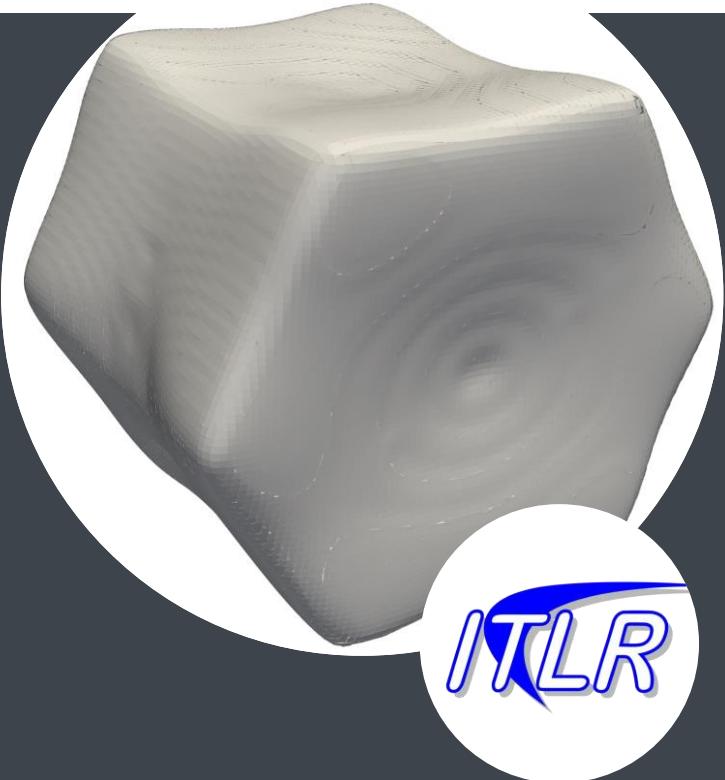


Numerical modelling of phase change processes in clouds

Challenges and Approaches

Martin Reitzle
Bernard Weigand



Introduction

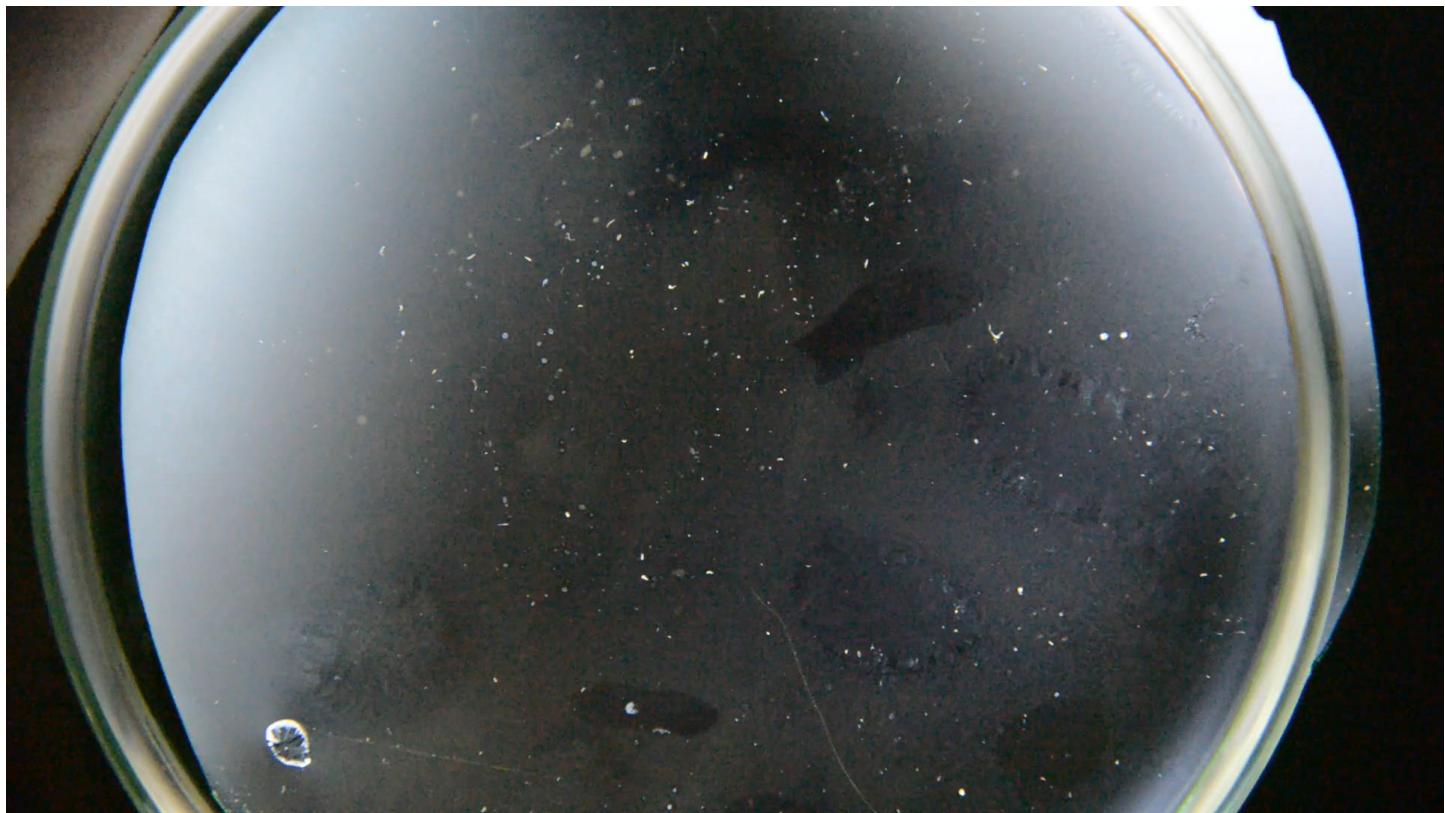
Institute of Aerospace Thermodynamics

- The ITLR is part of the faculty of aviation and aerospace engineering and geodesy at the University of Stuttgart.
- Two professors are associated to the ITLR. The institute has about 39 research associates and about 22 non-scientific employees (technicians, designer etc).
- Research topics (numerical & experimental) of the institute are:
 - heat transfer
 - aerothermodynamics
 - droplet dynamics
