



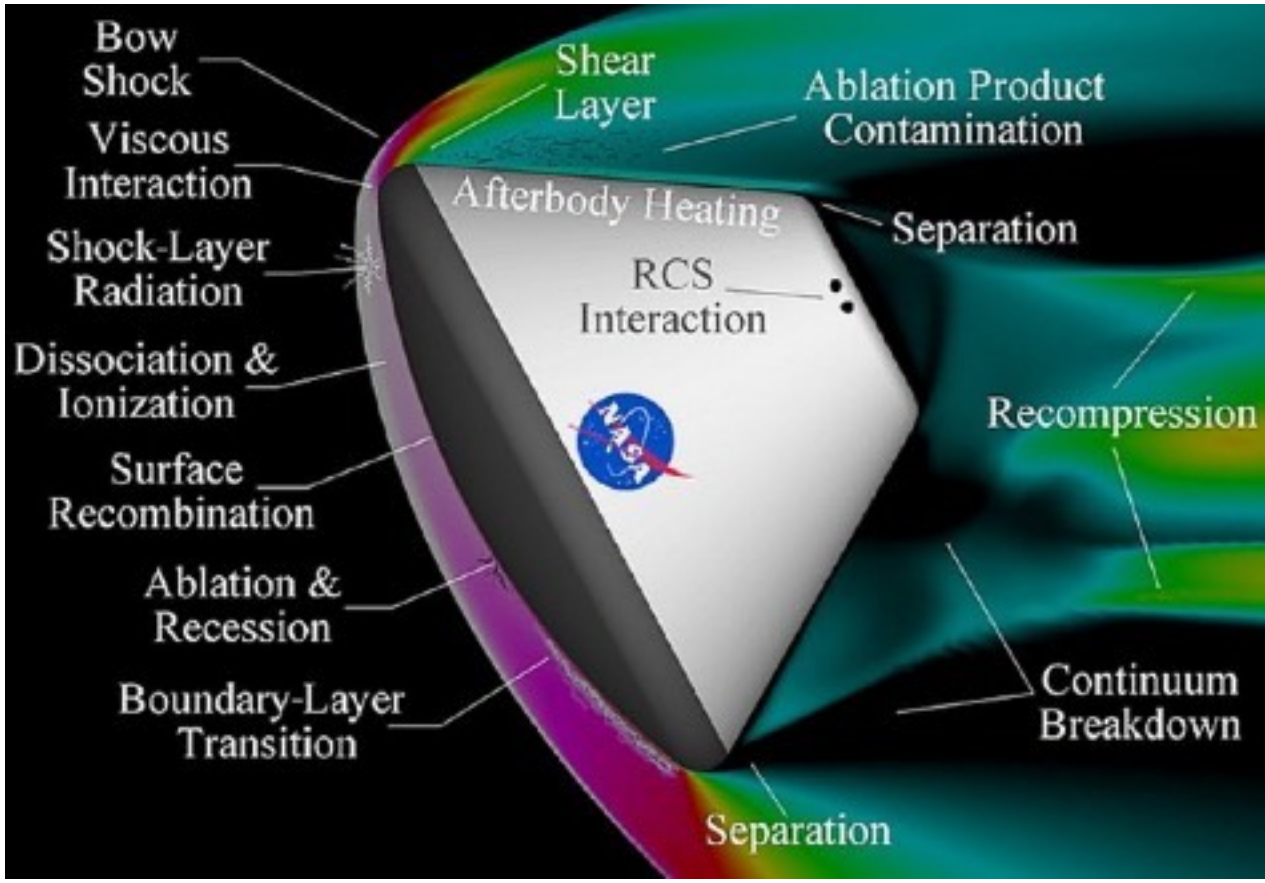






# Motivation: Non-Equilibrium Flows





# Shock Layer Temperature:

~100000K





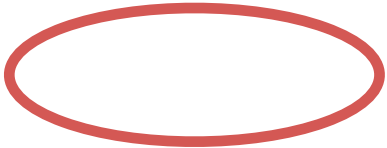


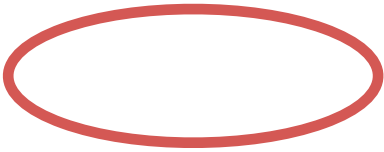


**(Re)-Entry Velocities:**

**4.5km/s / 11.0km/s**

- ◆ 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.



