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Ab initio simulation of normal shock waves in argon

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Abstract. The structure of a normal shock wave is calculated in a wide range of Mach numbers applying the direct simulation Monte Carlo method based on the *ab initio* potential for argon and for hard sphere molecules. The distributions of density and temperature in the shock wave and its thickness are calculated with the numerical accuracy of 0.5%. The numerical data are compared with other theoretical and experimental data.

Palavras-chave. shock waves, *ab initio* potential, direct simulation Monte Carlo, argon.

1 Introduction

Shock waves are mechanical waves that occurs when matter is subjected to a rapid compression. There is an abrupt change in all thermodynamic properties of the gas across the shock, that happens through a very narrow region, of the order of the mean free path, i. e., the distance that a flow particle travels between two successive intermolecular collisions. Because of the geometrical simplicity this flow can be an important benchmark problem to verify methods for computing kinetic process in gases. At the same time, this gas flow is of practical interest in aerospace engineering to develop and design space vehicles, to model the reentry into atmosphere of satellites, to calculate supersonic flows in high power jet engines etc.

A numerical modeling of phenomena with a higher precision in these technological fields requires a continuous improvement of numerical methods of rarefied gas dynamics. All these methods are based on a model of intermolecular interaction potential. The most used model is the hard spheres (HS) molecules, which has a fixed collision cross-section and yields a non-physical dependence of the gas viscosity on its temperature. Other collision models, like the variable hard spheres (VHS) and the variable soft spheres (VSS) were proposed to overcome this difficulty, see e.g. Ref. [2]. These models provide more physical results, but they are strongly dependent on adjustable parameters.

Recently, a technique to implement an arbitrary potential into the direct simulation Monte Carlo (DSMC) method was proposed in Ref. [5]. This technique allows us to implement the *ab initio* potential and to avoid the use of any adjustable parameter. Also,

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the computational time is of the same order of the DSMC based on the hard sphere potential. To verify the influence of the intermolecular potential on the shock wave structure problem, the same calculations were carried out for the *ab initio* potential for argon and the hard sphere potential.

2 Statement of the problem

Consider a one-dimensional stationary shock wave propagating in argon. The gas is uniform outside of the shock region and, in a coordinate system in which the shock front is at rest, the relation between the temperature T, pressure p and density ρ on both sides of the shock are the Rankine-Hugoniot relations:

$$\frac{p_2}{p_1} = \frac{2\gamma M_1^2 - (\gamma - 1)}{\gamma + 1}, \tag{1}$$

$$\frac{T_2}{T_1} = \frac{(2 + (\gamma - 1)M_1^2)(2\gamma M_1^2 - (\gamma - 1))}{M_1^2(\gamma + 1)^2}, \tag{2}$$

$$\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} = \frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2}. \tag{3}$$

Here the subscripts 1 and 2 are referred respectively to the gas state before and after the shock front, γ is the ratio of specific heats and is equal to 5/3 for a monatomic gas, M_1 is the upstream Mach number, which is defined as the ratio of the speed of shock wave front and the speed of sound in a gas before the front.

2.1 Potential

The hard sphere (HS) potential is given as

$$U(r)_{HS} = \begin{cases} \infty, & \text{quando } r < d, \\ 0, & \text{quando } r > d, \end{cases} \tag{4}$$

where d is the sphere diameter.

The AI potential for argon was calculated in Ref. [6] and is given by

$$\frac{U(r)_{AI}}{k_B} = A \exp\left[a_1 r + a_2 r^2 + \frac{a_3}{r} + \frac{a_4}{r^2}\right] - \sum_{n=3}^{8} \frac{C_{2n}}{r^{2n}} \left(1 - e^{-br} \sum_{k=0}^{2n} \frac{(br)^k}{k!}\right). \tag{5}$$

The parameters of the equation 5 are reported in Ref. [6].

