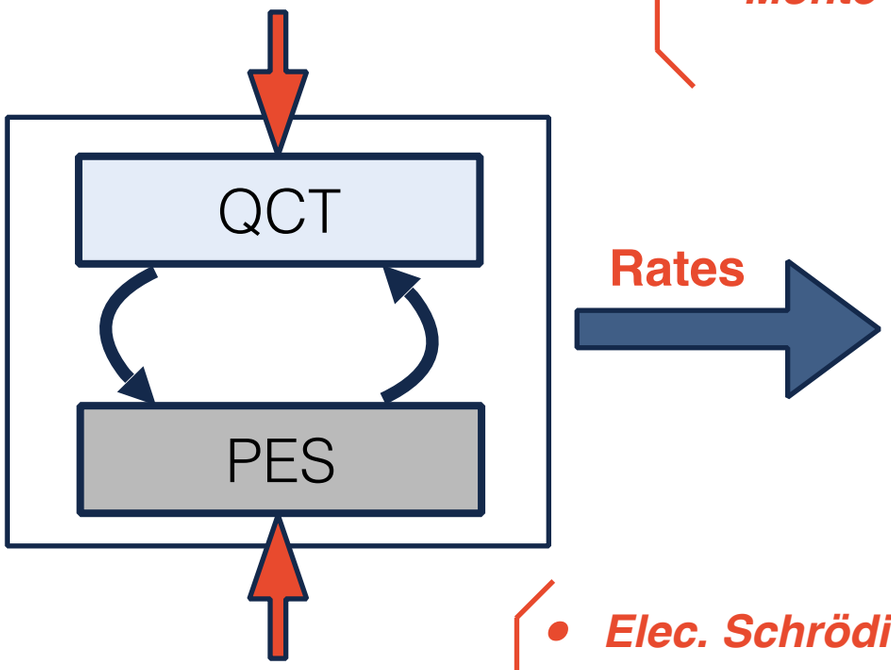
Motivation: Effects of PES Uncertainty

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

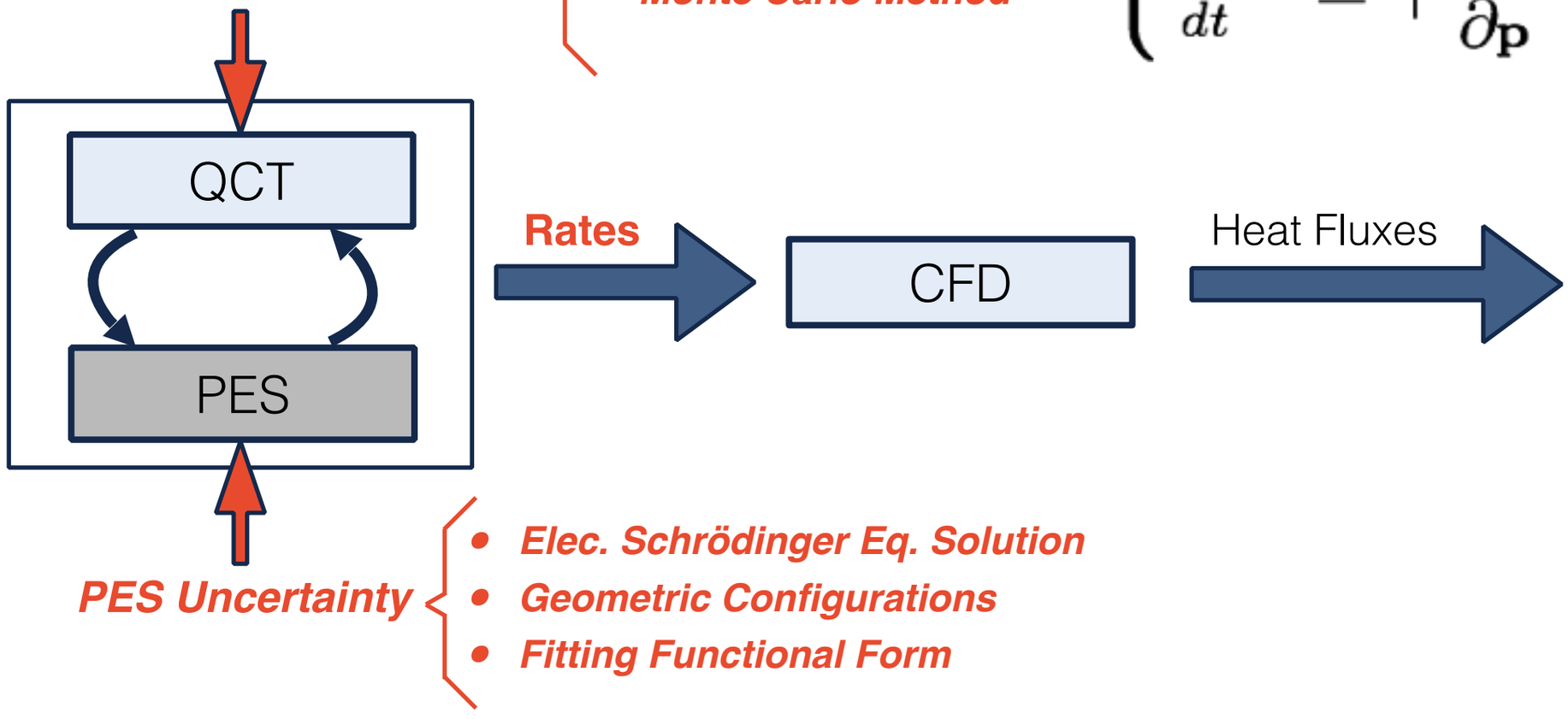
- *Elec. Schrödinger Eq. Solution*
- *Geometric Configurations*
- *Fitting Functional Form*

Motivation: Effects of PES Uncertainty

Collisional Dynamics Uncertainty

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

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



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?