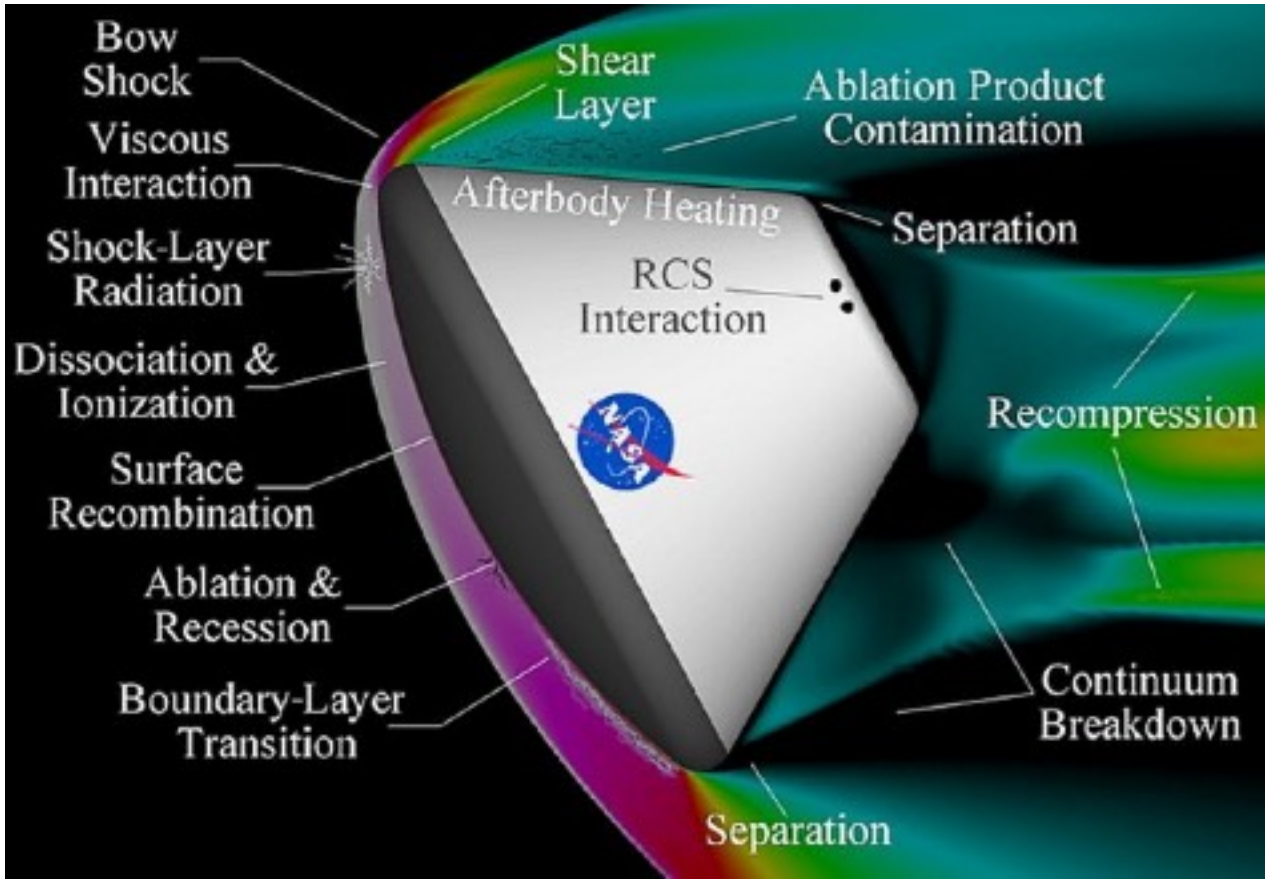
# Motivation: Non-Equilibrium Flows

8


Bow Shock
Viscous Interaction
Shock-Layer Radiation
Dissociation & Ionization
Surface Recombination
Ablation & Recession
Boundary-Layer Transition
Shear Layer
Ablation Product Contamination
Afterbody Heating
Separation
RCS Interaction
Recompression
Continuum Breakdown
Separation