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3 Numerical Scheme

The shock wave problem was solved by the direct simulation Monte Carlo, using the NTC (no time counter) method, proposed and described by Bird [2]. The gas flow region is divided into a one dimensional structure of cells and the time is advanced in discrete steps of magnitude Δt. The particle motion and the collisions are uncoupled over the time interval. In each time step, the number of pairs to be selected for intermolecular collisions in each cell is calculated as

$$N_{colM} = \frac{N_p(N_p-1)F_N\sigma_T g_{r,max}\Delta t}{2V_c}, \tag{6}$$

where N_p is the number of simulated particles in each cell during the time interval Δt, F_N is the number of real particles represented by one simulated particle, $g_{r,max}$ is the maximum relative velocity of two particles, σ_T is the total cross-section of particles and V_c is the cell volume. The collision cross-section is given by

$$\sigma_T = \pi b_{max}^2, \tag{7}$$

where b_{max} is equal to the diameter d of the sphere for the hard sphere model and for the *ab initio* potential it is the potential cut-off, i. e., it is assumed a maximum impact parameter b_{max} when a collision happens and the collision cross-section is constant.

The deflection angle in a collision is calculated considering a binary elastic collision. For the HS potential, the deflection angle is determined by the impact parameter b as

$$\chi_{HS} = 2\arccos(b/d). \tag{8}$$

For the *ab initio* potential, the technique proposed in [5] is used. A matrix of deflection angles $\chi_{i,j}$ is precalculated for N_e values of energy and N_b values of the impact parameter, and it is stored in computer memory. The energy and impact parameter values are distributed according to the expressions,

$$E_j = (j-0.5)E_{max}/N_e, \quad b_i = b_{max}\sqrt{(i-0.5)/N_b}, \tag{9}$$

where $1 \le j \le N_e$, N_e and N_b are integers and E_{max} is the maximum energy. To choose the deflection angle from the matrix for a specific collision, the following rules are used

$$i = N_b R_f + 1, \quad j = (E/E_{max})N_e + 1, \tag{10}$$

where R_f is a random number varying from 0 to 1.

The DSMC computations with open boundaries conditions were carried out under the following conditions: the space interval is $-30 \le x \le 30$ for Mach number from 1.1 to 3 and $-10 \le x \le 10$ for Mach number from 4 to 10, and the flow region is divided into 1000 cells and 2000 cells; the number of model particles fluctuates near 10^7; the time step is $\Delta t = 0.002$. The results are for argon at $T_1 = 300$ K. For AI potential $b_{max} = 3r_0$ where r_0 is the distance corresponding to the zero potential, which is equal to $6.375a_0$ for argon, where $a_0 = 5.2917721092 \times 10^{-11}m$ is the Bohr radius. The deflection matrix was calculated for $N_e = 5000$, $N_b = 900$ and $E_{max} = 200k_BT_1$.

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4 Results

The results for the density and temperature profiles for some Mach numbers are shown in figures 1 and 2.

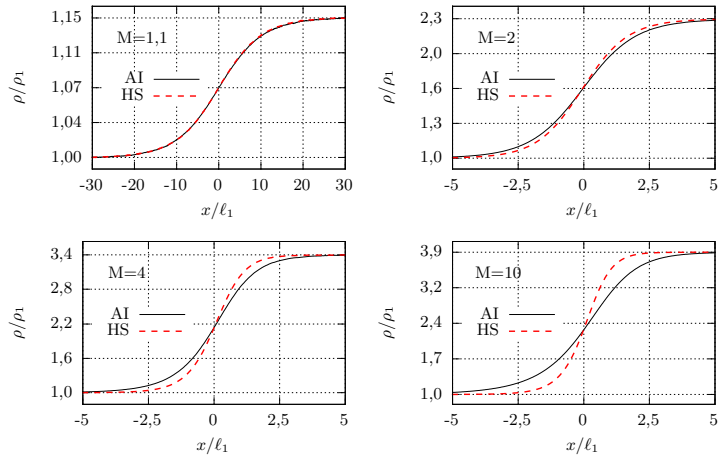

Figure 1: Density profiles.

