
An Introduction to Uncertainty Quantification for Predictive Science Part II

Simone Venturi

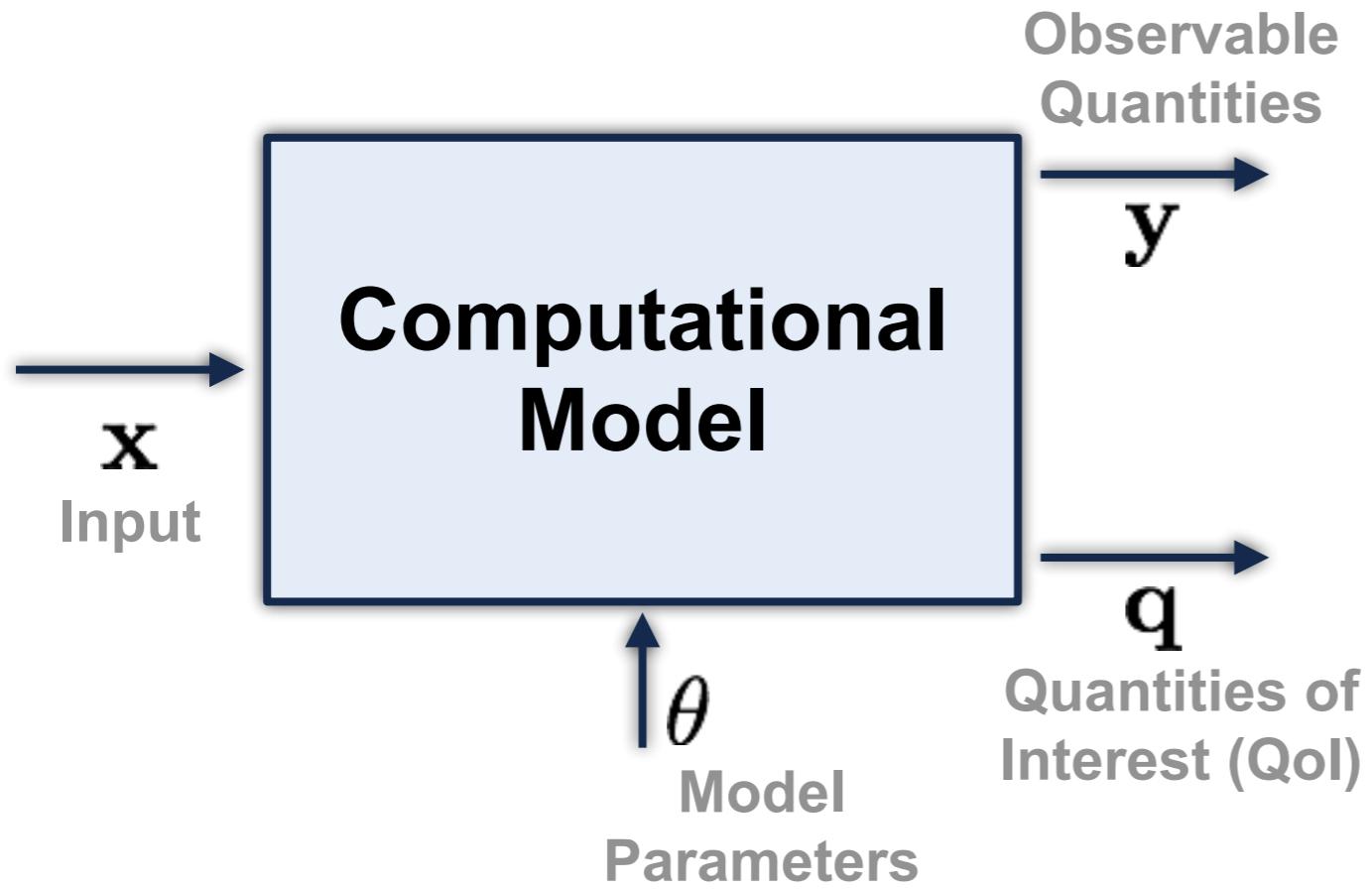
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Prof. Panesi's UQ Class, Fall 2019
September, 6th

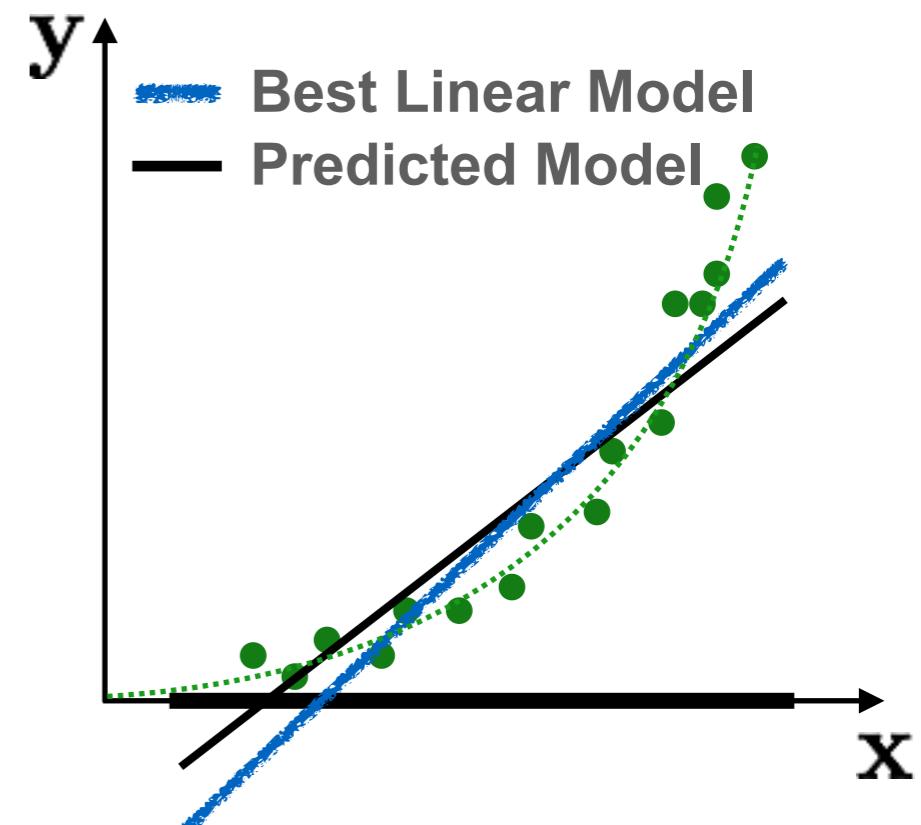


Last Class ...

“The ultimate purpose of most computational models is to make predictions, commonly in support of some decision-making process (e.g, for design of operation of some system).” [1]



- Experimental or Measurement or Observation Error: ● vs - - -
 - Model Uncertainty or Structural Inadequacy: - - - vs ●
 - Parameter Uncertainty: — vs —
- Due to Embedded Model!



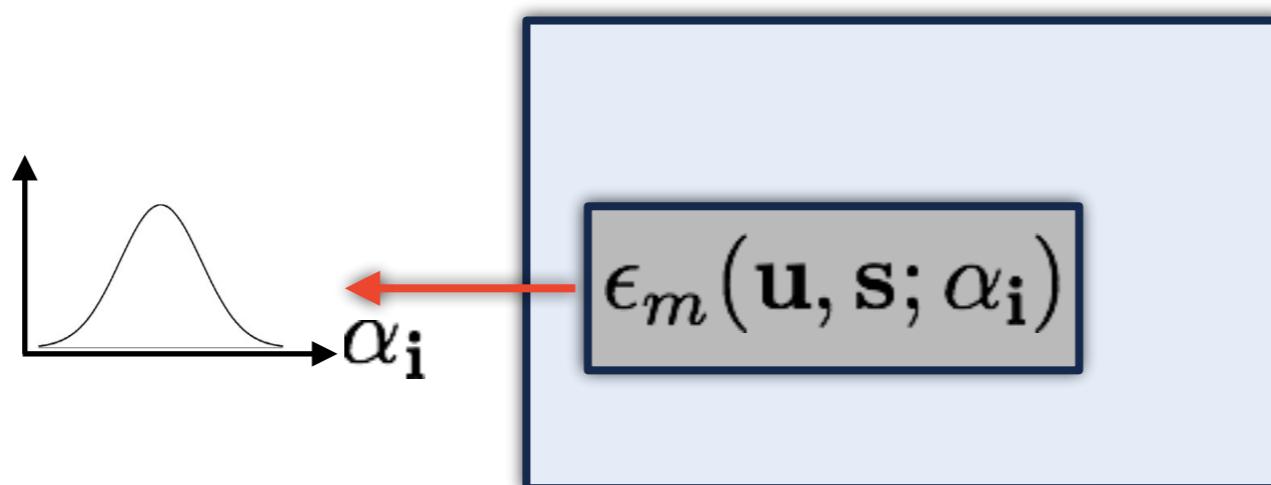
[1] Oliver et al., “Validating Predictions of Unobserved Quantities”, Computer Methods in Applied Mechanics and Engineering, Vol. 283, 2015.

Last Class ...

- Calibration or Inverse Problem

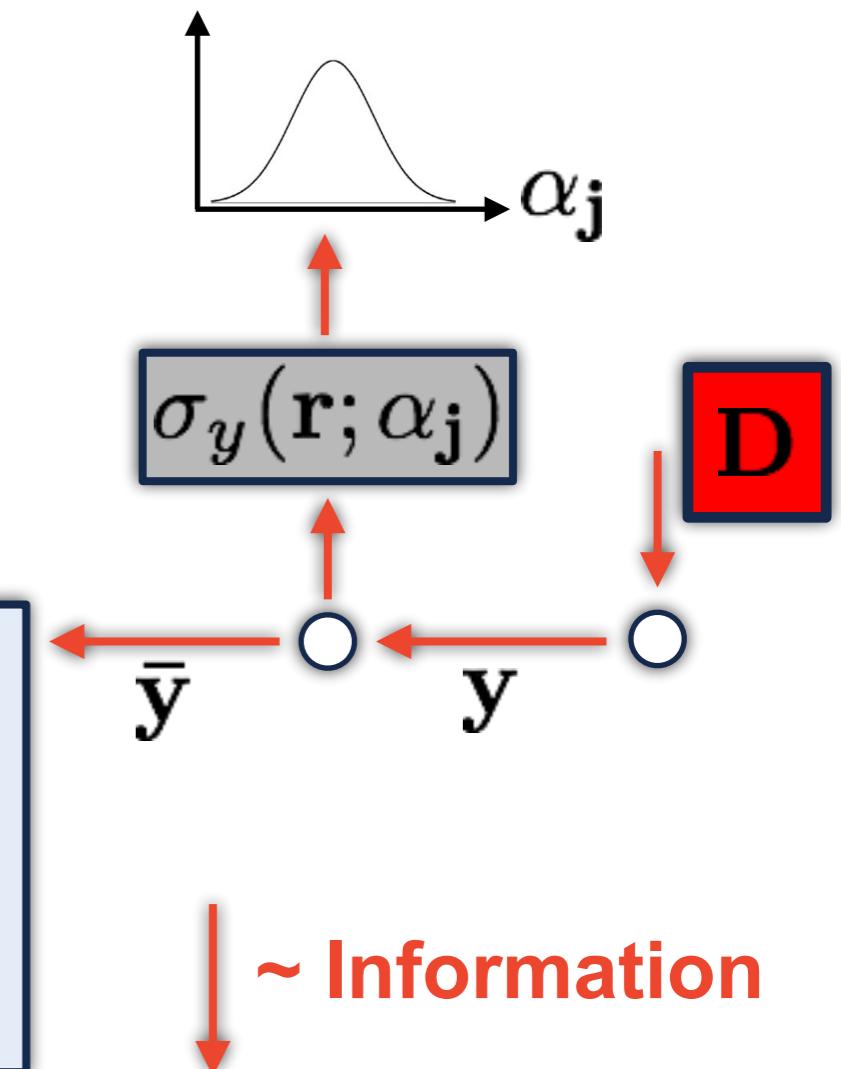
- Validation
- Predictive Assessment

The model is **informed by data**. Parameter values and their uncertainties are inferred from available observations by **solving an inverse problem**.

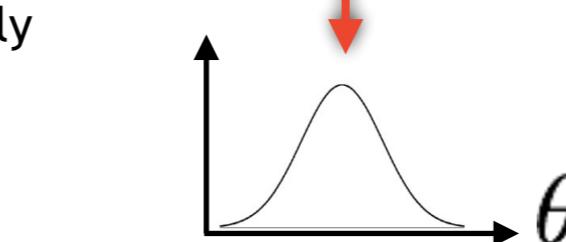


The use of probability to represent uncertainty naturally leads to the formulation of the calibration problem as Bayesian (**Bayesian Inference**):

$$p(\theta, \alpha | \mathbf{D}, \mathcal{M}) = \frac{\mathcal{L}(\theta, \alpha; \mathbf{D}, \mathcal{M}) p(\theta, \alpha | \mathcal{M})}{\int \mathcal{L}(\theta, \alpha; \mathbf{D}, \mathcal{M}) p(\theta, \alpha | \mathcal{M}) d\theta d\alpha}$$



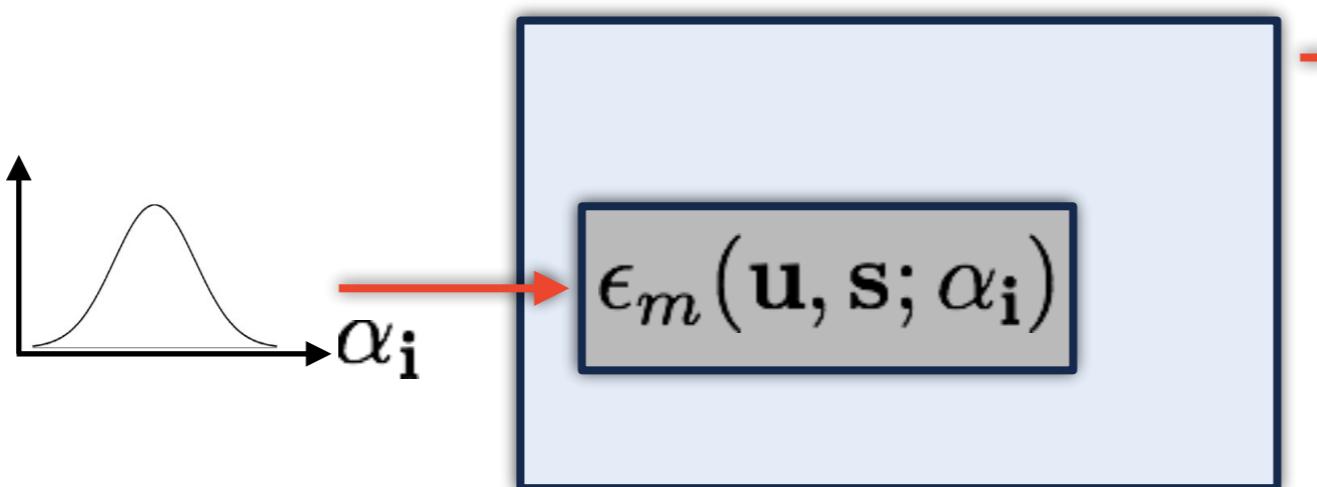
~ Information



Last Class ...