# Shock Layer Temperature:

~10000K

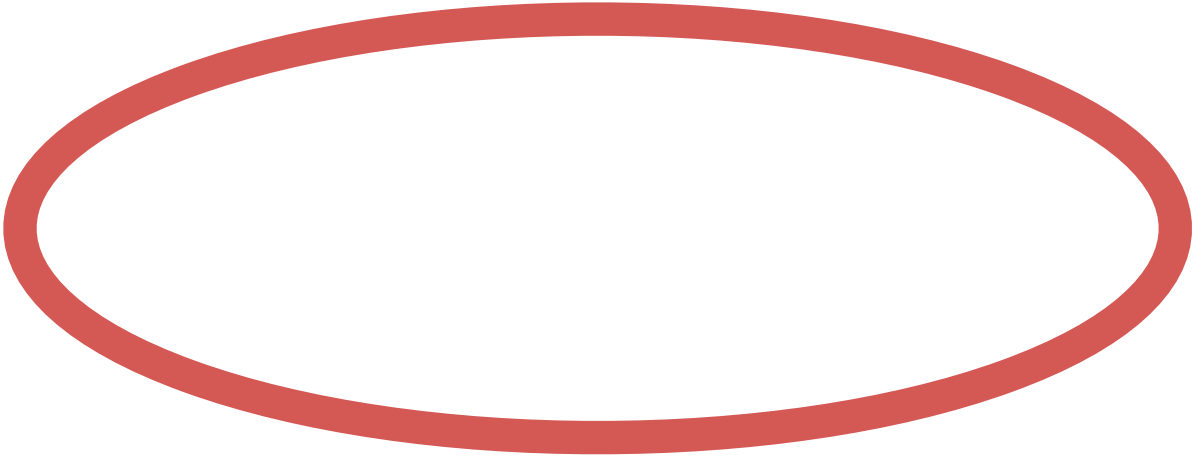
# (Re)-Entry Velocities:

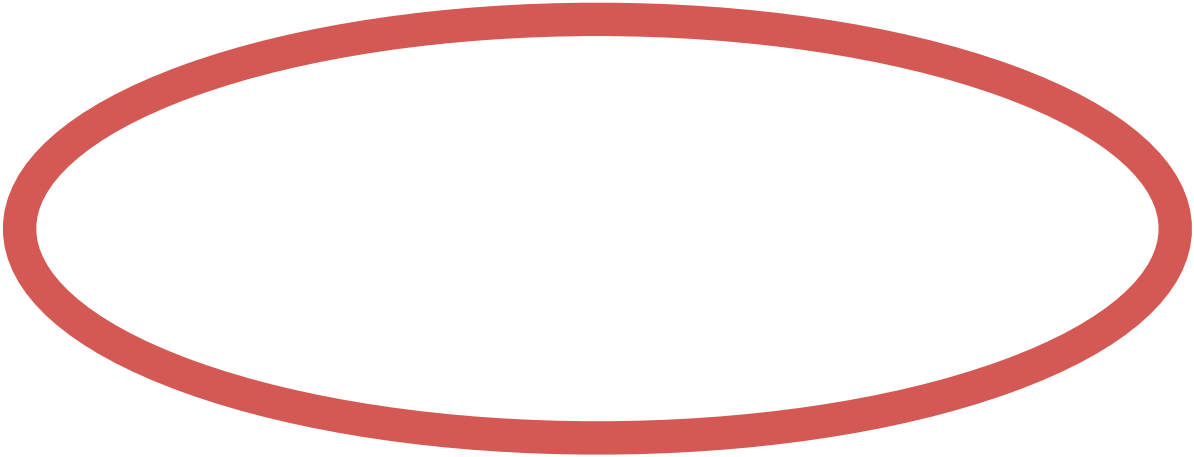
4.5km/s / 11.0km/s

- The mixture is **thermally and chemically reacting**, and the fluid in the shock layer cannot be modeled as a perfect gas.

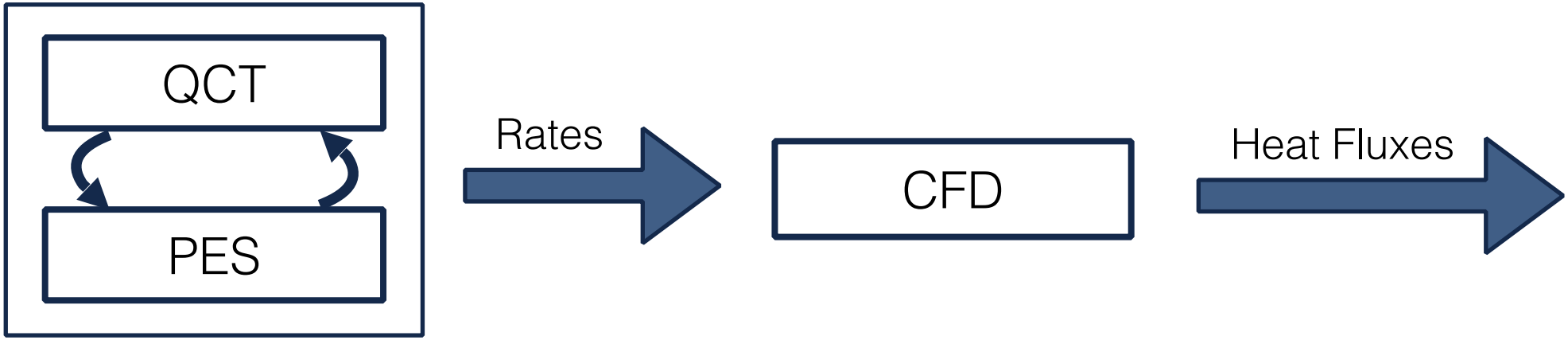
- It is necessary to understand how the energy of the flow is stored in its internal modes and is affected by the chemistry.

