5th International Conference on Computational Engineering

ICCE2024

September 30–October 2, 2024 Technische Universität Darmstadt, Darmstadt, Germany

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Welcome

We are very happy to welcome all participants at the 5th International Conference on Computational Engineering in the City of Science Darmstadt. The event continues the series of the previous four editions of this conference that were held in Herrsching (October 2009), Darmstadt (October 2011 and September 2017) and Stuttgart (October 2014).

The conference is intended to provide an interdisciplinary meeting place for researchers and practitioners working on computational methods in all disciplines of engineering, applied mathematics and computer science. The aim of the conference is to discuss the state of the art in this vibrant field, exchange experiences, develop promising perspectives for future research and initiate further cooperation.

The conference program comprises 45 contributed papers covering current research topics in the different areas of Computational Engineering as well as 21 presentations within an integrated students' conference. The program is complemented by five invited lectures from internationally well-known experts in the field.

The conference is jointly organized by the Graduate School of Computational Engineering and the Profile Topic CE at TU Darmstadt, the Center for Computational Engineering Science at RWTH Aachen University, the TUM School of Computation, Information and Technology at TU München and the Stuttgart Center for Simulation Science at University of Stuttgart.

Selected papers of the conference will be published in an issue of *Springer's Lecture Notes in Computational Science and Engineering*.

The chairpersons would like to thank all invited speakers, contributors and organizers of the conference. We are looking forward to a stimulating and fruitful event of high scientific quality.

Darmstadt, September 2024

Michael Schäfer

on behalf of the chairpersons:

Marek Behr, RWTH Aachen University
Hans-Joachim Bungartz, TU München
Michael Schäfer, TU Darmstadt
Sebastian Schöps, TU Darmstadt
Miriam Schulte, University of Stuttgart
Manuel Torrilhon, RWTH Aachen University
Oliver Weeger, TU Darmstadt

Timetable

Monday, September 30

	Room "Bonn": Plenum and parallel sessions	Room "Hannover": Parallel sessions
12:00–13:00	**Registration**	
13:00–13:05	**Welcome**	
13:05–14:05	**David Keyes** KAUST, Thuwal, Kingdom of Saudi Arabia Chair: Michael Schäfer	*Efficient Computation through Tuned Approximation*
14:05–15:05	**Session 1: Design/life-cycle simulation** Chair: Michael Schäfer	**Session 2: Multi-physics and aerodynamics simulation** Chair: Herbert De Gersem
	Maximilian Kannapinn *Digital twin inference from multi-physical simulation data of additive manufacturing processes: proof of concept study*	**Imane Fadli** *Multi-level aeroshape optimization using Active Subspace*
	Jascha Brötzmann *Data-driven and physics-based Structural Health Monitoring*	**Benjamin Rodenberg** *Verification and debugging of partitioned multiphysics simulation with preCICE and open-source solvers*
	Oliver Weeger *Immersed isogeometric analysis with boundary conformal quadrature for finite deformation problems*	**Tarik Corbo** *Transient plasma actuator force determination and its computational validation*
	Leon Blumrich *Efficient Design Strategies for Variable Speed Electric Motors: Integrating Finite-Element Analysis and Analytical Post-Processing*	**Steffen Gröninger** *Comparative assessment of different turbulence modelling approaches for the simulation of twin-jet impingement*
15:05–15:30	**Coffee break**	

Each talk in the parallel sessions is expected to take 15 min including discussion and questions (i. e. 10–12 min remain for the talk itself).

Clicking on the title of any talk scrolls to the corresponding abstract.

15:30–16:30	**Session 3: Numerics** Chair: Manuel Torrilhon	**Session 4: (High-performance) Computations** Chair: Maximilian Kannapinn
	Hendrik Wilka *Adaptive sparse grid collocation methods for uncertainty quantification in gas networks*	**Hendrik Nicolai** *Ammonia combustion modelling enabled by high-performance GPU computing*
	Michal Mika *Matrix-free inexact preconditioning techniques for discretizations on structured grids*	**Muhammed Toprak** *Cell agglomeration for cut cells in eXtended discontinuous Galerkin methods*
	Xiang Ye *High-Order Simulations for Fluid-Soft Substrate Interaction through Euler-Lagrange and Euler-Euler Frameworks*	**Luis Gall** *Tuning of Vectorization Parameters for Molecular Dynamics Simulations in AutoPas*
	Jan-Magnus Christmann *Combination of the Harmonic Balance FEM with Homogenization Techniques*	**David Martin** *The Multiple Time-Stepping Method for Three-Body Interactions in High Performance Molecular Dynamics Simulations*
starting 18:00	**Conference dinner at Orangerie**	