- Calibration
- **Validation**
- Predictive Assessment

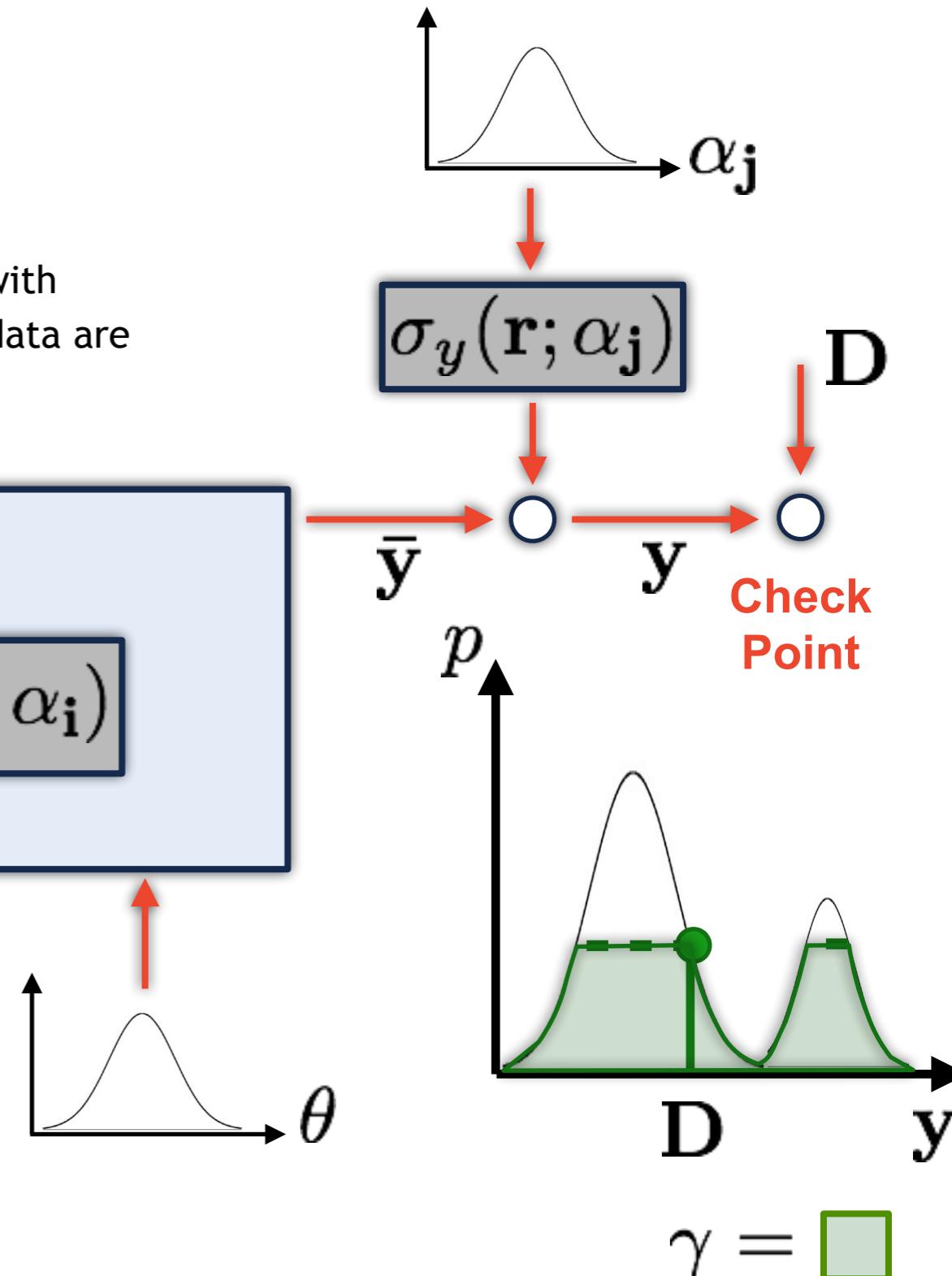
Outputs from a calibrated model are checked for consistency with available observation. We must assess whether the validation data are plausible according to the model.



There are number of possibilities for quantifying this plausibility, as the Bayesian credible intervals.

For example, we can use **highest posterior density (HPD)** credibility intervals.

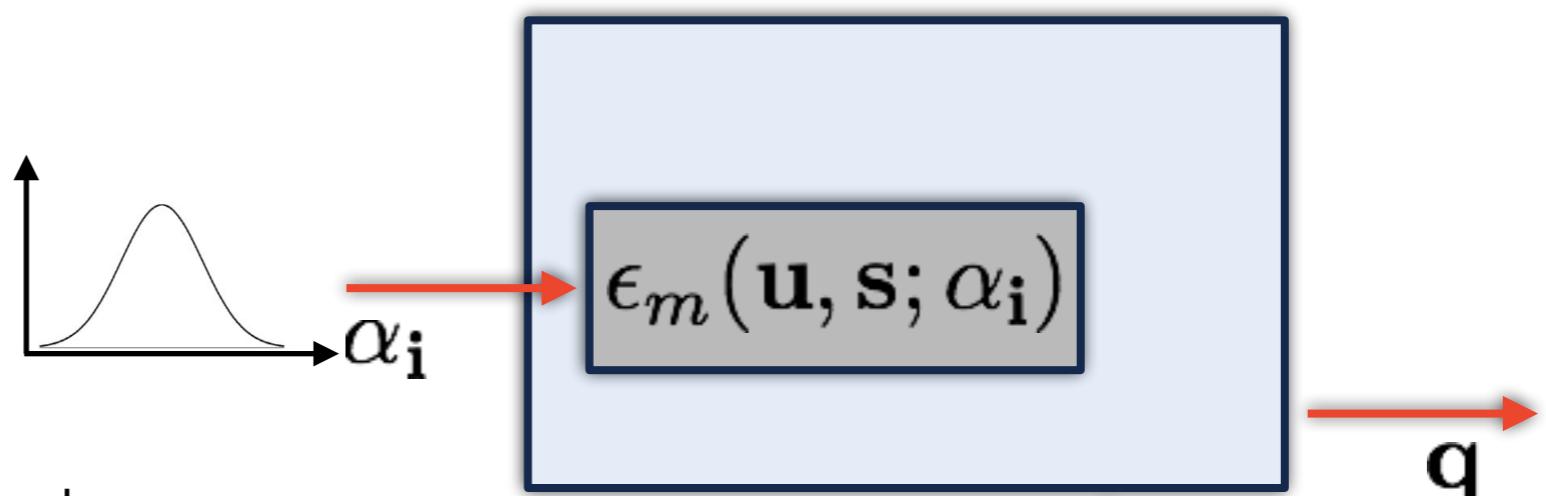
When γ is smaller than some tolerance (e.g., 1.e-3), the data are considered an implausible outcome of the model.



Last Class ...

- Calibration or Inverse Problem
- Validation
- **Predictive Assessment**

Determines whether the calibration and validation phases were sufficiently informative and challenging to provide confidence in the reliability of the predictions of the Qols.



Two primary questions need to be addressed:

- Are Qols sensitive to aspects of the overall model that have not been effectively informed?
- Is the overall model being used outside the domain of applicability?

Moreover, is the prediction is determined to be credible, does it have sufficiently small uncertainty for our purposes?

Last Class ...

Example: Mass-Spring-Damper, Real World System

Reliable Physical Theory

$$\mathcal{R}(\mathbf{u}, \tau; \mathbf{r}) = \mathbf{0}$$

$$m\ddot{x} + c\dot{x} + kx = 0$$

$$\mathbf{u} = \begin{bmatrix} x \\ \dot{x} \end{bmatrix} \quad \tau = \begin{bmatrix} c \\ k \end{bmatrix} \quad \mathbf{r} = \begin{bmatrix} m \\ x(0) \\ \dot{x}(0) \end{bmatrix}$$

Real World Embedded Model

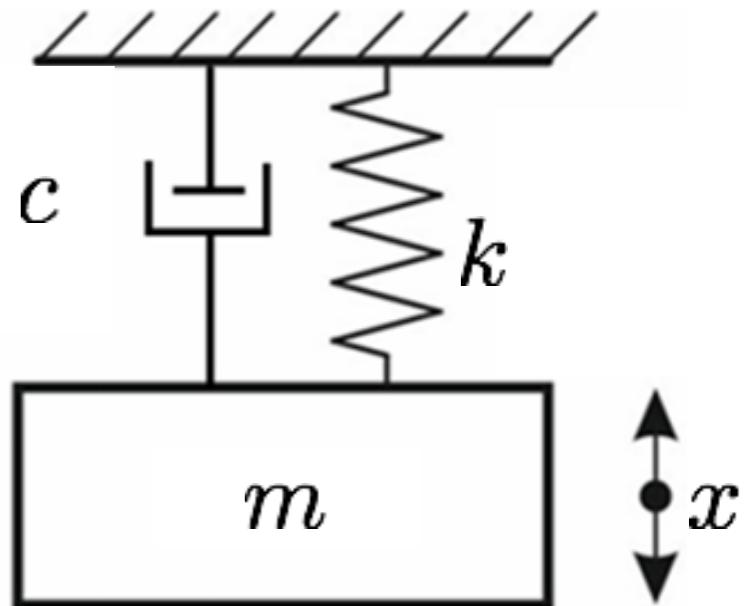
$$\tau = (\mathbf{u}, \mathbf{v}, \mathbf{s}, \theta)$$

$$k = \text{const}$$

$$c(T) = \exp\left(\frac{T_0}{T} - 1\right)$$

$$\dot{T} = c(T)\dot{x}^2 - \frac{T - T_0}{t_T}$$

$$\mathbf{v} = T \quad \mathbf{s} = \begin{bmatrix} T_0 \\ t_T \end{bmatrix} \quad \theta = k$$



$$\mathbf{y} = x$$
$$\mathbf{q} = \max(\dot{x})$$

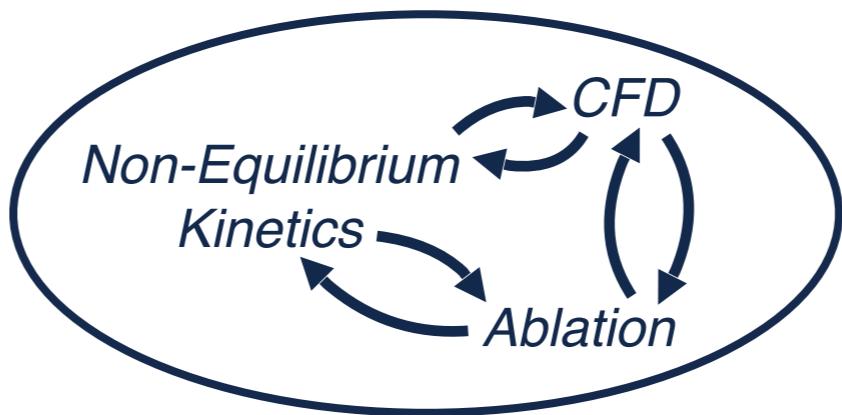
Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces [2]

[2] S. Venturi, R. L. Jaffe, and M. Panesi, “Bayesian Machine Learning Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces”, *The Journal of Physical Chemistry A*, Special Virtual Issue “Machine Learning in Physical Chemistry”, Vol. 124, No. 25 (2020)

Motivation: TPS

Thermal Protection System (TPS) is a set of safety-critical components that protects a vehicle traveling at hypersonic speed from heating.

- ◆ TPS is a **single point-of-failure**
- ◆ Predicting the **heat fluxes** experienced by the vehicle and modeling the **material response** are **challenging tasks**, mainly due to:
 - Multiple scales involved;
 - Multidisciplinarity of the problem;
 - Presence of coupling effects;
 - Hard to be replicated in labs.

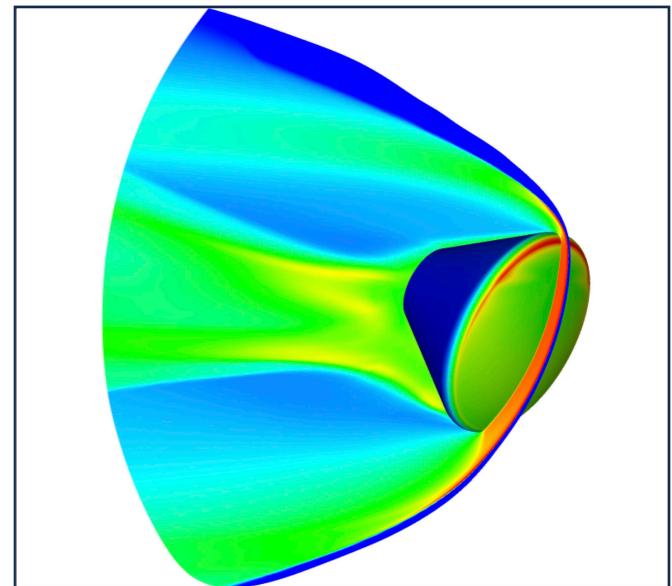


Substantial **margins of safety** are applied during TPS design, in order to account for the uncertainties in the quantity of interest predictions.