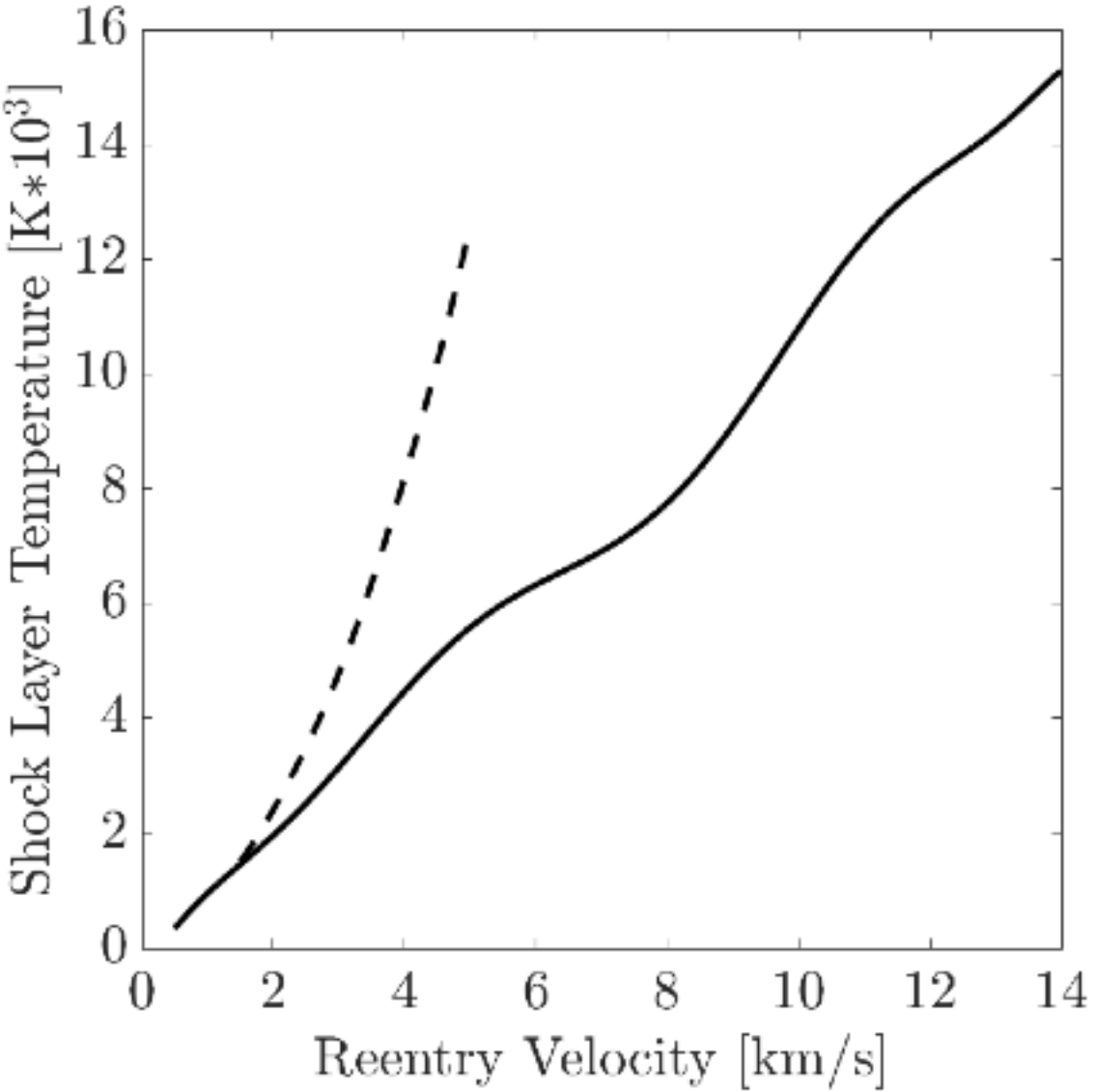
- A resolution up to the atomic and molecular scale is required.





