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A HYBRID GAUSSIAN MIXTURE-DSMC APPROACH APPLIED TO THE FOURIER THERMAL PROBLEM

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KEYWORDS

Rarefied gas, molecular dynamics (MD) simulation, gas-surface interaction, unsupervised machine learning, Gaussian Mixture model, DSMC

ABSTRACT

In rarefied gas dynamics, gas-surface scattering kernels play an important role in evaluating the gas flow field properties since they include crucial information about the effects of the physical and chemical properties of the gas-surface interface on the gas scattering process. In our previous work [1,2], an unsupervised machine learning approach, the Gaussian Mixture (GM) approach, is employed to establish a statistical gas-surface scattering model. In this paper, the GM- scattering kernel is coupled to a Direct Simulation Monte Carlo (DSMC) solver as a boundary model to study the Fourier thermal problem. Two gas-solid pairs are considered here: the Ar-Au and H_2-Ni systems. The schematic diagram of the simulation setup is shown in Fig. 1.

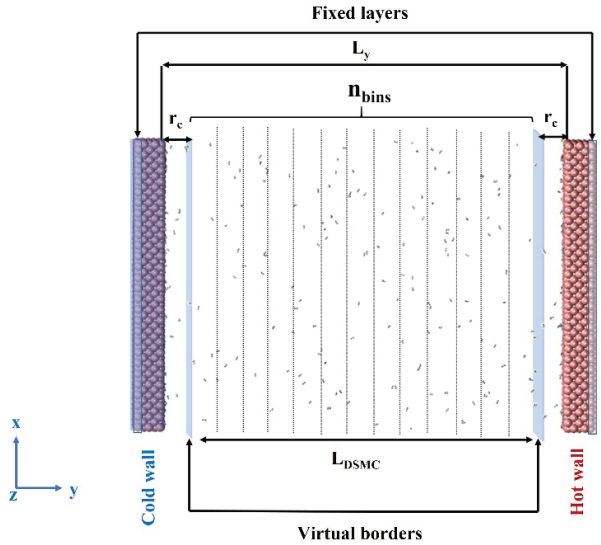

Fig. 1: Schematic representation of the system under consideration for the MD and DSMC simulations. L_y: distance between the two walls that are kept at constant temperatures $T_{Cold} = 300$ K and $T_{Hot} = 500$ K.

In the MD setup, each wall is constructed with five layers of FCC planes. Periodic boundary conditions are considered along x- and z-directions. Two cases are studied: a monatomic case, Ar-Au, and a diatomic case, H_2-Ni. In both cases, the Fourier thermal problem is considered in which the cold wall is kept at T_{Cold} = 300 K, while the hot plate is kept at T_{Hot} = 500 K. The distance between the two walls is L_y=12 nm, for the Ar-Au system, and L_y=30 nm for the H_2-Ni system. The interactions between the solid Au and Ni atoms located in the walls are models using the corresponding embedded atom model (EAM) potentials developed by Sheng *et al.* [3] and Foiles *et al*. [4], respectively. For the Ar-Au system, the non-bonded gas-gas, and gas-wall interactions are modeled by 12-6 Lennard-Jones (LJ) potentials ($\varepsilon_{Ar-Ar} = 1.22\ 10^{-2}$ eV; $\sigma_{Ar-Ar} = 3.35$ Å; $\varepsilon_{Ar-Au} = 1.14\ 10^{-2}$ eV; $\sigma_{Ar-Au} = 3.819$ Å). For the H_2-Ni system, the non-bonded interactions are modeled using COMPASS force field [5], which is an LJ 9-6 function ($\varepsilon_{\mathrm{H-Ni}} = 1.19\ 10^{-2}$ eV; $\sigma_{\mathrm{H-Ni}} = 2.016$ Å), is applied. For the hydrogen gas-gas interaction the 12-6 Lennard-Jones potential is used ($\varepsilon_{\mathrm{H-H}} = 9.29\ 10^{-4}$ eV; $\sigma_{\mathrm{H-H}} = 1.421$ Å). In the case of the Ar-Au system, each wall has a cross-sectional area of 10 nm × 10 nm, while for the H_2-Ni system, the cross-sectional area is 10.8 nm × 10.8 nm. In each wall, the outermost layer is constrained to prevent the translational motion of the wall in the normal direction. The same setup is also used for the DSMC simulations.