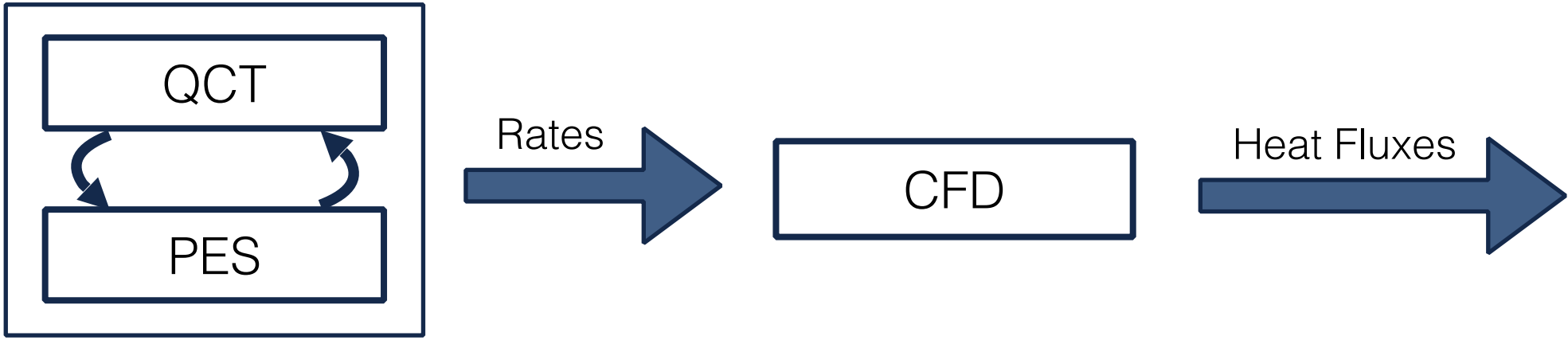




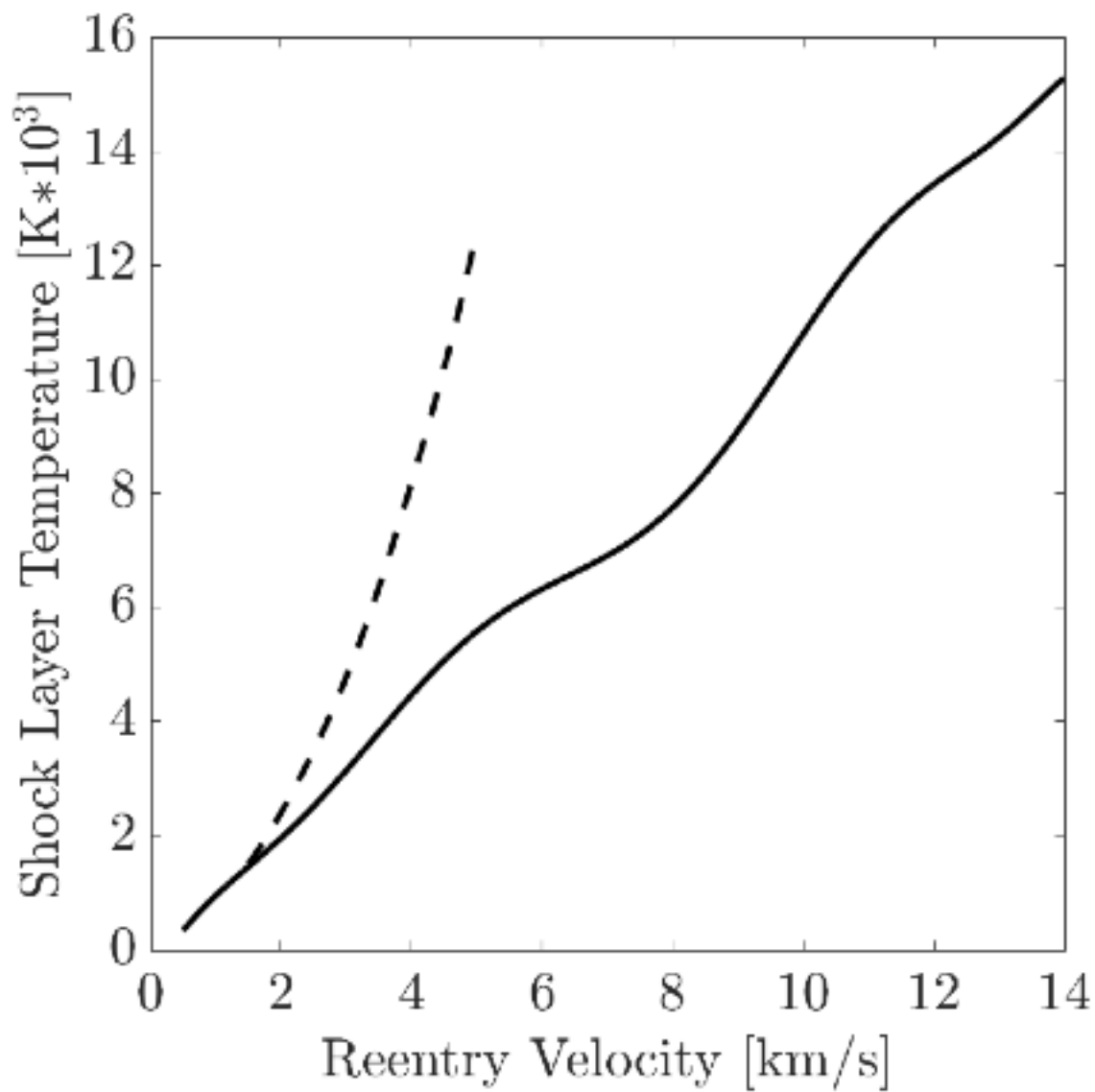




Ab-Initio Calculations: Design Goals are computed starting from the first principles of Quantum Chemistry







