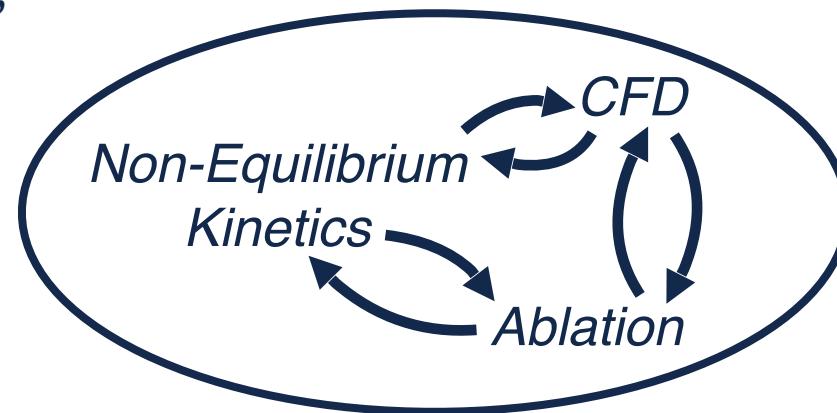

Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces [2]

[2] S. Venturi, R. L. Jaffe, and M. Panesi, “Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces”, The Journal of Physical Chemistry A, Special Virtual Issue “Machine Learning in Physical Chemistry”, Vol. 124, No. 25 (2020)

Motivation: TPS

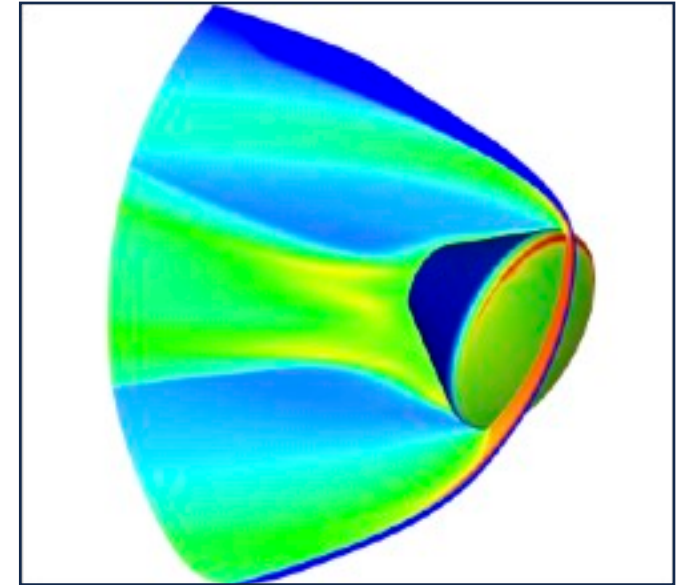
Thermal Protection System (TPS) is a set of safety-critical components that protects a vehicle traveling at hypersonic speed from heating.

- ◆ TPS is a **single point-of-failure**
- ◆ Predicting the **heat fluxes** experienced by the vehicle and modeling the **material response** are **challenging tasks**, mainly due to:
 - Multiple scales involved;
 - Multidisciplinary of the problem;
 - Presence of coupling effects;
 - Hard to be replicated in labs.



Substantial **margins of safety** are applied during TPS design, in order to account for the **uncertainties** in the quantity of interest predictions.

The more reliable the quantifications of such **uncertainties** are proved to be,
the more accurate such margins end up being,
reducing the risk of failures
OR
generating relevant profits from vehicle mass and mission costs points of view



Courtesy of NASA



Courtesy of NASA