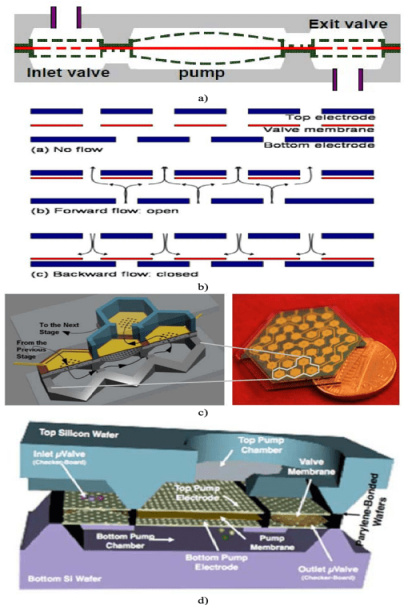
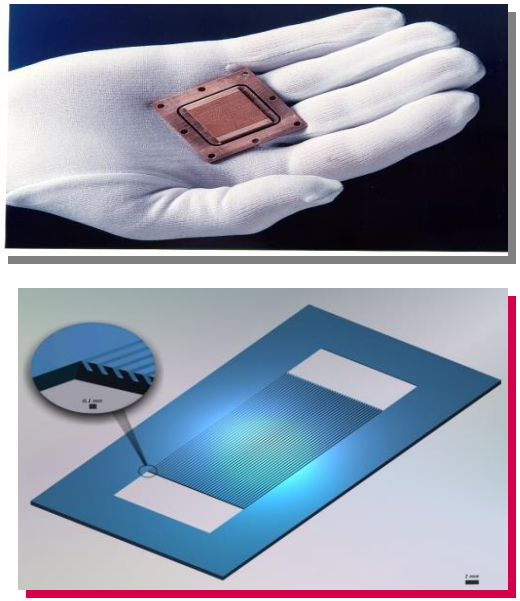
Machine learning based models for rarefied gas flow: Physics of interfaces.

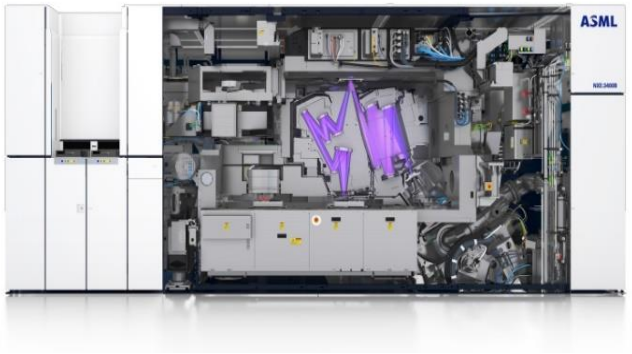
Application fields:



•Vacuum pumps/technology



MEMS/NEMS ->cooling.



Aerospace and EUV lithography

•In all these applications gas flows are highly rarefied. This implies that the molecular mean free path (λ) of gas molecules is large compared to the characteristic length scale (**L**) of the system. The degree of rarefaction is characterized by the **Knudsen number** as **Kn = λ/L**. **Phase boundaries, physics of interfaces becomes dominant!**

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Simulation models and techniques

