Direct Molecular Simulation of 1D Normal Shock Waves with a Neural Network Collision Model

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Motivation

- We aim to use machine learning models of collisions in rarefied gases to speed up simulations.
- Boltzmann equation of rarefied gas dynamics usually solved using Direct Simulation Monte-Carlo, a stochastic method.
- This method usually uses phenomenological models fitted to data to generate the outcome of a collision between particles, rather than resolving the dynamics.
- Doing this fully is computationally expensive, so we ask if machine learning can be used instead, starting with the simple case of monatomic Argon.

Background - Continuum Physics

- Aerodynamics modelling is usually done with the Navier-Stokes equations, valid for small Knudsen numbers,

$$Kn = \frac{\lambda_{mfp}}{L} \lesssim 0.01, \text{ (continuum flow)} \tag{1}$$

  where the *mean free path* is the average distance travelled by a molecule between collisions.

- However, for applications such as re-entry in the upper atmosphere, λ_{mfp} can be very large, so that Kn is > 1.

- Alternatively in nanoscale devices where L is very small, $Kn > 1$ at standard temperature and pressure.

Background - Boltzmann Equation

- Need a kinetic description - instead of velocity field, describe gas in terms of the distribution function $f(x, v, t)$ - density of particles at x, with velocity v, at time t.
- Under some assumptions (two-body collisions, particles un-correlated before a collision,...), can semi-rigorously derive from Hamiltonian system the famous Boltzmann equation for the distribution function:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f, f) \tag{2}$$

$$Q(f, f) = \int dv_* \int d\Omega \left[f' f'_* - f f_* \right] B(\Omega, |v - v'|) \tag{3}$$

- Introduced by Bird in 1970s, now the most commonly used method for simulating Boltzmann.
- Stochastic particle method - distribution function is represented by particles with a given velocity v and internal state I which allows the modelling of rotational or vibrational energy.
- At each time step, pairs of particles i, j in the same physical cell are selected to undergo collisions, with probability proportional to the cross section,

$$\sigma(|v_i - v_j|, I_i, I_j) \tag{4}$$

- Particles accepted undergo an elastic, hard sphere collision and velocities are updated.
- After collisions have occurred, particles move according to their velocities for a time Δt.
- A steady solution is obtained by time averaging quantities of interest, after waiting for transient behaviour to die down.
- Most common model for collisions is Variable Hard Spheres, $\sigma = |v_i - v_j|^{1-\omega}$.

Molecular Dynamics

- The equations of motion are integrated for every individual atom in a gas.
- Trustworthy results when using realistic interatomic potentials such as the Lennard-Jones interaction.
- However... easily $O(10^5)$ particles even for simple test cases and so extremely computationally expensive.
- Requires massively parallel computing to simulate a real gas, even with tricks such as the Event-Driven/Time-Driven algorithm.

Direct Molecular Simulation

- What if we use the standard DSMC algorithm to select collision pairs, but then fully resolve the dynamics of the collision by integrating particle trajectories?
- Can save computational cost vs MD with the same accuracy.
- How do we carry out the trajectory calculations?

Two particle collisions

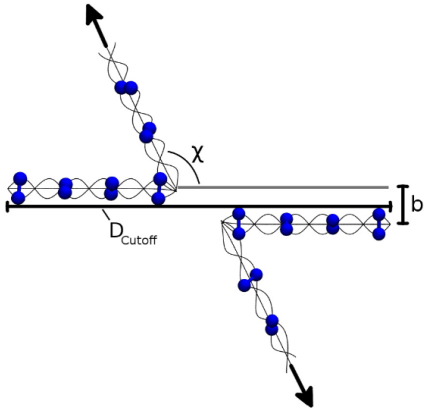


Figure: Diagram of representative two body collision

Norman, Valentini and Schwartzentruber, 2012, [1]

Ar-Ar Collisions

- In monatomic Argon, a collision is completely specified by the collision energy e and impact parameter b.
- Final result depends only on the scattering angle χ.
- So to do DSMC with real collisions, we need:
  - a model for the cross section σ, to decide which collisions to simulate,
  - a method of choosing an impact parameter b,
  - a function $(e, b) \mapsto \chi$.

Trajectory Calculations

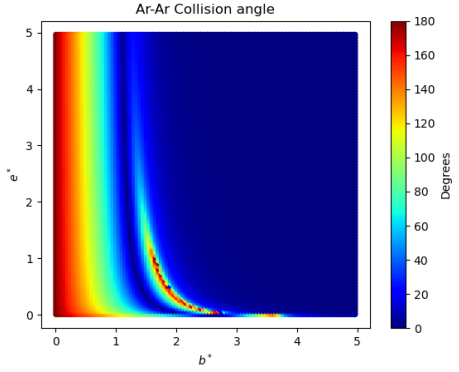


Figure: Generating a representative sample of trajectories suggests answers to all three questions...