In general, DSMC is a promising tool for obtaining accurate gas transport properties outside the gas-solid surface interaction layer, defined by the cutoff distance of the interatomic potential. In fact, near-surface effects, such as the presence of the adsorption layer caused by the attractive part of the interaction potential, cannot be captured by most DSMC codes. To overcome this shortcoming, here, a modified boundary condition is used at a distance r_c from the wall, where r_c is the gas-wall interaction cut-off distance. Therefore, the DSMC domain size, $L_{DSMC} = L_y\text{-}2r_c$, covers only the distance between the virtual borders (Fig. 1). To fully examine the coupling mechanism between the GM scattering kernel and the DSMC approach, a one-to-one correspondence between MD and DSMC particles is considered here. Therefore, the number of DSMC particles, N_{DSMC}, has to be corrected as follows:

$$N_{DSMC} = N_{MD} - N_{ads}$$

where N_{MD} is the number of particles used in the MD simulation and N_{ads} is the number of gas particles adsorbed on the surfaces. The value of N_{ads} is determined on basis of the results of the full MD simulation and the corresponding gas-wall cut-off radius r_c.

Benchmarked by MD results, the performance of the Gaussian Mixture model coupled to DSMC (GM-DSMC) is assessed against the Cercignani-Lampis-Lord (CLL) kernel [6,7] incorporated into DSMC simulation (CLL-DSMC). The number density and temperature profiles between two walls are utilized to assess the applied scattering kernels' performance. The accuracy of the simulation results is determined by measuring the deviations of the DSMC results from full MD simulation results. Considering x_{y-DSMC} as the predicted number density or temperature in a spatial bin for a DSMC model coupled to the scattering kernel of type y, the deviations are computed by

$$dev_{y-DMSC} = \sqrt{(x_{y-DSMC} - x_{MD})^2}/x_{MD}$$

where x_{MD} refers to the corresponding property obtained from the MD simulation.

In Fig. 2, the variation of the local number density and temperature observed in the MD simulation and the predicted trends by the GM-DSMC and CLL-DSMC for the Ar-Au case study are presented (N_{ads}= 222, N_{DSMC}=578). Regarding the number density (see Fig. 2a), the predicted results by DSMC incorporating both scattering models are consistent with the MD data. Here, the average deviations of the predicted results are 0.6% for both GM-DSMC and CLL-DSMC approaches. In the case of the temperature profile (see Fig.2b), the trend predicted by the GM-DSMC in the bulk of the domain

matches well the pure MD results. Here, the deviations are 0.2%. On the other hand, in most parts of the simulation domain, the results predicted by the CLL-DSMC method deviate from the MD results, observing the highest deviation close to the top wall, which is 4%.

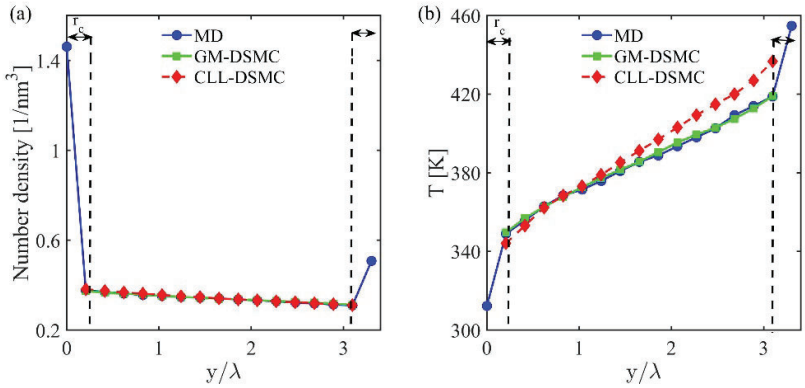

Fig 2. Variation of the macroscopic quantities for the Ar-Au system obtained from the pure MD simulation and DSMC simulations combined with the GM and CLL scattering models. (a) number density, (b) temperature. The positions are scaled by the corresponding mean free path length λ.