1) Continuum: Navier Stokes equation

Shear stress ↓ $\tau_{xy} = \mu \frac{dV_x}{dy}$ Newton

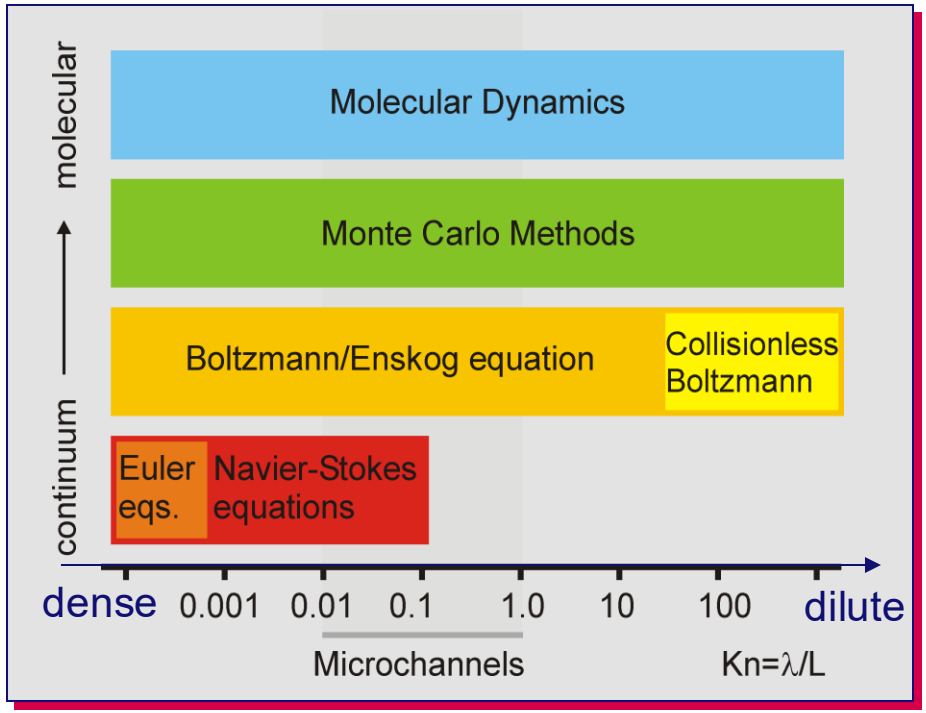
Heat flux ↓ $q_x = -k \frac{dT}{dx}$ Fourier

2) Boltzmann/ Enskog equation

velocity ↓ Collision term ↙

$$\frac{\partial F}{\partial T} + \xi \circ \nabla F = J_E(F,F)$$

$F(x,\xi,t) =$ One-particle distribution function of velocity



3) Monte Carlo Methods :

Disadvantages: stochastic collisions, less accurate

Advantages: computational faster, large systems, larger time intervals

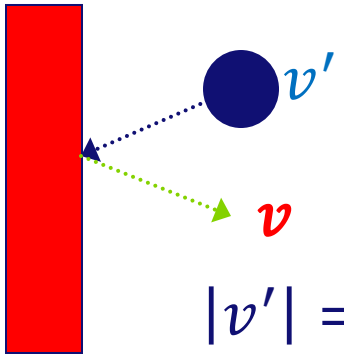
4) Molecular Dynamics: solve Newton's equations of motion $(\vec{F} = m\vec{a})$

Disadvantages: computational demanding, limited space and time scale

Advantages: Accurate Deterministic, Gas, liquid, solid

Modelling fluid-wall interactions

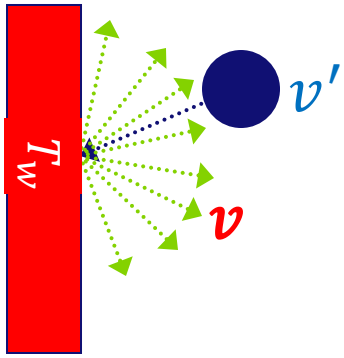
Specular wall / reflecting wall



$$|v'| = |v|$$

No energy exchange with wall

Thermal wall / diffusive wall



Energy exchange from wall to particle

Diffusive-specular wall

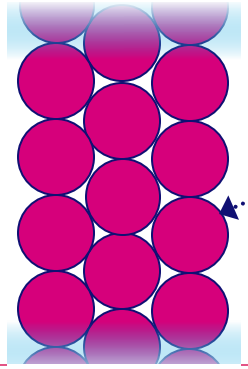
=

α Diffusive wall

+

(1-α) Specular wall

Explicit MD wall



$$F = -\nabla V$$

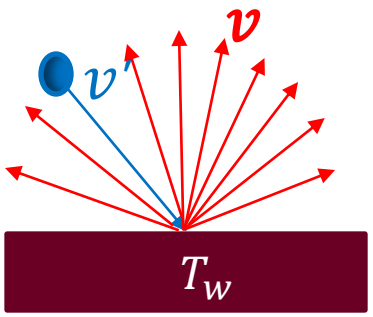
Energy exchange between wall and particle