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

Calorically  
Perfect Gas

Equilibrium Chemically  
Reacting Gas











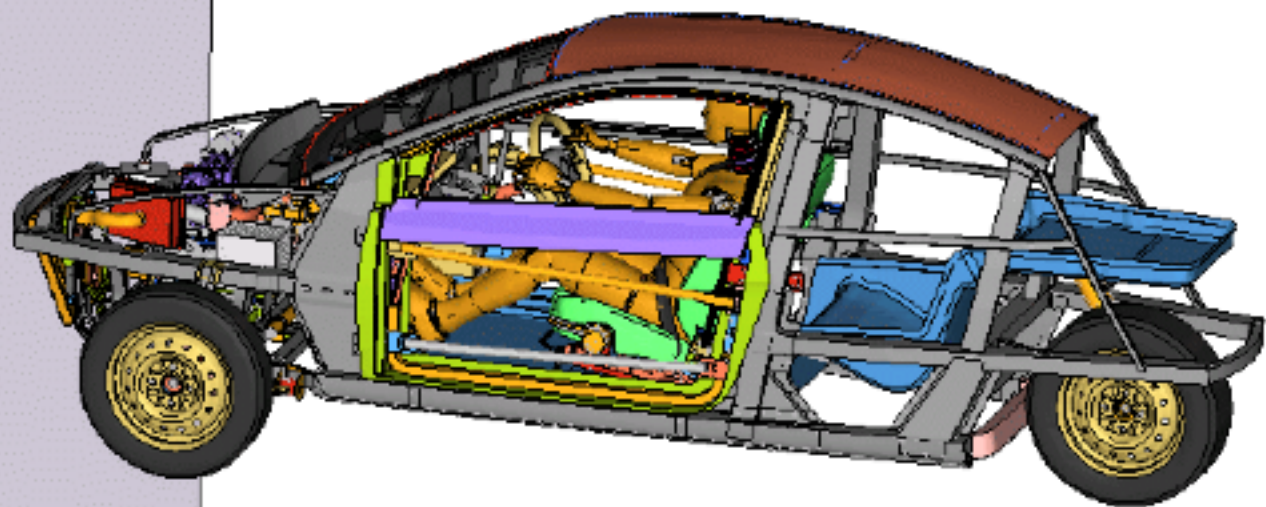


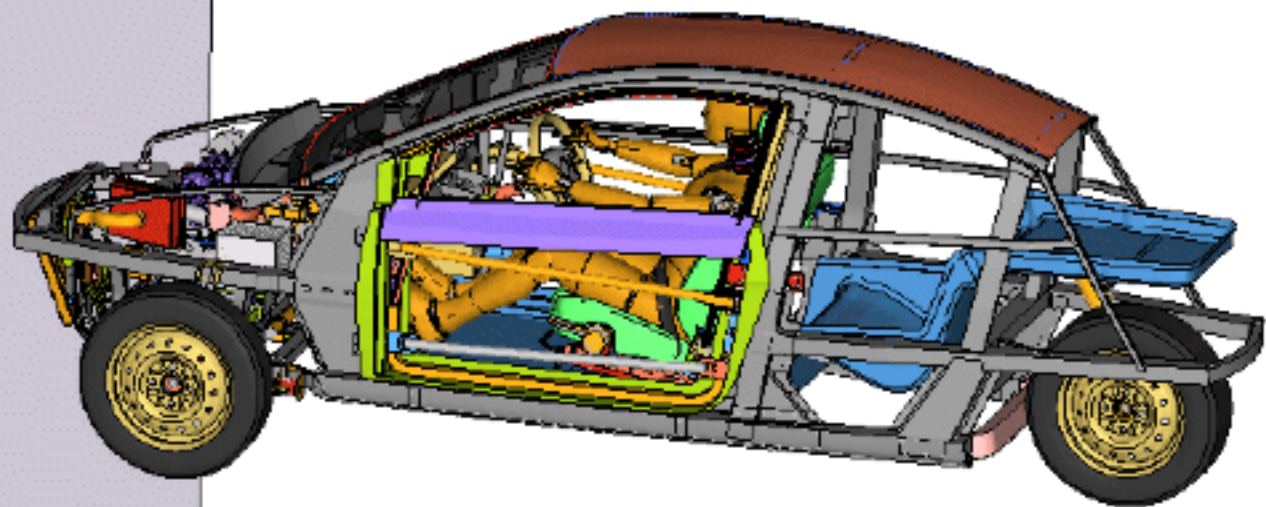