Tuesday, October 1

09:00–10:00	**Joris Degroote** Ghent University, Ghent, Belgium Chair: Miriam Schulte	*Recent advances in quasi-Newton methods for partitioned simulation of fluid-structure interaction*
10:00–10:30	**Coffee break**	
10:30–12:00	**Session 5: Mechanics modeling/IGA** Chair: Miriam Schulte	**Session 6: Computational models for fluid simulation** Chair: Magnus Kircher
	Juan Camilo Alzate Cobo *Thermo- and chemo-elastic beam modeling and simulation with isogeometric collocation methods*	**Matthias Rieckmann** *Numerical influence of model contradictions for non-material two-phase flow*
	Marco ten Eikelder *Phase-field mixture flows: modeling and isogeometric discretization*	**Irina Shishkina** *Wetting simulation of the porous structure of a heat pipe using an eXtended Discontinuous Galerkin method and a parameterized level-set*
	Nils Plückhahn *Accelerating Computation of Sealing Deformation – A Physics-Informed Neural Network Framework for Hyperelastic Deformation*	**Patrick Antony** *Adaptive Refinement for Multi-Phase Flow on Moving Domains*
	Felix Rutsch *Modelling and optimizing the grayscale masked stereolithography 3D printing process*	**Ullika Scholz** *Dispersive Shallow Water Moment Equations*
	Mohammad Shojaee *Multiscale modeling for vibration analysis of metamaterial beams via micromorphic theory*	**Muhammad Tayyab Bin Saghir** *Numerical Stabilization on the Simulation of Elastoviscoplastic Fluid*
	Bai-Xiang Xu *A finite strain isogeometric chemo-mechanical solid-beam element towards simulations of microlattice structured Li-ion battery electrodes*	**Satyvir Singh** *High-order discontinuous Galerkin scheme for capturing Richymyer-Meshkov instability at polygonal interfaces*
12:00–13:00	**Lunch break**	

13:00–14:00	**Somdatta Goswami** Johns Hopkins University, Baltimore (MD), USA Chair: Marek Behr	*Employing Machine Learning Approaches to solve PDEs in "Mechanics" within Big-data Regime*
14:00–15:00	**Session 7: Electromagnetic simulation** Chair: Marek Behr	**Session 8: (Reduced order) Modeling techniques** Chair: Sebastian Schöps
	Laura D'Angelo *Modeling Screening Currents in a Reduced Magnetic Vector Potential Formulation with Higher-Order Magnetic Moments*	**Ahsan Ali Siddiqui** *Reduced order modeling of blood perfusion in liver lobules with high dimensional parameter space*
	Mario Mally *On Domain Decomposition for Electromagnetic Problems in 3D*	**Vladimir Dunic** *Critical total strain-based Phase-Field Damage Model implementation for ductile fatigue*
	Thuc Pham Phu *Computational modeling of flexoelectric effects in microscale piezoelectric metamaterials*	**Nicolas Lepage** *Hybrid Autoencoder/Galerkin approach for nonlinear reduced order modelling*
	Jonas Christ *A Self-Consistent Model for Wakefield and Space Charge Calculations*	**Eda Yilmaz** *The Challenge of Modeling Rarefied Gases: Kinetic Theory, Moment Equations, and Closure Relations*
	Students' session 1	
15:00–15:30	**Short presentations of topics**	
15:30–16:00		**Project desks**
15:30–16:00	**Coffee break**	
	Students' session 2	
16:00–16:30	**Short presentations of topics**	
16:30–17:00		**Project desks**
17:00–17:45	**Stefan Turek** TU Dortmund, Dortmund, Germany Chair: Sebastian Schöps	*The Future of CFD Simulations (from a numerical & computational perspective) – Faster and more reliable predictions and new benchmark concepts are needed to compete with AI*

Detailed program of the students' sessions:

	Students' session 1	
15:00–15:30	**Short presentations of topics** Chair: Carsten Wesp, Eike Rehwald	
	Matthias Geratz (RWTH)	*Initial Investigation into Automatic AD Mission Pipeline Execution*
	Yacine Tayeb (RWTH)	*Efficient Interface Reconstruction On Polyhedral Meshes*
	Faris Begic (TUDa)	*Sensitized RANS-RSM simulations of flow and thermal fields in a concentric annulus*
	Jonas Fey (TUDa)	*Nonlinear inelastic constitutive modeling with physics-augmented neural networks*
	Georg Puntigam (RWTH)	*Comparison of evolutionary neural networks and optimization methods for function minimization*
	Yuki Nishizawa (RUB)	*Mixed finite element for numerical dynamic simulation of flexoelectric materials*
	Fabian Roth (TUDa)	*Physics-Guided Neural Networks for Lyapunov-Stable Dynamic System Identification*
	Jonas Bünning (RWTH)	*Efficiency estimation for melting probes subject to different ambient ice temperatures and different gravitational forces*
	Paul Hollmann (TUDa)	*Spectral Chebyshev Collocation Methods for Eigenvalue Problems in Linear Flow Stability Analysis*
	Runchao Wang (TUDa)	*Real-time Monitoring and Alert System for Building Material Storage*
15:30–16:00		**Project desks**

RWTH = RWTH Aachen University, TUDa = TU Darmstadt, TUM = Technical University of Munich, RUB = Ruhr-University Bochum

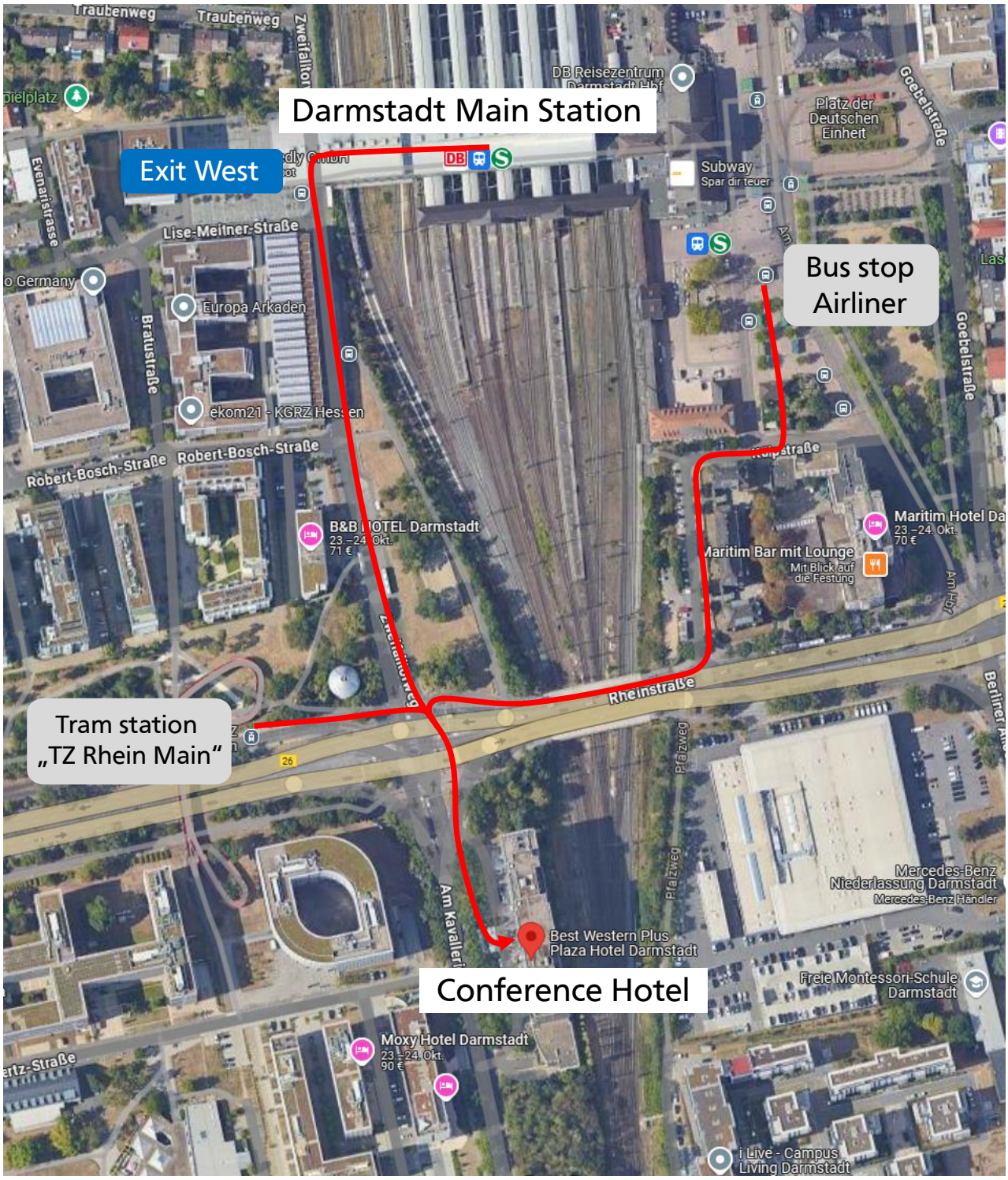
	Students' session 2	
16:00–16:30	**Short presentations of topics** Chair: Matthias Geratz	
	Piyush Karki (TUM)	*Coupling of Discontinuous Galerkin Numerical Solvers in ExaHyPE 2*
	Antonia Bähr (TUDa)	*Analysis of Ammonia-Hydrogen Combustion using Large-Eddy Simulation and detailed chemistry*
	Jiahui Yong (TUDa)	*Exploiting Neural Networks with Algorithm Unrolling for ARMA Parameter Estimation*
	Christian Berwanger (RWTH)	*Investigation of erythrocyte damage in aortic flow during aortic valve stenosis using Lagrangian blood damage analysis*
	Marc Hoffmann (TUDa)	*A posteriori error estimates for finite volume schemes for Keller-Segel systems*
	Pálma Emese Inczeffy (RWTH)	*Enhancing Magnetic Field Homogeneity by Optimal Magnet Positioning*
	Arthur Harger (TUDa)	*Phase field model of indentation-induced crack propagation in glass*
	Sneha Iyer (RWTH)	*Limitations of a 1D Advection-Diffusion Finite Difference Model for Sea Ice*
	Sathyamurthy Hegde (RWTH)	*Framework for Bayesian Inference with HPCs*
	Paul Liebenow (TUDa)	*Multilevel and Adaptive Training of Neural Network*
	Carsten Wesp, Eike Rehwald (TUDa)	*A simple crane simulation using the finite element method*
16:30–17:00		**Project desks**