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


QCT
PES
Rates
CFD
Heat Fluxes


Shock Layer Temperature [K*10^3]
16
14
12
10
8
6
4
2
0
0
2
4
6
8
10
12
14
Reentry Velocity [km/s]

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

# Calorically Perfect Gas

# Equilibrium Chemically Reacting Gas

Orbital

# Lunar

# Mars

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

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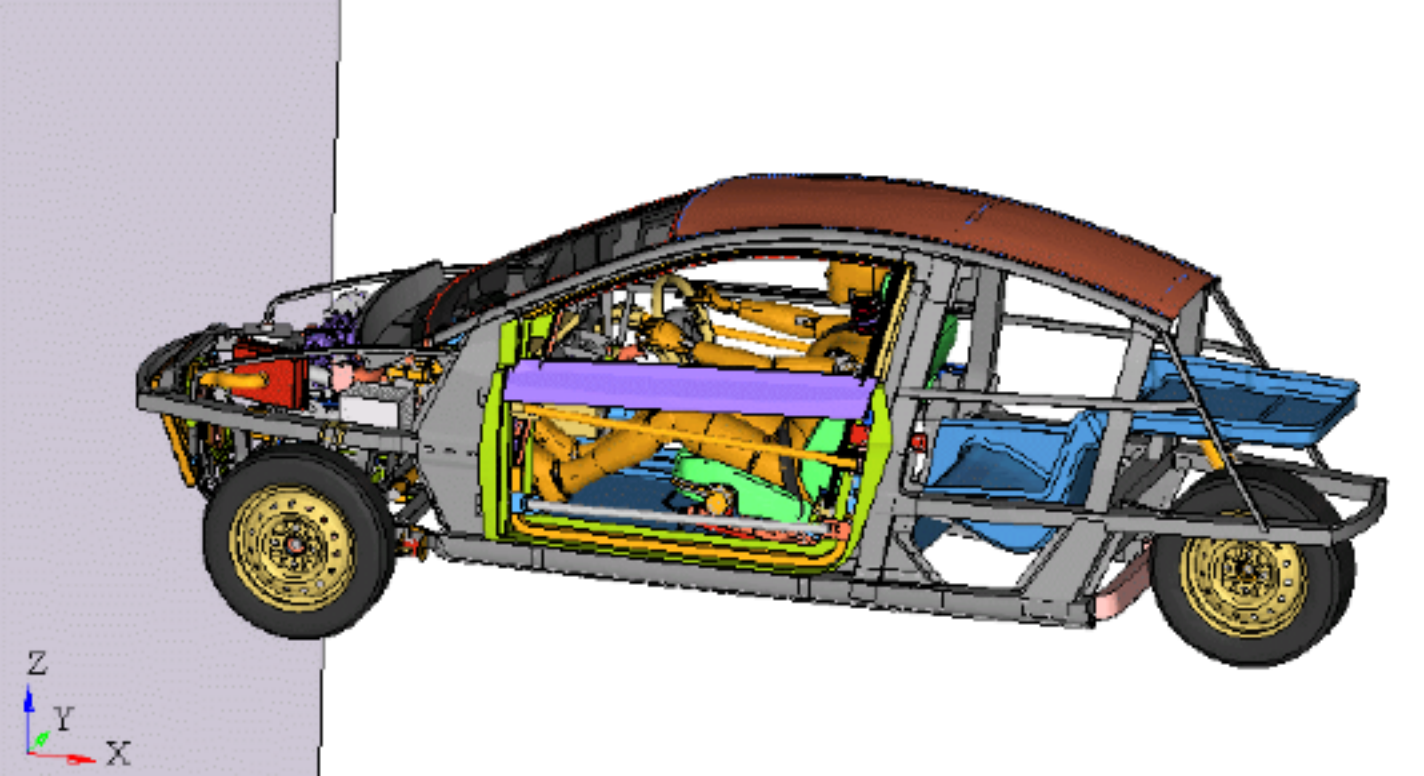
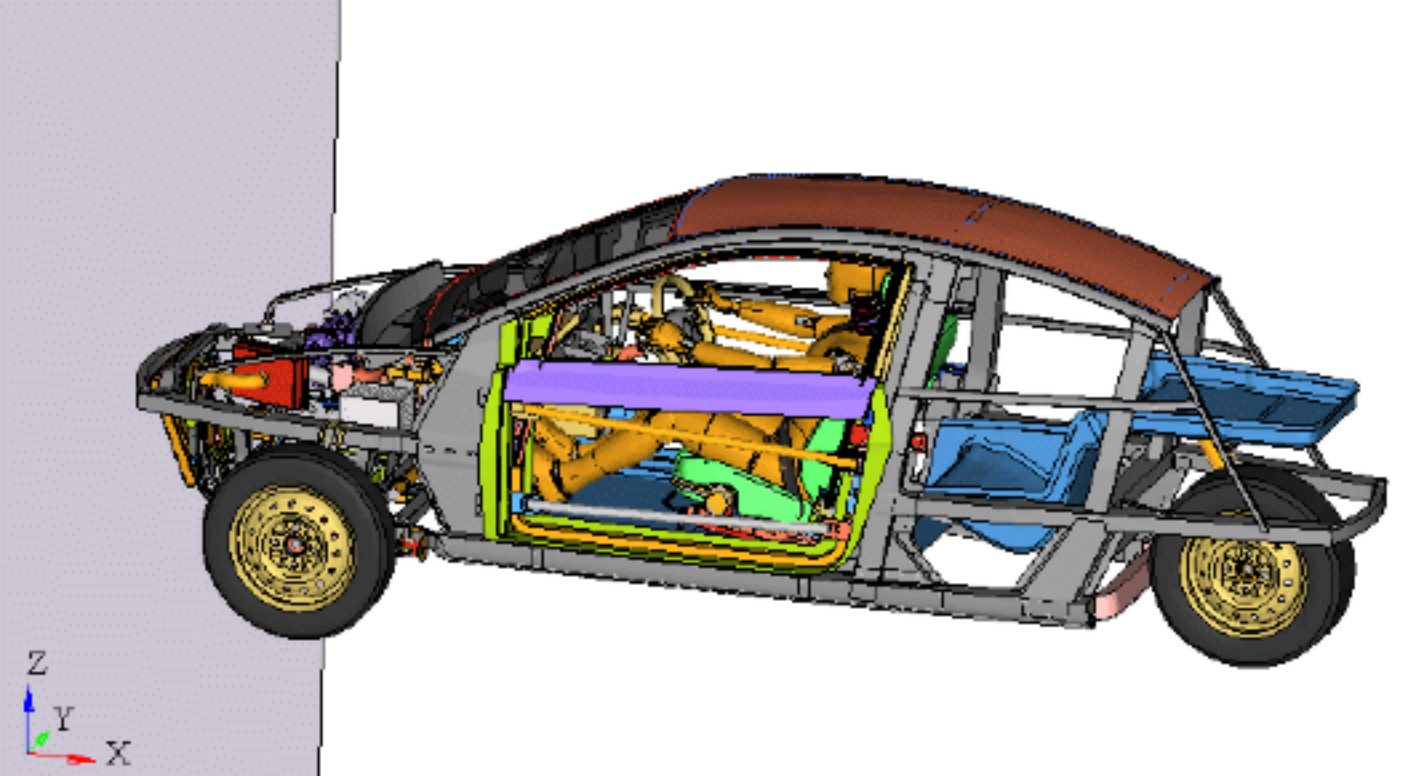
Low accuracy on deformations in a crash test Computational Simulation


