

Data-driven thermochemical model for simulating hypersonic reacting flows

Clément Scherding^{*,1}, Taraneh Sayadi¹, Georgios Rigas², Denis Sipp³ and Peter J. Schmid⁴

¹ Jean le Rond d'Alembert Institute, CNRS/Sorbonne University, Paris, France

² Department of Aeronautics, Imperial College London, London SW7 2AZ, UK

³ DAAA, ONERA, Université Paris Saclay, 92190 Meudon, France

⁴ Department of Mechanical Engineering, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Keywords: *Hypersonics, Thermochemical non-equilibrium, Machine Learning*

Hypersonic flows are of great interest in a wide range of aerospace applications and are a critical component of many technological advances. Accurate simulations of these flows in thermodynamic (non)-equilibrium (accounting for high temperature effects), rely on detailed thermochemical gas models [1]. While accurate these models dramatically increase the cost of such calculations. As a result, a light-weight and efficient alternative would be highly beneficial in making these calculations relevant in real applications. In addition, such strategies will be of use in other fields, such as reactive flows for example, where similar models capturing the reactive chemistry are employed.

In this work, we present a novel model-agnostic machine-learning technique to learn an a priori thermochemical model of any gas mixture. A first simulation gathers all relevant thermodynamic states and the corresponding gas properties through a given model. The states are clustered and embedded separately in a low-dimensional space to account for regions with different levels of thermochemical (non)-equilibrium. Each cluster is bootstrapped and a surrogate surface from the reduced cluster space to the output space is generated using radial basis function networks.

The method is validated with the simulation of a hypersonic flat-plate boundary layer including finite-rate chemistry. The gas properties of the reactive air mixture are initially modeled using the open-source Mutation++ library [2]. Substituting Mutation++ with the light-weight learned alternative, however, improves the performance of the solver while maintaining the overall accuracy.

REFERENCES

- [1] Candler, Graham V. *Rate effects in hypersonic flows*. Annual Review of Fluid Mechanics, 2019, vol. **51**, p. 379-402.
- [2] Scoggins, James B., Leroy, Vincent, Bellas-Chatzigeorgis, Georgios, et al. *Mutation++: Multicomponent thermodynamic and transport properties for ionized gases in C++*. SoftwareX, 2020, vol. **12**, p. 100575.