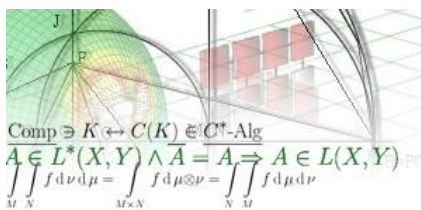


# GAMM Activity Group CSE

## Workshop 2017

Forschungszentrum Jülich  
19 – 20 October 2017



GESELLSCHAFT für  
ANGEWANDTE MATHEMATIK und MECHANIK  
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS

**Andreas Lintermann**  
**Robert Speck**

## Abstracts

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[www.fz-juelich.de/ias/jsc/gamm-cse-2017](http://www.fz-juelich.de/ias/jsc/gamm-cse-2017)



## Welcome!

We like to welcome you to the GAMM CSE Workshop 2017 at Jülich Supercomputing Centre! Together with a long-standing tradition of research on computational mechanics, the fields of mathematical modelling, numerics and scientific computing are key topics of the Gesellschaft für Angewandte Mathematik und Mechanik e.V. (GAMM). They form the basis of modern computational science and engineering (CSE), requiring interdisciplinary and international research collaborations across traditional boundaries.

The workshop program consists of 16 talks covering a variety of topics from the broad field of computational science and engineering. Yet, the focus of this event is on “coupling”: Finding strategies to efficiently couple models, methods and software to solve for the individual physics is a challenging task and a highly active field of research. In particular, regarding upcoming exascale systems, the scalability of such coupled software solutions is key to code sustainability and code applicability to solve even more complex multi-physics problems in the future. The talks are accompanied by our activity group meeting Thursday afternoon.

Coffee breaks and lunches will be served and on Thursday evening a workshop dinner takes place at Burg Obbendorf. When staying at the Hotel Kaiserhof in Jülich, a shuttle will take you from there to the workshop location at JSC’s rotunda, building 16.4, and back (with a detour to Burg Obbendorf on Thursday evening, of course).

We wish you a pleasant and productive workshop here at Jülich Supercomputing Centre!

Your organizers

Andreas Lintermann & Robert Speck



## Thursday, 19 October 2017

- 08:15 Shuttle from Hotel Kaiserhof to JSC
- 08:30-09:00 Registration
- 09:00-09:15 Opening
- 09:15-10:00 **Well-Balanced Meshless Methods for the Shallow-Water Equations**  
*Scott MacLachlan*  
Department of Mathematics and Statistics, Memorial University of Newfoundland, Canada
- 10:00-10:15 Coffee break
- 10:15-12:15 **Fourth Order Accuracy for the Lattice Boltzmann Method Using Only the Nearest Neighbor Stencil: Is It Possible?**  
*Martin Geier*  
Institute for Computational Modeling in Civil Engineering (iRMB), TU Braunschweig
- Aero-Structural Coupling Using Lattice Boltzmann Method**  
*Deepali Singh*  
Aerospace Applications, Exa GmbH, Stuttgart
- Median Filtering and Its Extensions for Color Images**  
*Andreas Kleefeld*  
Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH
- Computing Interior Transmission Eigenvalues**  
*Lukas Pieronek*  
Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH
- 12:15-13:15 Lunch break
- 13:15-14:15 Business meeting
- 14:15-15:00 **HPC-Based Cardiovascular Computational Modelling**  
*Mariano Vázquez*  
Engineering (CASE) Department, Barcelona Supercomputing Center, Spain
- 15:00-15:30 Coffee break
- 15:30-17:30 **Variational Space-Time Elements for Large-Scale Systems**  
*Christian Hesch*  
Chair of Computational Mechanics, University of Siegen
- Towards the Virtual Product**  
*Stephen Longshaw*  
Scientific Computing Department, Science and Technology Facilities Council (STFC), Warrington, Great Britain
- Multi-Physics Coupling and Uncertainty Quantification in Heat Transfer Applications**  
*Alex Skillen*  
Scientific Computing Department, Science and Technology Facilities Council (STFC), Warrington, Great Britain
- Gradient-Based Shape Optimisation of the TU Berlin Stator Using a Differentiated CAD Kernel**  
*Mladen Banovic*  
Institute for Mathematics, Paderborn University
- 18:15 Shuttle from JSC to Burg Obbendorf
- 18:30-21:30 Dinner
- 21:30 Shuttle from Burg Obbendorf to Hotel Kaiserhof