Fig. 3 shows the number density and temperature profile for the H_2-Ni system (N_{ads}= 84, N_{DSMC}=806). Regarding the number density variation, it is observed that within the bulk of the simulation domain, the GM-DSMC approach results match well the MD data. Here, the deviations of the GM-DSMC results are around 0.6% on average. However, a notable discrepancy between the density profiles obtained from the MD and CLL-DSMC is observed in the current case study. In this case, the highest deviation is measured near the top wall, which is 8%. In Fig. 3b, it is depicted that the predicted temperature profiles based on both GM-DSMC and CLL-DSMC approaches deviate from the reference MD results. Nevertheless, the GM-DSMC approach still outperforms the CLL-DSMC approach. Herein, the highest deviations based on the GM-DSMC approach are measured at the first and last bins, which are 2% and 1%, respectively. On the other hand, using the CLL-DSMC approach, the deviations on the same bins are 9% and 10%, respectively.

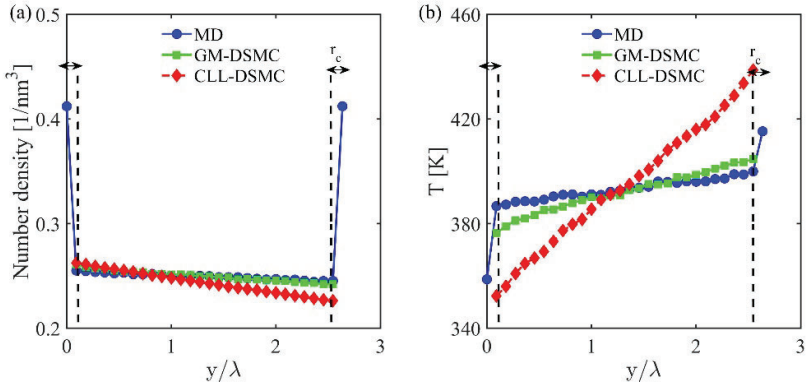

Fig 3. Variation of the macroscopic quantities for the H_2-Ni system obtained from the pure MD simulation and DSMC simulations combined with the GM and CLL scattering models. (a) number density, (b) temperature. The positions are scaled by the corresponding mean free path length λ.

CONCLUSIONS

In both test cases, a better performance of the GM-DSMC approach compared to the CLL-DSMC approach, especially for the diatomic systems, is seen. By employing the GM-DSMC technique, we obtained an energy exchange model that is almost as accurate as MD simulations, but for only a fraction of the computational cost.

ACKNOWLEDGEMENTS

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REFERENCES

[1] Mohammad Nejad, S., Iype, E., Nedea, S., Frijns, A. and Smeulders, D., 2021. Modeling rarefied gas-solid surface interactions for Couette flow with different wall temperatures using an unsupervised machine learning technique. *Physical Review E*, *104*(1), 015309, https://doi.org/10.1103/PhysRevE.104.015309

[2] Mohammad Nejad, S., Nedea, S.V., Frijns, A.J.H. and Smeulders, D., 2022. Development of a scattering model for diatomic gas-solid surface interactions by an unsupervised machine learning approach. *Physics of Fluids,* 34, 117122*;* https://doi.org/10.1063/5.0110117

[3] Sheng, H., Kramer, H., Cadien, A., Fujita, T. and Chen, M. (2011) Highly optimized embedded-atom method potentials for fourteen fcc metals, *Physical Review B,* 83, 134118.

[4] Foiles, S. Baskes, M. and Daw, M. S. (1986) Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys, *Physical review B*, 33, 7983.

[5] Sun, H. (1998) Compass: an ab initio force-field optimized for condensed-phase applications overview with details on alkane and benzene compounds, *The Journal of Physical Chemistry B*, 102, 7338–7364.

[6] Lord, R. (1991). Some extensions to the Cercignani–Lampis gas–surface scattering kernel, *Physics of Fluids A: Fluid Dynamics,* 3, 706–710.

[7] Hossein Gorji, M. and Jenny, P. (2014). A gas-surface interaction kernel for diatomic rarefied gas flows based on the Cercignani-Lampis-Lord model, *Physics of Fluids*, 26, 122004.