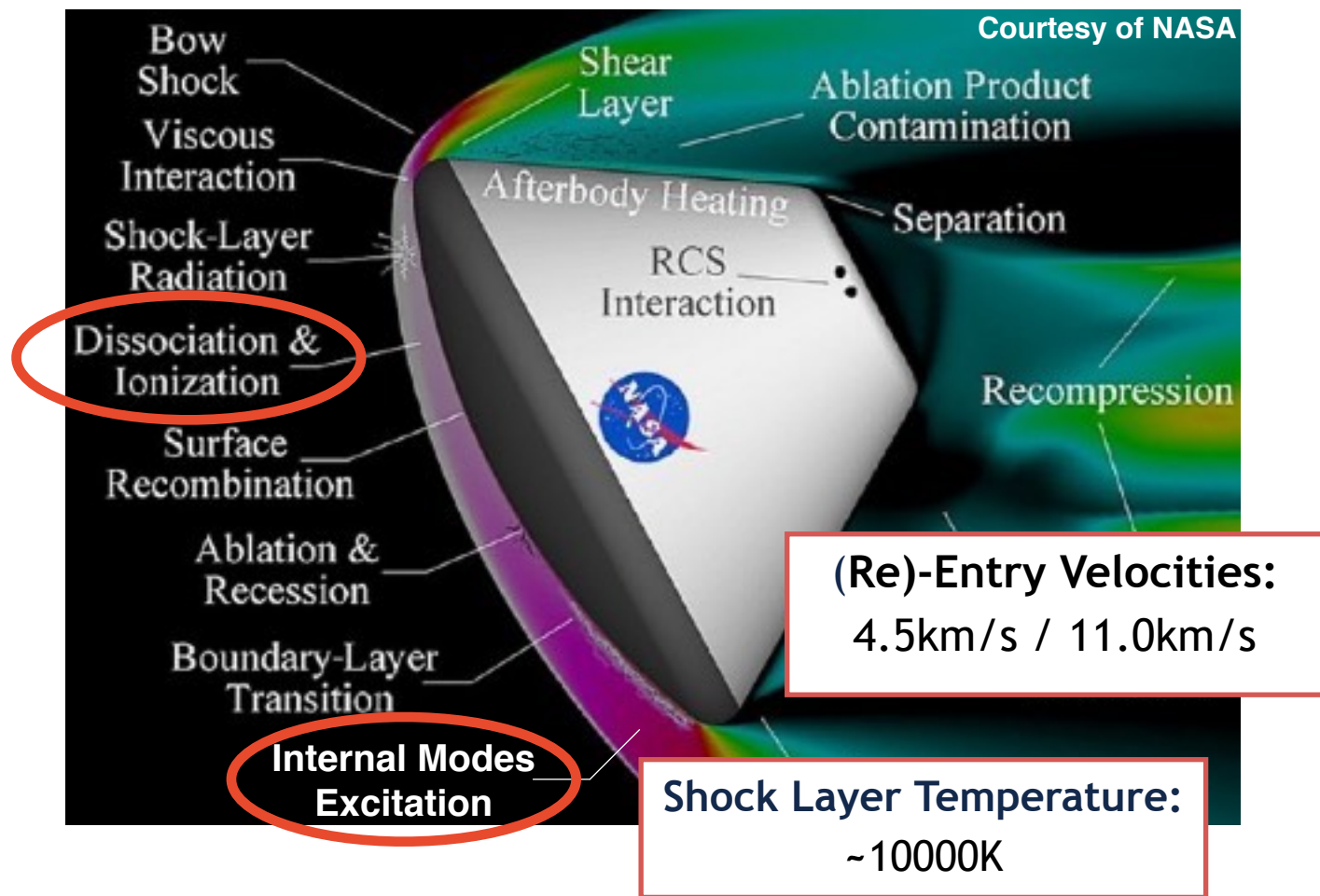
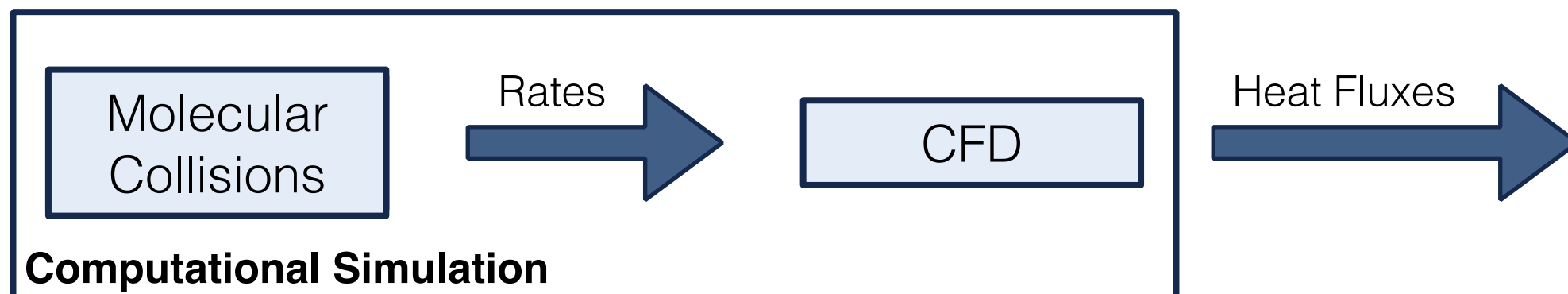