## Friday, 20 October 2017

- 08:45 Shuttle from Hotel Kaiserhof to JSC
- 09:15-10:00 **Modular Parallel Multi-Physics Simulation**  
*Miriam Mehl*  
Institute for Parallel and Distributed Systems, University of Stuttgart
- 10:00-10:15 Coffee break
- 10:15-12:15 **Coupling Molecular Dynamics and Dissipative Particle Dynamics Methods Using Adaptive Resolution Scheme**  
*Julija Zavadlav*  
Chair for Computational Science, ETH Zürich, Switzerland
- Towards Fully-Coupled CAA Simulations to Analyze Chevron Nozzle Noise**  
*Ansgar Niemöller*  
Institute of Aerodynamics, RWTH Aachen
- Time Stepping for Partitioned Multi-Physics**  
*Benjamin Rüth*  
Department of Informatics, Technical University of Munich (TUM)
- Coupled Simulation of LHC's Quench Protection System**  
*Sebastian Schöps*  
Department of Electrical Engineering and Information Technology, TU Darmstadt
- 12:15-13:15 Lunch break
- 13:15-14:15 **Adjoint-Based Data Assimilation for Compressible and Reactive Flows**  
*Jörn Lothar Sesterhenn*  
Institute of Fluid Dynamics and Technical Acoustics (ISTA), TU Berlin
- Transient Multi-Instance Molecular-Continuum Flow Simulation on Supercomputers**  
*Philipp Neumann*  
Department of Informatics, University of Hamburg
- 14:15 Closing remarks





# Abstracts



## **Well-Balanced Meshless Methods for the Shallow-Water Equations**

**Scott MacLachlan**

Department of Mathematics and Statistics, Memorial University of Newfoundland, Canada,  
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In this talk, I will present recent work on meshless discretizations for the nonlinear shallow-water equations and discuss their application to tsunami models. Meshless methods are attractive for modelling both coastal and river flooding, due to the unstructured nature of real-world topographic data, but standard meshless finite-difference approaches fail even for very simple test cases. This motivates the development of a mimetic scheme for the spatial derivative and averaging operators to realize well-balanced meshless discretizations. We couple this approach with a radial basis function based extrapolation method for the inundation model, giving an accurate and efficient simulation scheme for the shallow-water equations. This is joint work with Jörn Behrens (Universität Hamburg) and Alex Bihlo (Memorial University of Newfoundland), along with students Rüdiger Brecht and Ben Morrison.

## **Fourth Order Accuracy for the Lattice Boltzmann Method Using Only the Nearest Neighbor Stencil: Is It Possible?**

**Martin Geier**

Institute for Computational Modeling in Civil Engineering (iRMB), TU Braunschweig,  
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After our recent demonstration that the diffusion term in the lattice Boltzmann method for the Navier-Stokes equation can be made fourth order accurate [Journal of Computational Physics vol. 348, p. 862], which were also presented at the previous GAMM-CSE meeting, we show here that also advection can be made fourth order accurate without increasing the size of the stencil beyond next neighbors. The approach is based on an asymptotic analysis up to the fourth order, the utilization of quartic parameters and the recovery of some second order derivatives of velocity from third and fifth order cumulants. The approach is demonstrated to yield fourth order accurate results while the range of stability compared to the second order accurate lattice Boltzmann method is reduced.



## **Aero-Structural Coupling Using Lattice Boltzmann Method**

**Deepali Singh**

Aerospace Applications, Exa GmbH, Stuttgart, *deepali@exa.com*

The simulation of one-way coupled aero-structural problems using the Lattice Boltzmann method (LBM) and a finite element structural code is discussed. The unsteady fluid loads are calculated using the LBM based solver PowerFLOW, which are exported to Finite Element method based solver Nastran to calculate the time dependent structural displacement and deformation modes of the body. The transfer of unsteady surface pressure data from the fluid computation to the structural mesh is performed through an interpolation tool called PowerEXPORT. Special care is taken to ensure conservation of integrated forces and moments.

The one-way coupling method has the advantage of requiring significantly lower computational time compared to two-way coupled approaches, as well as a constant fluid mesh that ensures consistency in the mesh quality. It is suited for cases involving unsteady loads which cause small displacements, e.g., an open landing gear door during takeoff or landing of a typical passenger aircraft, which is test case used for the present study. The flow around such test case is already very unsteady even for zero yaw angle of attack. On the other hand, due to the low body deformation obtained using realistic material properties, it is assumed that for this particular application, the one-way coupling approach would be appropriate to provide reasonable results for preliminary designs. Results in both time and frequency domain, along with a discussion on other possible industrial applications of such an approach will be presented.