Existing Gas-surface interaction models

- **Maxwell** model

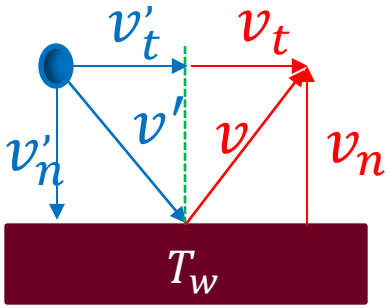
$$P(\boldsymbol{v}'|\boldsymbol{v}) = \underbrace{\boldsymbol{\alpha_K}\frac{1}{2\pi}\left(\frac{m_g}{kT_w}\right)^2 v_n \exp\left(\frac{-m_g\boldsymbol{v}^2}{2kT_w}\right)}_{\text{Diffusive reflection}} + \underbrace{(1-\boldsymbol{\alpha_K})\delta(\boldsymbol{v}' - \boldsymbol{v} + 2v_n\boldsymbol{N})}_{\text{Specular reflection}}$$

Diffusive reflection



- **Cercignani-Lampis-Lord (CLL)** model

Specular reflection

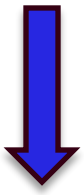


$$P(v_t'|v_t) = \sqrt{\frac{m_g}{2\pi kT_w\boldsymbol{\alpha_{TM}}(2-\boldsymbol{\alpha_{TM}})}}\exp\left[-\frac{m_g}{2kT_w}\frac{(v_t-(1-\boldsymbol{\alpha_{TM}})v_t')^2}{\boldsymbol{\alpha_{TM}}(2-\boldsymbol{\alpha_{TM}})}\right]$$

$$P(v_n'|v_n) = \frac{m_g v_n}{kT_w\boldsymbol{\alpha_{NE}}}\exp\left[-\frac{m_g}{2kT_w}\frac{v_n^2+(1-\boldsymbol{\alpha_{NE}})v_n'^2}{\boldsymbol{\alpha_{NE}}}\right]I_0\left(\frac{m_g}{kT_w}\frac{\sqrt{1-\boldsymbol{\alpha_{NE}}}v_n'v_n}{\boldsymbol{\alpha_{NE}}}\right)$$

Challenge

- Accommodation Coefficient (α_K) **is a measure to quantify the momentum or energy exchange** at the gas-solid interface
  - **Experimental determination** of α_K is a **very challenging task**



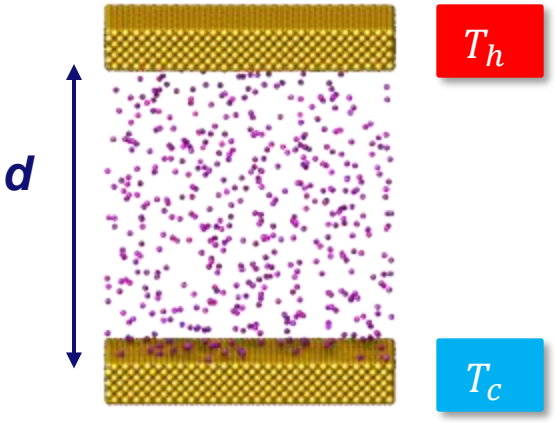
  - α_K depends on many factors:

i. Temperature (gas & surface)

