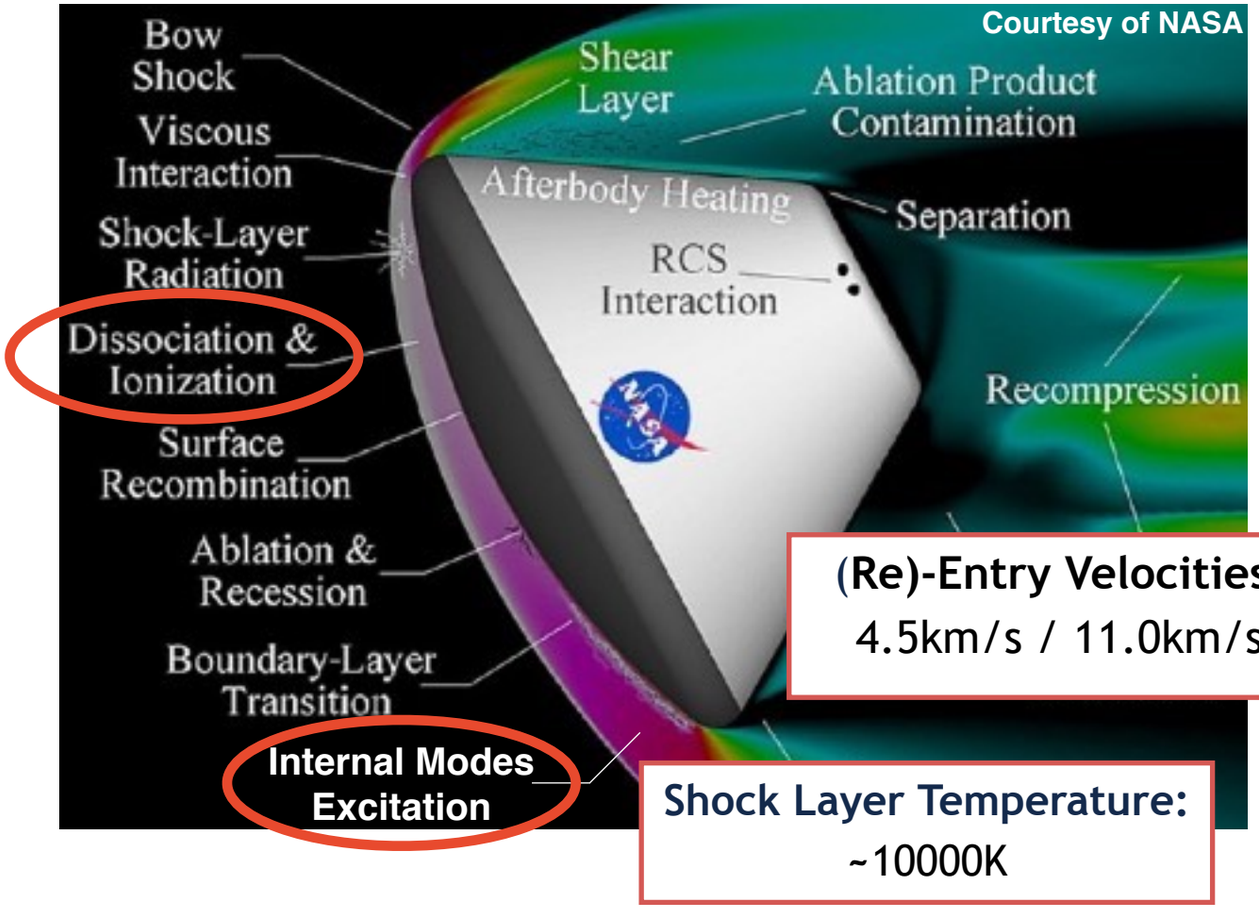
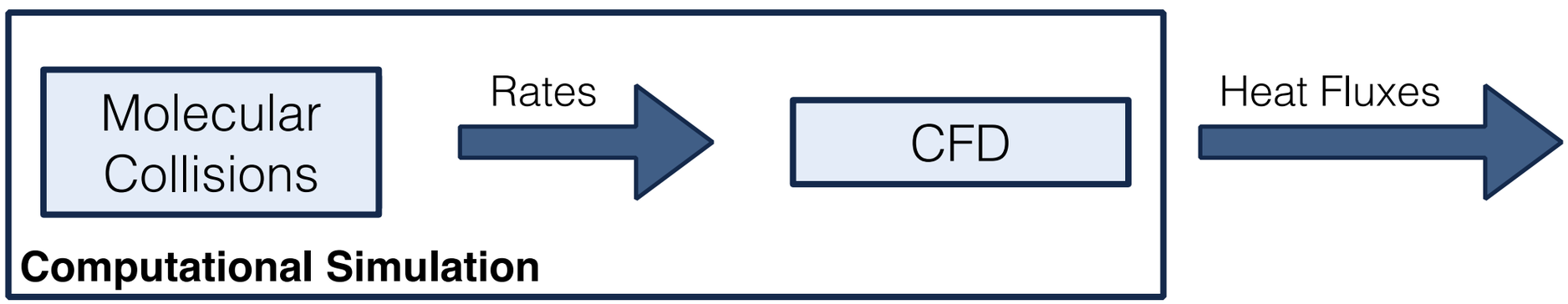
Motivation: Non-Equilibrium Flows



