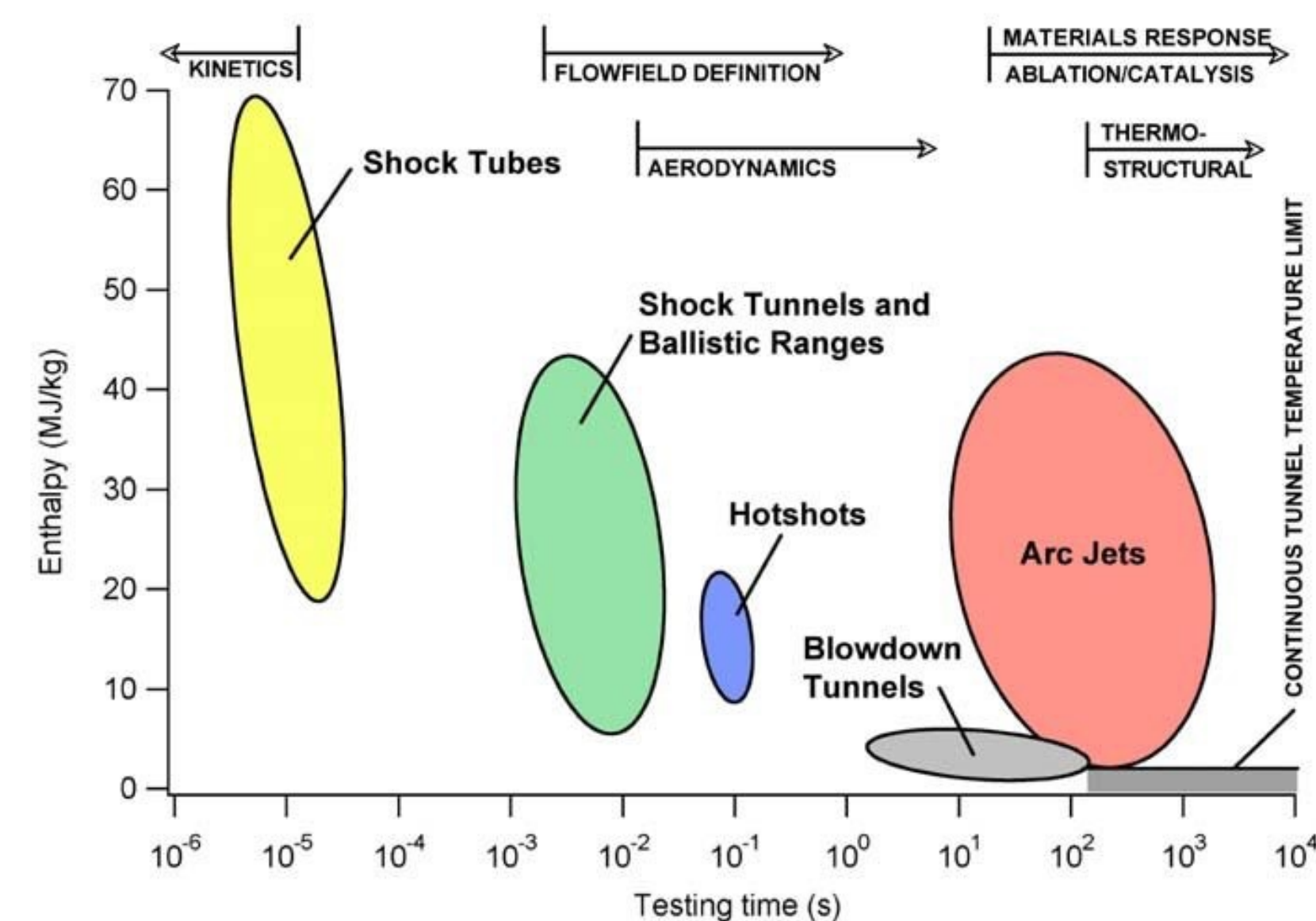# Vibrational State-to-State Nonequilibrium Modeling

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Introduction

The successful development of hypersonic vehicles requires detailed knowledge of the flow physics around the vehicle. Specifically, an understanding of the thermochemical nonequilibrium behavior is crucial for this flight regime.
The hypersonic flight regime involves an extremely high level of energy so a small error in the modeling of the energy processes can result in drastic changes in the vehicle design, which motivates modeling the physics involved at a high fidelity.
Behind a strong shock wave, the gas reaches a significantly high temperature which results in thermochemical nonequilbrium. It is difficult to experimentally model hypersonic conditions due to limitations on the amount of heat able to be generated and the testing time of the experiments, as shown below. Increased understanding of the hypersonic gas dynamics will help the modeling of re-entry vehicles in planetary atmospheres as gas interactions with the vehicles surfaces can be better understood.