 - hypersonic combustion
 - shock tube research.



Motivation

Phase change processes in clouds



Outline

- Motivation
- Introduction to multiphase code FS3D
- Numerical challenges for phase change problems
- Illustrative example
- Solution strategies
 - “Physical” approach
 - Numerical approach

Introduction to multiphase code FS3D

Introduction to multiphase code FS3D

General information

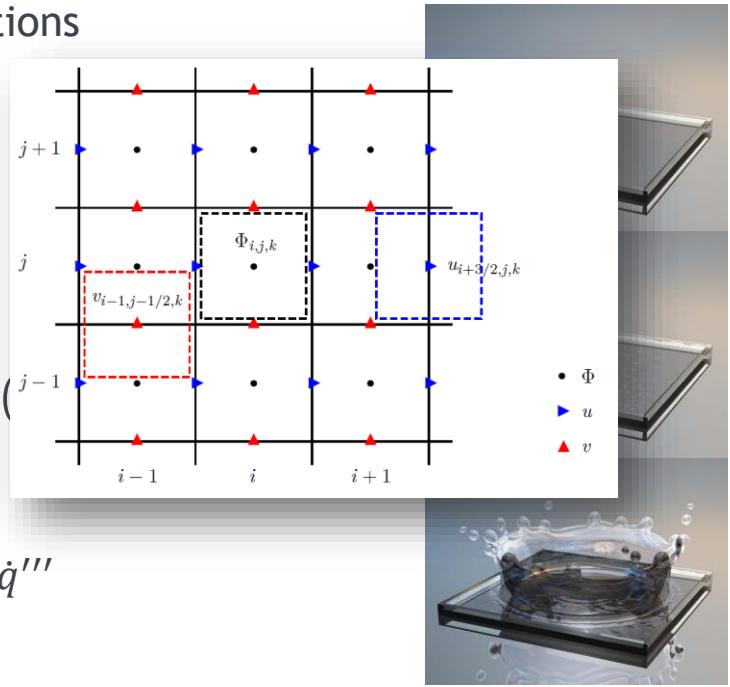
- In-house CFD code of ITLR written in Fortran
- Finite Volume discretization of incompressible Navier-Stokes equations
- Marker-and-Cell scheme
- Conservation of mass
- $\nabla \cdot \mathbf{u} = 0$
- Conservation of momentum

