

Extraction of moment closures for strongly non-equilibrium flows via machine learning

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We introduce a machine learning (ML) framework for moment-equation modeling of rarefied gas flows, addressing strongly non-equilibrium conditions inaccessible to conventional computational fluid dynamics. Our approach utilizes high-order moments and collision integrals—highly sensitive to non-equilibrium effects—as key predictive variables. Training datasets are created from one-dimensional steady shock simulations, and a methodology of computing collision integrals is developed. By learning thermodynamically consistent closures directly from direct simulation Monte Carlo (DSMC) data, our regularized 13 moment (R13)-ML model, combined with a discontinuous Galerkin solver for the transfer equations of moments, preserves physical structure and accurately predicts normal shock structures and generalizes to hypersonic and some unsteady, one-dimensional wave scenarios. This work bridges machine learning with continuum mechanics, offering a road map for high-fidelity aerothermal predictions in next-generation supersonic vehicles.