Vibrational State-to-State Modeling

The state-to-state (STS) approach is a higher fidelity model for describing the nonequilibrium energy transfer. The STS model is computationally expensive since it directly simulates the population of each internal state. In the case of this research, each vibrational energy state is simulated. The conservation of vibrational energy in the STS model is formulated for each vibrational energy level. This approach significantly increases the number of equations to be solved, however it eliminates highly-averaged parameters such as vibrational relaxation time that can vary drastically for each vibrational energy level.
At hypersonic speeds, the behavior of gas molecules becomes more complex. As shown in the figure at the bottom of the middle column, as velocity increases, more chemical effects come into play, such as vibrational excitation the dissociation of O_2 and N_2 air molecules, and the ionization of molecules. This research focuses on the modeling of this chemical phenomena.
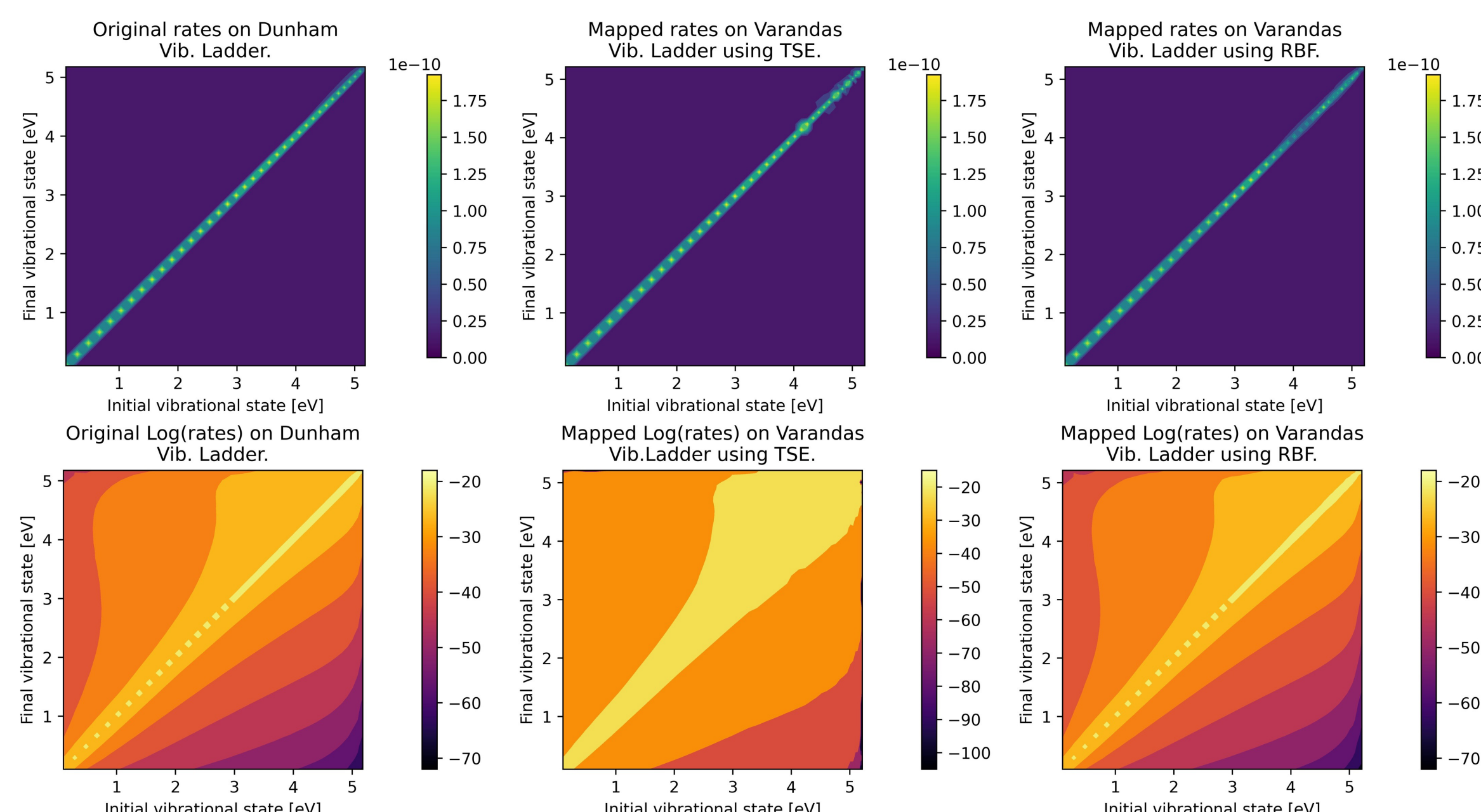
Rate Mapping Between Energy Surfaces

