip Pan, Fabian Pieck, Hendrik Weiske, and Ralf Tonner-Zech

Theoretische Chemie komplexer Systeme, Universität Leipzig

[FCSS poster as pdf](#)

Hyperpolarizabilities of LiNbO₃, LiTaO₃ and KNbO₃ calculated from first principles
Mike N. Pionteck, Felix Bernhardt, Christof Dues, Kevin Eberheim, Christa Fink, Kris Holtgrewe, Florian A. Pfeiffer, Nils A. Schäfer, Leonard M. Verhoff, Ferdinand Ziese, and Simone Sanna
Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

--- Materials Research ---

[CDD poster as pdf](#)

Dislocation configuration in microwires under torsion analyzed by nonlocal three-dimensional crystal plasticity simulations
Katrin Schulz and Kolja Zoller
Institute of Applied Materials - Reliability and Microstructure, Karlsruhe Institute of Technology

[DiHu poster as pdf](#)

Status report DiHu - Towards a digital human
David Schneider, Dominik Göttsche, Felix Huber, Thomas Klotz, Benjamin Maier, Oliver Röhrle, Miriam Schulte, and Benjamin Uekermann
Institute for Parallel and Distributed Systems, University of Stuttgart

--- Physics ---

[BNSMIC poster as pdf](#)

Microphysical aspects of binary neutron star mergers
Michail Chabanov, Alejandro Cruz-Orsorio, Christian Ecker, Claudio Meringolo, Luciano Rezzolla, Samuel Tootle, and Konrad Topolski
Institute for Theoretical Physics, Goethe University Frankfurt

[Flexadfg poster as pdf](#)

Molecular dynamics simulations of the structure of lipid-based nanomaterials
Giovanni Settanni and Friederike Schmid
Institute of Physics, Johannes-Gutenberg University Mainz

[INTRHYGUE poster as pdf](#)

INTRHYGUE: simulations of intermediate mass-ratio and hyperbolic binary black-hole mergers
Simone Albanesi, Sebastiano Bernuzzi, Boris Daszuta, Georgios Doulis, Rossella Gamba, Alessandro Nagar, and Francesco Zappa
Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena

[MCTDHB poster as pdf](#)

Correlations, Shapes, and Fragmentations of ultracold matter
A. U. J. Lode, O. E. Alon, A. Bhowmik, M. Büttner, L. S. Cederbaum, R. Chitra, S. Dutta, D. Jaksch, H. Kessler, C. Lévêque, R. Lin, P. Mognini, L. Papariello, M. C. Tsatsos, and J. Xiang
Institute of Physics, University of Freiburg

--- Structural Mechanics ---

[ANNdirect poster as pdf](#)

A new machine learning based method to determine directly validated material model parameters for sheet metal forming simulations

Celalettin Karadogan and Patrick Cyron

Institute for Metal Forming Technology, University of Stuttgart

18:00 Break

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

Wednesday, October 5th, 2022

Session 4: Molecules, Interfaces, and Solids

Chairman:

9:15 ECHO

The role of chemistry and bias in (photo)-electrochemical applications:

ECHO (Electro-Catalysis for H₂O Oxidation) and beyond

Detre Teschner and Travis Jones

Department of Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin

9:35 PhoMatY

Polaron formation dynamics in lithium niobate from massively parallel ab-initio simulations

M. Krenz, A. Bocchini, T. Biktagirow, A. Kozub, S. Badalov, S. Neufeld, I.A. Ruiz Alvarado,

U. Gerstmann, and W.G. Schmidt

Lehrstuhl für Theoretische Materialphysik, Universität Paderborn

9:55 AiMat

Artificial Intelligence for Materials Science

André Eberhard, Tobias Schlöder, and Pascal Friederich

Institut für Theoretische Informatik, Karlsruhe Institute of Technology (KIT)

10:15 QMAG

First-principles study of NV centers near extended defects

Reyhaneh Ghassemizadeh, Wolfgang Körner, Daniel F. Urban, and Christian Elsässer

Fraunhofer Institut für Werkstoffmechanik (IWM), Fraunhofer, Freiburg

10:35 Break

Session 5: Physics

Chairman:

10:55 GWanalysis

Simulating Binary Neutron Star Mergers

Tim Dietrich, Parikshit Biswat, Bernd Brüggemann, Swami Vivekanandji Chaurasia,

Mattia Emma, Francesco Maria Fabbri, Henrique Leonhard Gieg, Maximilian Kölsch,

Nina Kunert, Michele Mattei, Anna Neuweiler, Henrik Rose, Peter Tsun Ho Pang,

Federico Schianchi, and Maximiliano Ujevic

Institute for Physics and Astronomy, University of Potsdam

11:15 **GCS-denseqgp & GCS-wprecision**

- Bulk features of the quark gluon plasma at finite density
S. Borsanyi, Z. Fodor, J. Günther, S. D. Katz, A. Pasztor, P. Parotto, R. Kara, C. Ratti, and K. K. Szabó
- Lattice QCD with high precision
Zoltan Fodor, Fabian Frech, Christian Hoelbling, and Balint Toth
Department of Physics, University of Wuppertal

11:50 **Lunch Break**

12:50 **Awarding of [Golden Spikes of HLRS](#)**

13:00 **End**

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

anytime [HLRS - Virtual Reality](#)