The more reliable the quantifications of such uncertainties are proved to be,
the more accurate such margins end up being,
reducing the risk of failures

OR

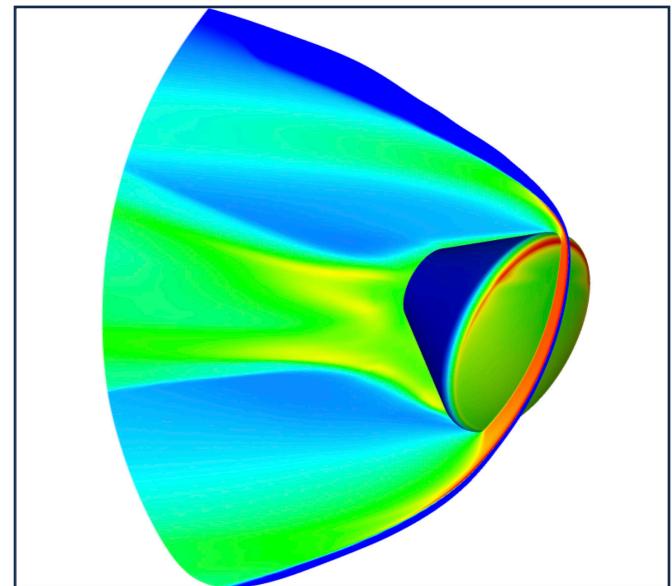
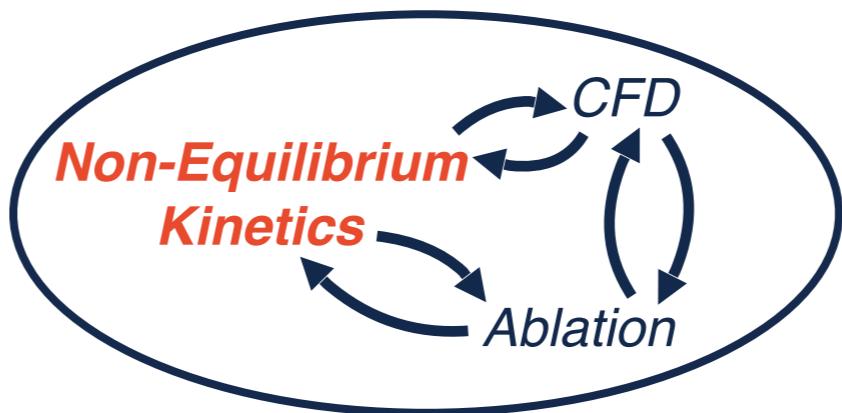
generating relevant profits from vehicle mass and mission costs points of view



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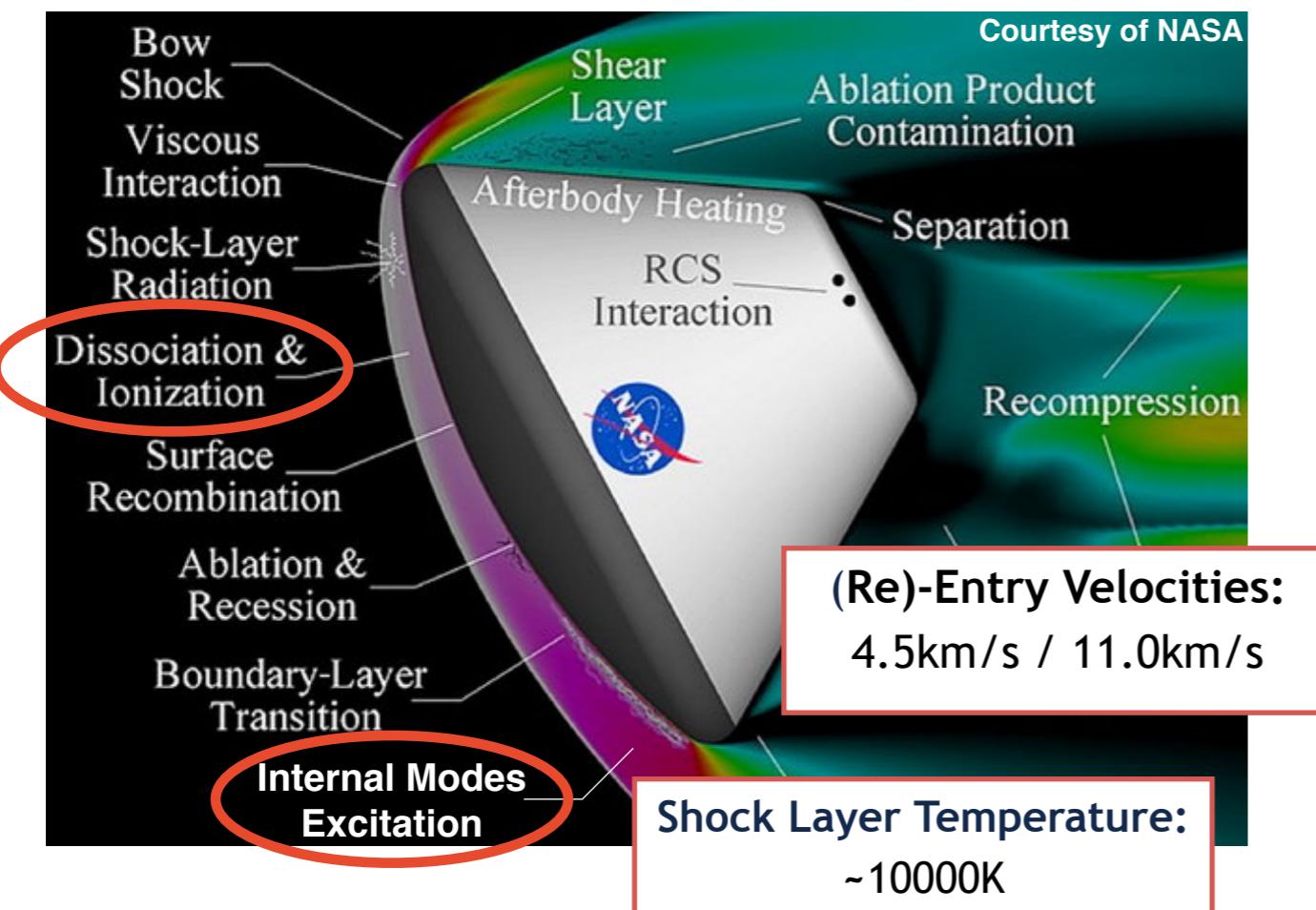
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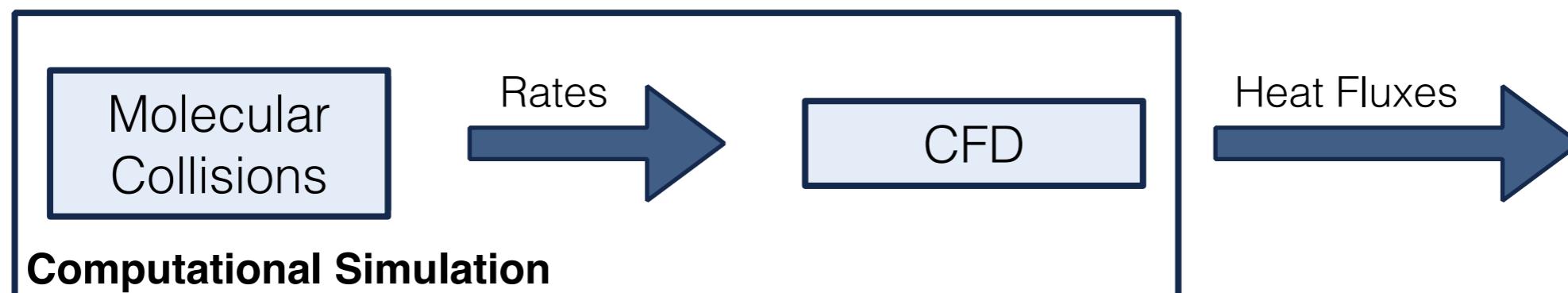


Motivation: Non-Equilibrium Flows

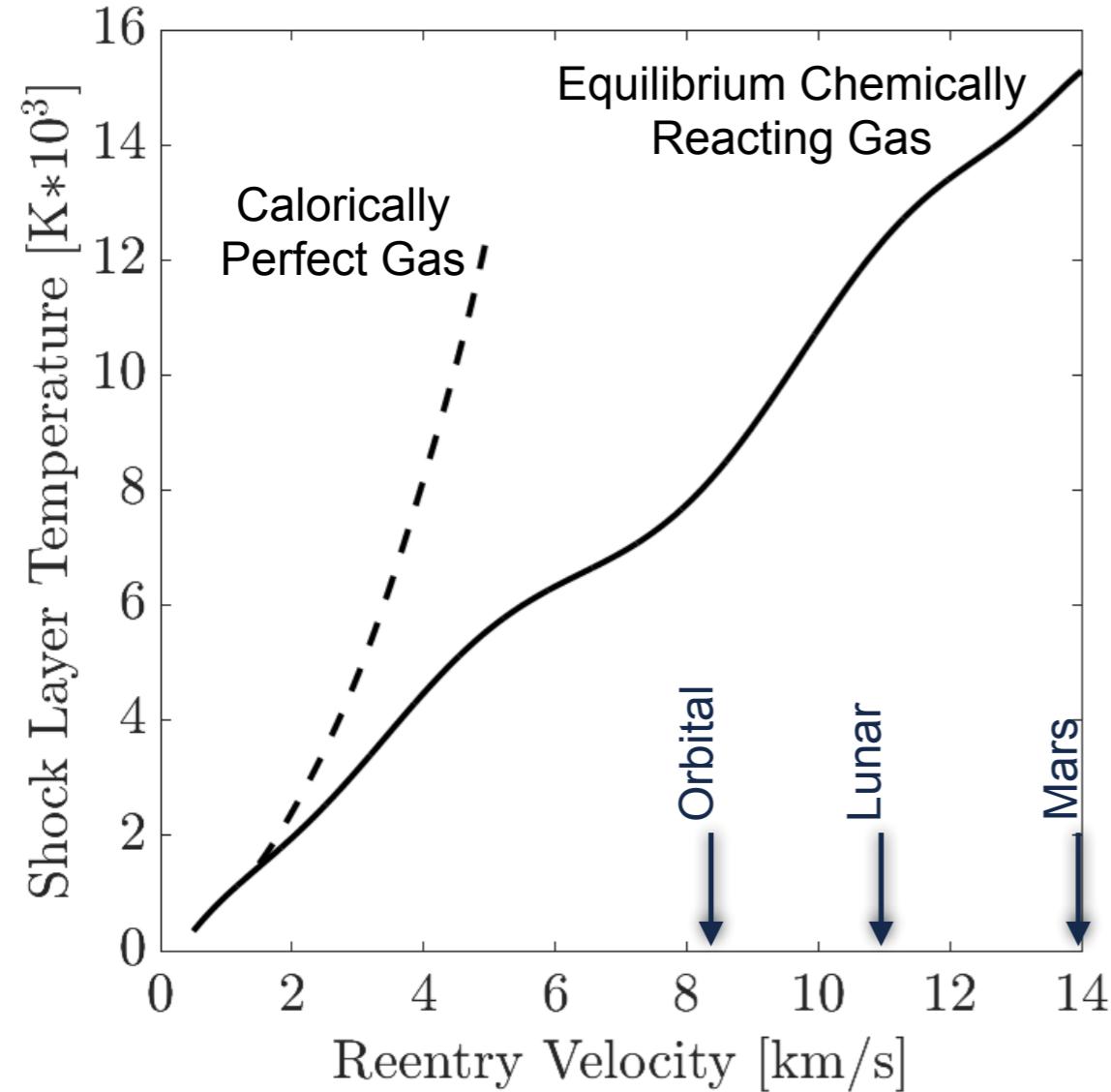


- ◆ The mixture is **thermally and chemically reacting**, and the fluid in the shock layer cannot be modeled as a perfect gas.
- ◆ It is necessary to understand how the energy of the flow is stored in its internal modes and is affected by the chemistry.
- ◆ A resolution up to the atomic and molecular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