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot (\rho\mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mu[($$

- Conservation of energy

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p T \mathbf{u}) = \nabla \cdot (\lambda \nabla T) + \dot{q}'''$$

FS3D



Introduction to multiphase code FS3D

Treatment of multiple phases - Volume of Fluid method (VOF)

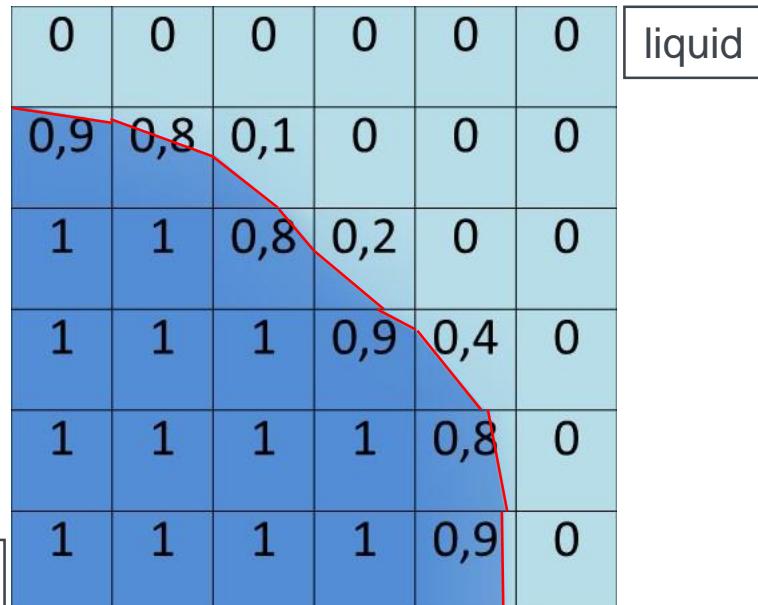
- Volume tracking using an additional scalar field

$$f_3(\mathbf{x}, t) = \begin{cases} 0 & \text{in the continuous phase} \\ 0 < f_3 < 1 & \text{at the interface} \\ 1 & \text{in the disperse phase} \end{cases}$$

- Reconstruction of the interface (PLIC)
- Additional conservation equation
- One-field formulation for material properties, e.g.

$$\rho(\mathbf{x}, t) = \rho_s f_3(\mathbf{x}, t) + \rho_l (1 - f_3(\mathbf{x}, t))$$

solid



Introduction to multiphase code FS3D

Numerical methods

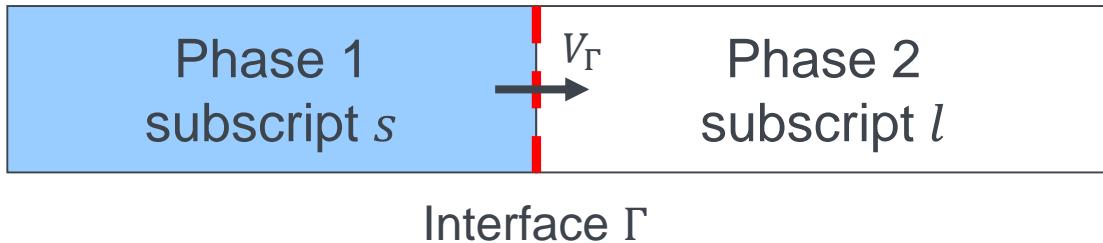
- Finite Volumes discretization
 - Convective terms: 2nd order upwind scheme
 - Diffusive terms: 2nd order central differences
 - Fluxes: Godunov type schemes with TVD Flux Limiter
 - Advection: Strang-Splitting or 3D unsplit
 - Poisson Equation: Red-Black Gauss-Seidel multigrid Solver
 - Time integration: 1st order explicit Euler,
2nd order explicit Runge-Kutta
 - MPI domain decomposition + OpenMP parallelization on loop level