## **Median Filtering and Its Extensions for Color Images**

**Andreas Kleefeld**

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The construction of structure-preserving denoising filters for color images is a challenging task. A new approach is presented that is based on a recently proposed transformation from the RGB color space to the space of symmetric  $2 \times 2$  matrices (Burgeth, B., Kleefeld A. (2014) An approach to color-morphology based on Einstein addition and Loewner order, Pattern Recognition Letters, 47, 29-39.). This new framework coupled with spatial adaptivity via morphological amoebas offers excellent capabilities for structure-preserving filtering of color images. Additionally, a generalization of the median-based concept is proposed leading to color-valued amoeba M-smoothers. Numerical experiments confirm the applicability and the potential of this novel approach (Kleefeld, A. et al. (2015) Adaptive Filters for Color Images: Median Filtering and its Extensions, Lecture Notes in Computer Science, Springer, Berlin, 9016, 149-158.).



## Computing Interior Transmission Eigenvalues

**Lukas Pieronek**

Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, *l.pieronek@fz-juelich.de*

Interior transmission eigenvalues (ITEs) arise in the study of inverse acoustic scattering problems and are related to non-scattering responses of a given penetrable object by specific incident waves. As such, ITEs can be seen as fingerprints of an opaque object which recover information about its interior, for example the existence of inner integrities and abnormalities, since heterogeneous composites affect the magnitudes of ITEs in an individual manner. Their accurate and fast calculation is therefore a challenging but desired task and can be mathematically translated into a non-linear eigenproblem whose eigenvalues coincide with the ITEs. In this talk we present a new solver for the efficient calculation of these eigenvalues based on the method of fundamental solutions which distinguishes from most of the currently applicable methods as it is both mesh- and integration free. The essential issue we needed to cope with in the discrete case was the ill-posedness of the underlying abstract problem which could be circumvented by an extended orthogonalization procedure suggested by Trefethen and Betcke within a related context. We will provide an introduction to the modelling framework and embellish our analysis with a variety of numerical examples which proves our approach for ITE recovery to be more than competitive with those known from the literature.

## HPC-Based Cardiovascular Computational Modelling

**Mariano Vázquez**

Computer Applications in Science and Engineering Department(CASE), Barcelona Supercomputing Center, Spain, *mariano.vazquez@bsc.es*

In this talk I will describe the use of HPC to simulate the complex multi-physics problems found in computational cardiovascular mechanics. I will focus on simulations at tissue and organ levels, involving fluid mechanics, non-linear solid mechanics and electrophysiology, all fields tightly coupled, in scenarios like arteries or the heart itself.

## Variational Space-Time Elements for Large-Scale Systems

**Christian Hesch**

Chair of Computational Mechanics, University of Siegen, *christian.hesch@uni-siegen.de*

In this talk, we introduce a new Galerkin based formulation for transient continuum problems, governed by partial differential equations in space and time. Therefore, we aim at a direct finite element discretization of the space-time, suitable for massive parallel analysis of the arising large-scale problem. In particular, novel finite elements for thermal, mechanical and fluid systems as well as higher order formulations for problems in material science have been developed in a joint project between the Chair of Computational Mechanics in Siegen, the Institute of Nonlinear Mechanics in Stuttgart and the Institute of Computational Science in Lugano. Eventually, we will demonstrate the applicability of the proposed formulations to a wide range of problems.





## **Towards The Virtual Product**

**Stephen Longshaw**

Scientific Computing Department, Science and Technology Facilities Council (STFC),  
Warrington, Great Britain, *stephen.longshaw@stfc.ac.uk*

This talk will look at current work happening within STFC involving a number of industrial and academic partners. The overall goal is to further the state of the art with regards to code coupling on HPC systems in order to enable a future where the concept of the virtual product is actually a reality. The grand vision involves more than just coupled simulations, it looks to a future where a jet engine, for example, is designed entirely in-silico. The immediate challenges however revolve around multi-physics and multi-scale simulation on large HPC systems.

This talk will present the coupling approach being taken by STFC in the form of lightweight, MPI-based inter-solver communication through the "Multiscale Universal Interface" library, as well as other similar approaches. It will briefly touch on other existing approaches and talk about some of the issues expected on modern HPC systems in terms of scheduling and resource use.

## **Multi-Physics Coupling and Uncertainty Quantification in Heat Transfer Applications**

**Alex Skillen**

Scientific Computing Department, Science and Technology Facilities Council (STFC),  
Warrington, Great Britain, *alex.skillen@stfc.ac.uk*

This talk will build on the talk of Stephen Longshaw. We will outline the status of the large scale coupling project that is currently underway at STFC. Stephen's talk will focus on the coupling methodology and HPC aspects, while this talk will focus on the applications. We will present our work on the conjugate heat transfer within a power transformer, and the coupling of a neutronics code to a CFD code.

