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Representation Learning as a Clustering Paradigm for Combustion: A Progress Variable Perspective

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Chemical kinetics is a challenging problem to model, producing significant computational overheads; nowadays, the increased popularity of Machine Learning (ML) techniques and their implementation for Combustion Science has provided significant advances, leading to the development of Combustion Machine Learning. However, it is important to remember that ML techniques are ingrained in mathematical considerations, reason why the embedding of physical laws in such approaches is key. Regardless of this, it is important to visualize other ways in which the application of Combustion Machine Learning can be enhanced, specifically, with the consideration of modelization concepts, i.e. combustion progress variable, mixture fraction, and so on. This work explores the idea of using a combustion progress variable as a clustering parameter. In fact, combustion dynamics can be fully parameterized with this variable [1], and therefore processes that have similar behavior in the progress of variable behavior are likely to share similar characteristics in combustion development, allowing the discussion of clustering techniques. Due to the non-dimensional characteristics of the progress variable, a subset of chemical species is used to project the progress variable dynamics into the thermochemical space. These chemical species are selected by making use of Time-lag Autoencoders (TAE)[2], allowing for a non-linear dimensionality reduction; additionally, sparse data considerations are implemented, leading to the conceptualization of “Gappy-Autoencoders”. This methodology is applied to methane combustion with the GRI-Mech 2.11 mechanism, consisting of 31 reactive species and 279 reactions; the resulting model enables efficient projection of the thermochemical states while using 9 chemical species as inputs, significantly reducing the thermochemical state dimensionality. Therefore, the results can be associated with the effectiveness of the TAE-identified chemical species as input features for the description of chemical kinetics, but principally, due to the clustering effects in model convergence.

References

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