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MD-Informed Gas-Surface Interaction Kernel for LEO/VLEO Atmospheres

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Abstract

This work presents our ongoing effort to develop a physically informed gas-surface interaction (GSI) model for rarefied flows by integrating molecular dynamics (MD) data into the widely used Cercignani-Lampis-Lord (CLL) scattering kernel. The study focuses on improving the aerodynamic modeling of satellite surfaces in very low Earth orbit (VLEO), where atomic oxygen (AO) is the most dominant atmospheric species. Silica-based materials are selected for resistance to AO-driven erosion, making them highly relevant for future spacecraft surface designs.

Molecular dynamics (MD) is used to understand the interactions of AO with an SiO2 surface, and the resulting information is used to minimally modify the CLL model. While traditional CLL models are computationally convenient, they are not inherently linked to the surface chemistry or scattering physics of specific material-gas pairs. This work introduces a systematic approach to inform CLL models using MD-derived velocity distributions and energy-momentum accommodation characteristics.

MD scattering simulations were performed for pristine and AO-saturated silica surfaces to capture the impact of surface conditions on energy and momentum transfer. From these simulations, energy and momentum accommodation coefficients were extracted and used as input to standard CLL models implemented in DSMC solvers. The initial results show that with its existing assumptions, the original CLL model fails to fully capture the scattering characteristics revealed in the MD data as expected, particularly the post-collision angular and energy distributions. These observed gaps highlight the need for a refined model.

In the current phase, we propose a set of physically motivated and computationally simple modifications to the CLL algorithm that incorporate MD-informed trends. These updates aim to preserve the structure of the CLL model while improving its accuracy for VLEO-relevant GSI phenomena. Model development and testing are actively in progress, with DSMC integration underway. Future phases will expand the scope to explore the effects of surface chemistry further.