Z
Y
X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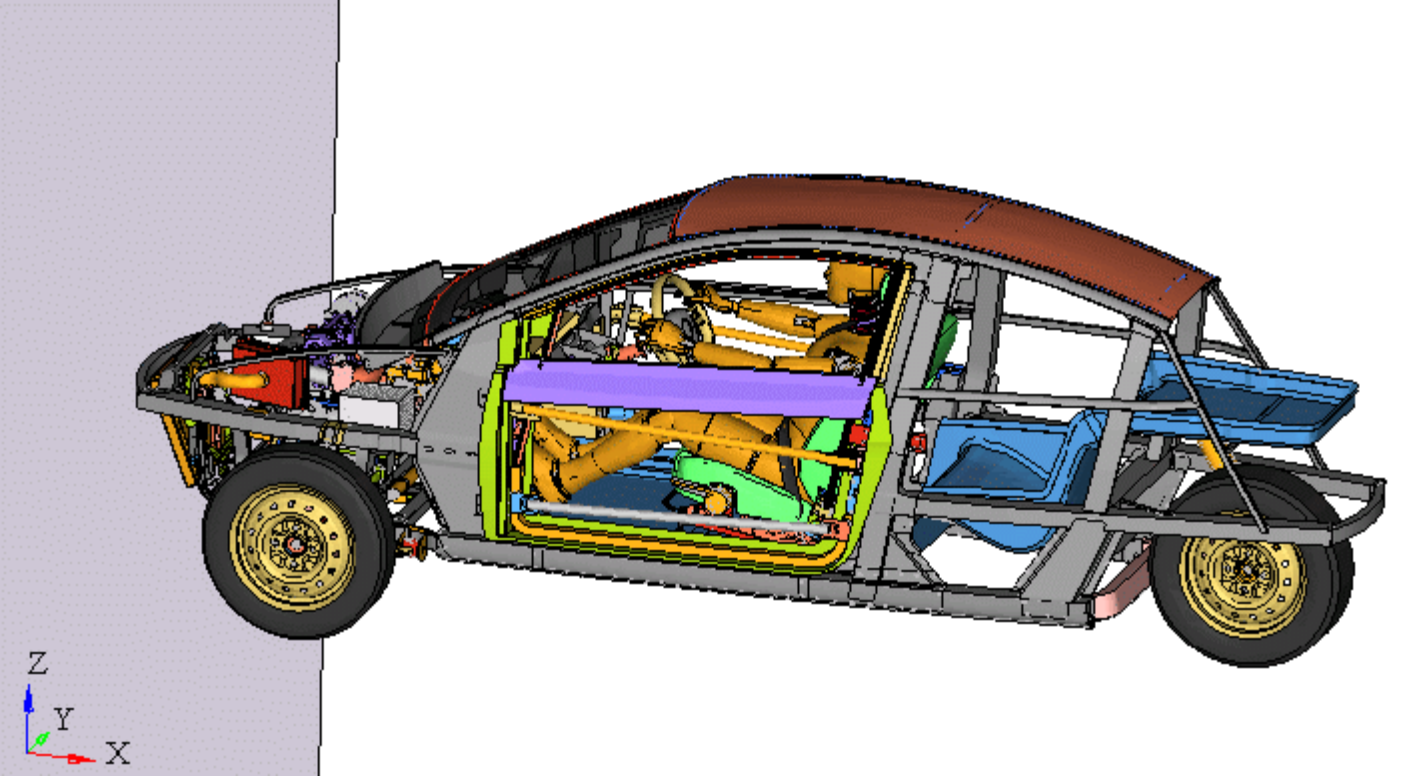
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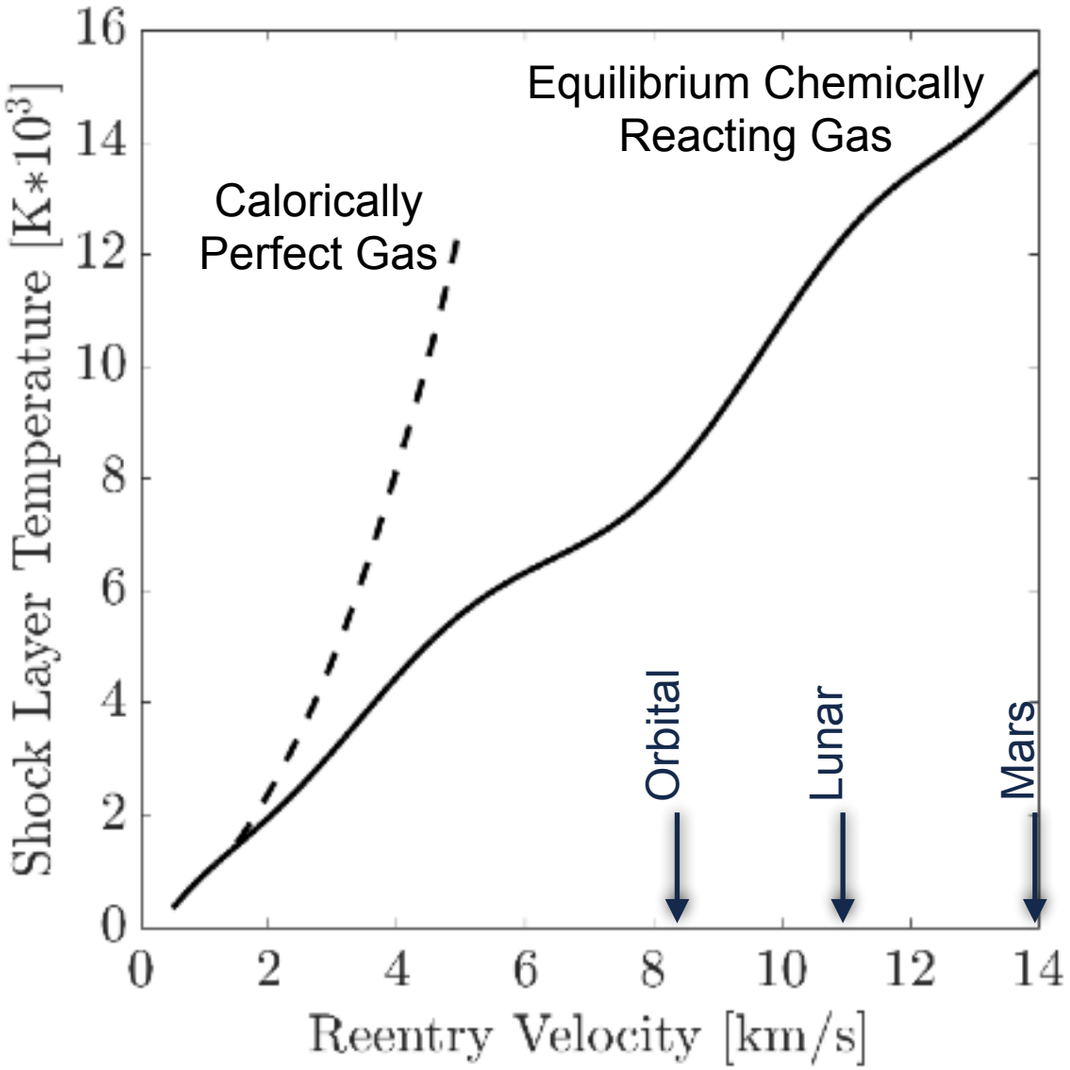


