


Model Order Reduction of Rarefied Gases Using Neural Networks

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Outline

Introduction

The BGK-Model

Sod’s shock tube

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Governing equations

- The Boltzmann equation approximated by ***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 ***Kn*** with

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

1

[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

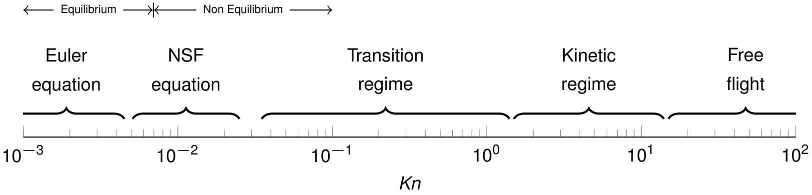

Figure: Partitioning of Kn, the Knudsen number, into levels of rarefaction.

[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

- Collision invariants $\Phi(v) = [1, v, \frac{1}{2}v^2]$
- The first moment/ Density is

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

- the second moment/ Momentum is

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

- the third moment/ kinetic Energy is

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

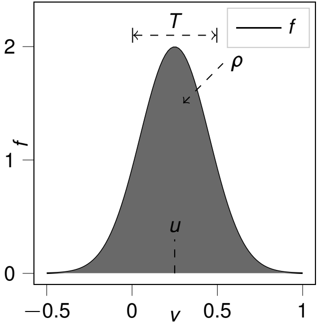

Figure: Illustration of the linkage between the macroscopic quantities of the gas flow and the distribution function f.

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Sod's shock tube

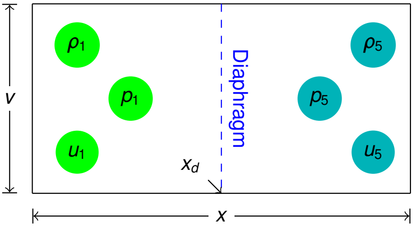
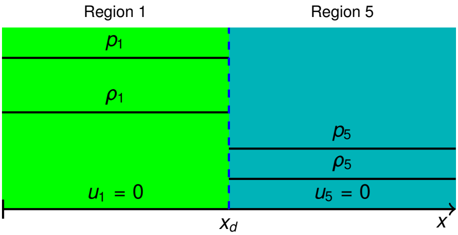


Figure: Problem setup of Sod's shock tube for the BGK model in 1D at $t = 0s$.

- 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 results expecially **resolution of discontinuities**

Sod's shock tube



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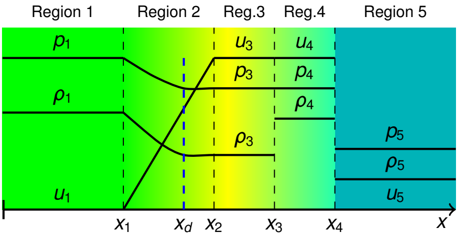

Figure: Problem setup of Sod's shock tube for the BGK model in 1D at $t > 0s$.

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  - Solve problem numerically
  - Compare results expecially **resolution of discontinuities**
    - » $\mathbf{x_1}$ head of rarefaction wave
    - » $\mathbf{x_2}$ tail of rarefaction wave
    - » $\mathbf{x_3}$ contact discontinuity
    - » $\mathbf{x_4}$ position of shockwave

Two Case Studies

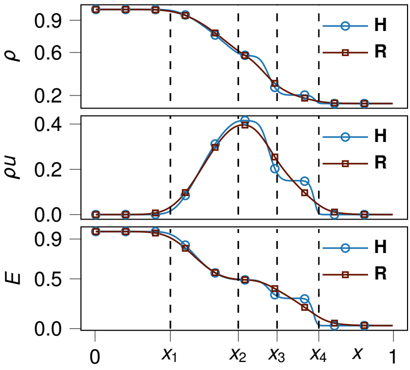


Figure: Moments of **H** and **R** at $t = 0.12s$ and $v = v_0$ in Sod's shock tube.

– Two solutions of the BGK model in Sod's shock tube

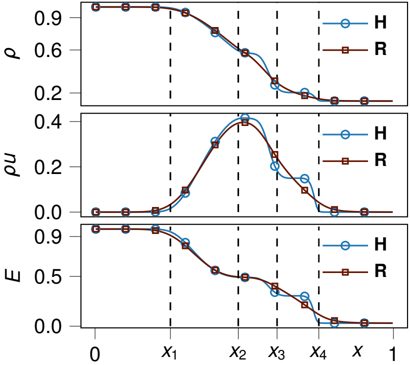
– Two levels of rarefaction

- **H**, $Kn = 0.00001$, "Continuum Flow"
- **R**, $Kn = 0.001$, "Slip flow"

– Present discontinuities

H	**R**
• x_1	• x_1
• x_2	• x_2
• x_3	• x_3
• x_4	• x_4

Two Case Studies



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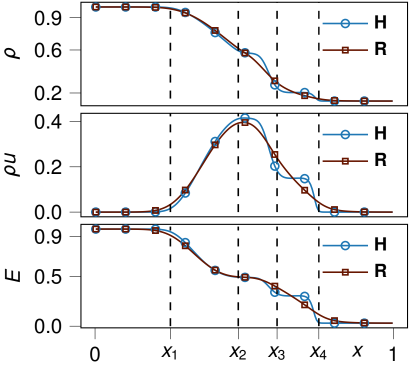

