

Physics-assisted neural network based modeling of the dynamics of the velocity gradient tensor in incompressible and compressible turbulence

Abstract

This thesis investigates the development of machine learning--based closure models for velocity gradient dynamics in both incompressible and compressible flows. The velocity gradient tensor contains detailed information about nonlinear turbulent processes and is fundamental to understanding small-scale flow physics. Its evolution is governed by two unclosed terms - the pressure Hessian and the viscous Laplacian - which account for pressure-related and viscous effects, respectively. Tracking the velocity gradient tensor along a fluid particle therefore requires closure models or additional evolution equations for these terms. For incompressible flows, a range of phenomenological and data-driven models has been proposed in recent years to approximate these unclosed contributions. In contrast, similar modeling efforts for compressible flows remain relatively limited. Furthermore, to the best of our knowledge, no existing models for compressible velocity gradient dynamics incorporate the effects of vibrational non-equilibrium.

This work develops a machine learning-based framework for modeling velocity gradient dynamics in compressible flows, explicitly accounting for the effects of vibrational non-equilibrium on pressure Hessian evolution. As an initial step, we focus on improving existing neural network-based models for the pressure Hessian in incompressible flows. Building on these developments, the modeling framework is subsequently extended to compressible regimes, providing a novel data-driven approach to address the complexities of high-speed and non-equilibrium flow physics. The objectives of this research are organized into four interrelated studies, as outlined below:

1. Study A: Development of an augmented invariants-based closure model for the pressure Hessian tensor in incompressible turbulent flows.
2. Study B: Development of neural network-based closures for vibrational non-equilibrium effects influencing the evolution of the pressure Hessian tensor in compressible turbulent flows.
3. Study C: Development of neural network-based closures for the non-symmetric mechanisms governing the evolution of the pressure Hessian tensor in compressible turbulent flows.
4. Study D: Integration of the developed neural network-based closures into a fully dynamical closure framework for the velocity gradient tensor in compressible turbulent flows with vibrational non-equilibrium effects.

All processes considered in this work can be represented mathematically as second-order tensors. A unified modeling framework is proposed in which two separate neural networks are employed: one to predict the alignment of the eigenvectors of the target tensor, and the other to predict its magnitude. This decomposition enables the formulation of mathematically optimal and physics-assisted loss functions, tailored separately for alignment and magnitude predictions.

In Study A, the anisotropic part of the pressure Hessian tensor for incompressible flows is modeled using a combinations of two different physics-embedded deep neural networks. Even though the training of the two networks is performed using direct numerical simulation (DNS) database of an incompressible stationary isotropic turbulence at a particular Reynolds number,

we extensively evaluate the model at different Reynolds numbers and in different kinds of flow fields. In incompressible flows, the proposed model shows significant improvements over the existing phenomenological model (the recent fluid deformation closure model or the RFD model) of the pressure Hessian tensor. While the improvements in the alignment tendencies are convincingly evident in the shapes of the probability density functions of the cosines of various angles between eigenvectors, the improvements in the prediction of the magnitude of the pressure Hessian tensor using the new model is quantifiable in the range of 28% - 89% (depending on the type of flow field.) compared to the RFD model.

Studies B, C, and D focus on the modeling of compressible flows with vibrational non-equilibrium effects. In compressible flows, pressure evolves as a thermodynamic variable; consequently, the pressure Hessian tensor satisfies its own evolution equation containing several unclosed terms. This makes the modeling significantly more challenging than in incompressible flows. As the Mach number of the compressible flow field further increases, turbulent flows start experiencing many additional non-equilibrium effects. The shock fronts and the

high-temperature zones that exist in hypersonic flow fields ($>800\text{K}$) trigger vibrational excitation of the constituent air molecules. Even though these vibrationally excited molecules have a natural tendency to relax and attain a state of equilibrium with the evolving temperature field in several hypersonic flows, the time scale of this relaxation may be comparable to the time scale over which the turbulent velocity field itself evolves. This raises additional complexity in the flow field and makes the modeling more challenging because the vibrational energy of the flow field must now be tracked separately in addition to the internal energy incumbent in the temperature field of the flow.

The approach adopted in this work first models the individual unclosed processes appearing in the governing equations of the pressure Hessian tensor using neural networks, followed by the development of a fully coupled dynamical framework. In Study B, the effects of vibrational non-equilibrium on the pressure Hessian tensor are modeled. In Study C, non-symmetric mechanisms governing its evolution are modeled using a tensor-basis neural network architecture. A complete and physically consistent set of tensor bases and scalar invariants is derived to represent general second-order non-symmetric tensors. The networks are trained on data from a single direct numerical simulation (DNS) and validated against multiple datasets, demonstrating strong generalizability within the studied parameter space.

In Study D, a fully dynamical model for the evolution of the velocity gradient tensor in compressible turbulent flows with vibrational non-equilibrium effects is developed. The framework incorporates both symmetric and non-symmetric mechanisms governing the pressure Hessian evolution. Existing phenomenological closures are retained for symmetric components, while neural network--based closures developed in Studies B and C are used for non-symmetric and vibrational non-equilibrium contributions. The resulting framework combines phenomenological modeling with data-driven representations of various symmetric and non-symmetric mechanisms, referred to as the *hybrid enhanced homogenized Euler equation* (H-EHEE) model. Model predictions are evaluated across a range of flow regimes spanning from low to high turbulent Mach numbers, where vibrational non-equilibrium effects become significant. The performance of the H-EHEE model is compared with the direct numerical simulation (DNS) behavior and the existing compressible velocity-gradient dynamical model. The results demonstrate that the proposed framework exhibits close agreement with DNS statistics and consistently shows significant improvements upon the existing model, particularly in high-turbulent Mach number flows.