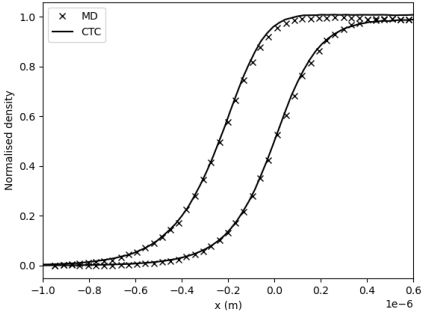
DMS Procedure

- a model for the cross section σ, to decide which collisions to simulate,
  - Choose $\sigma = \pi b_{max}^2$, using the largest impact parameter which results in a noticeable collision for a given e.
- a method of choosing an impact parameter b,
  - Choose b uniformly in $[0, b_{max}]$ for each collision
- a function $(e, b) \mapsto \chi$.
  - Either integrate the equations of motion with a Lennard-Jones potential to generate a trajectory (DMS), or use a neural network model (this work).

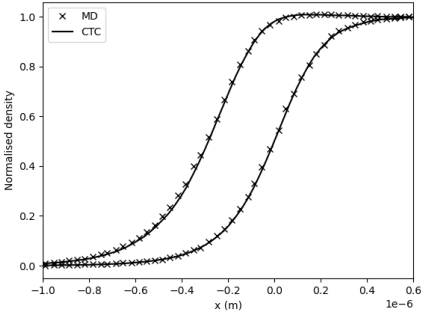
1D Shock Problem

- This is a simple test-case often used to validate DSMC implementations, and for which Molecular Dynamics results are available in the literature.
- Simulation initialised with a discontinuity in the macroscopic variables, which are fixed at the boundaries of a 1D domain.
- A travelling shock profile develops which is steady, but remains out of equilibrium, which is sensitive to the details of the collision dynamics.

DMS Results



(a) Mach 5



(b) Mach 9

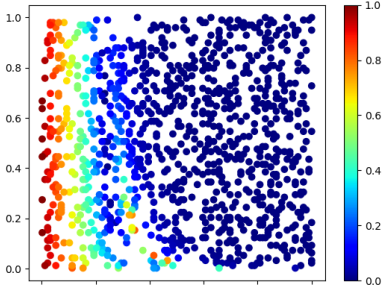
Figure: 1D shock at $\rho_L = 1\,\mathrm{kg\,m^{-3}}$, $T_L = 300\,\mathrm{K}$.

MD profiles from Valentini and Schwartzentruber, 2009 [2]

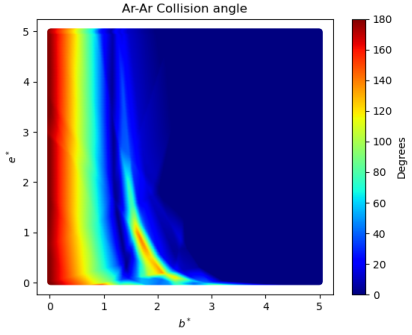
Neural network model

- Train one model for low energy collisions and another for high energies.
- Three fully connected ReLU layers, each with 50 units.
- 4,500 and 150 training epochs for the low and high energy networks respectively.
- Neural network simulation takes a few hours on a laptop CPU, whereas full DMS requires tens of hours on a high performance GPU.

Low Energy NN



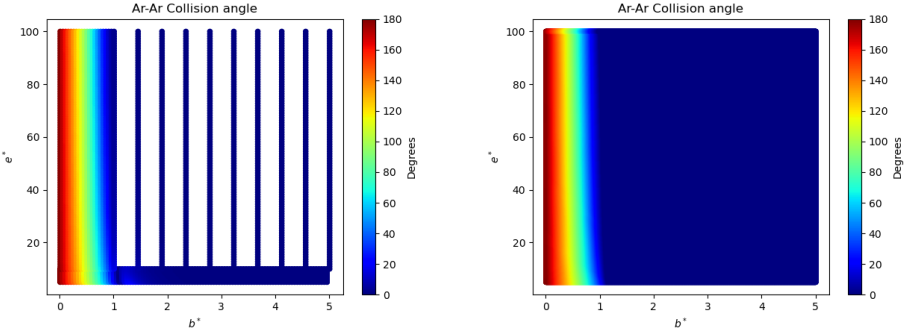
(a) "Low energy" training dataset



(b) "Low energy" model output

Figure: Reference data and model output for low energy neural network model.