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



Motivation: Non-Equilibrium Flows

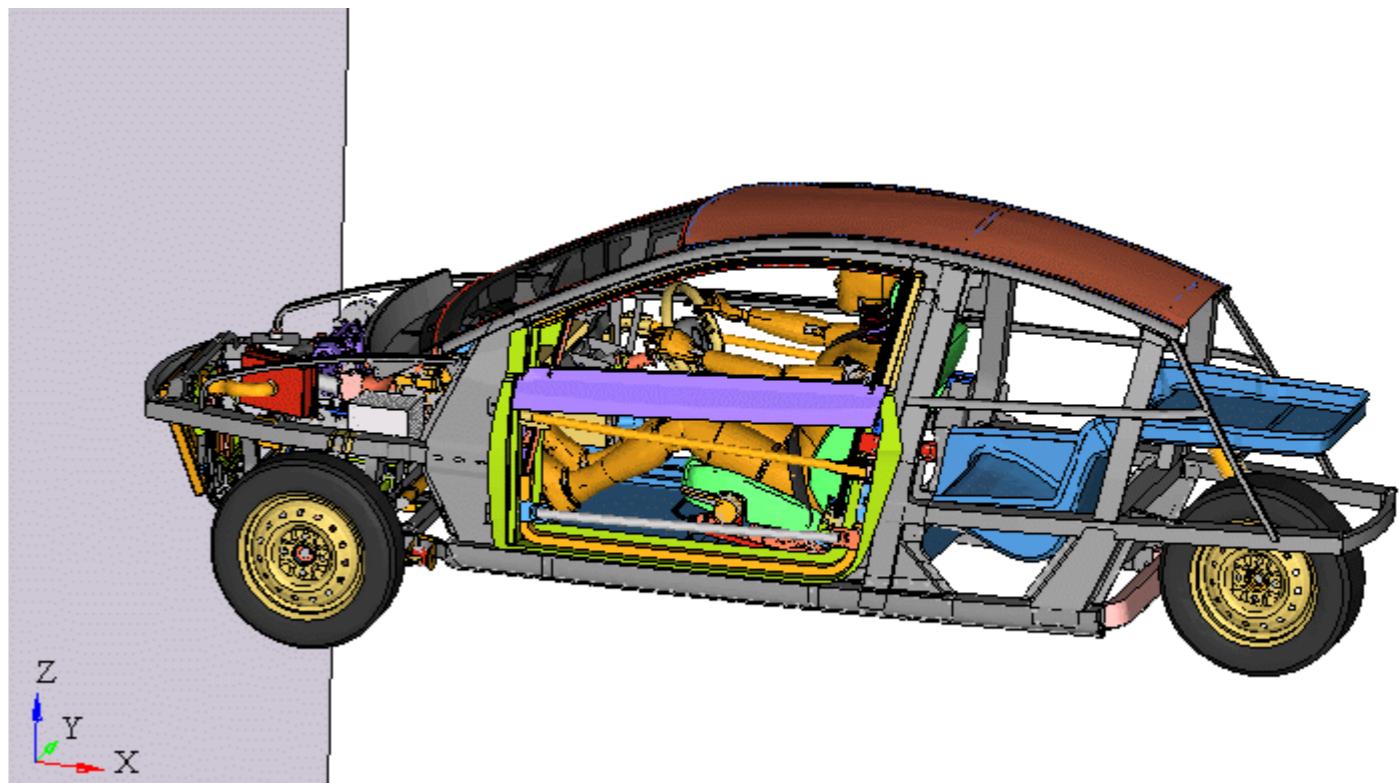


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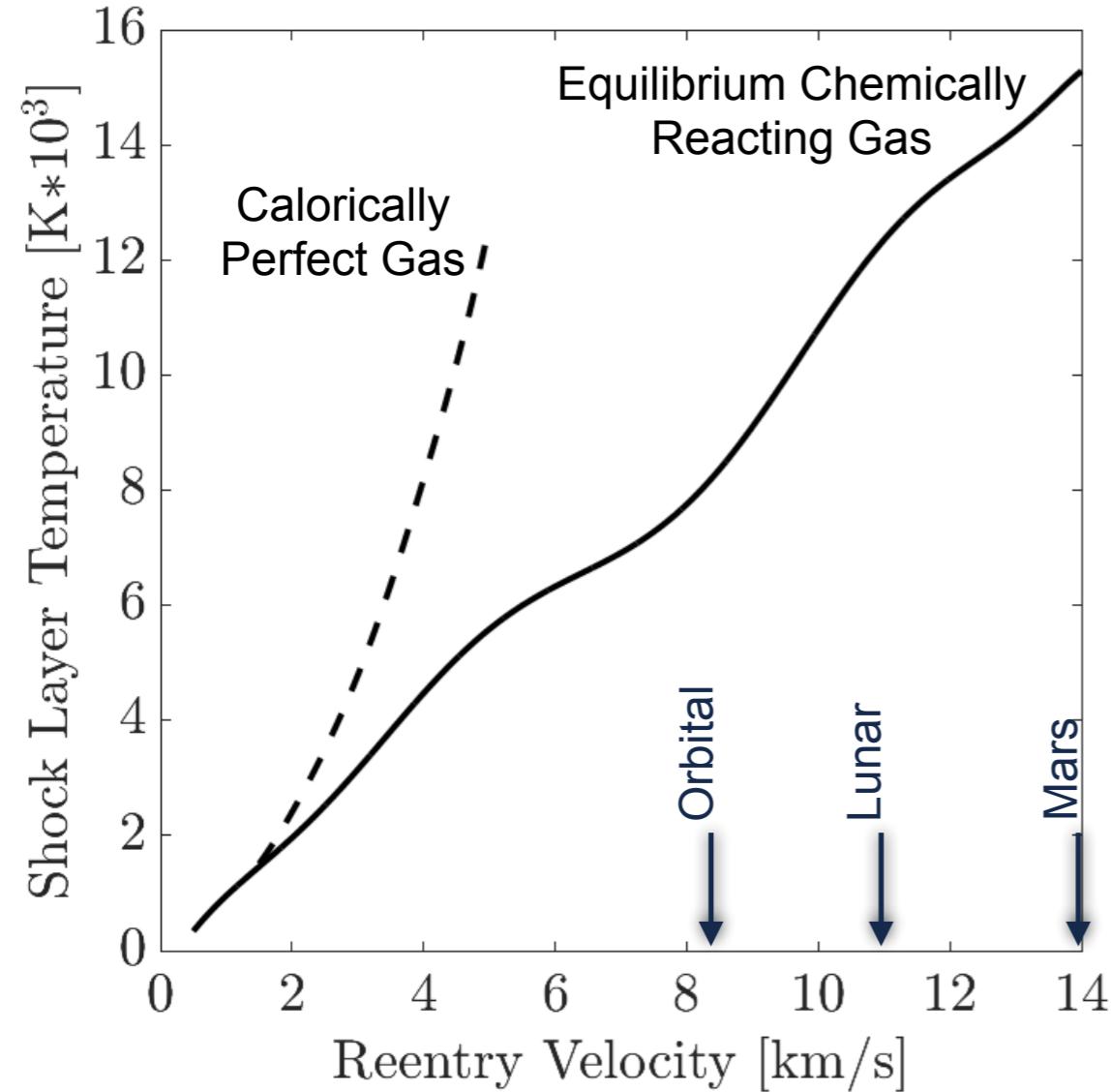
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gas behavior in Computational Hypersonics

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Low accuracy on deformations in a crash test
Computational Simulation



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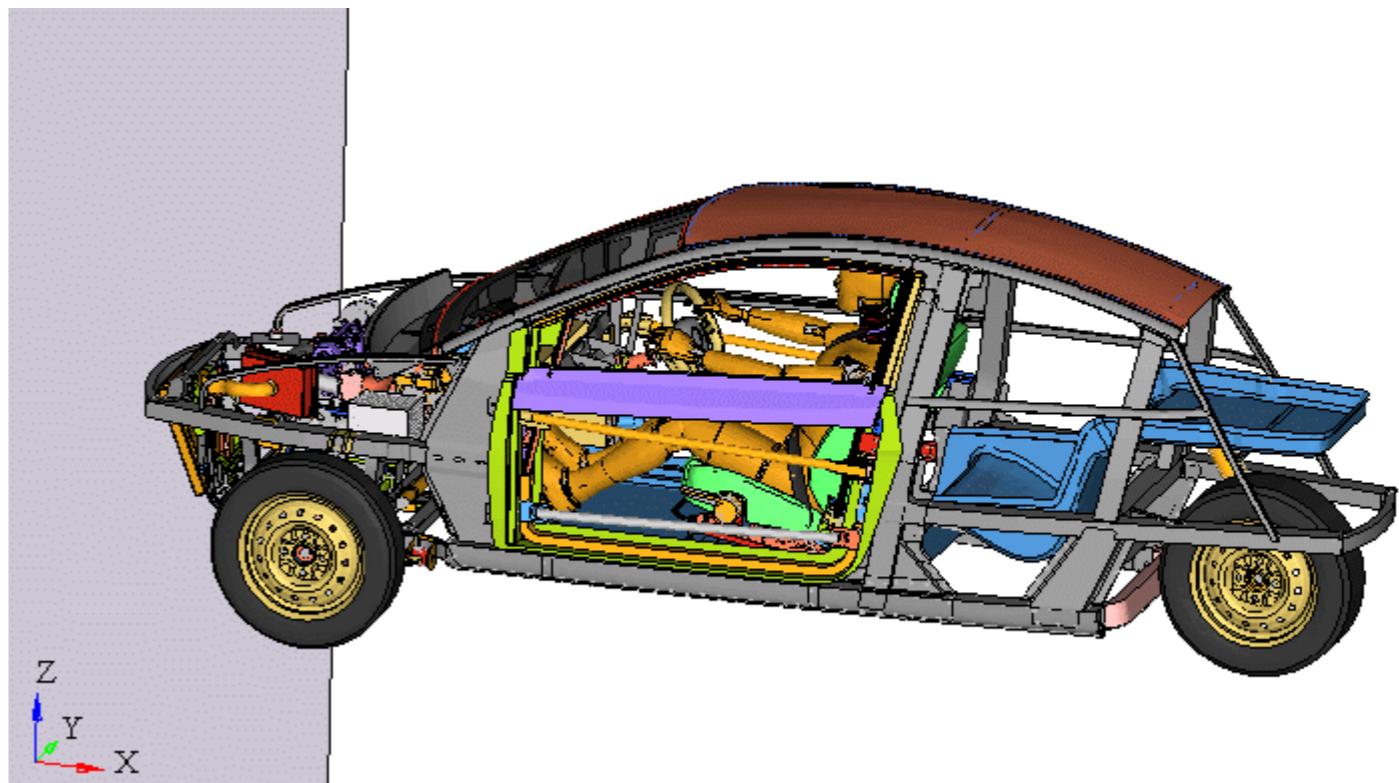


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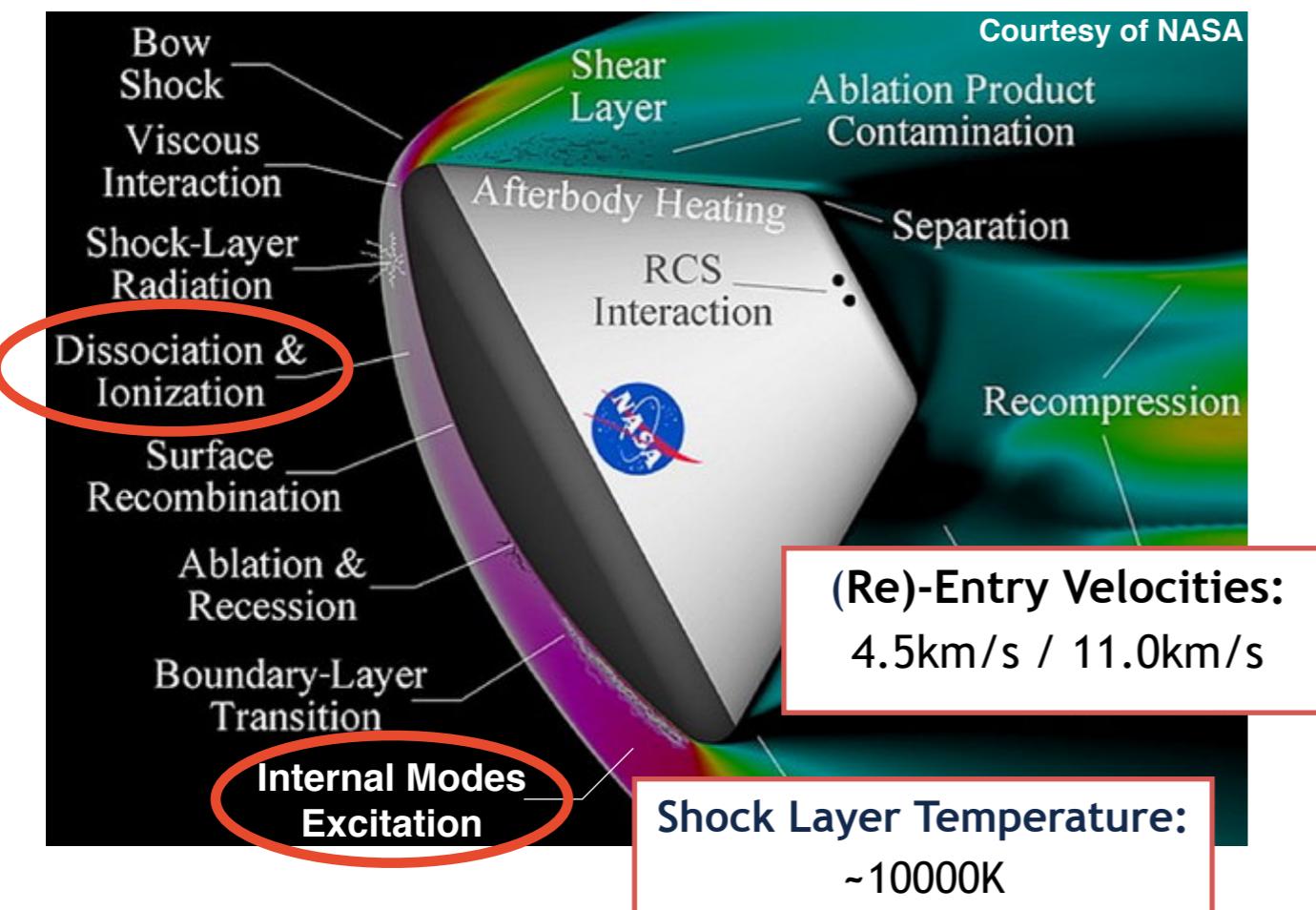
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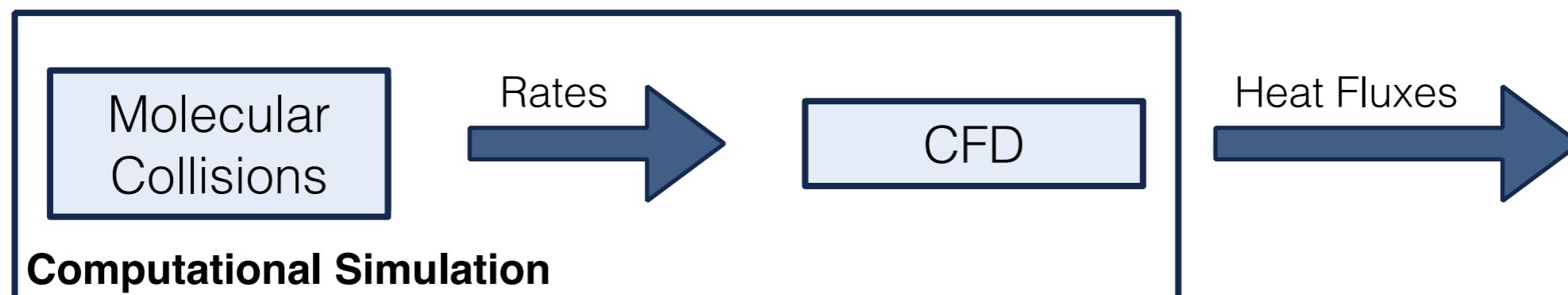


