Most numerical approaches to handle gas-fluid interactions are based on continuum methods. A main disadvantage is the necessity of continuum assumptions including local thermodynamic equilibrium or limitations to quasi-steady conditions. At the boundary layer between gas and a liquid droplet microscopic non-equilibrium effects can play a crucial role for the evaporation process. Therefore, within this project the interaction between gas flow and liquid droplet will be simulated using the Direct Simulation Monte Carlo (DSMC) method. The DSMC approximates the gas flow from a microscopic point of view and discrete simulation particles allow for a treatment of non-equilibrium effects. Consequently, a comparison between DSMC and existing analytical results will be of fundamental interest to analyse the effects of equilibrium assumptions and flow unsteadiness.

### Project Description

#### Objectives

- **Simulation of gas phase vicinity of nano-scale droplets.**
  - Capture and resolve deviations from thermodinamic equilibrium
  - Consider influences of droplet deformation
  - Provide results for comparison with analytic and continuum simulation results
  - Evaluate necessity of non-equilibrium approaches

#### Methodology

**Model gas phase by solving the Boltzmann equation with Direct Simulation Monte Carlo method** [1].

**Equation:**

\[
\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \frac{1}{m} \vec{F} \cdot \nabla f = \frac{\partial F}{\partial t}
\]

- Approximation of distribution function \( f(\vec{x}, \vec{v}, t) \)
- Distribution of \( N \) discrete particles \( \sum_{i=1}^{N} w_i (\vec{x} - \vec{x}_i(t)) \cdot (\vec{v} - \vec{v}_i(t)) \)
- Simulated particles are weighted \( \sum_{i=1}^{N} w_i \)
- Particle movement and collisions decoupled
- Statistical method
- Decisions with random numbers
- Macroscopic results are sampled from particle values
  - Number density \( n = \int f \, dv \)
  - Mass density \( \rho = \int f \, \vec{v} \, dv \)
  - Velocity \( \vec{u}_i = \frac{1}{\sqrt{m}} \int \vec{v} \, f \, dv \)
  - Temperature \( T = \frac{1}{2m} \int \vec{v} \cdot \vec{v} \, f \, dv \)
  - Force tensor \( \vec{F}_i = \frac{1}{\sqrt{m}} \int \vec{F} \, f \, dv \)
  - Heat flux \( q = \frac{1}{2} \int c_i \vec{F}_i \, dv \)

- Use flow solver PICLas [2]
- Flexible simulation tool for rarefied 3D plasma flows
- Cooperatively developed by Institute of Aerodynamics and Gasdynamics (IAG) and Institute of Space Systems (IRS) at University of Stuttgart
- Particle framework for coupling methods:
  - Particle in Cell (PIC): electromagnetic interactions
  - Direct Simulation Monte Carlo (DSMC): particle collisions

#### First Steps

**Implement gas-liquid boundary conditions into PICLas modeling evaporation and condensation processes.**

- Adaptation of boundary conditions for DSMC considering sub projects SP-A2 and SP-A4.
- Reconstruct microscopic surface interaction using a formulation of a distribution function derived from preliminary molecular dynamics (MD) studies [3].

**First results with implemented simple gas-liquid boundary**

- Use Hertz-Knudsen equation to estimate number of evaporating particles.
  \[
  \frac{\partial n}{\partial t} = -\frac{\partial n}{\partial x} + \frac{n}{\sigma} = \frac{1}{\sigma} \int n_i \frac{\partial f_i}{\partial t} \, dv
  \]
- Assumptions: Particles evaporate from liquid corresponding to Maxwell distribution at surface temperature and condensation coefficient \( \sigma = 1 \).

**Future Work**

- Consider moving nano-scale particles interacting with DSMC particles
- Add and combine moving boundaries with nano-scale particles
- Calculate fluxes on moving droplets
- Simulate decrease of droplet size
- Model liquid behaviour and droplet deformation
- Temperature / pressure distribution inside droplet
- Droplet size and shape
- Simulations with the implemented models evaluating microscopic effects on evaporation process

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**References**