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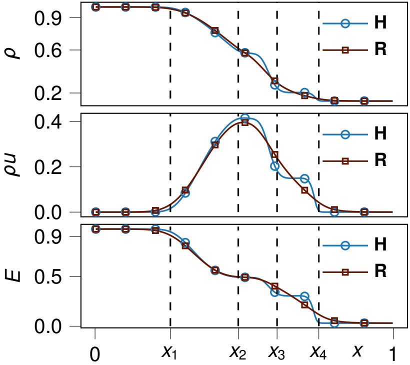

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H	**R**
x_1	x_1
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Two Case Studies

- Spatial resolution $J = 200$
- Temporal resolution $I = 25$
- Velocious resolution $K = 40$

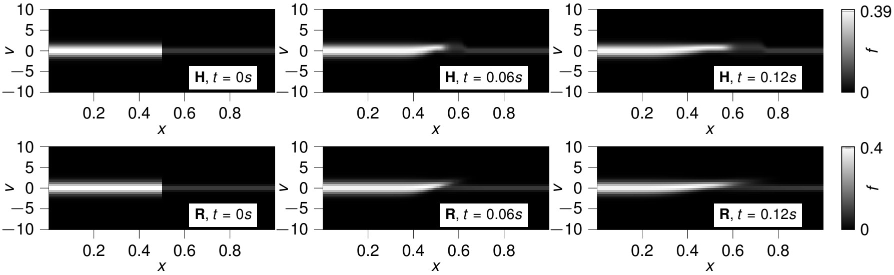

Figure: Solution f for **H** and **R** in x and v.

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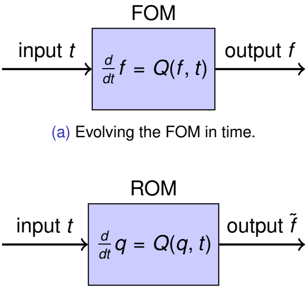
Model Order Reduction



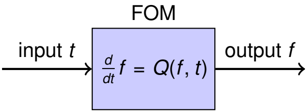
(a) Evolving the FOM in time.

(b) Evolving the ROM in time.

Figure: In the online phase the operator Q is different for the FOM and the ROM.

– **Goal**: Reduce computational cost

Model Order Reduction



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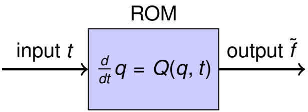

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  - $f(x, v, t)$ with KJ ODE's in time for 1D

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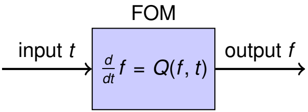

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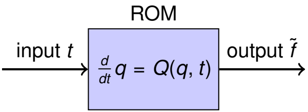

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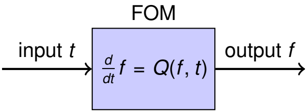

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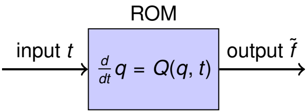

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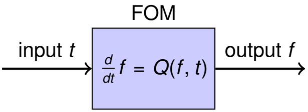

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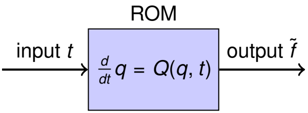

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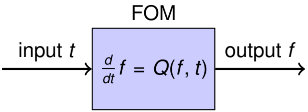

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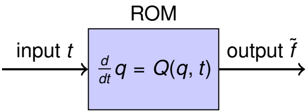

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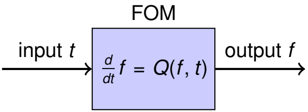

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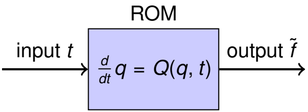

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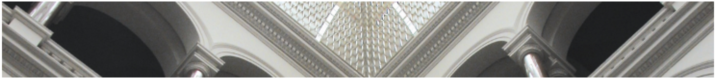

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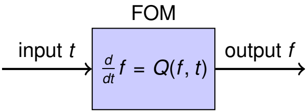

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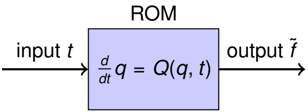

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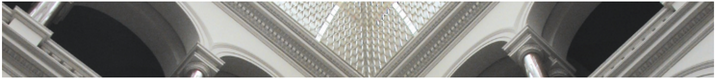

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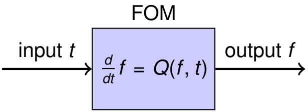
Model Order Reduction



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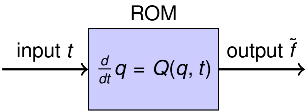

(b) Evolving the ROM in time.

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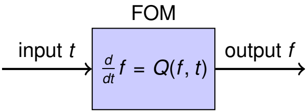
Model Order Reduction



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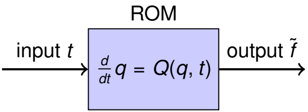

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Proper Orthogonal Decomposition

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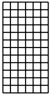
- How to get $\boxed{\Phi_i}$?
  - **Preprocessing**: Seperating the spatial and temporal axis of the solution $f(x, v, t)$
    - » $P =$ 

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ToDo

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