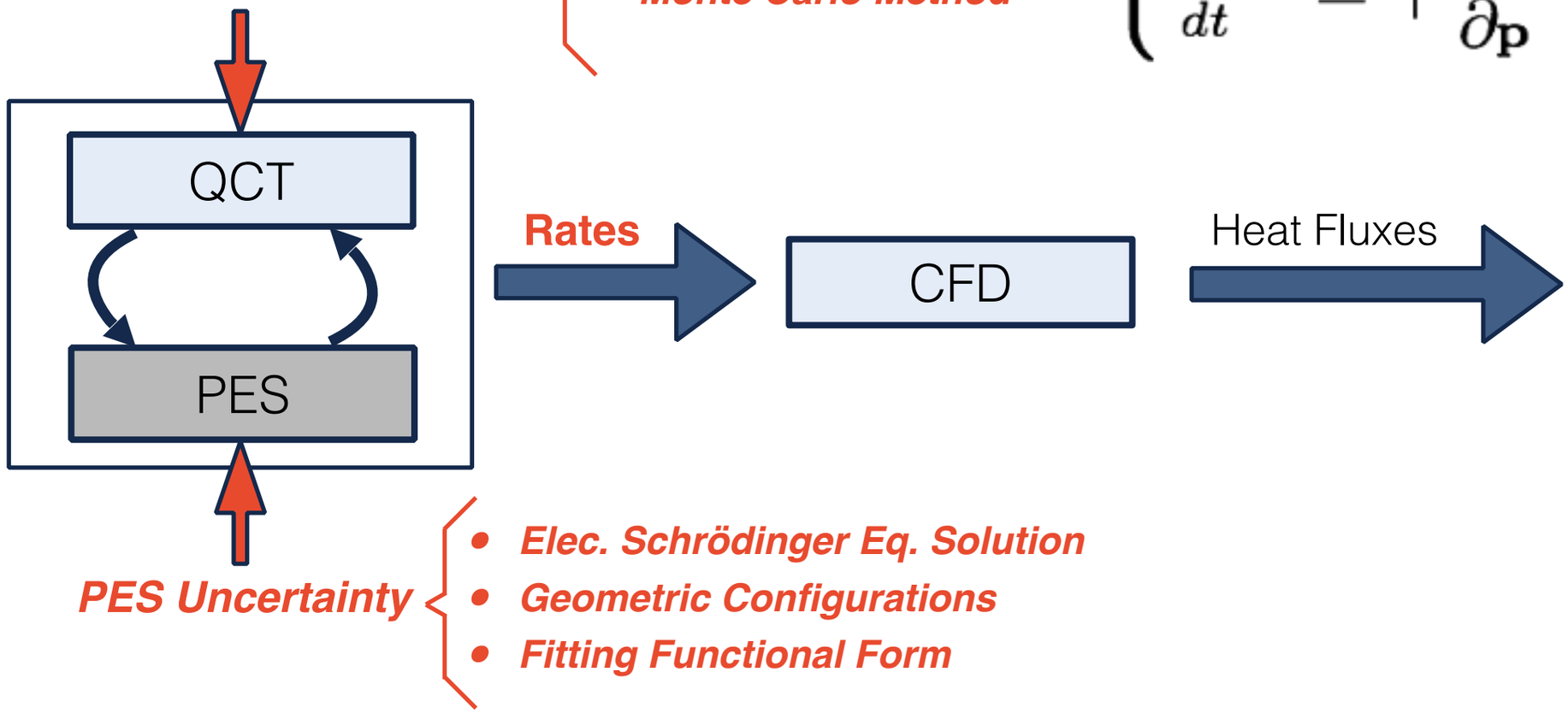
Motivation: Effects of PES Uncertainty

Collisional Dynamics Uncertainty

- ~~***Hamiltonian Mechanics***~~
- ~~***Monte Carlo Method***~~

$$\begin{cases} \frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \\ \frac{d\mathbf{q}}{dt} = +\frac{\partial \mathcal{H}}{\partial \mathbf{p}} \end{cases} \qquad \mathcal{H} = T + V$$



PES Uncertainty

- ***Elec. Schrödinger Eq. Solution***
- ***Geometric Configurations***
- ***Fitting Functional Form***

Can we use Machine Learning in oder to generate surrogate Potential Energy Surfaces for Hypersonic Applications?

What impact does the PES uncertainty have on the rate coefficients and, ultimately, on the capsule design?

ML for PESs: Introduction

In the last decade there has been an increasing effort in taking advantage of Machine Learning for constructing Potential Energy Surfaces. In particular, using:

- ✦ **Gaussian Processes**
- ✦ **Neural Network**

- ✦ "*Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes*", *J. Phys. Chem. A 2017*;
- ✦ "Comparison of permutationally invariant polynomials, neural networks, and Gaussianapproximation potentials in representingwater interactions through many-bodyexpansions", J. Chem. Phys. 2018;
- ✦ "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces", Phys. Rev. Lett. 2007;
- ✦ "Permutation invariant potential energy surfaces for polyatomic reactions using atomistic neural networks", J. Chem. Phys. 2016;
- ✦ …

However, almost the entire literature focuses on the relatively low energy part of the PES.

Through this work, we want to assess if the ML reconstruction can achieve reasonable accuracy for the region of the surface of Hypersonic interest.