Wednesday, October 2

09:00–10:00	**Angelika Humbert** Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research, Bremerhaven and University of Bremer Bremen, Germany Chair: Oliver Weeger	*Multi-physics simulations of the Greenland Ice Sheet – approaches and challenges in tackling a complex system*
10:00–10:30	**Coffee break**	
10:30–11:45	**Session 9: Fluid simulation applications** Chair: Michael Schäfer	**Session 10: Data-driven CE** Chair: Oliver Weeger
	Magnus Kircher *Multi-cycle LES of knocking combustion initiation in a spark ignition engine*	**Jonathan Stollberg** *Physics-augmented neural networks meet topology optimization*
	Julien Steib *Uncertainty analysis on an internal combustion engine fueled with hydrogen*	**Azzeddine Tiba** *Partitioned data-driven reduced order strategies for fluid-structure interaction problems*
	Donat Weniger *Numerical Methods for Rarefied Gas Phase Transitions*	**Dominik Klein** *Nonlinear electro-elastic finite element analysis with neural network constitutive models*
	Marthe de Crouy-Chanel *Uncertainty quantification for Large Eddy Simulations with Remeshed Vortex Methods*	**Qing Sun** *Solving wave equations with neural networks*
	Khaled Boulbrachene *Numerical simulation of discrete wind gusts generated by an adaptive nozzle using a dynamic immersed boundary method*	
11:50–12:00	**Final plenum**	
12:00	**End of Conference**	

Location & Conference Dinner

Location: Best Western Plus Plaza Hotel Darmstadt
Address: Am Kavalleriesand 6, 64295 Darmstadt



Conference Dinner: Orangerie, Darmstadt
Address: Bessunger Straße 44, 64285 Darmstadt

By tram (recommended): Enter tram 4 or 9 at station “TZ Rhein Main” (cf. map on previous page; directions “Kranichstein” respectively “Böllenfalltor”), change to line 3 or 7 at “Luisenplatz” (direction “Lichtenbergschule”) and exit at station “Orangerie”. Link to tram network plan of Darmstadt

By car: Use parking lot “Orangerie”, driveway is accessible through Orangerieallee.