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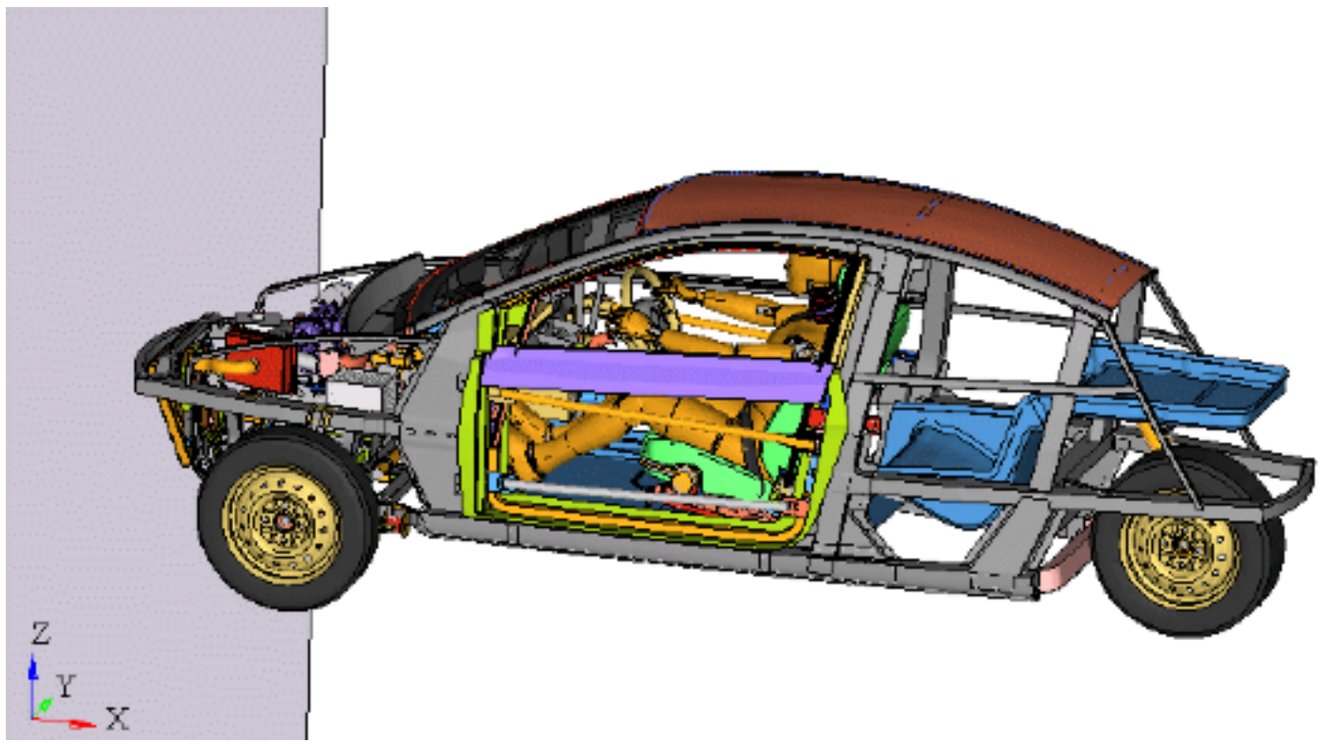