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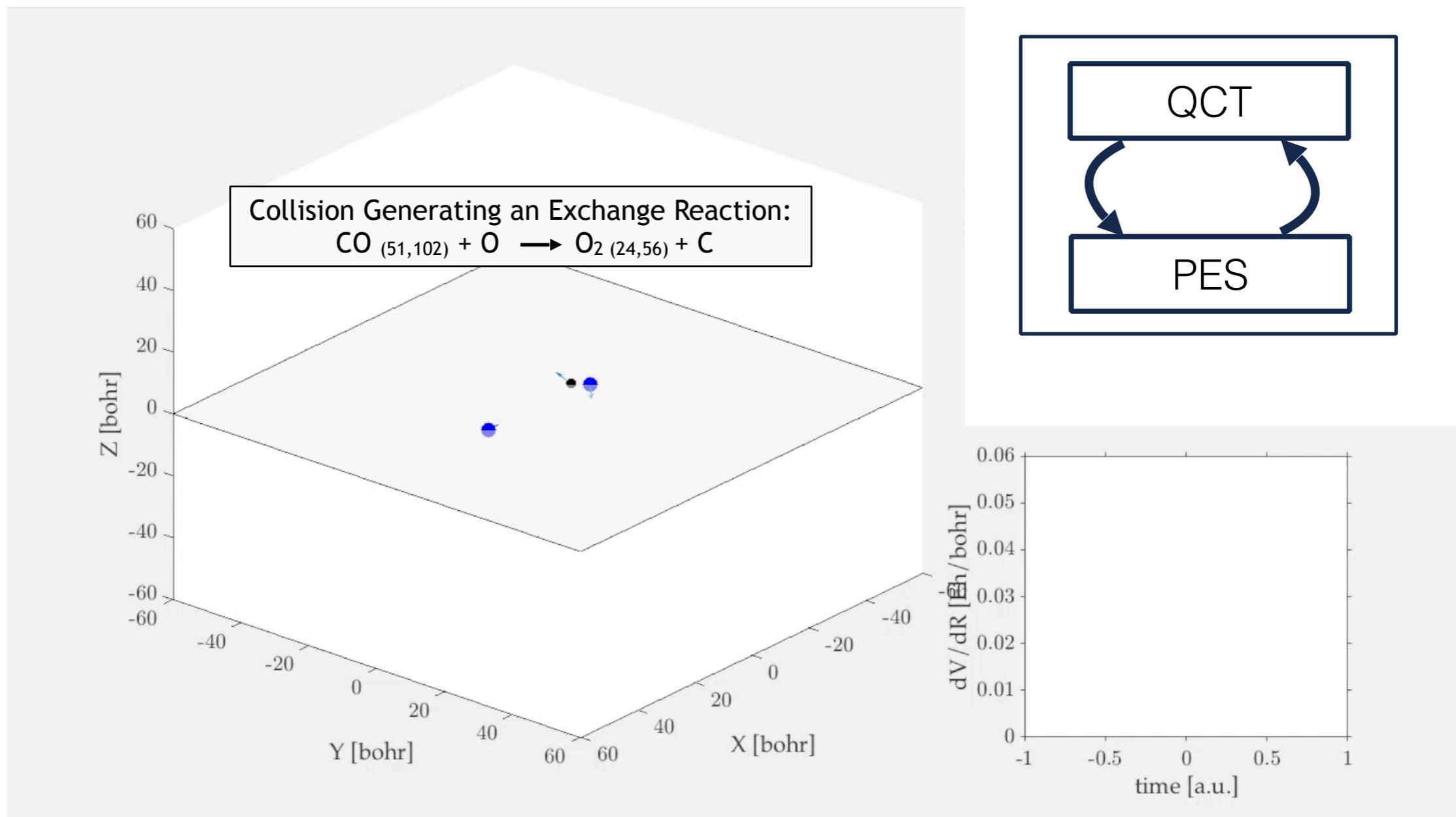


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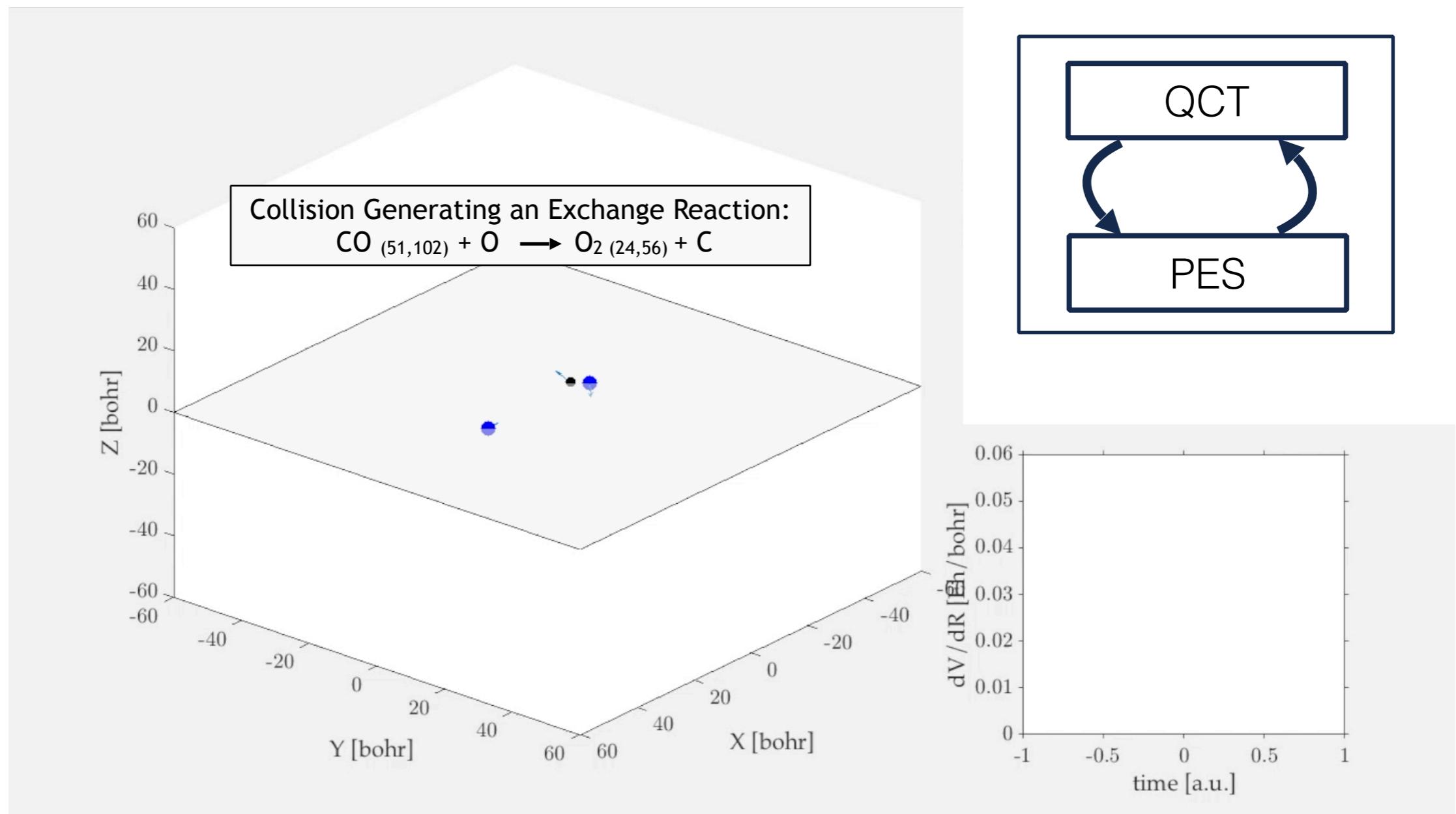


Motivation: PES-to-Rate Coeff.s Approach



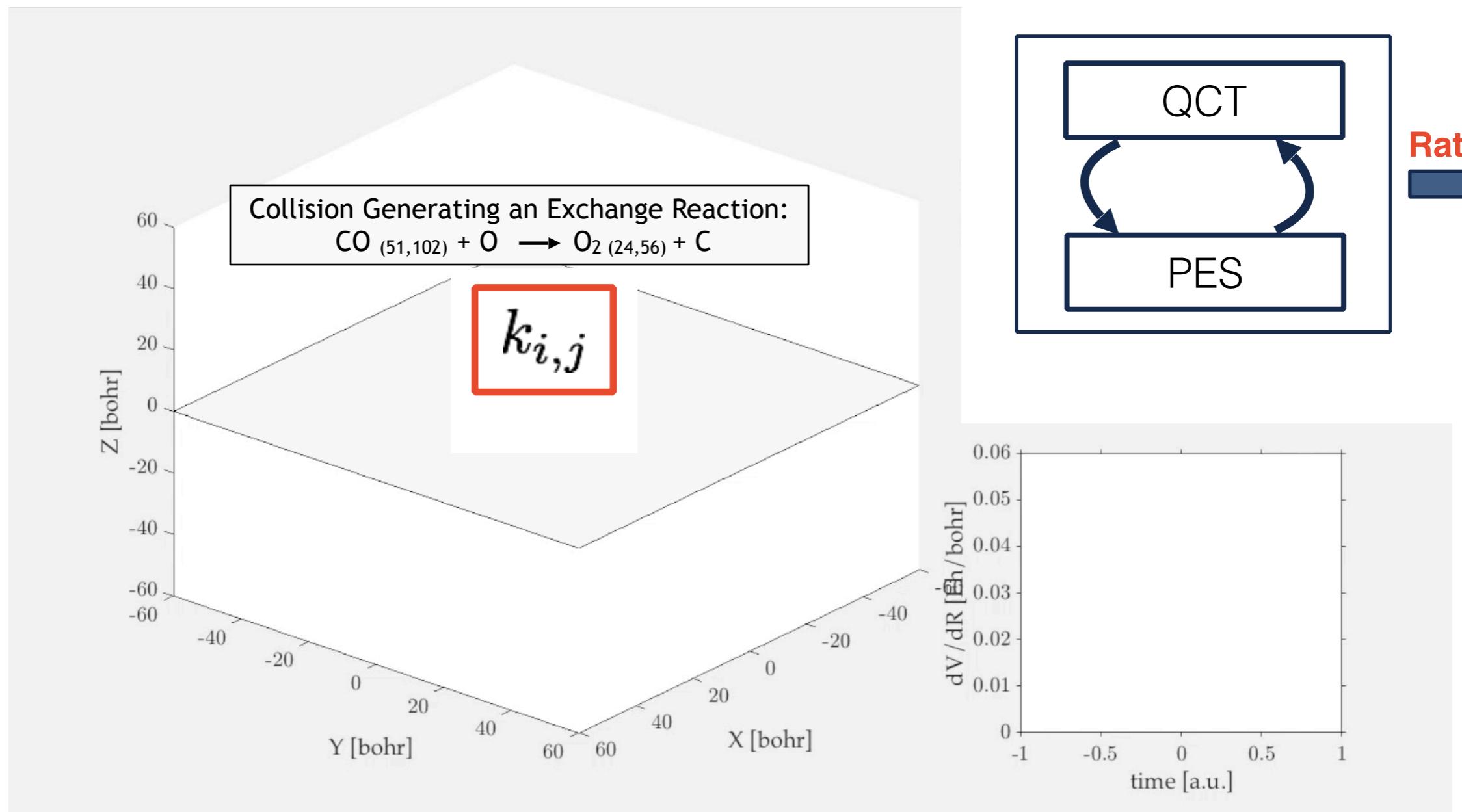
1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as source terms of the Hamiltonian Eq.s for the calculation of atom trajectories;