Solidification

Numerical challenges for phase change problems

Numerical challenges for phase change problems

A closer look on the energy balance equation



- Conservation of energy

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p T \mathbf{u}) = \nabla \cdot (\lambda \nabla T) + \dot{q}'''$$

- Stefan condition - local thermodynamic equilibrium

$$V_\Gamma \rho_s L = -\lambda_l \nabla T_l \cdot \mathbf{n}_\Gamma + \lambda_s \nabla T_s \cdot \mathbf{n}_\Gamma$$

- For the evaluation of the temperature gradients, the interface temperature T_Γ is needed.

Numerical challenges for phase change problems

Interface Temperature - Gibbs-Thomson effect

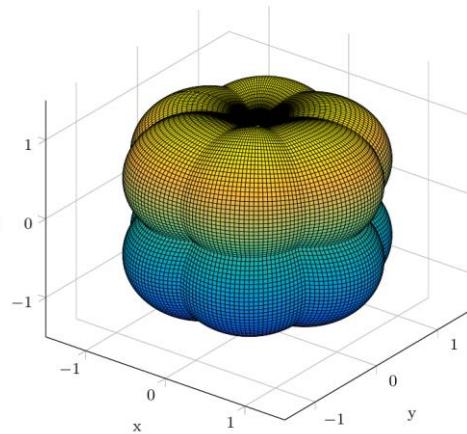
- Gibbs-Thomson relation

$$T_\Gamma = T_m \left(1 - \frac{1}{\rho_s L} \sigma_0 H_\gamma \right)$$

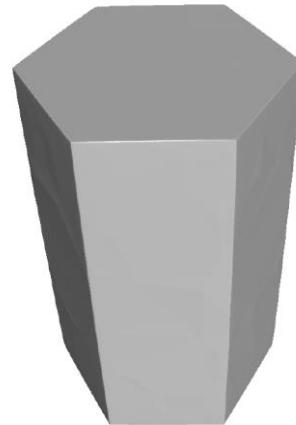
- With anisotropic mean curvature

$$H_\gamma = \sum_{i,j=1}^n \gamma_{p_i p_j} (\nabla v, -1) v_{x_i x_j}$$

Polar plot



Shape of crystal
in equilibrium



Numerical challenges for phase change problems

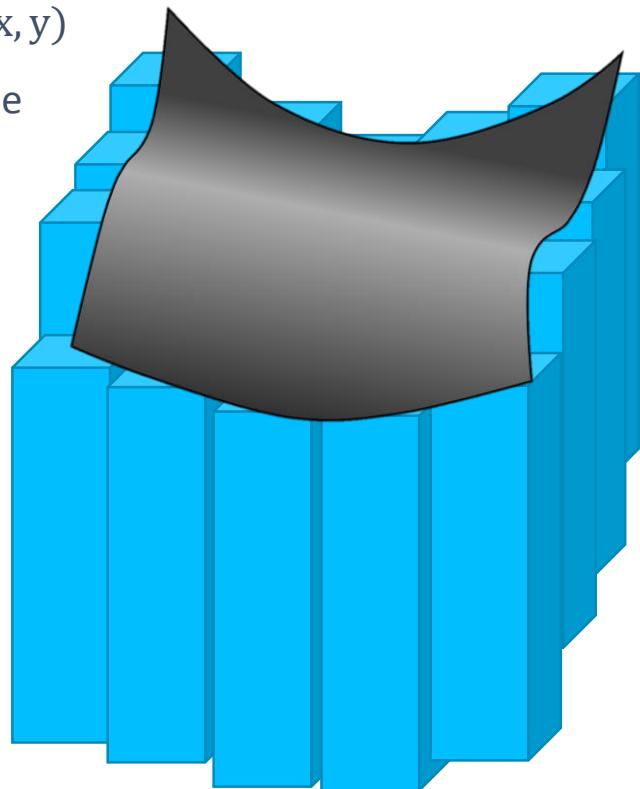
Reconstruct surface as a graph

- Use the height function method to parameterize the surface

$$v(x, y) \approx h_f(x, y)$$

- Coordinate transformations depending on the main direction of the height functions