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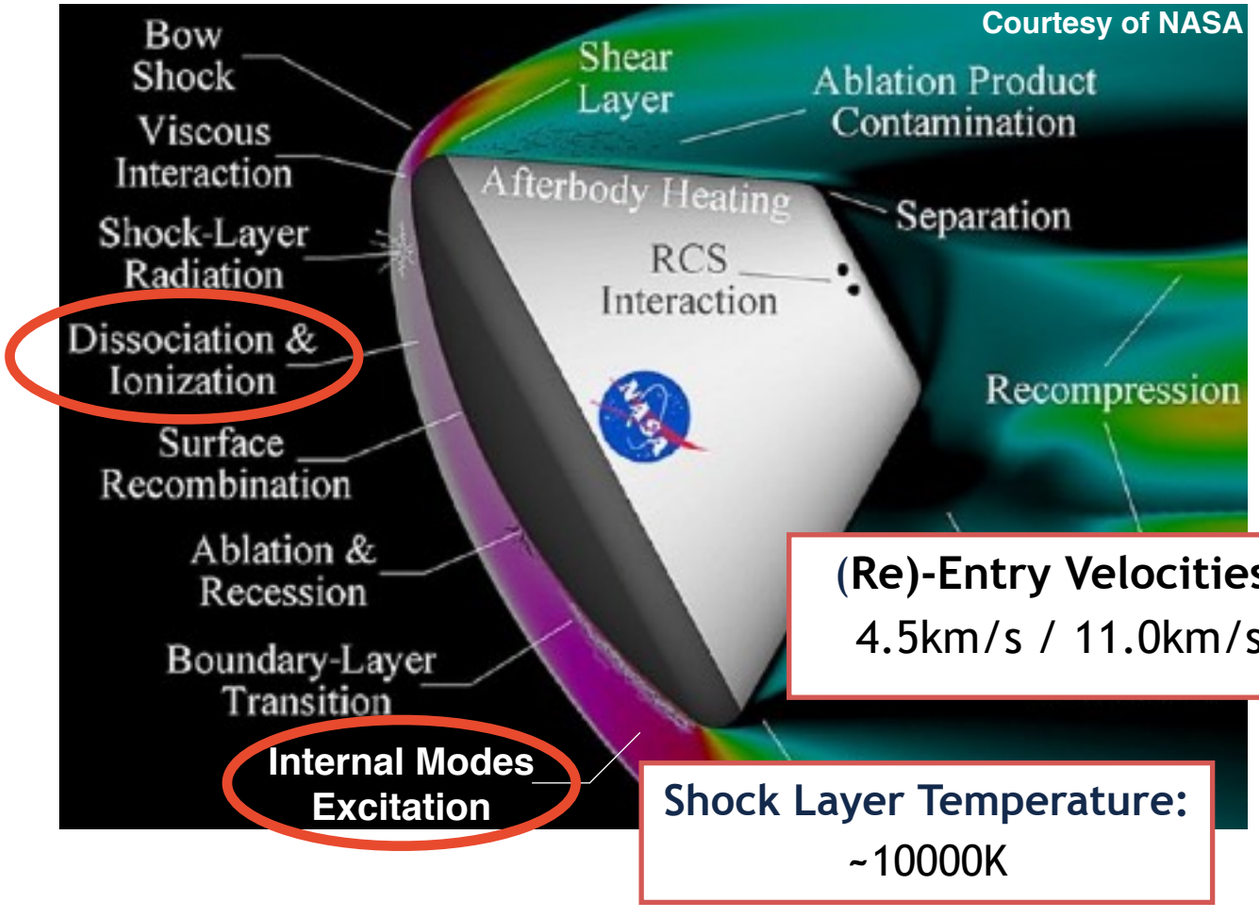