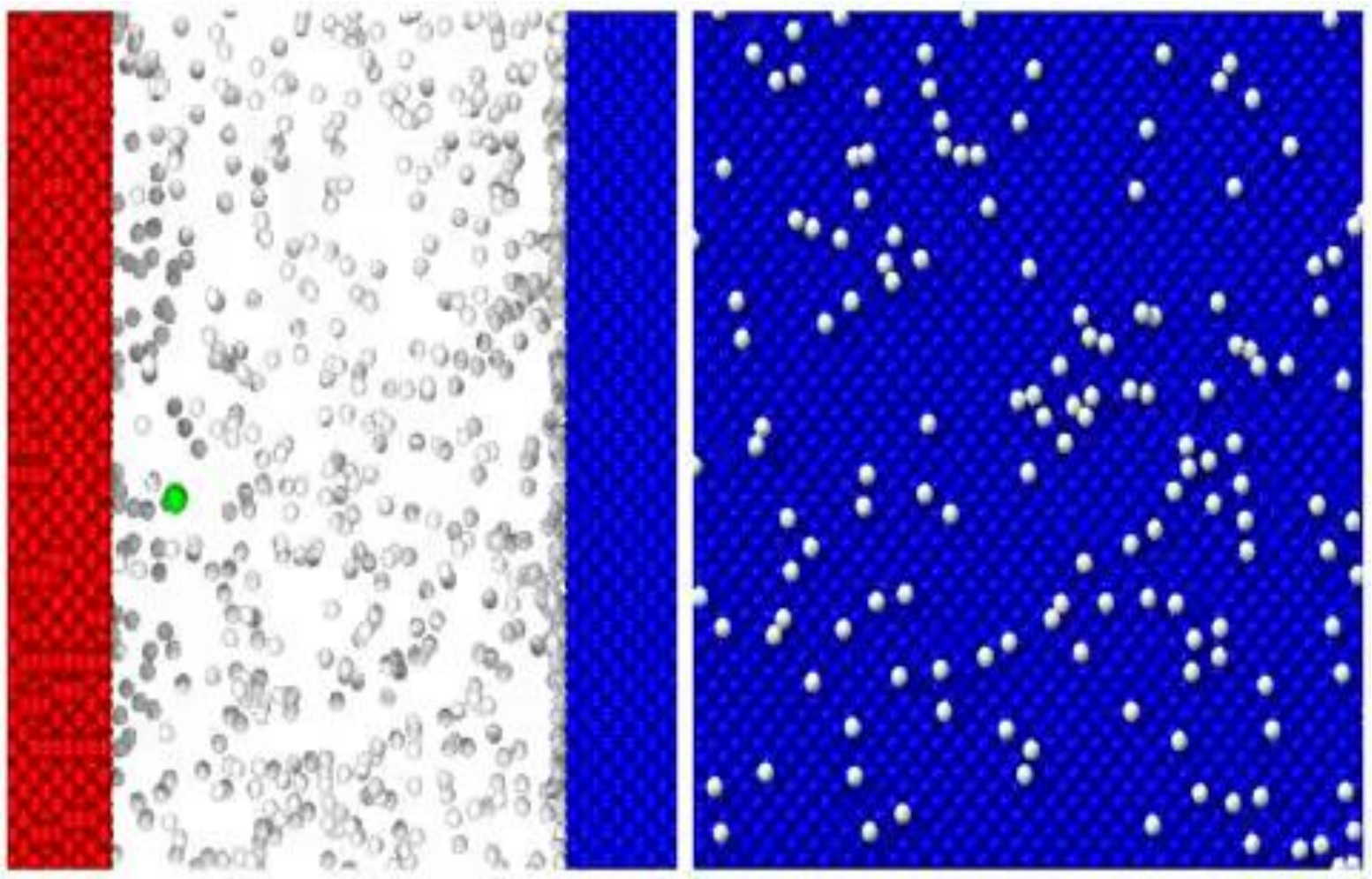
ii. Surface condition (cleanness & roughness)

iii. Gas-solid mass ratio

iv. Elastic module of the solid



MD scattering for computing thermal accommodation coefficients



Lennard Jones (12,6) potential

"Lennard-Jones (n,6) potential";

