DROPIT

SFB-TRR 75
Tropfendynamische Prozesse unter extremen Umgebungsbedingungen

Workshop

Mathematical and Numerical Modeling of Multiphase Flow

Thursday, 7th of November 2019
University of Stuttgart
Seminar Room, Basement U-1.039, at Institute for Aerodynamics and Gas Dynamics
Pfaffenwaldring 21

Organisation: C.-D. Munz, C. Rohde
Institute of Aerodynamics and Gas Dynamics (IAG), Institute of Applied and Numerical Mathematics (IANS)
University of Stuttgart

Program

9:00-9:45	M. Hantke (Halle) Analysis and Simulation of a New Multi-Component Two-Phase Flow Model with Phase Transition and Chemical Reactions
9:45-10:30	J. M. Winter (München) Sharp-Interface Modeling of Shock-Interface Interactions

Coffee

11:00-11:45	T. Hitz (Stuttgart) A Sharp-Interface Ghost-Fluid Method with Phase Transition
11:45-12:30	B. Fond (Magdeburg) Temperature measurement with thermographic particles

Lunch

13:30-14:15	M. Dumbser, E. Romenski (Trento-Novosibirsk) A unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics and its solution with high order ADER schemes
14:15-15:00	F. Thein (Magdeburg) The Riemann Problem for a Barotropic Two Fluid Model

Coffee

15:30-16:15	C. Müller (Stuttgart) A HLLC approach for the Euler equations with heat conduction based on the GRP model
16:15-17:00	J. Magiera (Stuttgart) A Molecular-Continuum Riemann Solver for Liquid-Vapor Flow
17:00-17:45	G. Warnecke (Magdeburg) Systems of two-phase mixture balance laws with phase transitions

Dinner

Analysis and Simulation of a New Multi-Component Two-Phase Flow Model with Phase Transition and Chemical Reactions

Maren Hantke
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For the modeling and simulation of multi-phase flows, Baer-Nunziato type models are frequently used. Usually this leads to several problems. A new multicomponent model introduced by Bothe and Dreyer can avoid these disadvantages of Baer-Nunziato type models. This model can be employed to simulate chemically reacting flows as well as phase transitions. In particular, we apply this model to two phases, where each phase is a simple multi-component mixture.

The available theory of conservation laws as well as numerical methods for these type of equations relies very much on the knowledge of eigenvalues and eigenvectors corresponding to the Jacobian of the inviscid fluxes. Although we cannot explicitly compute the eigenvalues and eigenvectors of the system, we are able to prove some analytical results that are essential for the implementation.

Using an explicit time stepping, the time steps are restricted by the characteristic velocities of the fluids. On the other hand, stiffness of the system is also introduced by the chemical reactions. Depending on the fluid state and the relaxation times, either the characteristic velocities of the fluid or the chemical relaxation rates will be dominating the CFL number.

We present numerical results where we consider a two-component flow with phase transition and a three-component flow with chemical reactions.

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Sharp-Interface Modeling of Shock-Interface Interactions

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The numerical simulation of compressible flow phenomena with several interacting gaseous and liquid phases has become an important tool in research and industry. These flows often involve singularities such as shocks and interfaces as well as instabilities driven by their interaction. The inherent highly nonlinear dynamics of those systems leads to a broad range of temporal and spatial scales that have to be resolved and properly modeled. Having adequate fluid models and related high-performance solvers at hand, the increasing computational power offered by large distributed-memory machines like the SuperMUC-NG at LRZ or the future HPE APOLLO 9000

HAWK system at HLRS enables large-scale simulations of complex compressible flow phenomena.

In this talk, we present our open-source multi-phase compressible flow simulation framework ALPACA [1], developed at the TUM Chair of Aerodynamics and Fluid Mechanics. Therein, the fully compressible Navier-Stokes equations are solved with a finite-volume approach and state-of-the-art low-dissipative shock capturing schemes. A conservative interface-interaction model accounts for the interaction between fluids. To describe the interface, we use a sharp-interface level-set method. Computational efficiency is achieved by an adaptive-local time-stepping scheme and multi-resolution approaches [2]. ALPACA is written in C++17 and uses the Message Passing Interface (MPI) for distributed-memory parallelization. Careful software design balances high-performance algorithms and compute kernels with modular and flexible user interfaces. This allows to easily switch between different numerical models without loss of computational efficiency. During the talk, we focus on the implemented flow models and numerical schemes. To demonstrate the capability of our solver, we show complex scenarios of shock waves interacting with fluid interfaces. The interaction of a helium bubble with a shock wave in air exhibits the appearance of small-scale interface instabilities and different vortex production mechanisms. Macroscopic breakup modes during secondary atomization of a water droplet are shown as a second example.