List of Abstracts – Talks

Critical total strain-based Phase-Field Damage Model implementation for ductile fatigue

V. Dunić[1], ***M. Živković***[1]

[1] University of Kragujevac, Faculty of Engineering, Kragujevac, Serbia

The Phase-Field Damage (PFD) method is an attractive approach for modeling damage in materials. Special attention is given to ductile behavior where a non-linear plastic stress-strain response occurs above the yield stress. The authors proposed the novel, critical total strain-based PFD implementation into in-house FEM software (PAK-DAM). The total strain internal energy consists of elastic, plastic and fracture contribution [1]: $W = W_e + W_p + W_f$. The fracture contribution is based on the work-density criterion with threshold [1]: $W_f = G_v \left(d + \frac{l_c^2}{2} |\nabla d|^2 \right)$ where G_v is the specific fracture energy per unit volume, l_c is the characteristic length, and d is the damage variable. The equilibrium of the internal and external potential energy gives the phase field damage evolution law [1,2]:

$$f\left(\bar{\alpha}(t)\right) G_V \left[d - l_c^2 \nabla^2 d\right] + g'\left(d\right) max\left(\psi^E + \psi^P - \frac{G_v}{2}\right) = 0$$

where $f\left(\bar{\alpha}(t)\right)$ is the fatigue function, $g'\left(d\right)$ is the derivative of degradation function, while ψ^E and ψ^P are the elastic and plastic strain energy density. The unit cube is loaded by prescribed displacement on one side, while the other side is restrained. The relationship between G_v and critical total strain value ε_{cr} is proposed where $\varepsilon_{cr} = 0.12$. Three loading-unloading cycles are performed up to strain: the first cycle = 2%, the second cycle = 3%, the third cycle 4%.

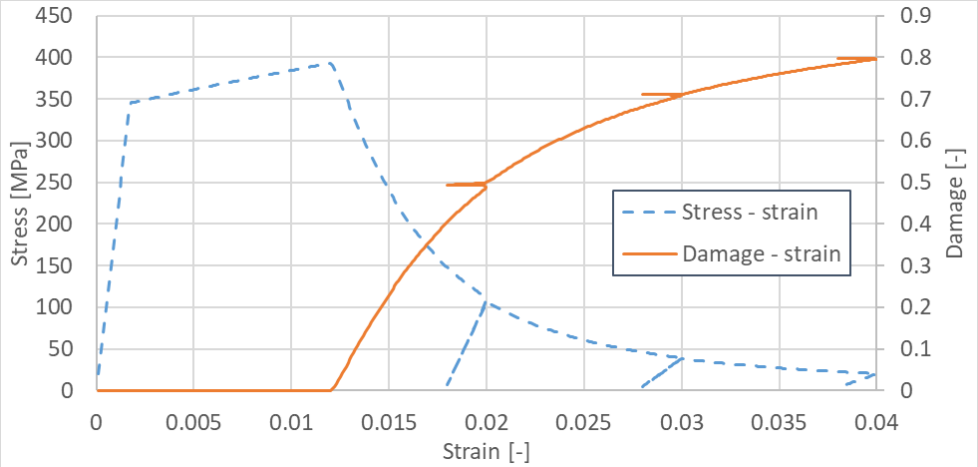


Figure 1: Stress-strain and damage-strain response for cyclic loading.

Acknowledgment

This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7475, Prediction of damage evolution in engineering structures - PROMINENT.

References

[1] C. Miehe, M. Hofacker, L.-M. Schanzel and F. Aldakheel (2015) Phase field modeling of fracture in multi-physics problems. Part II. CMAME, 294:486-522.

[2] M. Simoes, C. Braithwaite, A. Makaya, E. Martínez-Pañeda (2022) Modelling fatigue crack growth in shape memory alloys. Fatigue Fract Eng Mater Struct, 45(4):1243-1257

List of Participants

With all participants who give a talk or a presentation the stated pagenumber is linked to the corresponding abstract.