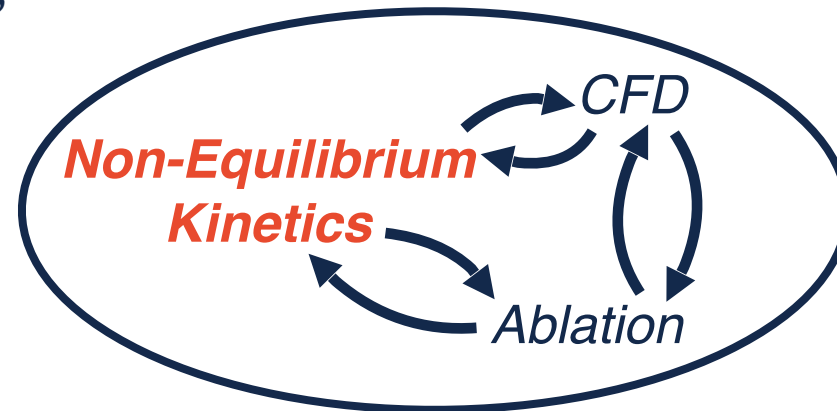


Motivation: TPS

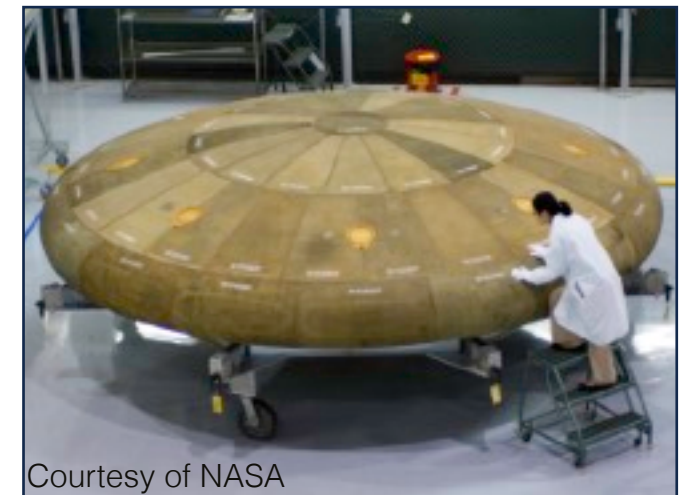
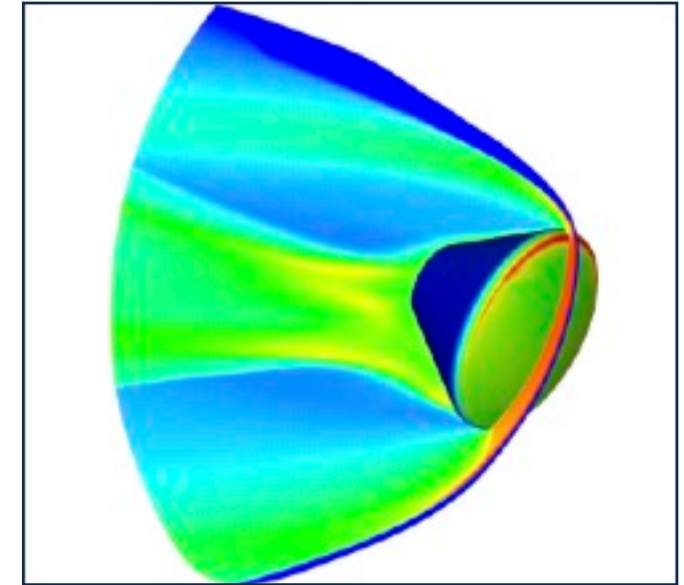
Thermal Protection System (TPS) is a set of safety-critical components that protects a vehicle traveling at hypersonic speed from heating.