References

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A Sharp-Interface Ghost-Fluid Method with Phase Transition

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Many technical applications that involve multiphase flow, such as rocket combustion chambers and Diesel engines, operate at high pressures and temperatures such that the environmental conditions may exceed the critical point of the liquid species. In these regimes, the assumption of incompressibility of the liquid is not valid any more, even when the flow Mach number is low. This is an inherent challenge for numerical simulations of flow phenomena in the near- and transcritical regimes. The governing flow equations, i.e. the compressible Navier-Stokes equations, are fully coupled as the thermodynamic pressure is linked to the internal energy of the fluid via a real gas equation of state (EOS).

In the present talk we introduce a sharp-interface method combined with a ghost-fluid method, based on the discontinuous Galerkin spectral element method (DGSEM) [1].

The phase boundary is represented by the zero iso-contour of a level-set function which allows for a high order representation of its geometry and, consequently, accurate calculation of normals and curvature [2]. The multiphase jump conditions across the phase boundary are maintained by the solution of the multiphase Riemann problem. The numerical flux is then applied for the liquid and vapour phases via the ghost fluid method [1]. For the accurate description of near critical fluid behaviour, tabulated real gas EOS are used [3], including state of the art EOS provided by the libraries CoolProp and RefProp.

Away from the phase interface we find a smooth solution and utilize the high order of accuracy of the discontinuous Galerkin method. In the vicinity of the phase interface, a local sub-cell formulation is introduced where we change to a second order accurate finite volume formulation to avoid stability issues and allow a more refined representation of the phase interface. Both methods are coupled by classical Riemann solvers in the bulk phases. The jump conditions at the phase interface are realized by means of special multiphase Riemann solvers. Approximate solvers are available for immiscible two phase flows. If phase transition is considered, the classical solution of the Riemann problem is complemented by an evaporation wave that represents the motion of the phase interface relative to the surrounding fluids. Interfacial heat flux and the latent heat of evaporation are taken into account by means of a subgrid resolution of the temperature profile, based on the solution of the diffusive generalized Riemann problem [5].

We present results for a variety of examples, such as shock-droplet interactions at high Mach numbers with the droplet being at rest or subject to a crossflow. Furthermore, using highly accurate real gas EOS, the method is validated against molecular dynamics simulations for several classical Riemann problems, e.g. a shock tube experiment and the expansion into vacuum.

References

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Thermographic phosphor particles as tracers for fluid temperature measurements.

Benoit Fond
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This presentation will discuss optical techniques for measuring fluid temperatures, which are based on thermographic phosphors. Phosphors are crystalline nano- to micro-scale particles consisting of a host compound that is normally doped with rare-earth or transition metal elements, lending the material temperature-dependent luminescence properties. Phosphor particles have similar physical properties than typical solid seed material for PIV such as TiO2 and can also be seeded into flows of interest. Following laser excitation, the luminescence signal of the particles is detected and the temperature may be derived using spectrally- or temporally-resolved methods. These diagnostics have several advantages. For example, they are easily combined with particle-based velocimetry approaches to acquire instantaneously correlated vector-scalar data necessary to characterise turbulent flows. Thermographic phosphors are often resistant to harsh, chemically-reacting environments. Furthermore, the near-infinite range of materials possess a rich variety of spectroscopic features that allow versatile tailoring of the technique to specific temperature ranges, including cryogenic temperatures, and demanding experimental conditions.

The presentation will include a short description of thermographic phosphors and basic principles of the thermometry method, followed by an application of the concept to the flow downstream of high pressure-ratio expansion confined in a channel. The observed temperature distribution results from a combination of compressible features, the real-gas Joule-Thomson effect and the wall-to-fluid heat transfer. Finally, recent developments toward higher precision and temporal/spatial resolution will be presented.

A unified first order hyperbolic formulation of Newtonian continuum mechanics coupled with electro-dynamics and its numerical solution

M. Dumbser[1] and E. Romenski[1,2]
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In this talk, we present a new unified first order hyperbolic model of Newtonian continuum mechanics coupled with electro-dynamics. The model is derived from the theory of hyper-elasticity and is able to describe the behavior of moving elasto-plastic dielectric solids as well as viscous and inviscid fluids in the presence of electro-magnetic fields. It is a peculiar feature of the proposed PDE system that viscous fluids are treated just as a special case of elasto-plastic solids. This is achieved by introducing a strain relaxation mechanism in the evolution equations of the distortion field **A**, which in the case of purely elastic solids maps the current configuration to the

