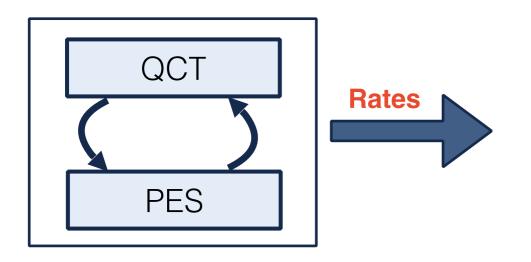
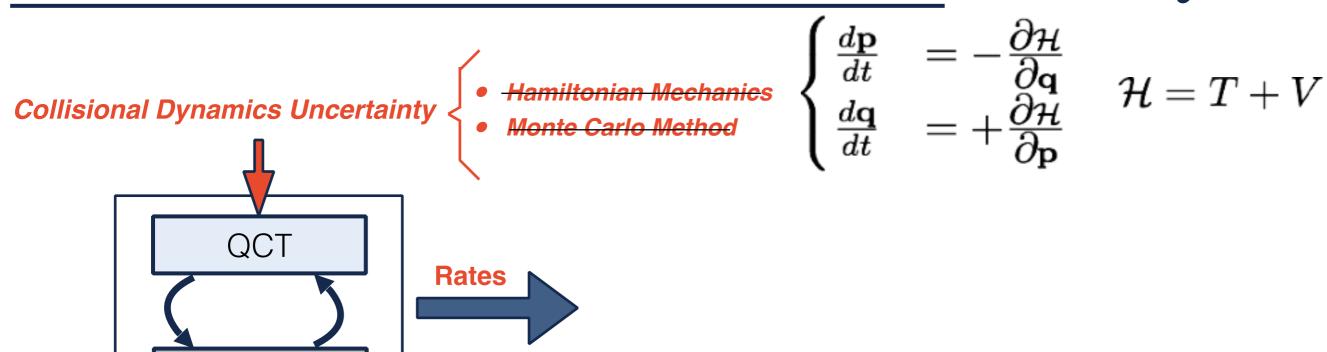
Motivation: Effects of PES Uncertainty

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



Motivation: Effects of PES Uncertainty



PES Uncertainty

PES

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