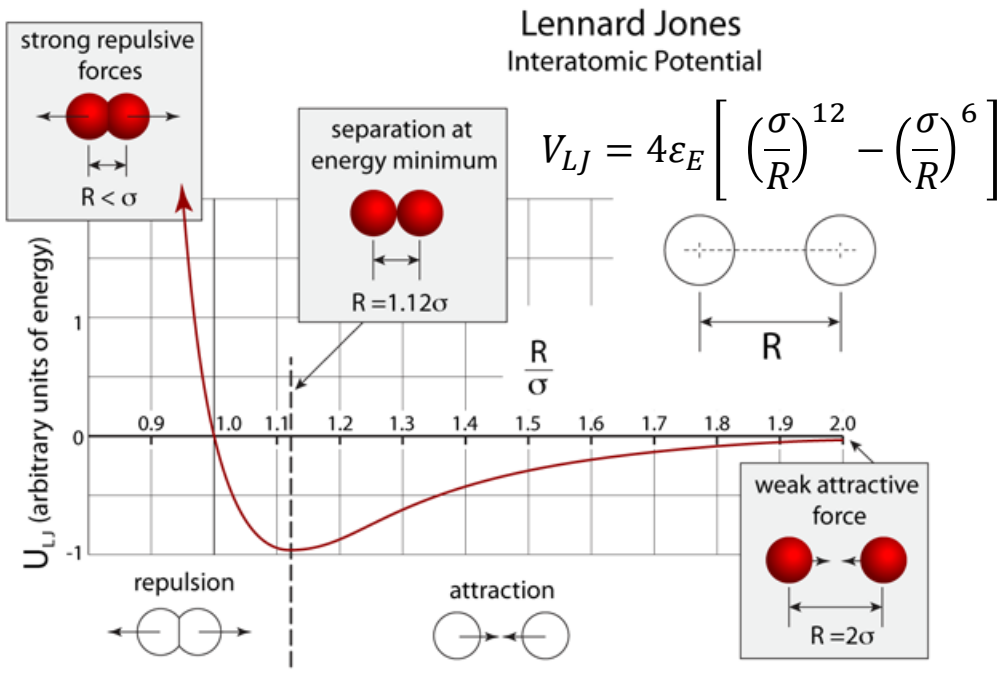
Mostly n=12 (for mathematical reasons)

$$V = 4\varepsilon_E \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

With ε depth of well and σ molecular diameter

Force: $F = -\frac{\partial V}{\partial r} = \frac{24\varepsilon_E}{r}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$

Minimum at $\frac{\partial V}{\partial r} = 0$ => $r_e = \sqrt[6]{2}\,\sigma = 1.12\,\sigma$



Source: http://www.atomsinmotion.com

The velocity-Verlet algorithm

Step 1:

$r(t + Delta*t) = r(t) + v(t) * Delta*t + 1/2 * a(t) * Delta * t \wedge 2$

$v(t + (Delta*t)/2) = v(t) + 1/2 * a(t) * Delta*t$

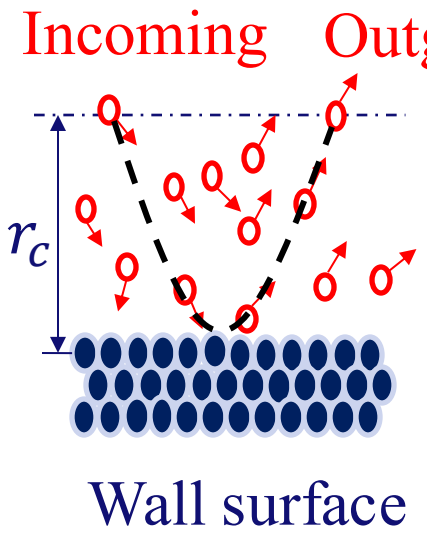
Step 2:

$a, (t+At) = m_1 - V_1 U(r(t+At))$

$v(t + Delta*t) = v(t + (Delta*t)/2) + 1/2 * a(t + Delta*t) * Delta*t$

Theoretical background

- Different approaches for computing accommodation coefficients from MD simulations