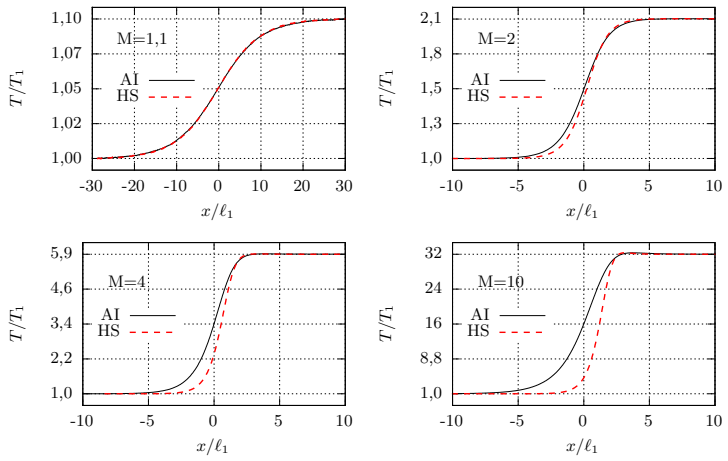

Figure 2: Temperature profiles.

The maximum slope of the density profile, in dimensionless form, is given by

$$D_\rho = \frac{\ell}{\rho_2 - \rho_1}\left(\frac{d\rho}{dx}\right)_{max}, \tag{11}$$

where ℓ is the equivalent free path, defined by

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$$\ell = \frac{\mu_1 v_{mp}}{p_1}, \quad v_{mp} = \sqrt{\frac{2k_B T_1}{m}}, \tag{12}$$

μ_1 is the viscosity at the temperature T_1, p_1 is the pressure and k_B is the Boltzmann constant.

The comparison between the results for AI and HS potentials and other results from the literature are presented in figure 3.

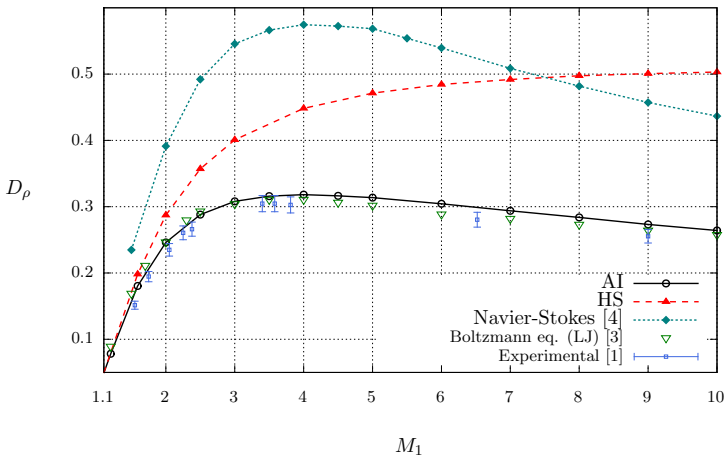

Figure 3: D_ρ as a function of the Mach number for *ab initio* (AI) and hard sphere (HS) potential, for argon.

For low Mach numbers the hard sphere model gives good agreement with experiment, but for higher Mach numbers it provides shocks waves thinner than the experimental results. The results for the AI potential agree to within the accuracy of the numerical solution of the Boltzmann equation for the Lennard-Jones potential [3], for the whole range of the Mach number. Good agreement is also found between the AI and the experimental results from [1]. As was expected, deviations of the Navier-Stokes solutions are found even for low Mach numbers.

5 Conclusions

The shock wave structure was obtained using DSMC method for the *ab initio* potential, without the use of any adjustable parameter from experimental data. The comparison shows that the hard sphere potential is not appropriate for such a problem, and realistic potentials must be used. Also, significant deviations of the Navier-Stokes results are found, which indicates that this problem must be treated through the kinetic theory. The reported results can be used as benchmark data to test model kinetic equations.

The same technique will soon be applied to obtain the structure of a shock wave in a mixture of gases, for those gases of which the AI potential is known.

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