Due to the differences in energy surfaces of the available data on state-resolved rates, we need to find a way to map the rates to be able to complete self-consistent simulations. We investigate two interpolation and extrapolation methods to be able to complete simulations on the same energy surface.
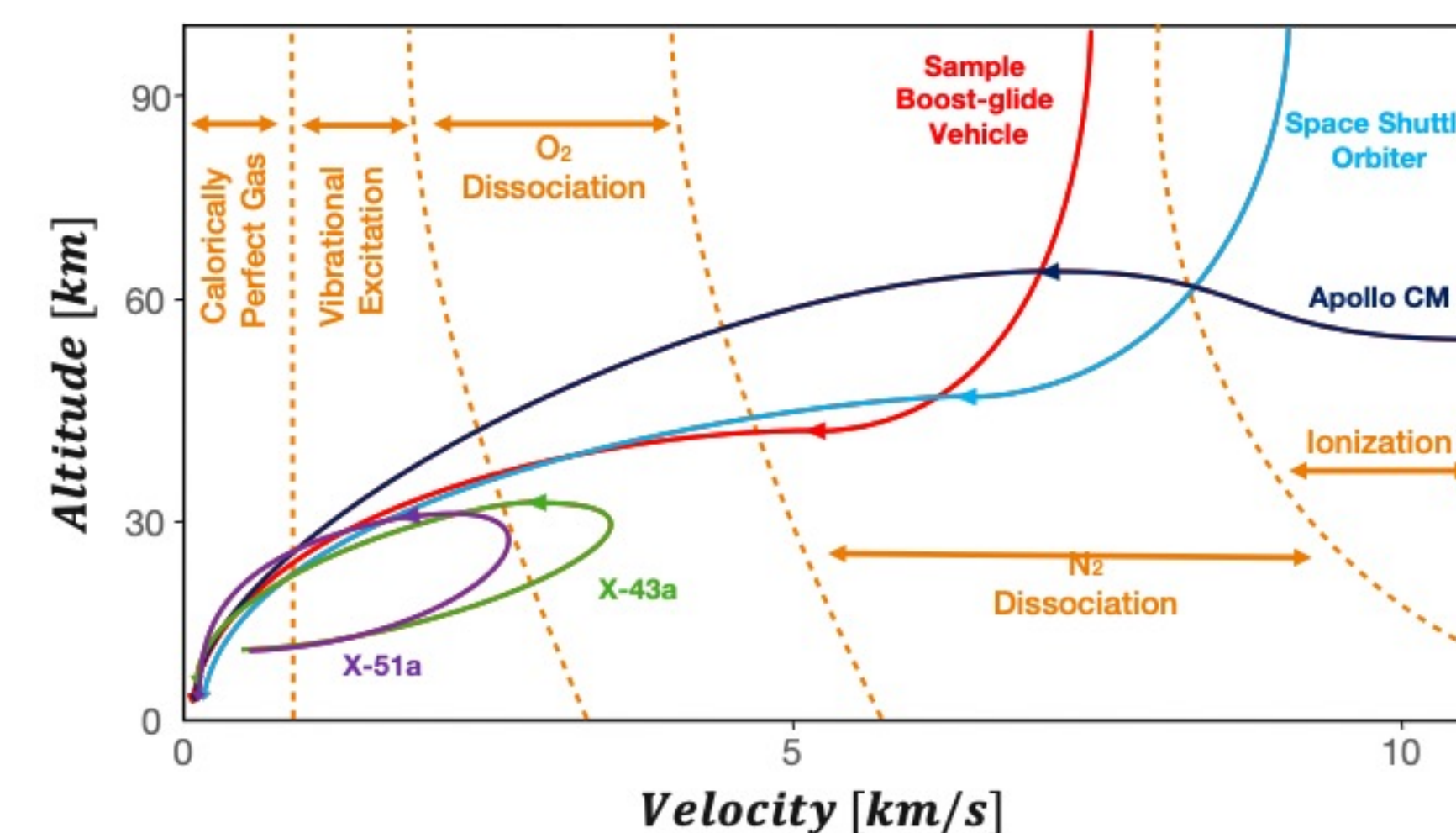
The first method employed is an algorithm that focuses on evaluating distances between points on the known vibrational ladder to each point on the unknown energy ladder. We will accomplish this using radial basis functions with the addition of a first-degree polynomial. We select our radial basis function to be the thin plate spline, defined as

$$\phi(r) = r^2 \log(r) \qquad r = \|\mathbf{v} - \mathbf{d}_i\|$$

We then calculate a weighted sum to calculate all of the unknown rates.