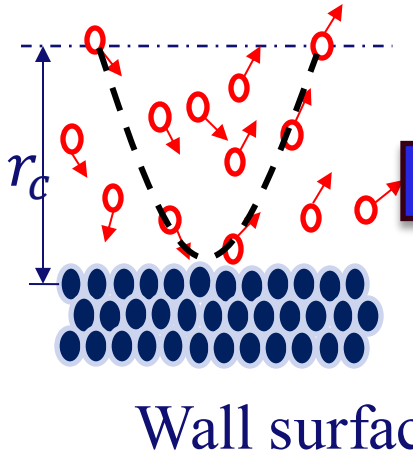


Collisional data

$$\alpha_K = \frac{\langle K_I \rangle - \langle K_O \rangle}{\langle K_I \rangle - \langle K_w \rangle}$$

Theoretical background

- Different approaches for computing accommodation coefficients from MD simulations



Collisional data

Classical method

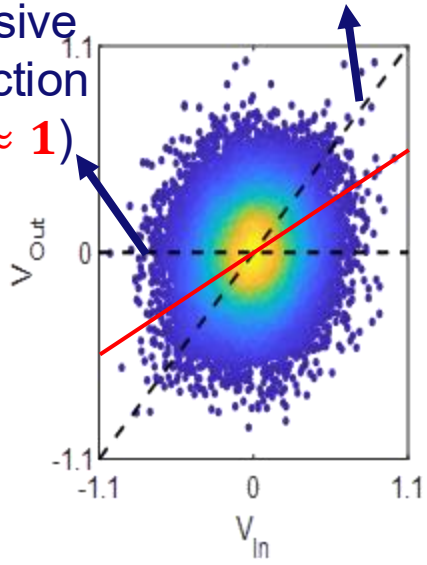
$$\alpha_K = \frac{\langle K_I \rangle - \langle K_O \rangle}{\langle K_I \rangle - \langle K_w \rangle}$$

Velocity-correlation method

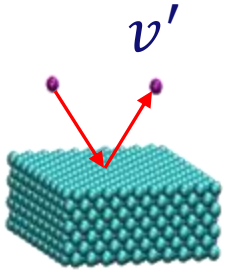
$$\alpha_k = 1 - \frac{\sum_i (K_I^i - \langle K_I \rangle)(K_O^i - \langle K_O \rangle)}{\sum_i (K_I^i - \langle K_I \rangle)^2}$$

Specular reflection ($\alpha_k \approx 0$)

Diffusive reflection ($\alpha_k \approx 1$)



Goal: Deriving a gas-wall interaction model using Machine Learning



Common Approach

Gathering collision data

Computing different ACs

Scattering kernels

New Approach

Deriving a gas-wall interaction model using Machine Learning

- We use the **Gaussian mixture model (GM)**[1], which is an unsupervised machine learning technique

Main Features

i. It uses **linear combination** of multiple **multidimensional Gaussians** to estimate the probability density function of collision data

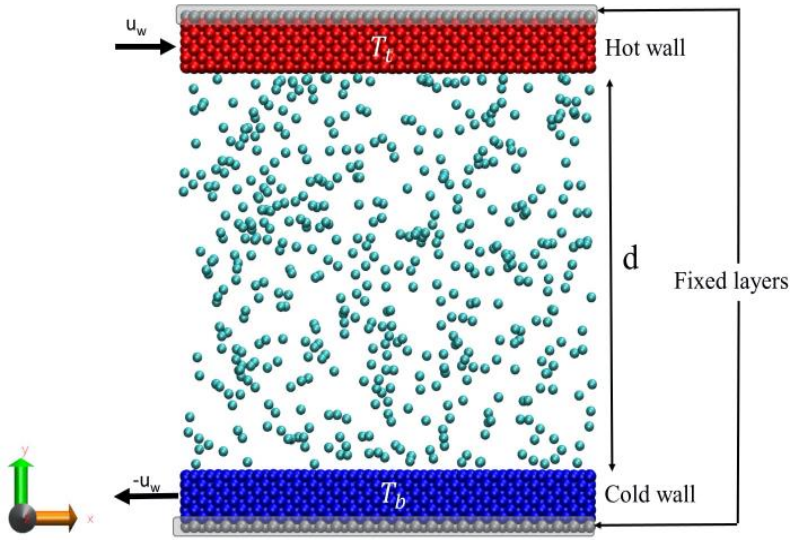
ii. The **correlation** between gas molecules velocity components is considered