- 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 QoIs are computed starting from the first principles of Quantum Chemistry



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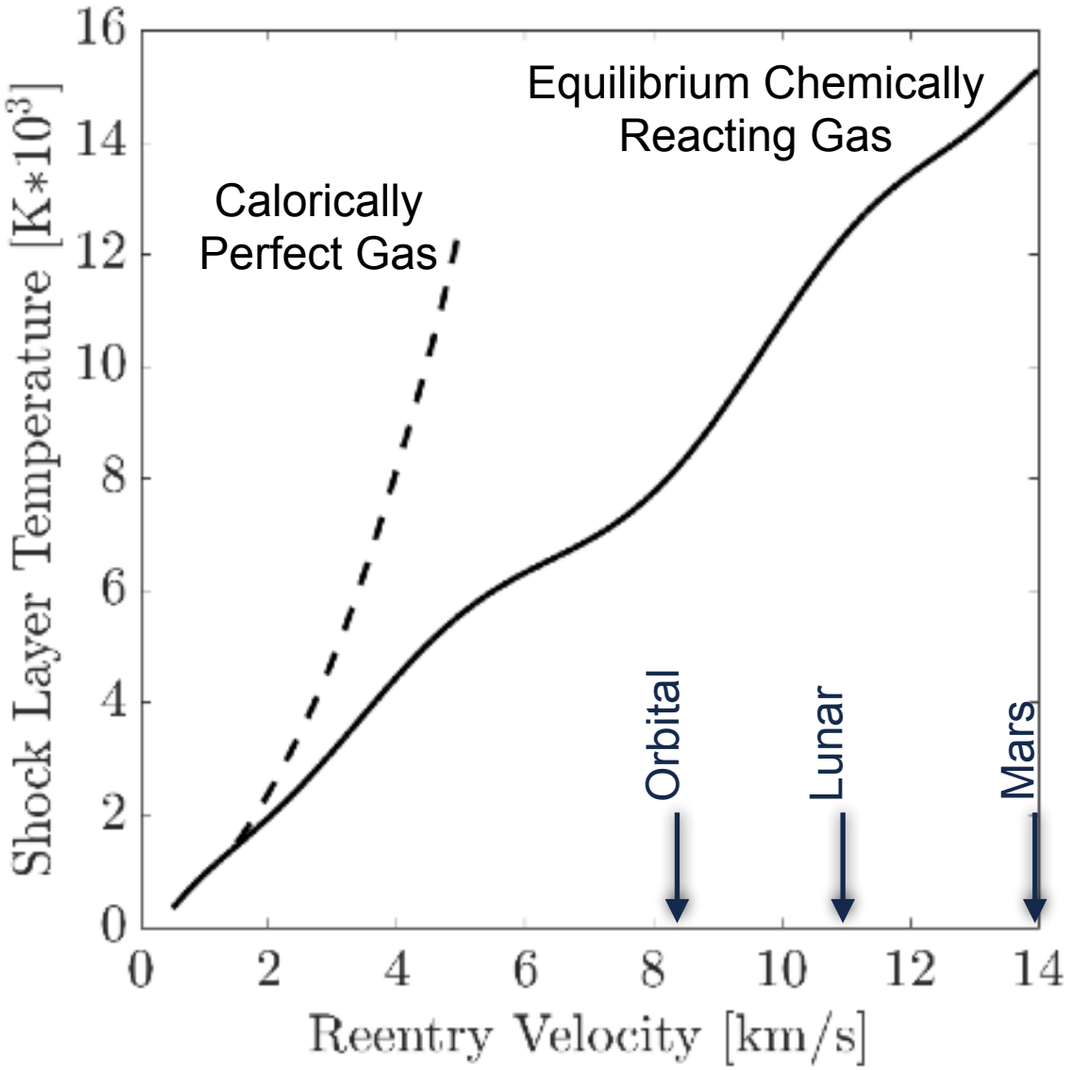

From J. D. Anderson, "*Hypersonic and High-temperature Gas Dynamics*", American Institute of Aeronautics and Astronautics, 2006.

Low accuracy on the non-ideal (+ non equilibrium) gas behavior in Computational Hypersonics

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Low accuracy on deformations in a crash test Computational Simulation