- ◆ 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

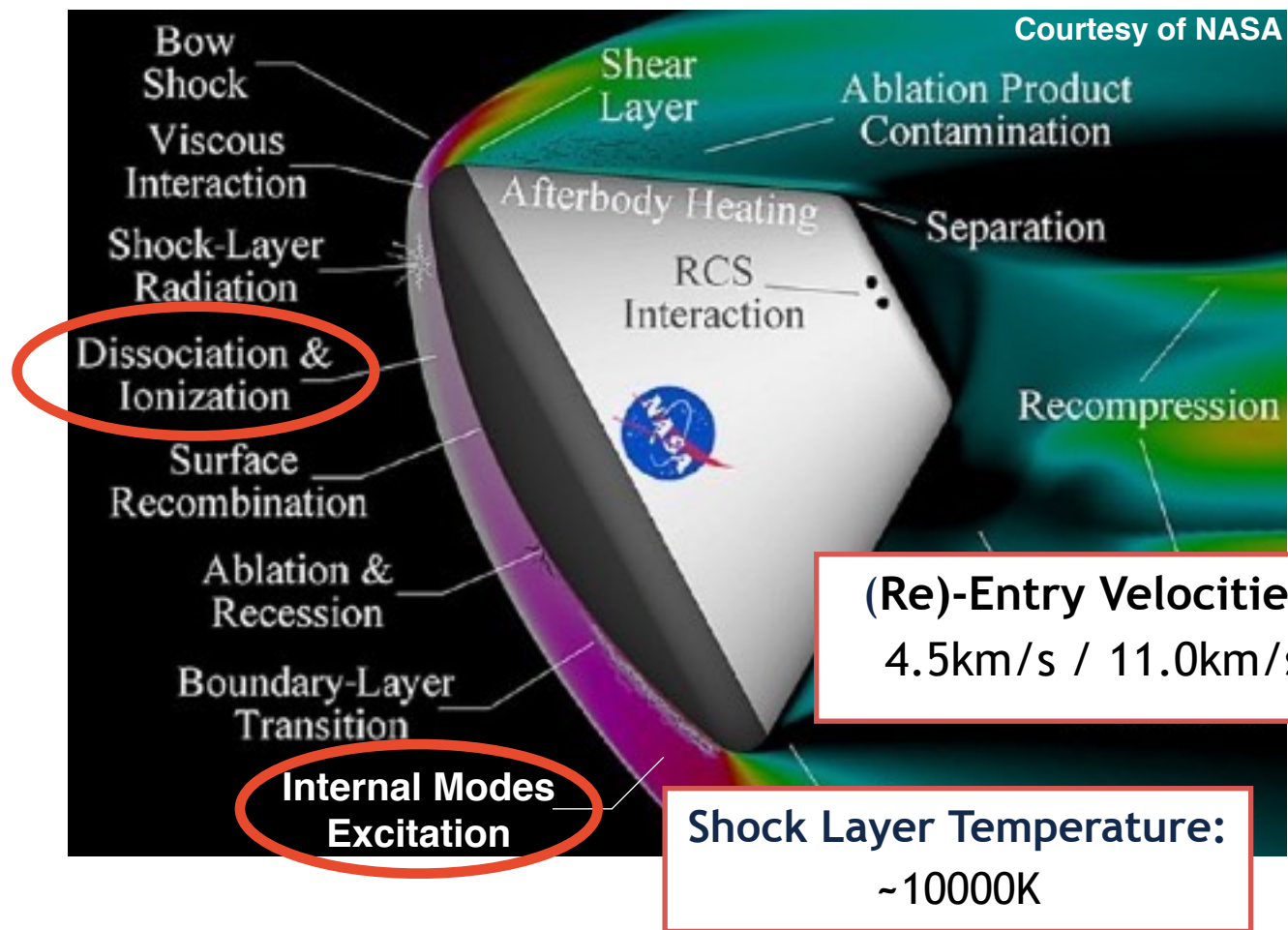


Courtesy of NASA



Courtesy of NASA

Motivation: Non-Equilibrium Flows



- ♦ The mixture is **thermally and chemically reacting**, and the fluid in the shock layer cannot be modeled as a perfect gas.
- ♦ It is necessary to understand how the energy of the flow is stored in its internal modes and is affected by the chemistry.
- ♦ A resolution up to the atomic and molecular scale is required.

- ♦ **Ab-Initio Calculations:** Design Qols are computed starting from the first principles of Quantum Chemistry