Motivation: Non-Equilibrium Flows

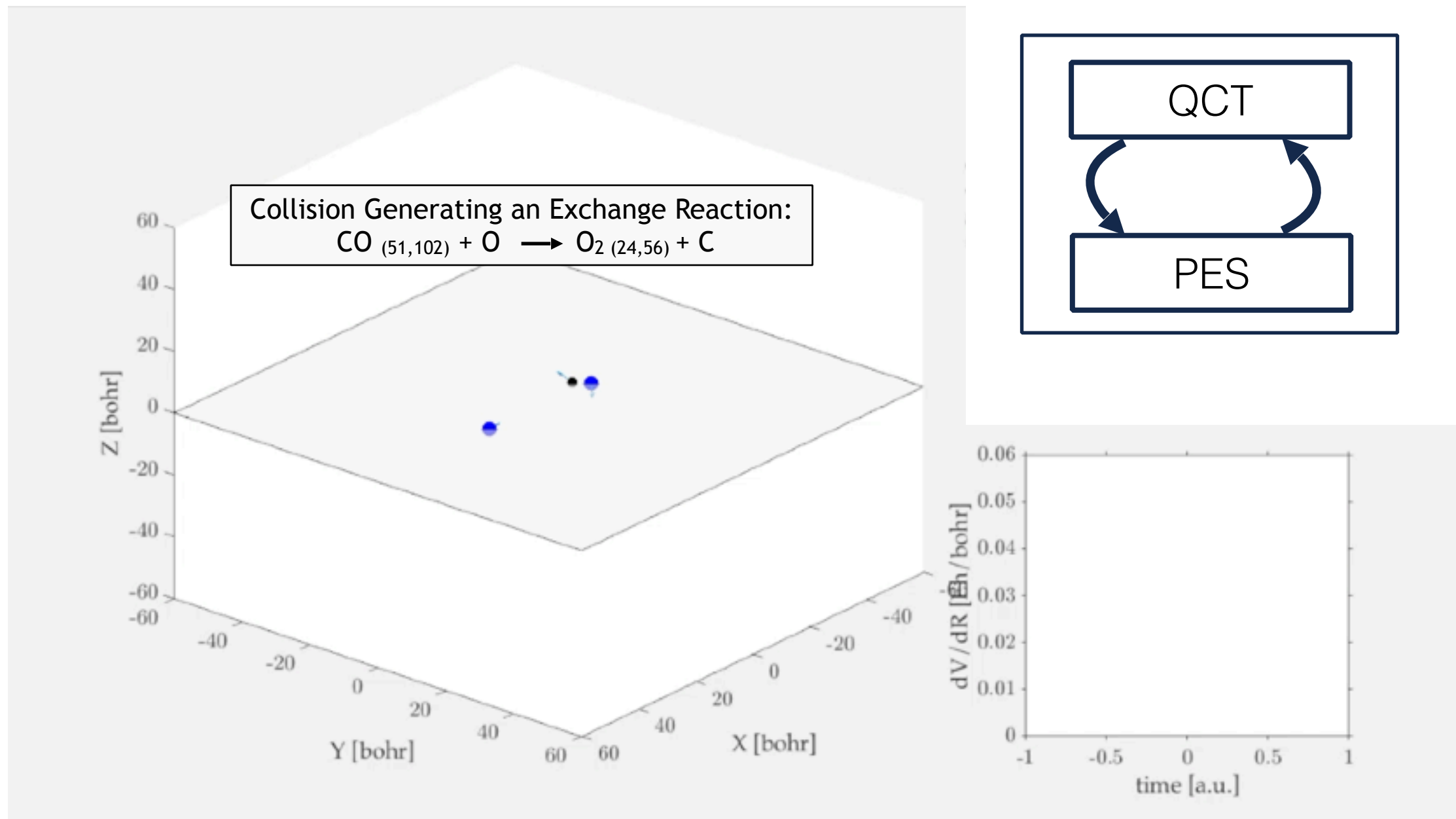


- ♦ The mixture is **thermally and chemically reacting**, and the fluid in the shock layer cannot be modeled as a perfect gas.
- ♦ It is necessary to understand how the **energy of the flow is stored in its internal modes and is affected by the chemistry.**
- ♦ A resolution up to the atomic and molecular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

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



Motivation: PES-to-Rate Coeff.s Approach



1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as **source terms of the Hamiltonian Eq.s** for the calculation of atom trajectories;