Low accuracy on the non-ideal ( + non equilibrium)  
gas behavior in Computational Hypersonics

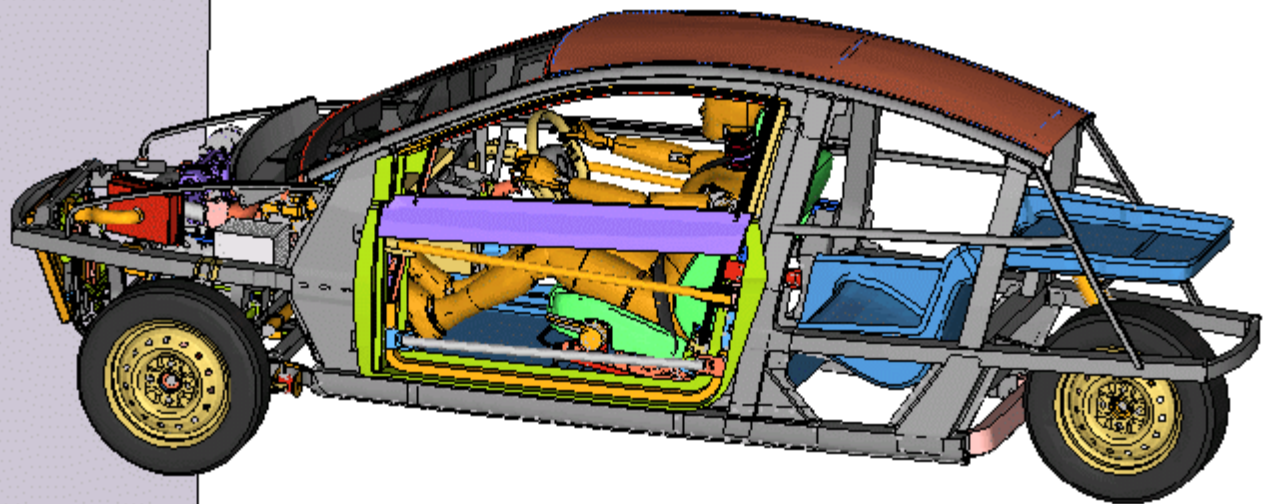
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Low accuracy on deformations in a crash test  
Computational Simulation

