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Model Order Reduction of Rarefied Gases Using Neural Networks

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Outline

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Governing equations

- The Boltzmann equation approximated by $\boldsymbol{Q}$ the BGK operator as a source term with

$$\partial_t f + v\partial_x f = \overbrace{\frac{1}{\tau}(M_f - f)}^{Q} \tag{1}$$

- The equilibrium solution is a Maxwellian distribution $\boldsymbol{M_f}$ with

$$M_f = \frac{\rho(x,t)}{(2\pi RT(x,t))^{\frac{3}{2}}} \exp\left(-\frac{(v - u(x,t))^2}{2RT(x,t)}\right) \tag{2}$$

- The duration to evolve into equilibrium is given by the relaxation time $\boldsymbol{\tau}$ with

$$\tau^{-1} = \frac{\rho(x,t)T^{1-\nu}(x,t)}{Kn} \tag{3}$$

- The rarefaction level is defined over the Knudsen number $\boldsymbol{Kn}$ with

$$Kn = \frac{\lambda}{l} \tag{4}$$

[1]

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[1] **PhysRev.94.511**.

Knudsen number

– Solution is $f(x, v, t)$ in 1D and $f(x, y, v_x, v_y, t)$ in 2D and $f(x, y, z, v_x, v_y, v_z, t)$ in 3D

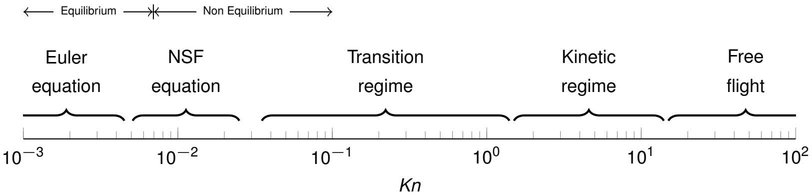

Figure: Partitioning of Kn, the Knudsen number, into levels of rarefaction.

[2]

[2] **NumaKUL**.

Discretization in space and velocity space in 1D

- Space and time discretization considering a uniform grid i.e.
  $x_j = j\Delta x$ and $j \in \mathbb{Z}$, $v_k = k\Delta v$ and $k \in \mathbb{Z}$, $t^i = i\Delta t$ and $t \in \mathbb{N}$,
- is leading from the full PDE to a set of ODE's in time

$$\partial_t f_{j,k} = -(v_k)_1 D_x f\big|_{j,k}(t) + \frac{1}{\tau}(M_{f\,j,k}(t) - f_{j,k}(t)). \tag{5}$$

- KJ first-order differential equations need to be evaluated when K and J are the number of gridpoints in space and velocity space.
- In 3D there are K^3J^3 first-order differential equations.
- The discretization in velocity space requires the computation of the moments of f.

Moments/ Expected values of *f*

- By multiplying the collision invariants $\Phi(v) = [1, v, \frac{1}{2}v^2]$ with f and integrating in velocity space v the moments are obtained.
- The first moment/ the Density is

$$\rho(x, t) = \int f \, \mathrm{d}v \, , \tag{6}$$

- the second moment/ the Momentum is

$$\rho(x, t) u(x, t) = \int v f \, \mathrm{d}v \, , \tag{7}$$

- the third moment/ the kinetic Energy is

$$E(x, t) = \int \frac{1}{2} v^2 f \, \mathrm{d}v \, . \tag{8}$$

Moments/ Expected values of f

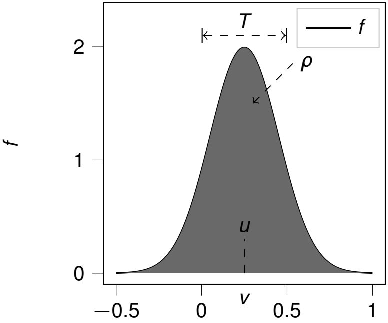

Figure: Illustration of the linkage between the macroscopic quantities of the gas flow and the distribution function f.

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Sod's shock tube

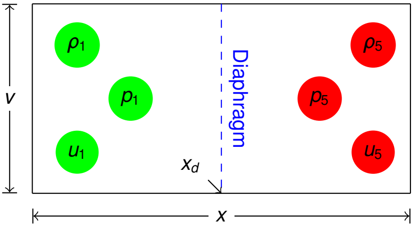

Figure: Problem setup of Sod's shock tube for the BGK model in 1D.

- Test case for numerical schemes solving
- **non-linear hyperbolic conservation laws** in gas dynamics (Gary A. Sod in 1978)
- **Idea**:
  - Solve problem analytically (Rankine-Hugoniot jump conditions)
  - Solve problem numerically
  - Compare resolution of discontinuities

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Sod’s shock tube

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ToDo

- **ToDo** schreiben
- **ToDo** abarbeiten