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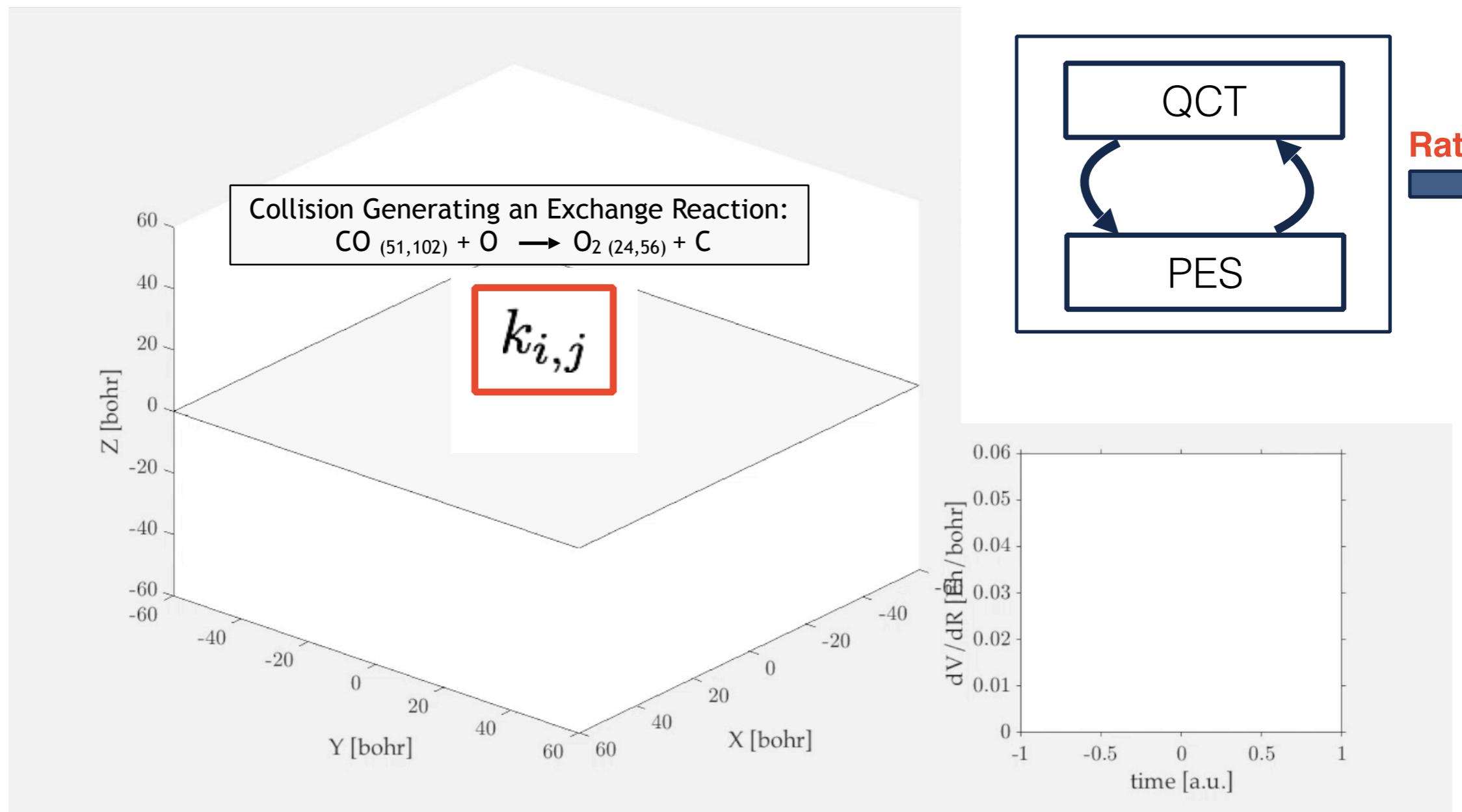
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1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as source terms of the Hamiltonian Eq.s for the calculation of atom trajectories;
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PESs drive the collision dynamics, and govern the values of rate coefficients

Motivation: PES-to-Rate Coeff.s Approach

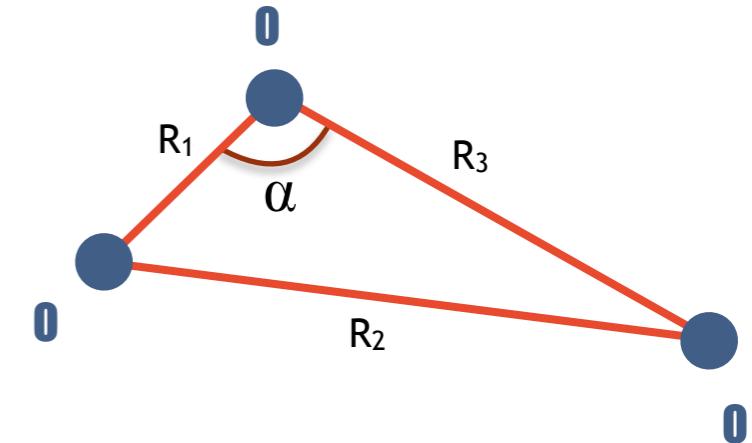
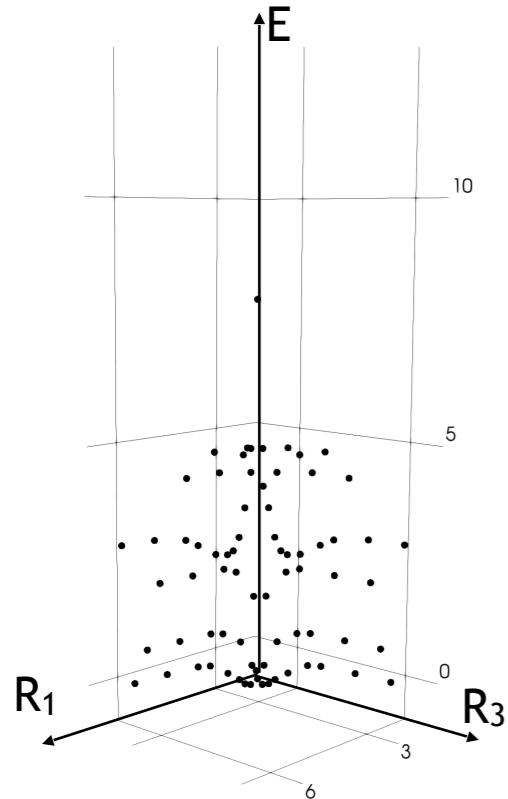


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Potential Energy Surfaces (PESs) are functions that describe the **quantum-physics interactions between atoms**.

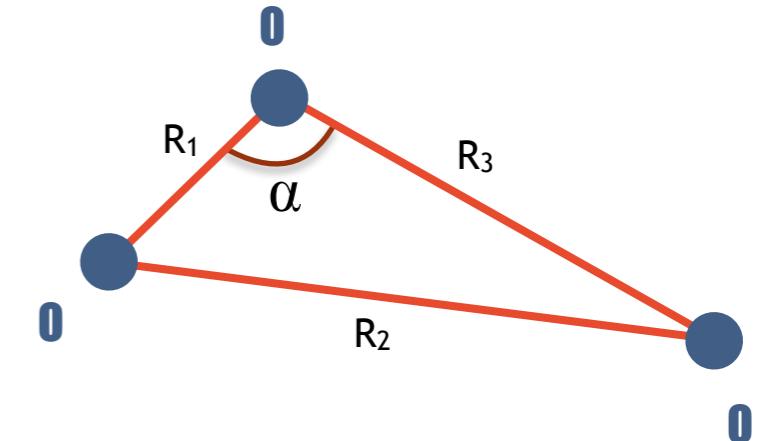
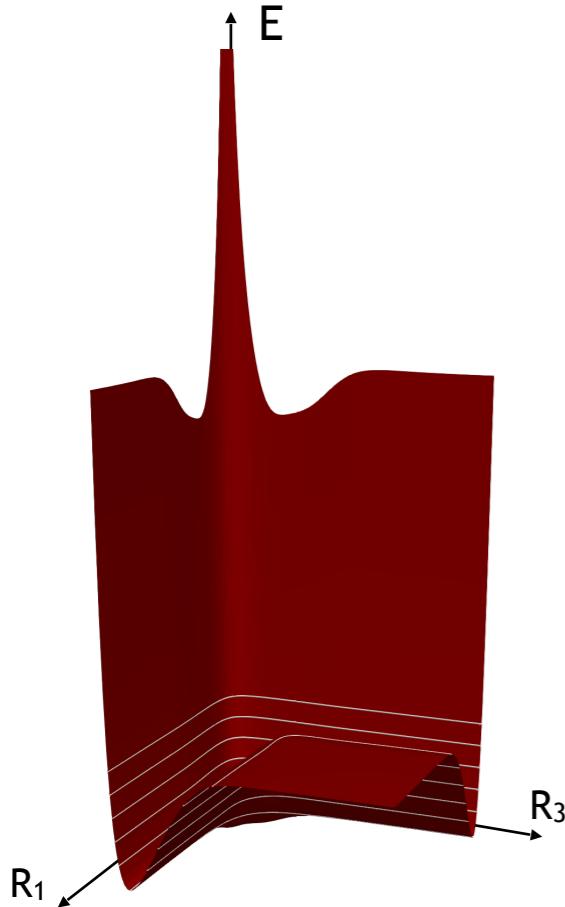


Ab-Initio PES Generation Process:

1. A large number of atom **geometric arrangements** (R_1, R_2, R_3) is selected;
2. **Electronic Schrödinger Eq.** is solved at such arrangements;
3. The resulting energies are **fit to analytical expressions**.

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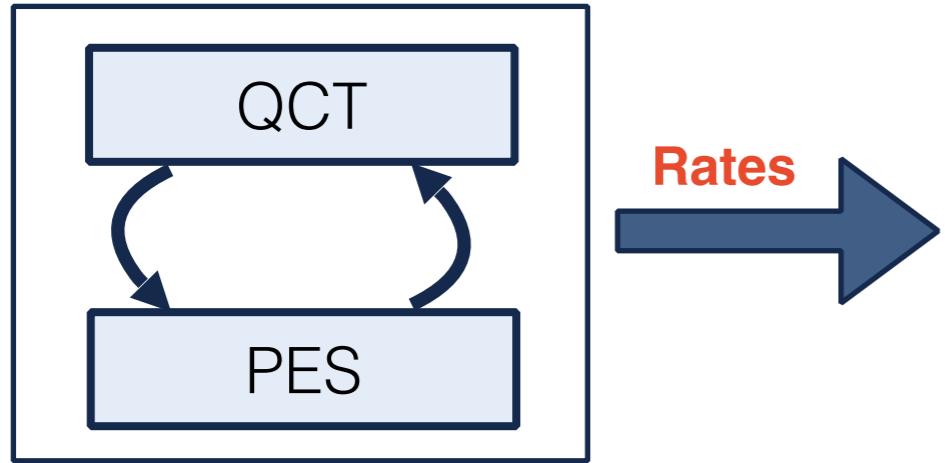
Each research group typically has its distinctive protocols to PES generations.

The result is that the surfaces for a given collisional system are diverse from one laboratory to the other.

- The process is extremely time consuming;
- There is no systematic approach in place in order to evaluate the “cost” of such differences.

Motivation: Effects of PES Uncertainty

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

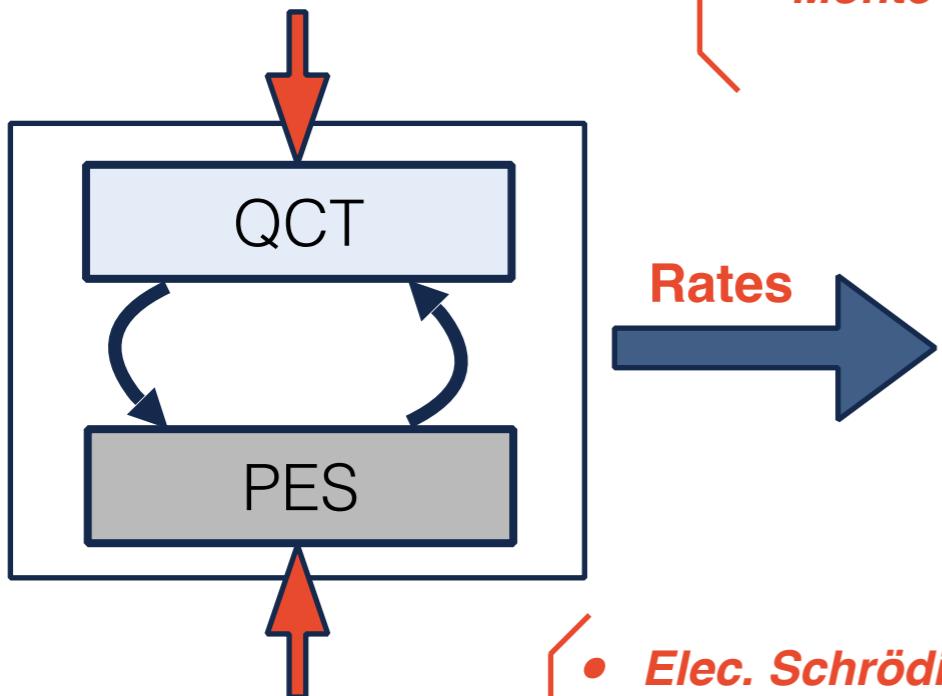


Motivation: Effects of PES Uncertainty

Collisional Dynamics Uncertainty

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

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



PES Uncertainty

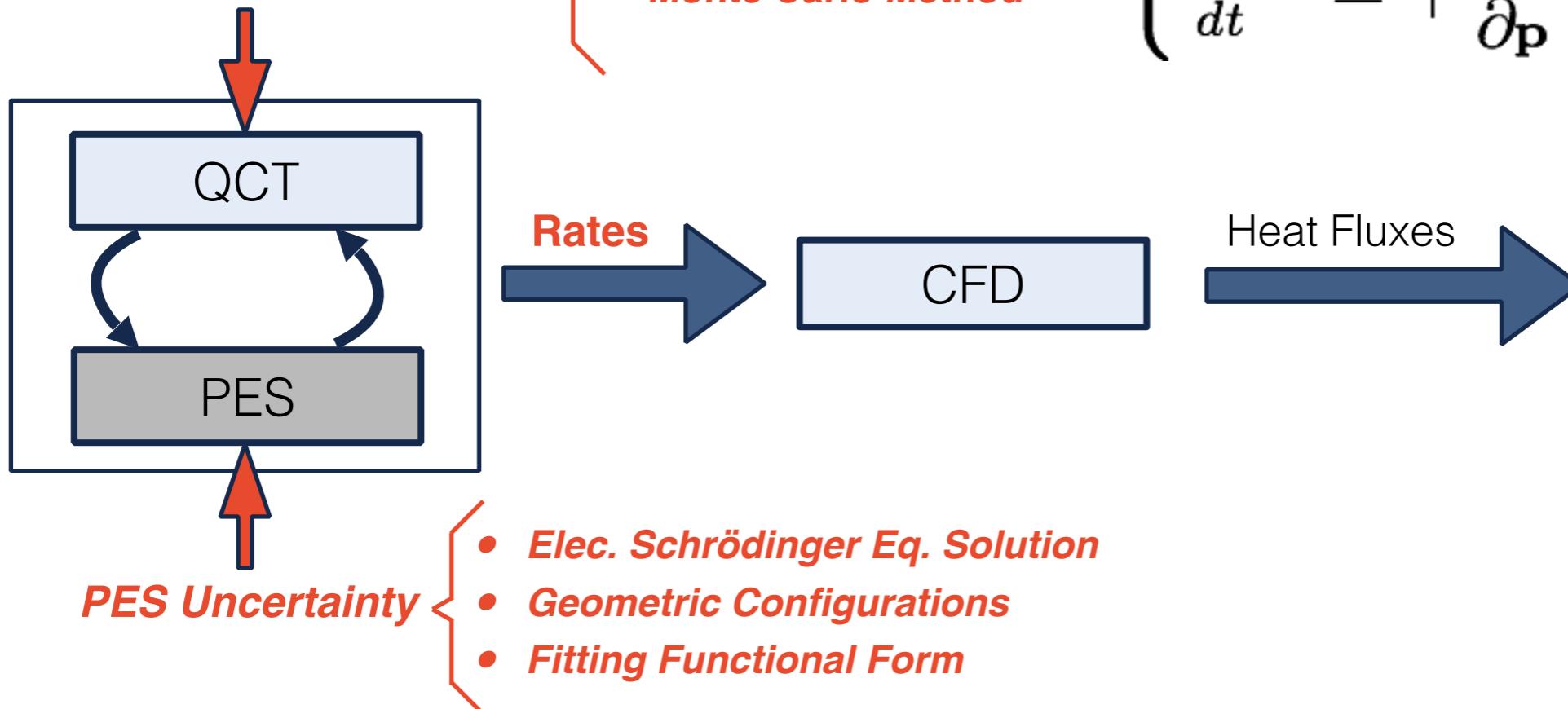
- *Elec. Schrödinger Eq. Solution*
- *Geometric Configurations*
- *Fitting Functional Form*

