Machine-learned Manifold-based Models for Large Eddy Simulation of Turbulent Combustion

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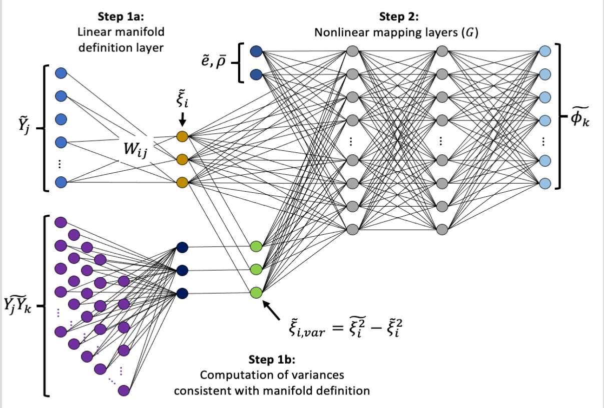
Reduced-order manifold models: lower computational cost by projecting the thermochemical state onto a manifold with $N_\xi \ll N_S$ dimensions. Both physics-based (Flamelet Generated Manifolds, FGM) and data-driven (Principal Component Analysis, PCA) approaches share the same three major steps:

Definition of manifold variables $\boldsymbol{\xi_i = W_{ij} Y_j}$ → ***Mapping to output variables – often using a neural network*** $\boldsymbol{\phi_k = (Y_j, T, \dot{\omega}_j, D, \mu, \ldots) = F(\xi_i)}$ → ***LES closure of filtered quantities*** $\boldsymbol{\tilde{\phi}_k = \widetilde{F(\xi_i)} = G(\tilde{\xi}_i, \xi_{i,var})}$

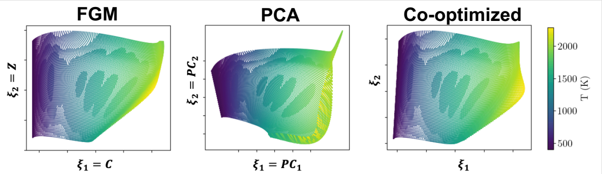
Co-optimized Machine-Learned Manifolds Approach: extend the neural network used for nonlinear mapping to allow simultaneous learning for all three steps

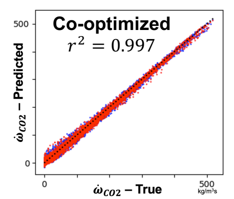
Proposed Neural Network Structure



Case 1: 1D Premixed Flame Data

CH4 (DRM19 mech.), ϕ = 0.5-1.5, 1 atm, T_0 = 400 K



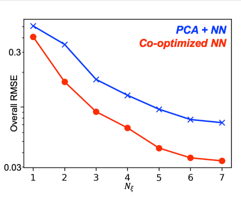


Manifold structure comparison: Co-optimized is similar to FGM, with improved prog. variable

More accurate nonlinear mapping than FGM ($r^2 = 0.992$) or PCA ($r^2 = 0.957$)

Case 2: Jet-A Ignition Kernel DNS Data

Data from Krisman et al., CNF, 2021



More efficient representation of thermochemical state than PCA

Accurate prediction of filtered DNS source terms

The proposed approach can flexibly incorporate thermochemical data from any source, yielding optimized versions of physics-based models in the appropriate limits, but also enabling accurate predictions by including additional data when physics-based manifold descriptions are not available

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