- Alternatively:
locally fit parabola to surface



Numerical challenges for phase change problems

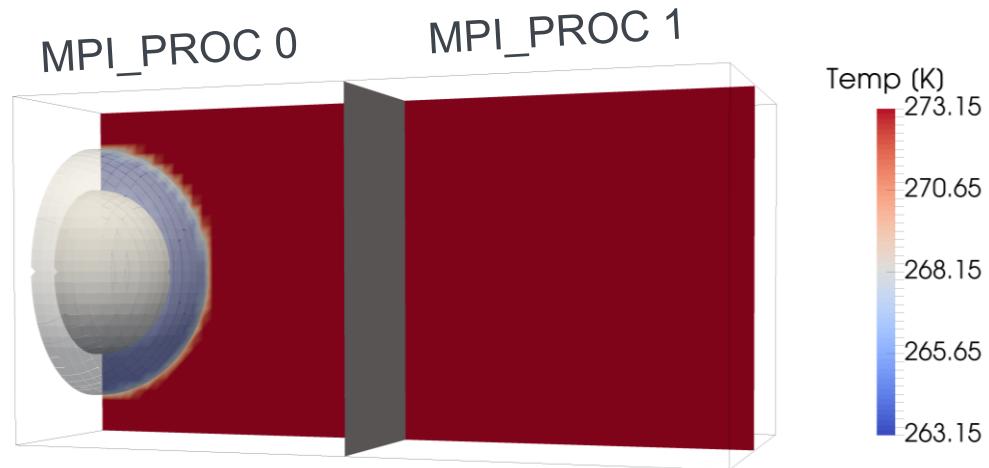
Summary - Solution algorithm

- - Calculation of ...
 - normal vectors
 - curvature
 - Evaluate surface temperature
 - Reconstruct surface as a graph
 - Calculate temperature gradients at interface
 - Solve heat conduction equation
 - Advance interface
- Furthermore ...
 - Asymmetrical and ill-conditioned matrices due to interface
 - High spatial resolution → small time steps

Illustrative example

Illustrative example

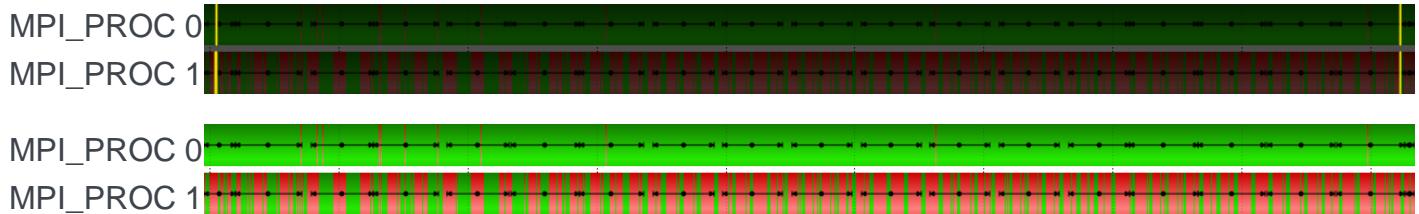
Setup



- Solid seed embedded in liquid droplet
- $T_{solid} < T_{liquid} < T_{gas}$
- Anisotropic phase change at solid-liquid interface
- Heat fluxes across all interfaces

Illustrative example

Tracing (Score-P + Vampir)



- MPI communication

MPI PROC	MPI_SENDRECV + MPI_ALLREDUCE [s]	Percentage of walltime of timestep
0	0.121	0.88%
1	8.891	64.46%