Motivation: Effects of PES Uncertainty

Collisional Dynamics Uncertainty

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Can we use Machine Learning in order 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:

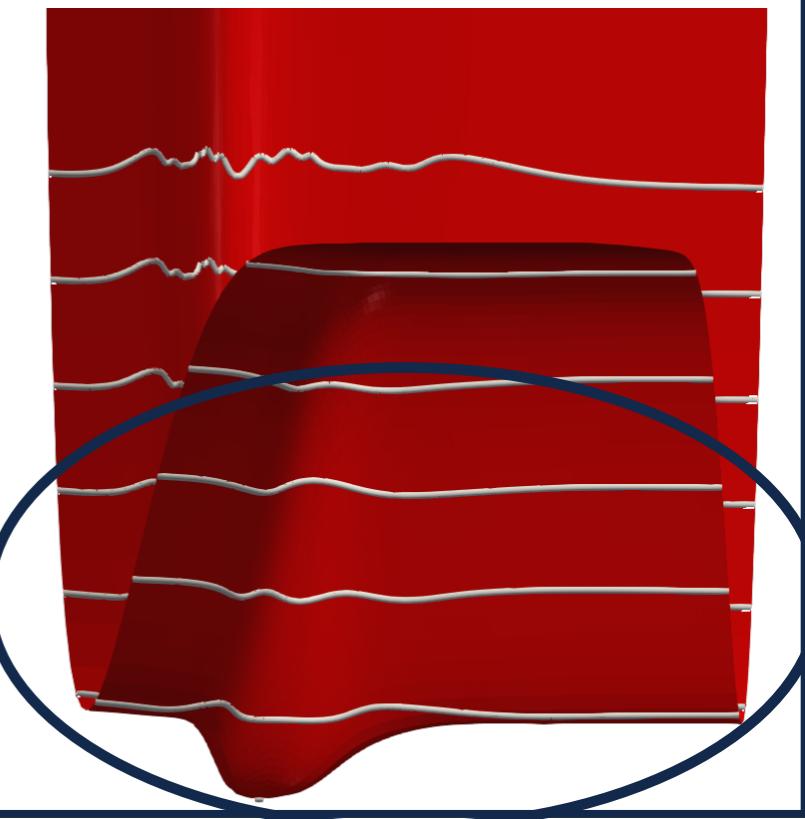
- ◆ Gaussian Processes

- ◆ Neural Network

- ◆ “*Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes*”, [*J. Phys. Chem. A* 2017](#);
- ◆ “Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions”, *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.



ANN for PESs: Methodology

Multi-layer feed-forward Neural Networks (NN) have been adopted as **fitting functional**:

- ◆ Easy to implement;
- ◆ Easy to train;
- ◆ Easy to generalize to new systems;
- ◆ Easy to differentiate in R;
- ◆ Cost effective;
- ◆ Easy to be refined;
- ◆ Widely tested;
- ◆ Easy to be extended to the stochastic case.

Permutation Invariant Polynomials Neural Networks (PIP-NN):

theano

Lasagne

1. A **Symmetrized Polynomial Vector (G)** is constructed, in order to account for the permutation symmetries; for example, for a A3-type system:

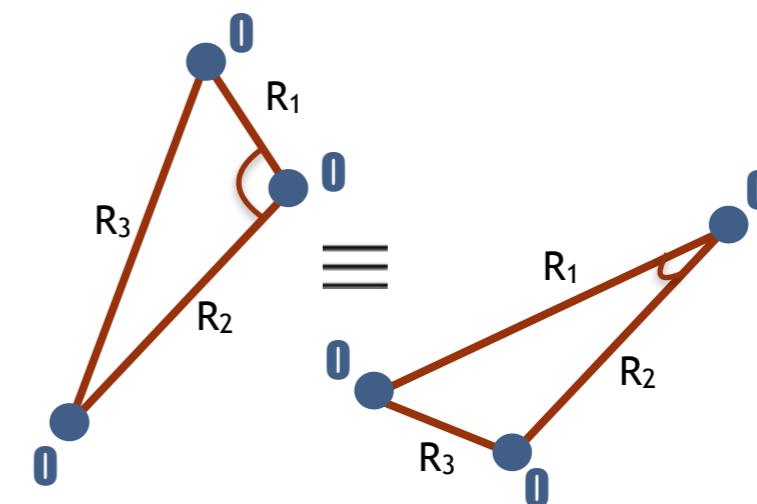
$$G_1 = p_1 + p_2 + p_3$$

$$G_2 = p_1 p_2 + p_2 p_3 + p_1 p_3$$

$$G_3 = p_1 p_2 p_3$$

where $p_i = \exp(-\lambda_i(R_i - r_{e_i}))$, being λ_i and r_{e_i} tunable parameters.

(R₁)
(R₂)
(R₃)
⋮
(R_N)



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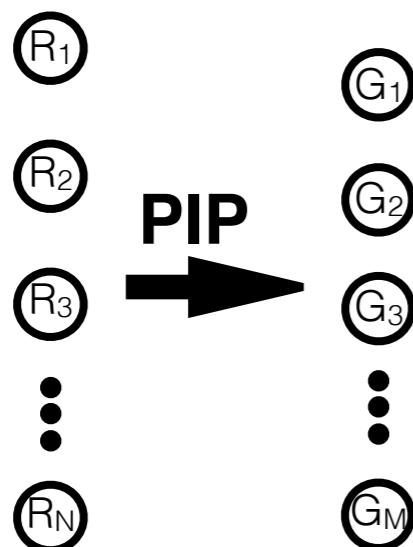
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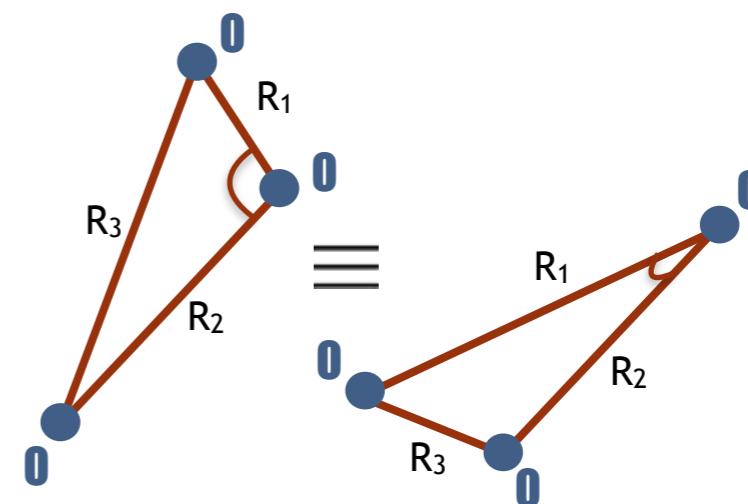


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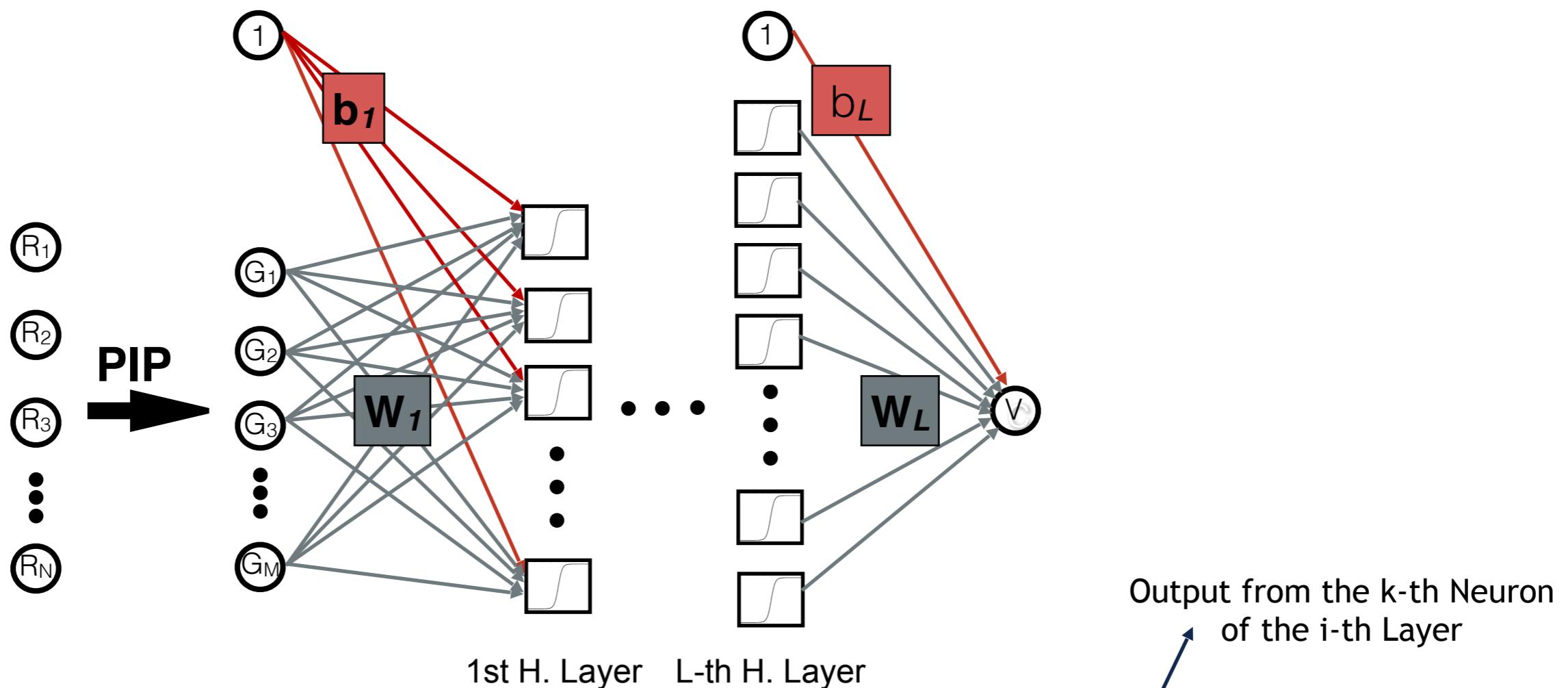
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Permutation Invariant Polynomials Neural Networks (PIP-NN):

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2. G is fed to a feed-forward neural network, and it flows through its layers as a series of weighted linear combinations alternated to non-linear functions

$$\begin{cases} z_i^k = \sum_{j=1}^{N_{i-1}} W_i^{jk} y_{i-1}^j + b_i^k \\ y_i^k = f_i(z_i^k) \end{cases}$$