The second method is to use Taylor Series Expansions[1] by computing gradients of known variables[2] on unstructured grids. This method focuses solving systems of equations that calculate weighted sums of the two closest points on the known energy ladder, as opposed to creating a weighted sum of all points.
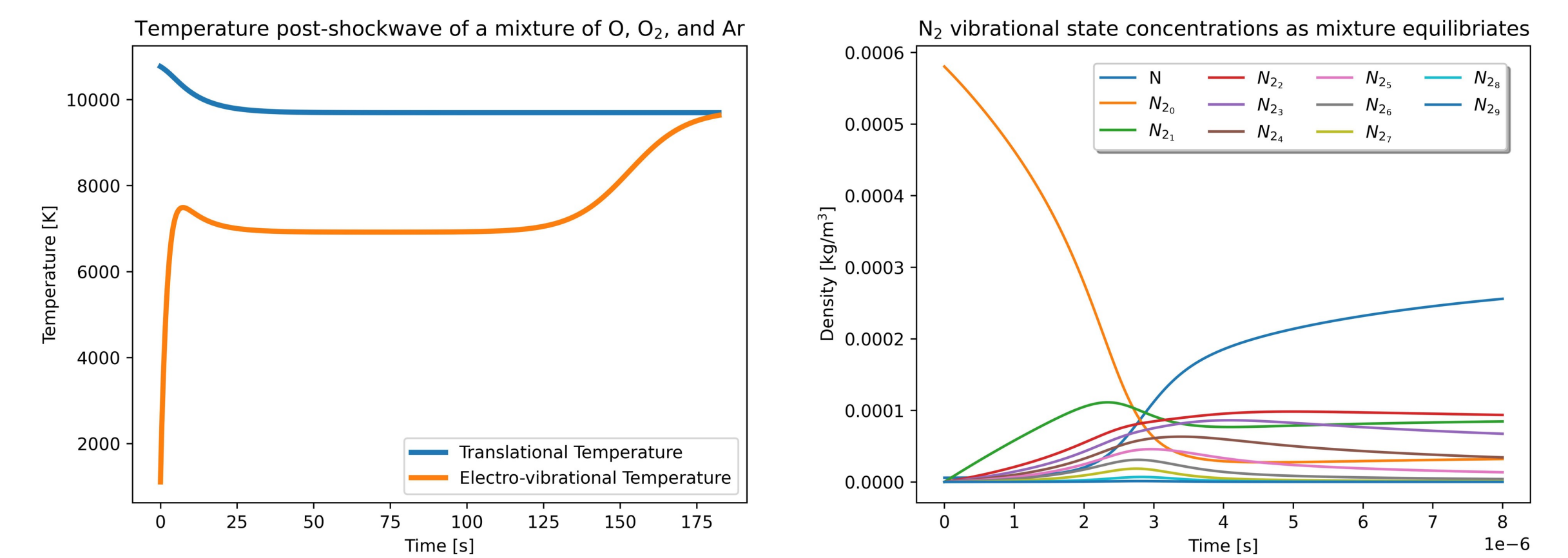

[1] Andrienko, D. A., and Boyd, I. D., "Kinetics of O2-N2 collisions at hypersonic temperatures," AIAA Aviation and Aeronautics Forum and Exposition, AIAA Paper 2018-3438, Atlanta, GA, 2018.
[2] Mavriplis, D. J., "Revisiting the least-squares procedure for gradient reconstruction on unstructured meshes," 16th AIAA Computational Fluid Dynamics Conference, AIAA Paper 2003-3986, 2003. https://doi.org/10.2514/6.2003-3986.

Chemical Kinetics Behind a Shockwave

As a normal shockwave passes through a fluid perpendicular to the flow direction, the static pressure, temperature, and gas density increase. At high temperatures, the molecular vibrational energy increases and contributes to the overall energy state of the gas. Thermal equilibrium occurs when there is no net transfer of of energy between the translational and vibrational modes. This is demonstrated in the figure on the left in a simulation of O, O_2, and Ar. The rates that different vibrational energy states are formed are described by reaction rates as seen in the figure in the middle column for O_2 at 3000 K. The equilibrium state of a system is described by when the rate of forming a certain vibrational mode is the same as the vibrational mode increasing or decreasing in energy. The figure on the right shows a mixture of Nitrogen placed in a system, the temperature of which remains constant the system is driven to equilibrium.

Conclusions

- The radial basis function mapping of the known reaction rates from the known energy ladder to the unknown energy ladder is visually more optimal as it maintains the same reaction rate surface levels and patterns

- In initial tests, as seen above, equilibrium can be reached using simulations of Oxygen (left), using the mapped reaction rates, and Nitrogen (right) mixtures

Future Work

- Further validation of the mapped reaction rates using radial basis functions

- Simulations of hypersonic flows in shock tubes and over complex geometries, such as a double cone

- The implementation of a reduced order model to calculate the temperature distribution across a surface