reference configuration. The model also contains a hyperbolic formulation of heat conduction as well as a dissipative source term in the evolution equations for the electric field given by Ohm's law. Via formal asymptotic analysis we show that in the stiff limit, the governing first order hyperbolic PDE system with relaxation source terms tends asymptotically to the viscous and resistive magnetohydrodynamics (MHD) equations. The governing PDE system is symmetric hyperbolic and satisfies the first and second principle of thermodynamics, hence it belongs to the so-called class of symmetric hyperbolic thermodynamically compatible systems (SHTC), which have been studied for the first time by Godunov in 1961 and later in a series of papers by Godunov and Romenski. An important feature of the proposed model is that the propagation speeds of all physical processes, including dissipative processes, are finite. The model is discretized using high order accurate ADER discontinuous Galerkin (DG) finite element schemes with a posteriori subcell finite volume limiters and using high order ADER-WENO finite volume schemes on fixed and moving meshes. We show numerical test problems that explore a rather large parameter space of the model ranging from Euler and Navier-Stokes flows over ideal MHD, viscous and resistive MHD and nonlinear large-strain solid mechanics of elasto-plastic materials to pure electro-dynamics and moving dielectric elastic solids in a magnetic field.

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The Riemann Problem for a Barotropic Two Fluid Model

F. Thein[1;2], M. Dumbser[2] and E. Romenski[2;3]

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In several previous works Godunov, Romenski and co-authors proposed a PDE model derived using fundamental principles, cf. [2, 3]. The governing PDE system belongs to the class of symmetric hyperbolic thermodynamically compatible systems (SHTC). Particular results on two fluid models were obtained by Romenski, Toro and others [5,

4]. Numerical results for this type of model can exemplary be found in recent works by Dumbser, Romenski et al. e.g. [1]. However, a distinguished analytical treatment is still far from being complete. As a first attempt we want to discuss the Riemann problem for the homogeneous barotropic (i.e. isentropic or isothermal) two fluid model derived from the SHTC system. We will present exact relations for the appearing waves and discuss the wave structure of the solution. Comparisons of numerical and exact solutions will be shown. Further we want to discuss this model in the context of two phase flows with phase transition.

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A sharp interface method with heat conduction and mass transfer based on the GPR model

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In this talk, we present a novel sharp interface method, that allows heat and mass transfer across the two-fluid interface. The sharp interface framework is based on the work of Fechter et al. [2]. It combines a level-set and a ghost-fluid method to transport the two-fluid interface in three space dimensions. The method is incorporated into a DG framework with finite-volume sub-cells to solve the flow in the bulk phases. A new model for in-viscid flow with heat transfer, the GPR model [1], is used. It models heat transfer hyperbolically. This allows the construction of an HLLC type multi-phase Riemann solver that handles heat transfer generically. It is extended to allow mass transfer across the two-fluid interface, so evaporation and condensation is possible. The capabilities of the new method are illustrated with several testcases.

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A Molecular–Continuum Riemann Solver for Liquid–Vapor Flow

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Using a sharp interface approach, compressible liquid–vapor flow can be described by the hyperbolic Euler equations in the bulk phases, provided that viscosity and heat conductivity can be neglected. For an accurate description of the liquid–vapor phase boundary it is important to account for the microscale properties of the fluid at the interface. To this end, the interface dynamics in normal direction can be described as a Riemann problem [2, 6], which is typically solved by nonstandard wave patterns, usually entailing an undercompressive wave, representing the phase boundary. Consequently, an additional algebraic relation is necessary, which is called a kinetic relation. However, the physically relevant choice of the kinetic relation is often unclear. With this as our motivation, we want to describe the interface dynamics by a molecular dynamics microscale model that does not rely on continuum-scale closure relations and related parameters. Instead, molecular dynamics models rely on accurate force-fields, which are already established, even for complex mixtures [7, 3].

In summary, we want to solve microscale Riemann problems with molecular dynamics and use the microscale Riemann solutions in our continuum-mechanical simulations, see e.g. [5]. In order to drastically reduce computational time constraint-preserving artificial neural networks [4] are employed. We employ a moving-mesh based front capturing algorithm [1] that resolves the position of the interface exactly, within the mesh. In this talk the aforementioned multiscale Riemann solver for liquid–vapor flow and numerical simulation results of the complete multiscale model are presented.

References

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Systems of two-phase mixture balance laws with phase transitions

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A model consisting of balance laws for two-phase mixture flows with phase tran-sitions is considered. It was derived by averaging techniques. The model equations are a first order systems of partial differential equations with source terms. They are weakly hyperbolic, i.e. they have real eigenvalues, but not a full set of eigenvectors. After a short introduction of the model we consider sub-models. We consider an isothermal subsystem of conservation laws that is also weakly hyperbolic. A further difficulty is that real applications with gas and liquid flow need appropriate equations of state.

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