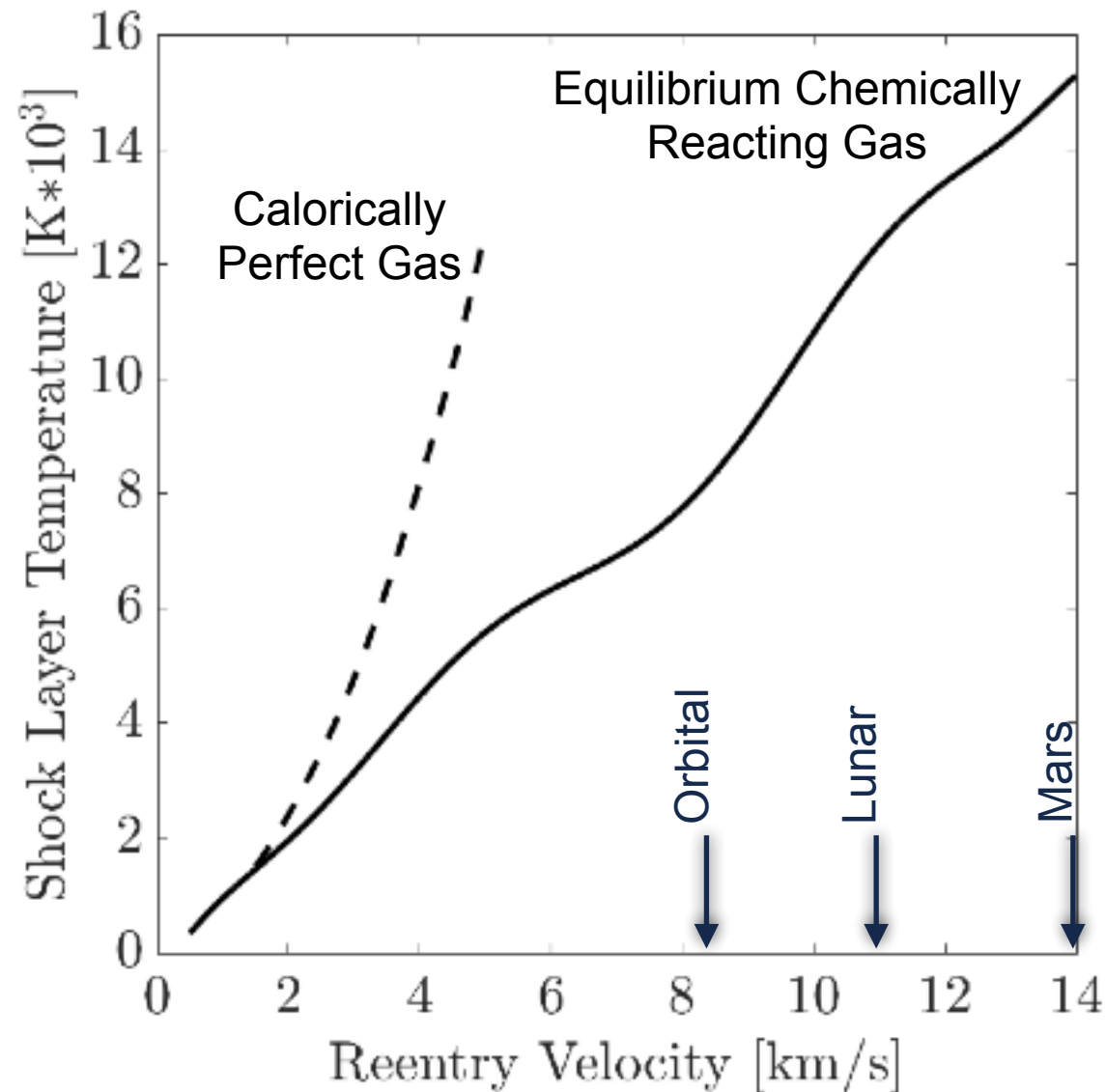








# Motivation: Non-Equilibrium Flows

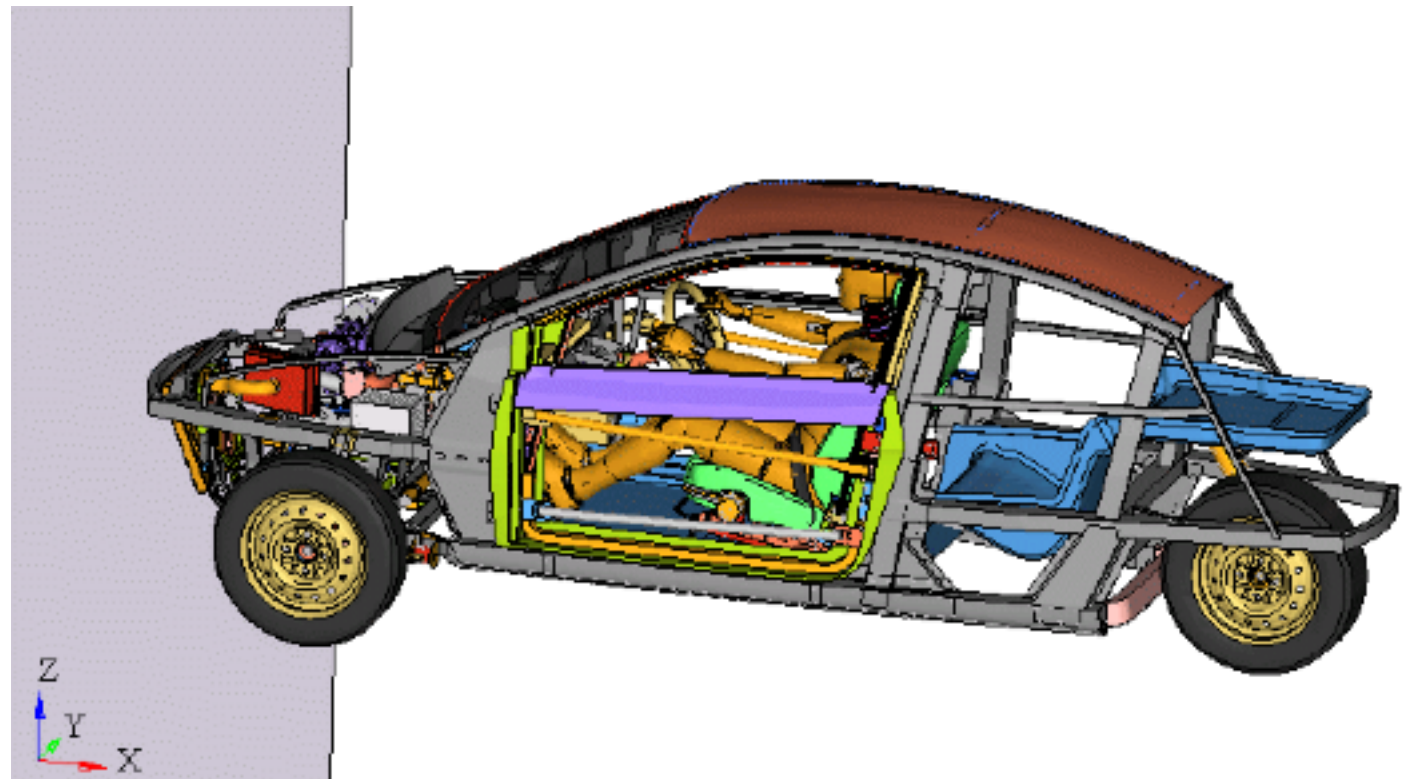


From J. D. Anderson, "*Hypersonic and High-temperature Gas Dynamics*", American Institute of Aeronautics and Astronautics, 2006.