## **Gradient-Based Shape Optimisation of the TU Berlin Stator Using a Differentiated CAD Kernel**

**Mladen Banovic**

Institute for Mathematics, Universität Paderborn, *mladen.banovic@math.uni-paderborn.de*

The open-source CAD kernel Open CASCADE Technology (OCCT) is algorithmically differentiated, in forward and reverse mode, using the AD software tool ADOL-C (Automatic Differentiation by Overloading in C++). The differentiated OCCT kernel is coupled with a discrete adjoint CFD solver, thus providing a fully differentiated design chain at hand.

This design chain is used to perform the gradient-based optimisation of the total pressure loss in the TU Berlin TurboLab Stator test-case. Furthermore, the optimised blade has to accommodate two cylinders that serve to mount the blade to the casing. Their optimal position is calculated using the differentiated OCCT kernel.



## Modular Parallel Multi-Physics Simulation

**Miriam Mehl**

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The underlying models for today's numerical simulation of technical and biological systems are mostly highly complex and, in particular, involve multiple types of equations, a property which we refer to as multi-physics. To achieve a high accuracy of the numerical solution of these models requires very large computational resources – as provided by supercomputers. However, the combination of model complexity and massively parallel and often heterogeneous systems raises many challenges – from the software challenge (How to write maintainable software in an acceptable development time for varying combinations of sub-models and solvers?) over the discretization challenge (How to provide a common stable, accurate and efficient discretization for models consisting of different types of equations) and the solver challenge (How to solve huge non-linear ill-conditioned discretized multi-physics systems) to the partitioning and load balancing challenge (How to measure and balance load over several heterogeneous parts of a simulation environment?). We present these challenges and solutions developed mainly in the German-Japanese ExaFSA (Exascale Simulation of Fluid-Structure-Interactions) project of the German priority program SPP1648 - Software for exa-scale computing.

## Coupling Molecular Dynamics and Dissipative Particle Dynamics Methods Using Adaptive Resolution Scheme

**Julija Zavadlav** and Matej Praprotnik

Chair for Computational Science, ETH Zürich, *julijaz@ethz.ch*

We present the hybrid coupling of the molecular dynamics (MD) and dissipative particle dynamics (DPD) methods, bridging the micro- and mesoscopic descriptions [1]. The interfacing is performed within the adaptive resolution scheme (AdResS) [2], which is a linear momentum conserving coupling technique. Our methodology is hence suitable to simulate fluids on the micro/mesoscopic scale, where hydrodynamics plays an important role. The presented approach is showcased for water at ambient conditions. The water molecules change their resolution back and forth between the MD and DPD scales according to their positions in the system. The supramolecular coupling is enabled by a recently developed clustering algorithm SWINGER [3] that assembles, disassembles and reassembles clusters as needed during the course of the simulation. This allows for a seamless coupling between standard atomistic MD and DPD models.

[1] J. Zavadlav, S. M. Praprotnik, *J. Chem. Phys.* 147, 114110, 2017.

[2] M. Praprotnik, L. Delle Site and K. Kremer, *Annu. Rev. Phys. Chem.* 59, 545, 2008.

[3] J. Zavadlav, S. J. Marrink, M. Praprotnik, *J. Chem. Theory Comput.* 12, 4138-4145, 2016.



## Towards Fully-Coupled CAA Simulations to Analyze Chevron Nozzle Noise

**Ansgar Niemöller**

Institute of Aerodynamics, RWTH Aachen University, *a.niemoeller@aia.rwth-aachen.de*

Various ideas exist to reduce jet noise, which is still one of the major noise sources at aircraft take-off. Serrated or chevron nozzles represent one approach, since the jet structures depend on the exit geometry of the nozzle and these flow structures define the noise sources of the jet.

Typically, hybrid methods are employed for the analysis of such kind of computational aeroacoustic applications. In general, these hybrid methods are based on a two-step approach consisting of two independent simulations for the prediction of the flow and the acoustic field. This allows the use of optimized algorithms and customized grids for each physical system. However, since the exchange of acoustic source term data takes place via disk I/O the scalability of the overall methodology is limited by both the available I/O bandwidth as well as the disk storage capacity.

The direct-hybrid method for computational aeroacoustics circumvents these issues by coupling both solvers in the same framework and running them simultaneously facilitates the exchange of source data directly in memory. Thereby, intensive I/O operations are avoided while the use of a joint hierarchical Cartesian grid allows for efficient parallelization, dynamic load balancing and local mesh refinement. Spatial interpolation by local Galerkin projection enables the use of non-conforming grids to satisfy differing resolution requirements.

