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MAE557: Simulation and Modeling of Fluid Flows
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Final Project Abstract:
Physics-Informed Neural Networks for Compressible Mixing

Traditional numerical methods for computational fluid dynamics (CFD), such as high-order finite-difference (FD) or finite-volume schemes, are foundational to fluid dynamics research but remain computationally intensive, particularly for turbulent flows requiring high resolution. Physics-Informed Neural Networks (PINNs) [8, 9, 10, 11] have recently emerged as a novel alternative, offering a mesh-free approach that leverages the approximation power of deep learning while enforcing physical laws.

This project proposes the development of a PINNs framework in `PyTorch` [1] to solve the 2-D compressible Navier-Stokes equations. The core of this approach is a feed-forward neural network that takes spatio-temporal coordinates (t, x, y) as input and outputs the primitive flow variables (ρ, u, v, P). The network's loss function is derived directly from the governing equations and the initial and boundary conditions. This "physics-informed" loss function represents the residual of the PDEs and the mismatch at the boundaries. The project methodology will proceed in four phases:

1) **Development**: A PINNs model will be developed, trained, and subjected to hyper-parameter tuning. The network parameters will be optimized by minimizing a composite loss function. This loss function encodes the governing physics and boundary conditions, requiring no *a priori* labeled training data. The partial differential operators in the equations will be computed using automatic differentiation (AD), a cornerstone of `PyTorch` that provides exact derivatives of the network's output with respect to its inputs.
2) **Validation in Lid-Driven Cavity Flow**: The PINNs framework will be validated on the 2-D lid-driven cavity problem. This steady-state flow is a canonical CFD benchmark. Success here will verify the core implementation of the network, the AD-based loss functions, and the training procedure.
3) **Application to Rayleigh-Taylor Instability**: The validated PINNs will then be applied to a 2-D Rayleigh-Taylor (RT) mixing problem. This case is of significant scientific interest [3] as the flow transitions from a quiescent (but unstable) initial state, through a linear growth phase, and into a self-similar turbulent mixing regime.
4) **Benchmark Comparison**: The PINN-generated flow fields will be quantitatively and qualitatively compared against high-fidelity data from `Miranda` [2, 5, 4, 6], a high-order finite-difference implicit large-eddy simulation (iLES) code.

A key hypothesis of this work is that the PINNs will face challenges in accurately resolving the turbulent spectrum. Neural networks are known to exhibit "spectral bias" [7], preferentially learning low-frequency features when trained with gradient descent and effectively filtering high-frequency components. Turbulence is an inherently broadband, high-frequency phenomenon. Therefore, it is anticipated that the PINNs solution may fail to capture the fine-scale turbulent structures characteristic of late-stage RT mixing, potentially yielding a solution that resembles a RANS (Reynolds-Averaged Navier-Stokes) solution, effectively filtering the turbulent fluctuations and capturing only the mean flow behavior.

The primary objective is to critically assess the PINN's capabilities and limitations. This work will investigate whether the PINNs can at least capture the early-stage linear growth and subsequent mean flow characteristics, such as the mixing layer growth rate and mixture fraction profiles, even if it fails to resolve the turbulence. This study will provide valuable insights into the practical applicability of PINNs for complex, unstable, and turbulent flow phenomena.

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