iii. Presence of many **fitting parameters** makes the model very flexible

[1] *M.Liao, et. al, Physical Review E 98, no. 4 (2018): 042104*

Assignment

Develop Machine Learning (ML) models to construct a statistical gas-surface scattering model based on the collisional data obtained from Molecular Dynamics (MD) simulations for hydrogen-nickel interactions in a micro/nano-system.



Goal: To study the isothermal and non-isothermal Couette flow of a diatomic gas (Hydrogen) confined between two parallel infinite Nickel walls.

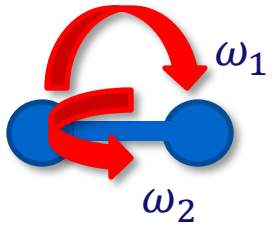
Structure:

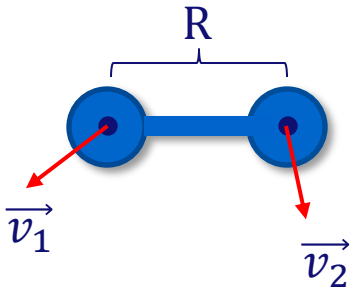
- Part A: ML for isothermal/non-isothermal H2-Ni interactions
- Part B :ML model for isothermal-non-isothermal Couette flow
- Part C: ML model for predicting the atomic angular velocity distributions and translational/rotational energy accommodation coefficients.
- Part D: Compare GM and Bayesian model/DNN on ACC predictions.

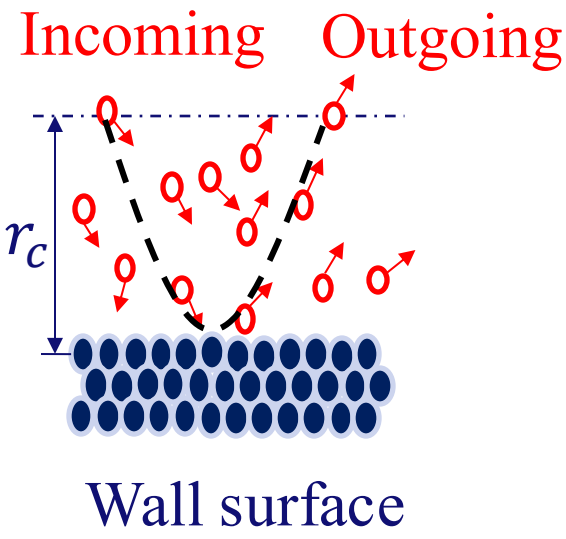
Q&A: Next: Tuesday (10.30h) and Thursday (14.30h), location: Vector. -> discuss on challenge, scripts, data, examples and documentation

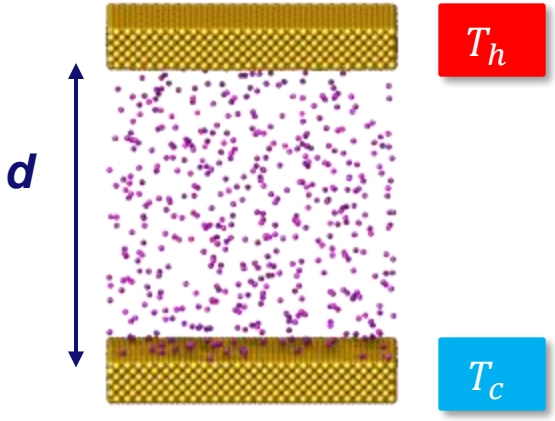
$$\boldsymbol{x_I} = (v_{t1}^I, v_{t2}^I, v_n^I, \omega_1^I, \omega_2^I)$$