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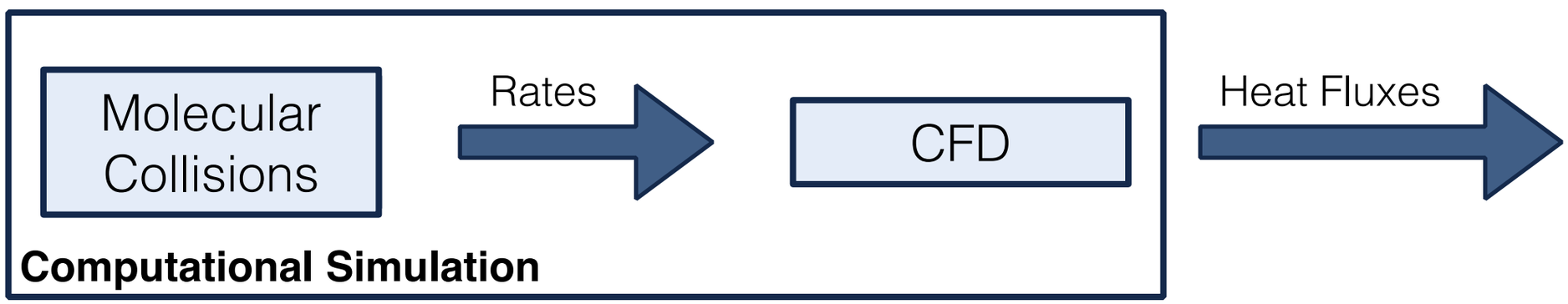
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