Therefore, the direct-hybrid method is a promising candidate for large-scale aeroacoustic simulations to target jet noise reduction through serrated engine nozzles.

## Time Stepping for Partitioned Multi-Physics

**Benjamin R uth** Department of Informatics, Technical University of Munich,  
*benjamin.rueth@tum.de*

Two different approaches exist for the simulation of multi-physics phenomena: Either a monolithic simulation framework is used to directly solve the system of equations describing the multi-physics setup, or in a partitioned approach multiple single-physics problems are solved independently and the coupling is enforced by iteratively solving a fixed-point problem.

We rely on a minimal invasive, partitioned approach, where multiple black-box solvers are coupled explicitly or implicitly. For non-matching spatial meshes interpolation methods are provided. However, the proper handling of non-matching temporal discretization is an open research question. Currently, identical time-steps are required for the single-physics solvers. Additionally, time-stepping schemes are reduced to first order and stability problems arise - even for A-stable solvers.

In this talk, the aforementioned phenomena are reproduced for a simple 1D model problem – two 1D heat transport equations with Dirichlet-Neumann coupling. Specialized strategies that maintain order and stability properties are described for different explicit and implicit time integration schemes. In the future we plan to develop a general mechanism for arbitrary time integration schemes. This finally enables us to solve complex multi-scale-multi-physics scenarios, such as turbulent fluid-structure interaction or fluid-structure-acoustics interaction.



## **Coupled Simulation of LHC's Quench Protection System**

**Sebastian Schöps**

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This contribution discusses the simulation of magnetothermal effects in superconducting magnets as used in particle accelerators, e.g. the LHC at CERN, Geneva. An iterative coupling scheme for a network of partial differential equations describing the electromagnetic, thermal and mechanical effects is demonstrated. The multiphysics, multirate and multiscale problem requires a consistent formulation and framework to tackle the challenging transient effects occurring at both system and device level.

## **Adjoint-Based Data Assimilation for Compressible and Reactive Flows**

**Jörn Lothar Sesterhenn**

Institute of Fluid Dynamics and Technical Acoustics (ISTA), Technische Universität Berlin, *joern.sesterhenn@tnt.tu-berlin.de*

The analysis of complex fluid mechanical phenomena is usually based on experimental and numerical analysis. Both approaches provide useful information. However, experimental data are usually incomplete, because not every state variable is accessible by measurements. On the other hand, numerical solutions are often affected by initial and boundary conditions, which do not fully match to the real flow conditions. To obtain a complete set of information of a real flow state, both approaches can be combined by means of data assimilation.

Most commonly, a variational approach is used. Parameters of a numerical model are adapted until the numerical solution match the experimental data. The required adaptation (gradient) is determined by adjoint equations. The assimilated numerical state contains the unknown/unmeasured quantities under the constraint of the applied model. Furthermore, the quality of experimental data is enhanced by means of a model-based filtering, which can reduce measurement noise.

The application of an adjoint-based data assimilation for compressible flows will be presented by means of three different applications. The first application considers the identification of sound sources. The second application deals with the determination of instantaneous pressure distributions based on PIV data. The third application is the analysis of reactive flow configurations.

The employed numerical framework and its requirements on the computational infrastructure are discussed in detail.





# Transient Multi-Instance Molecular-Continuum Flow Simulation on Supercomputers

**Philipp Neumann**

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Adaptive methods allow for fluid flow simulation of large and complex systems. Hence, the application of adaptive grids has become a well-established standard technique in open-source and commercial flow solvers. The same holds for multiscale approaches, such as turbulence models in CFD. These methods are, however, often limited to problems in which the scales of concern and consideration are well separated.

If the scales are not well separated or if molecular effects have to be incorporated directly via (potentially local) molecular dynamics (MD), hybrid molecular-continuum simulations close the gap between molecular and continuum description. The computational domain is divided into two overlapping regions: a continuum and a particle region. Both domains are coupled via exchange of relevant quantities such as mass and momentum. This yields a solution in the whole domain and locally accounts for molecular effects.

I present the macro-micro-coupling tool (MaMiCo) which allows for molecular-continuum simulation on both Desktop and supercomputers. Due to its modular and flexible software design, existing software packages, e.g. continuum or MD solvers, can be linked together and, thus, be reused. Both quasi steady-state and transient systems can be handled using MaMiCo. In the transient case, MaMiCo employs a novel multi-instance approach in which several quasi-identical particle systems are sampled and coupled to a single continuum solver. I present validation results and discuss parallel performance based on an in-house MD code and LAMMPS, including both MD and dissipative particle dynamics solvers.



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