High Energy NN

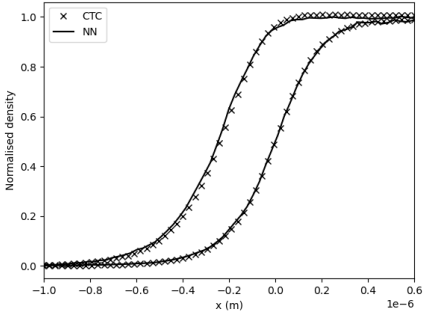


(a) "High energy" collision dataset

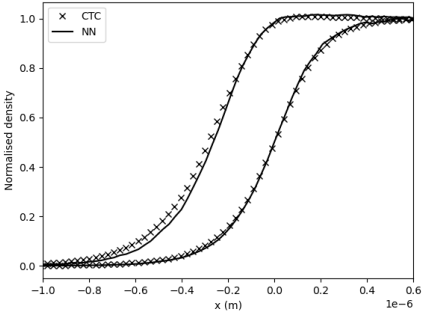
(b) "High energy" model output

Figure: Reference data and model output for high energy neural network model.

Offline NN Results



(a) Mach 5



(b) Mach 9

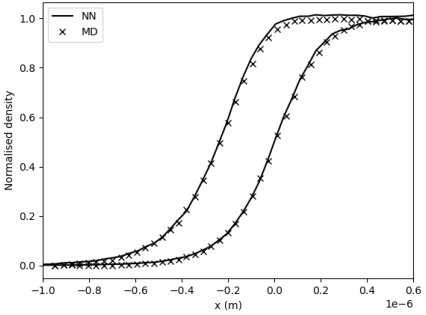
Figure: 1D shock at $\rho_L = 1\,\mathrm{kg\,m^{-3}}$, $T_L = 300\,\mathrm{K}$.

MD profiles from Valentini and Schwartzentruber, 2009 [2]

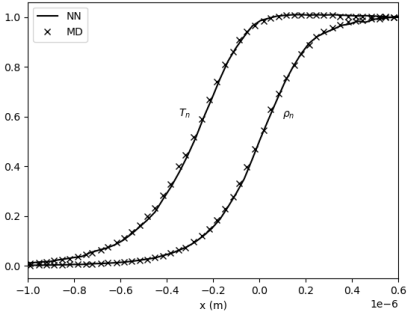
Online Training

- So a neural network model trained in advance can reproduce MD as long as it has been trained on the correct dataset.
- What if we ensure the dataset is correct by training the neural network alongside the DMS?
- Same simulation as before, except during the first 20 timesteps, a fraction of the collisions are fully resolved with DMS.
- The neural network undergoes 100 epochs of training at each step, before being used to simulate the rest of the collisions.

Online Training Results



(a) Mach 5



(b) Mach 9

Figure: Improved results for 1D shock at the same representative physical conditions.

MD profiles from Valentini and Schwartzentruber, 2009 [2]

Next Steps

- Argon-Argon collisions are simple - rotational energy transfer is more complex.
- In N_2 for example, the collision dynamics are now a function $(e, b, I_1, I_2) \mapsto (I_1', I_2', \chi)$, and additional random choices of molecular orientations are possible.

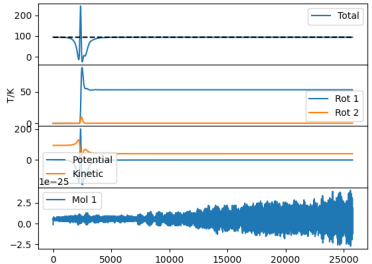


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Figure: Rotational and translational energies during a typical $N_2 - N_2$ collision

Summary

- Competing methods of simulating rarefied gases.
- Direct Molecular Simulation can reproduce Molecular Dynamics results - but is still computationally intensive.
- Neural networks can replace expensive trajectory calculations in simple cases.
- Can they do the same for polyatomic molecules?

Thank you for listening!

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Any questions?

References

[1] Paul Norman, Paolo Valentini, and Thomas Schwartzentruber. "GPU-accelerated Classical Trajectory Calculation Direct Simulation Monte Carlo applied to shock waves". In: *Journal of Computational Physics* 247 (2013), pp. 153–167. ISSN: 0021-9991. DOI: https://doi.org/10.1016/j.jcp.2013.03.060. URL: https://www.sciencedirect.com/science/article/pii/S0021999113002441.

[2] Thomas Schwartzentruber and Paolo Valentini. "Molecular Dynamics Simulations of Normal Shocks in Dilute Gases". In: *41st AIAA Thermophysics Conference*. DOI: 10.2514/6.2009-3602. eprint: https://arc.aiaa.org/doi/pdf/10.2514/6.2009-3602. URL: https://arc.aiaa.org/doi/abs/10.2514/6.2009-3602.