$$\boldsymbol{x_R} = (v_{t1}^R, v_{t2}^R, v_n^R, \omega_1^R, \omega_2^R)$$

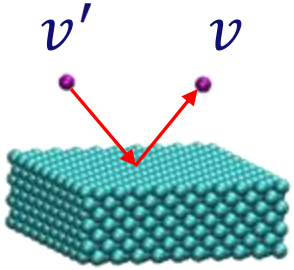








Goal: Deriving a gas-wall interaction model using Machine Learning



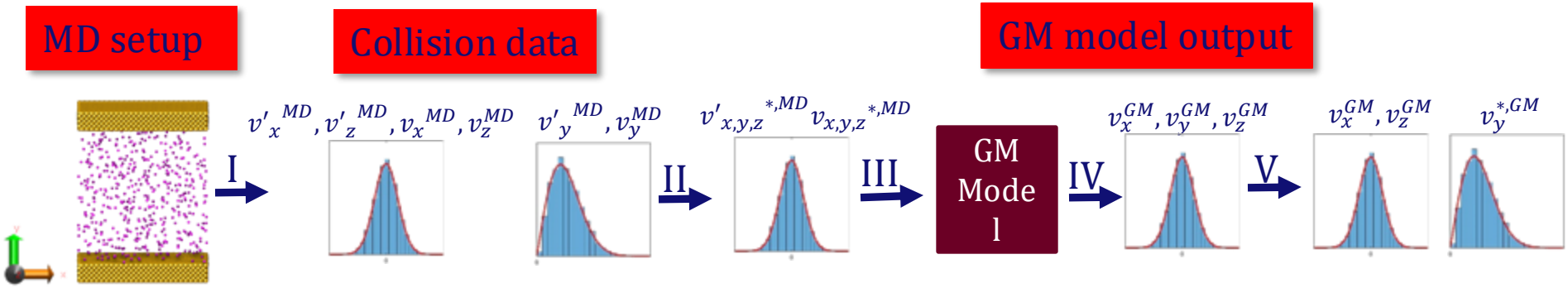
Common Approach

Gathering collision data → Computing different ACs → Scattering kernels

New Approach

Deriving a gas-wall interaction model using Machine Learning

- Application of the GM model in the case of monoatomic gas



$$\mathcal{T}(U) = \sqrt{2\theta}\,\mathrm{erf}^{-1}\left[1 - 2\exp\left(-\frac{U^2}{2\theta}\right)\right]$$

$$\mathcal{T}^{-1}(U) = \sqrt{-2\theta \ln\left[\frac{1}{2} - \frac{1}{2}\mathrm{erf}\left(\frac{U}{\sqrt{2\theta}}\right)\right]}$$

$$\boldsymbol{x}_R = \begin{bmatrix} c_x \\ c_y \\ \mathcal{T}(c_z) \end{bmatrix}, \quad \boldsymbol{x}_I = \begin{bmatrix} c'_x \\ c'_y \\ \mathcal{T}(c'_z) \end{bmatrix}$$

$$\boldsymbol{c} = \begin{bmatrix} x_{R1} \\ x_{R2} \\ \mathcal{T}^{-1}(x_{R3}) \end{bmatrix}, \quad \boldsymbol{c}' = \begin{bmatrix} x_{I1} \\ x_{I2} \\ -\mathcal{T}^{-1}(x_{I3}) \end{bmatrix}$$

$$\theta = \frac{k_B T_g}{m_g}$$

Either for Incoming or Outgoing gas molecules temperature

$$T_g = \frac{\langle v^2 \rangle m_g}{4k_B}$$