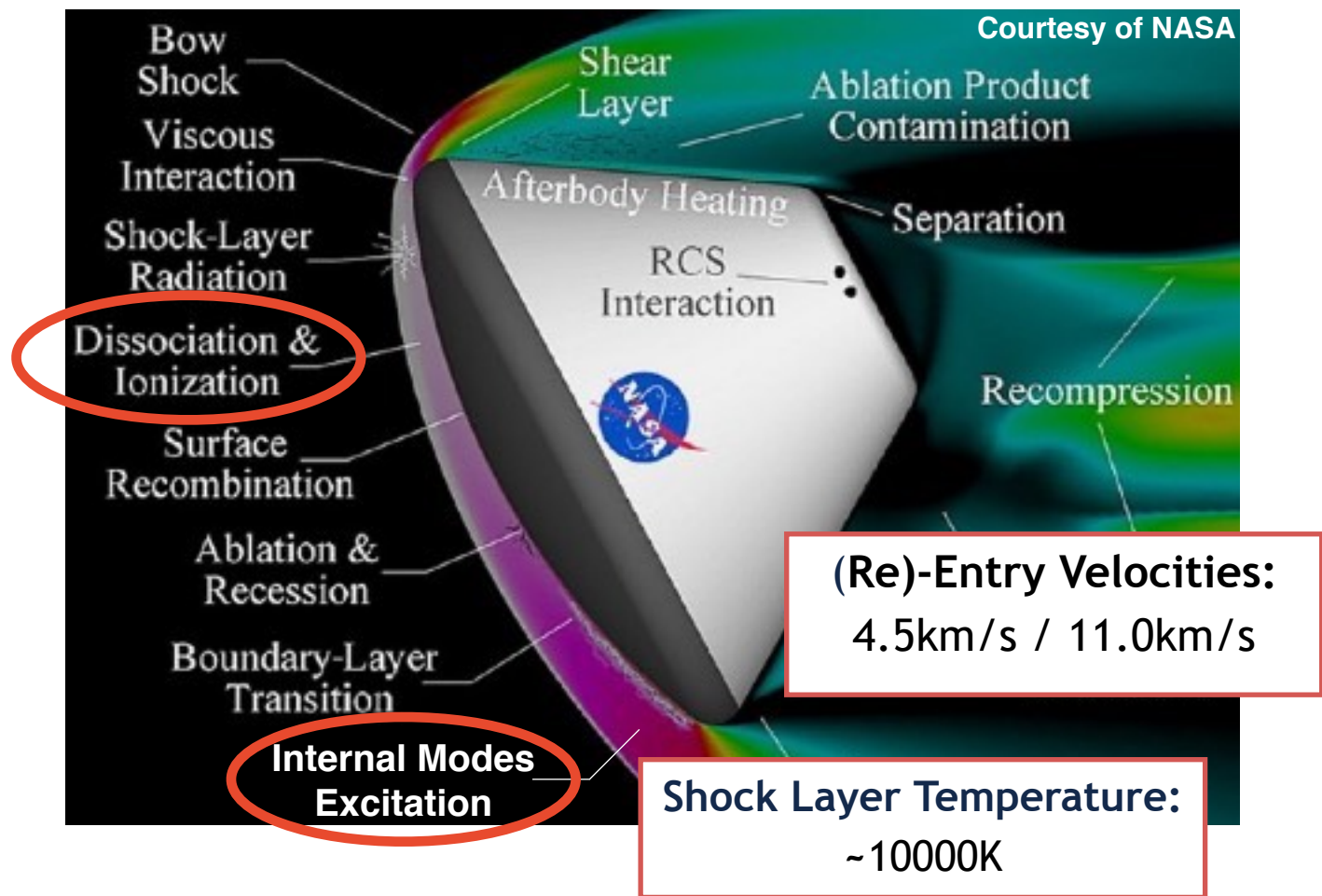
Low accuracy on the non-ideal ( + non equilibrium) gas behavior in Computational Hypersonics

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Low accuracy on deformations in a crash test Computational Simulation



# 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.

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