Solution strategies

Solution strategies

"Physical" approach

- Goal is to capture the “true” physics as closely as possible

Evaluate temperature at interface T_Γ
Gibbs-Thomson equation

Coupling of temperature fields at interface
 $V_\Gamma \rho_s L = \dot{q}_s + \dot{q}_l$

Use these heat fluxes as source terms in the heat conduction equation

Evaluate temperature at interface T_Γ

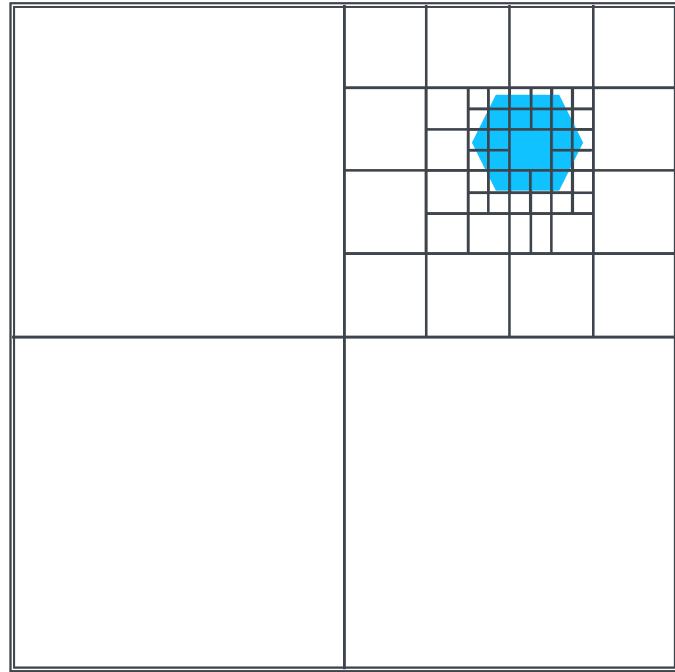
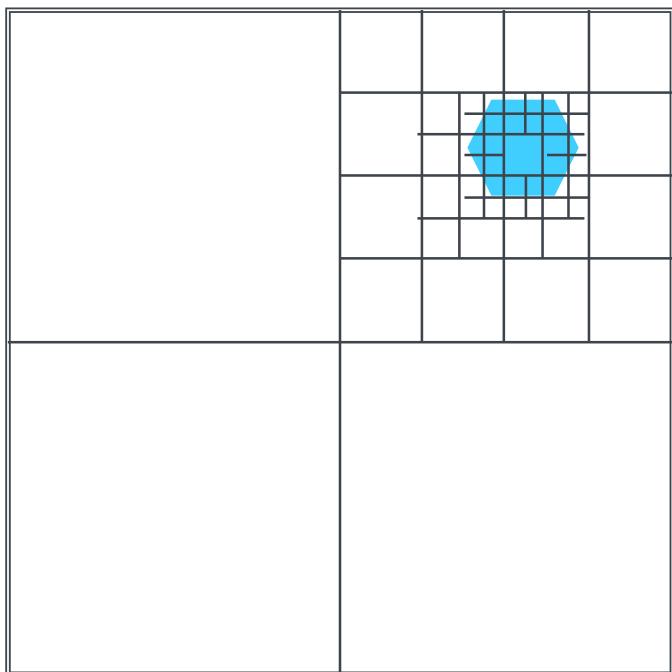
Use T_Γ as a boundary condition in heat conduction equation

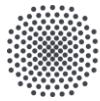
- Reduces number of inner iterations
- Especially at very fast transient processes better results are obtained

Solution strategies

Numerical approach

- Make use of highly optimized numerical methods
e.g. UG4 multigrid solver (Pressure Poisson equation)
- Next step: reduce load imbalances





University of Stuttgart

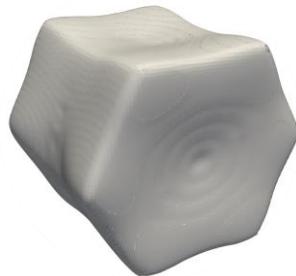
Institute of Aerospace Thermodynamics



SFB-TRR 75

Tropfendynamische Prozesse unter
extremen Umgebungsbedingungen

Thank you!



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