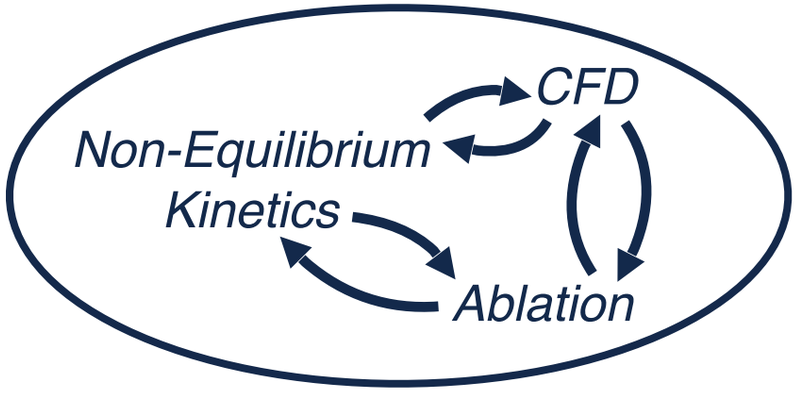
A Bayesian Neural Network Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces

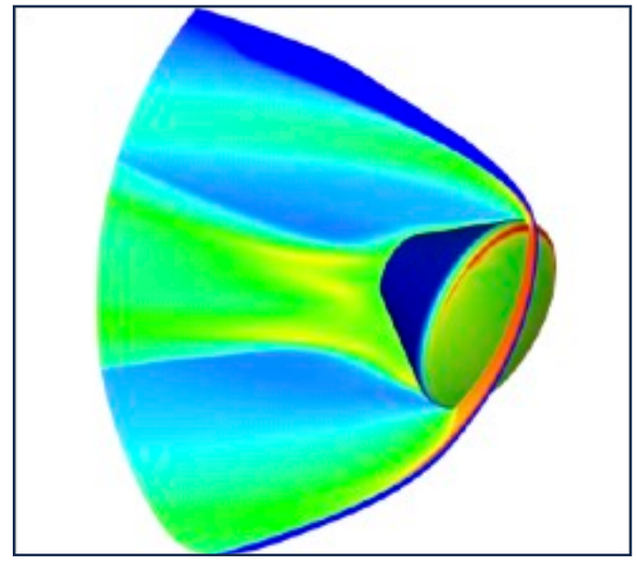
Motivation: TPS

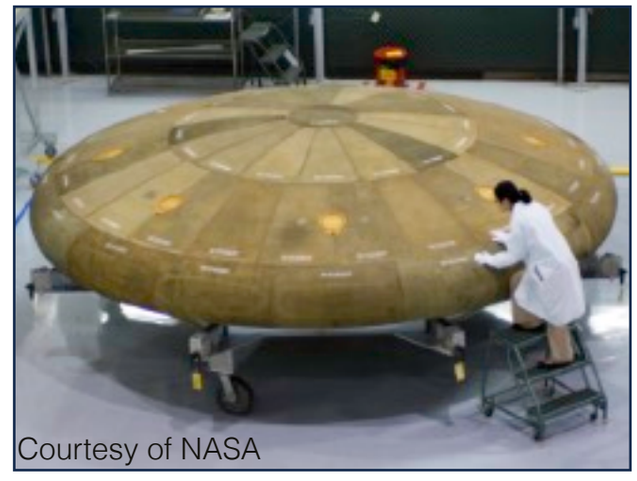
Thermal Protection System (TPS) is a set of safety-critical components that protects a vehicle traveling at hypersonic speed from heating.

- 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;
  - Multidisciplinarity of the problem;
  - Presence of coupling effects;
  - Hard to be replicated in labs.






Courtesy of NASA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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