ANN for PESs: Methodology

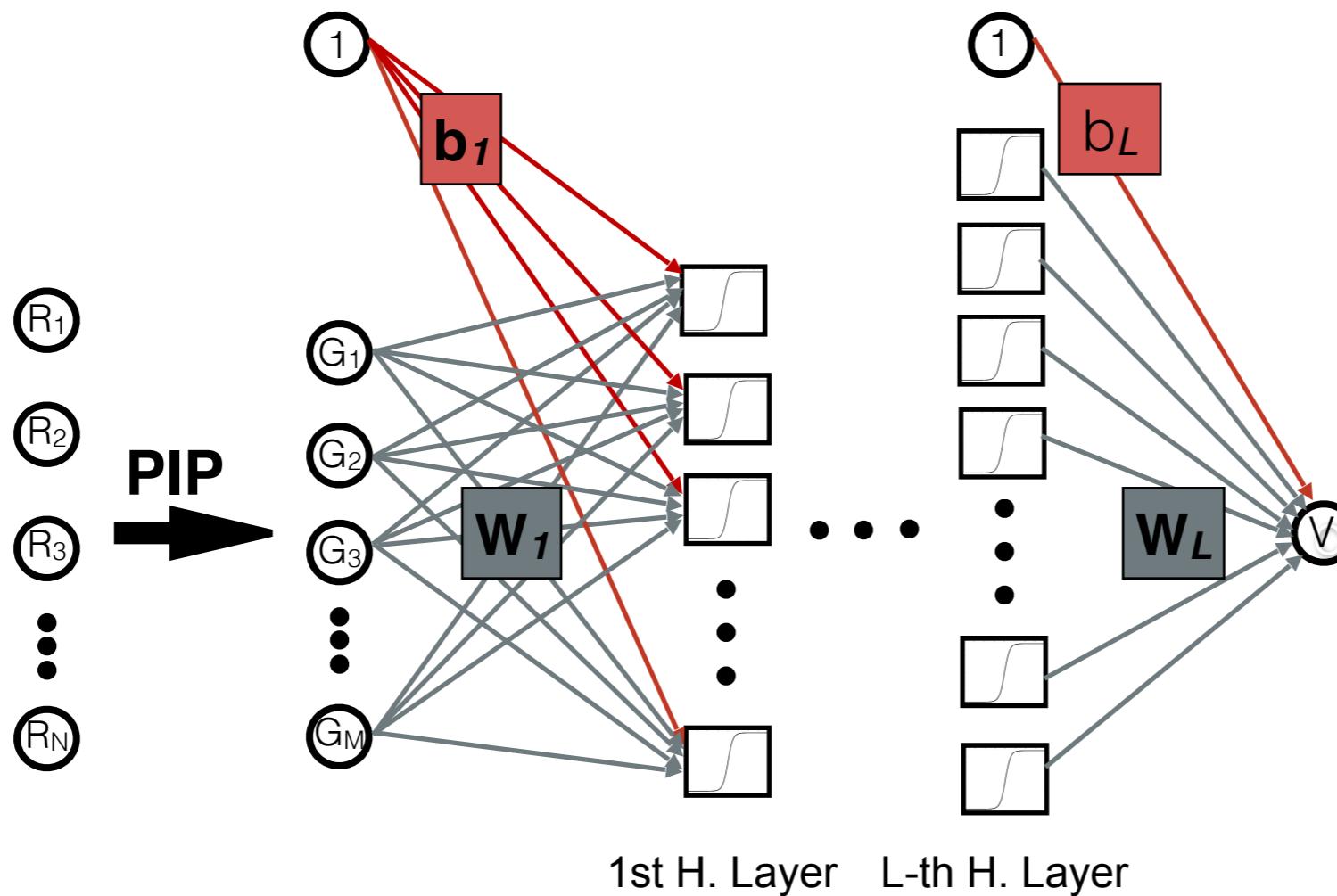
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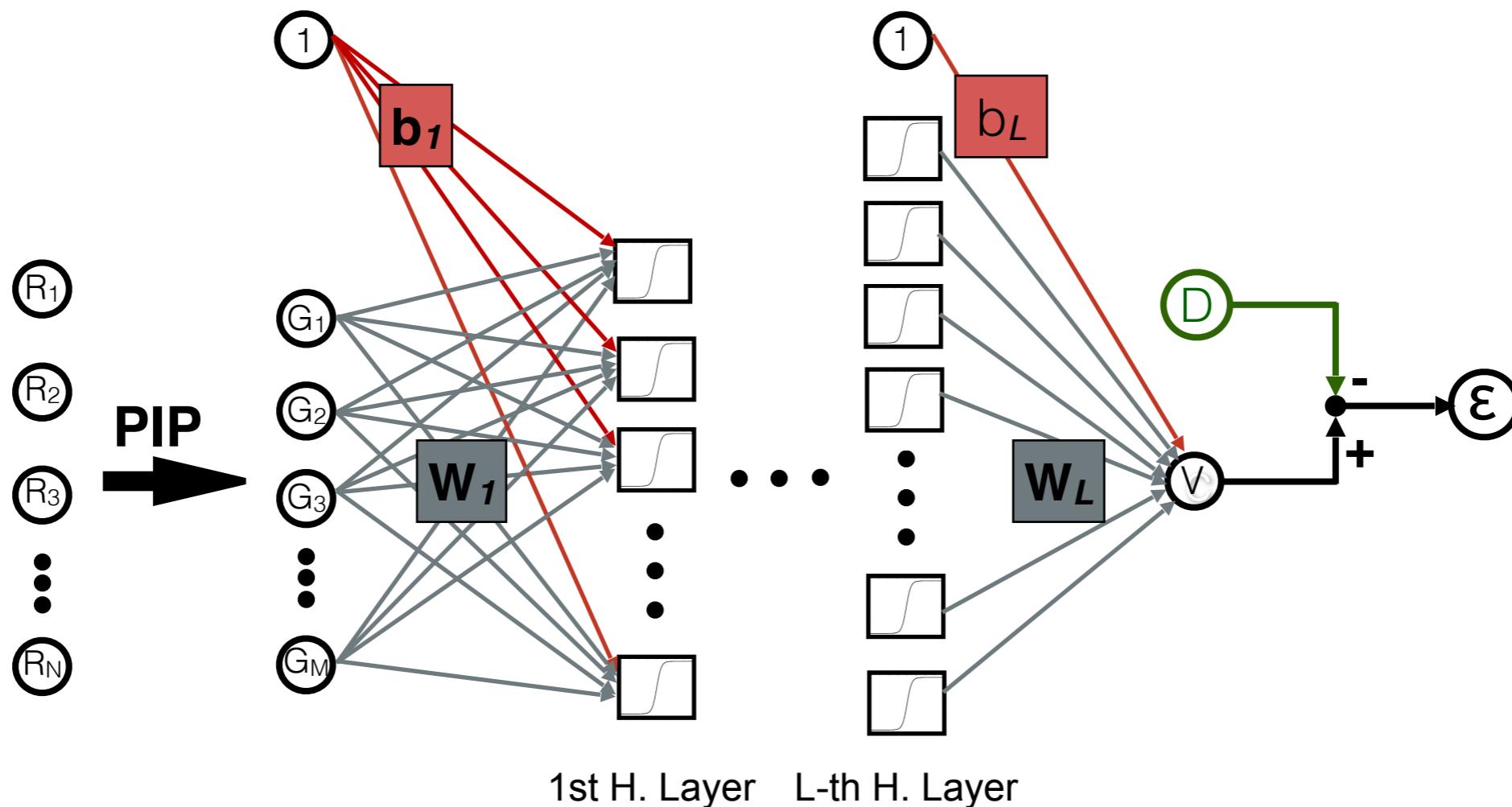
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3. E is compared with some ab-initio data (D), in order to estimate the error in the prediction (ε).

The values of W_i and b_i are then learnt through an optimization algorithm (e.g., adadelta, rmsprop, ...), which minimizes a loss function by cycles of forward propagations, error estimates and weights updates.

From Deterministic To Stochastic

In a classic approach to ML, the error is known only at the data points. What can we say about the reliability of the fit at a generic location?

Plus ... 3 main concerns about the deterministic PIP-NN deterministic approach ...

- ◆ The uncertainty on the data points (Schrödinger Eq. solutions) has not been taken into account;
- ◆ Overfitting Risk;
- ◆ Committee of Neural Networks can produce significantly different results:

No. of fit points N_{pts}	NN		GP	
	1 NN	$\langle 10 \text{ NN} \rangle$	1 GP	$\langle 10 \text{ GP} \rangle$
313	198.00/103.93/87.77	119.11/53.97/43.90	29.09	17.18
625	21.12/12.91/12.03	13.36/7.52/6.53	5.98	3.87
1250	9.29/5.74/4.38	5.74/3.36/2.54	2.17	1.13
2500	4.59/2.43/1.12	2.27/1.23/0.86	1.08	0.62

Fig.1: RMSEs for multiple NN configurations. From: “Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy”, J. Chem. Phys. 148, March 2018

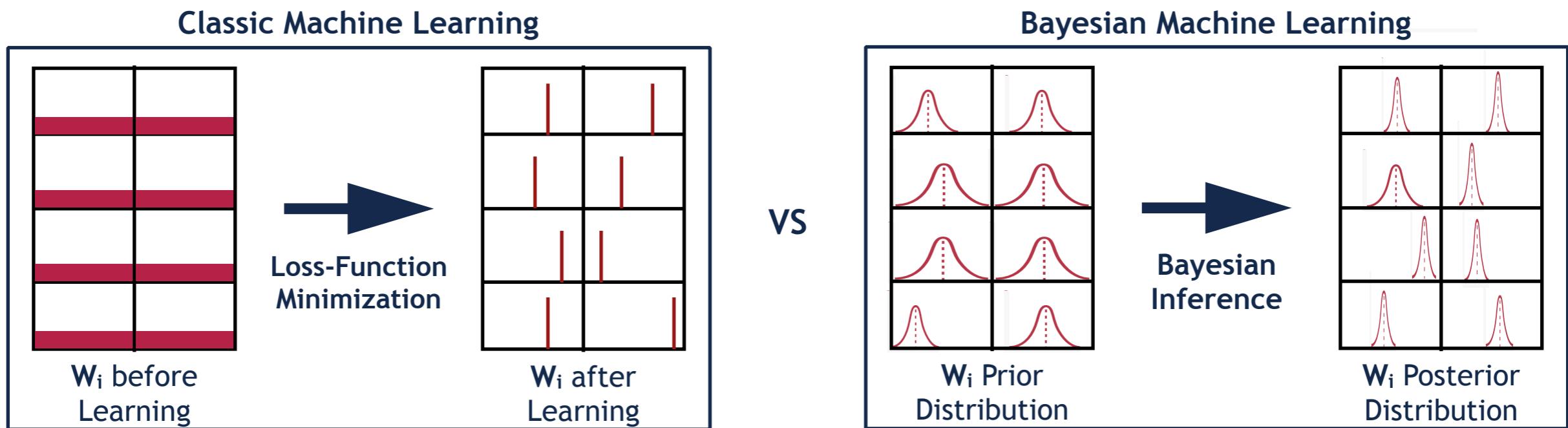
From Deterministic To Stochastic

We propose the construction of a **stochastic PES**, which condenses the inaccuracy content related to both the grid of atom configuration chosen and the fitting function adopted.

Thus, we extend the ANN to **Bayesian Neural Networks (BNNs)**, following the work initiated by R. Neal and recently pursued by C. Blundell *et al.*

Non-Deterministic attribute of BNNs is a consequence of:

- ◆ Functional parameters treated as random variables (parameter uncertainty):



Bayes Theorem:

$$\frac{p(\mathbf{W}_i, \mathbf{b}_i | D, M)}{\text{Posterior}} \propto \frac{p(D | \mathbf{W}_i, \mathbf{b}_i, M) p(\mathbf{W}_i, \mathbf{b}_i | M)}{\text{Likelihood} \quad \text{Prior}}$$

Prior: $p(\mathbf{W}_i, \mathbf{b}_i | M) \sim \mathcal{N}(\mu = \dots, \sigma = \dots)$

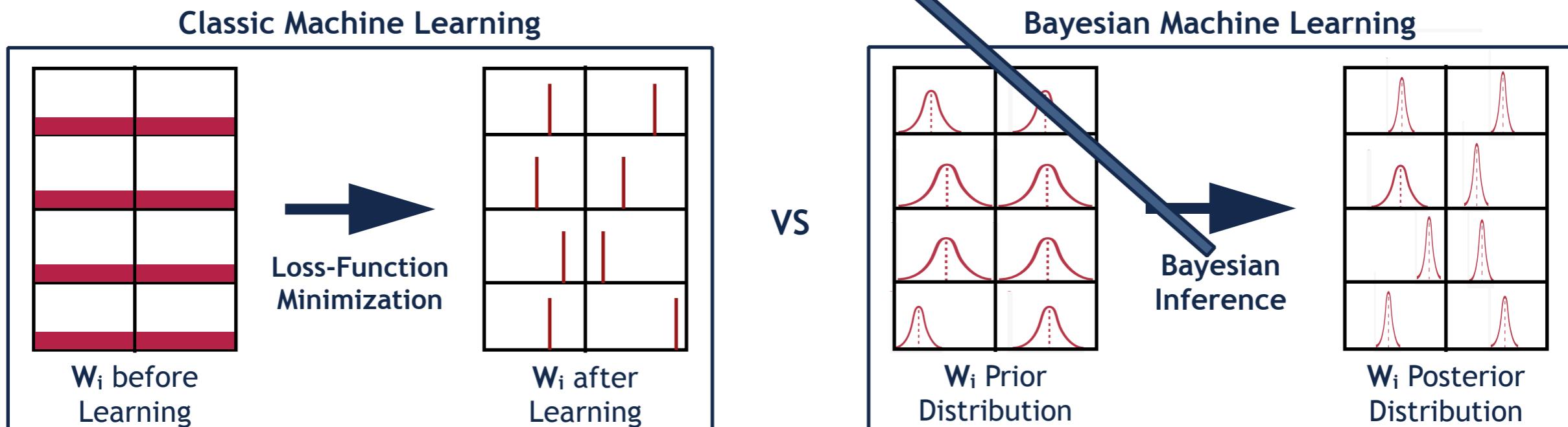
$$\text{Likelihood: } p(D | \mathbf{W}_i, \mathbf{b}_i, M) = \frac{1}{\sqrt{2\pi\sigma_L^2}} \exp\left(\sum_j \frac{(\log(V_j) - \log(D_j))^2}{2\sigma_L^2}\right)$$

Posterior distributions have been computed through the Automatic Differentiation Variational Inference (ADVI) algorithm.



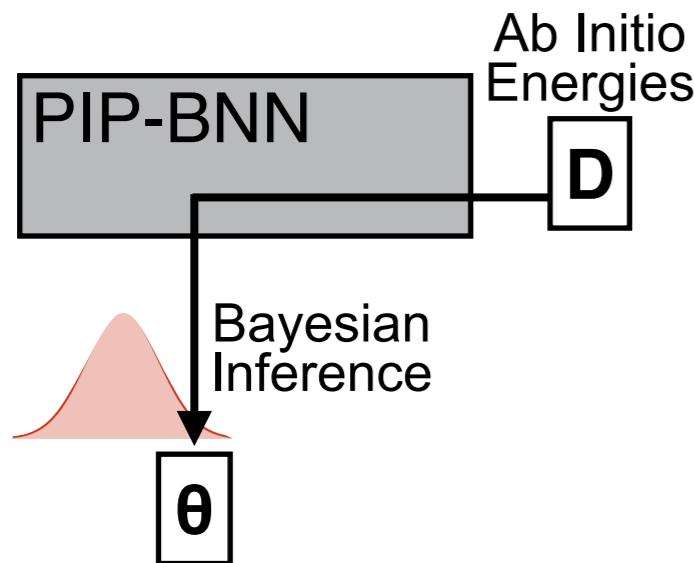
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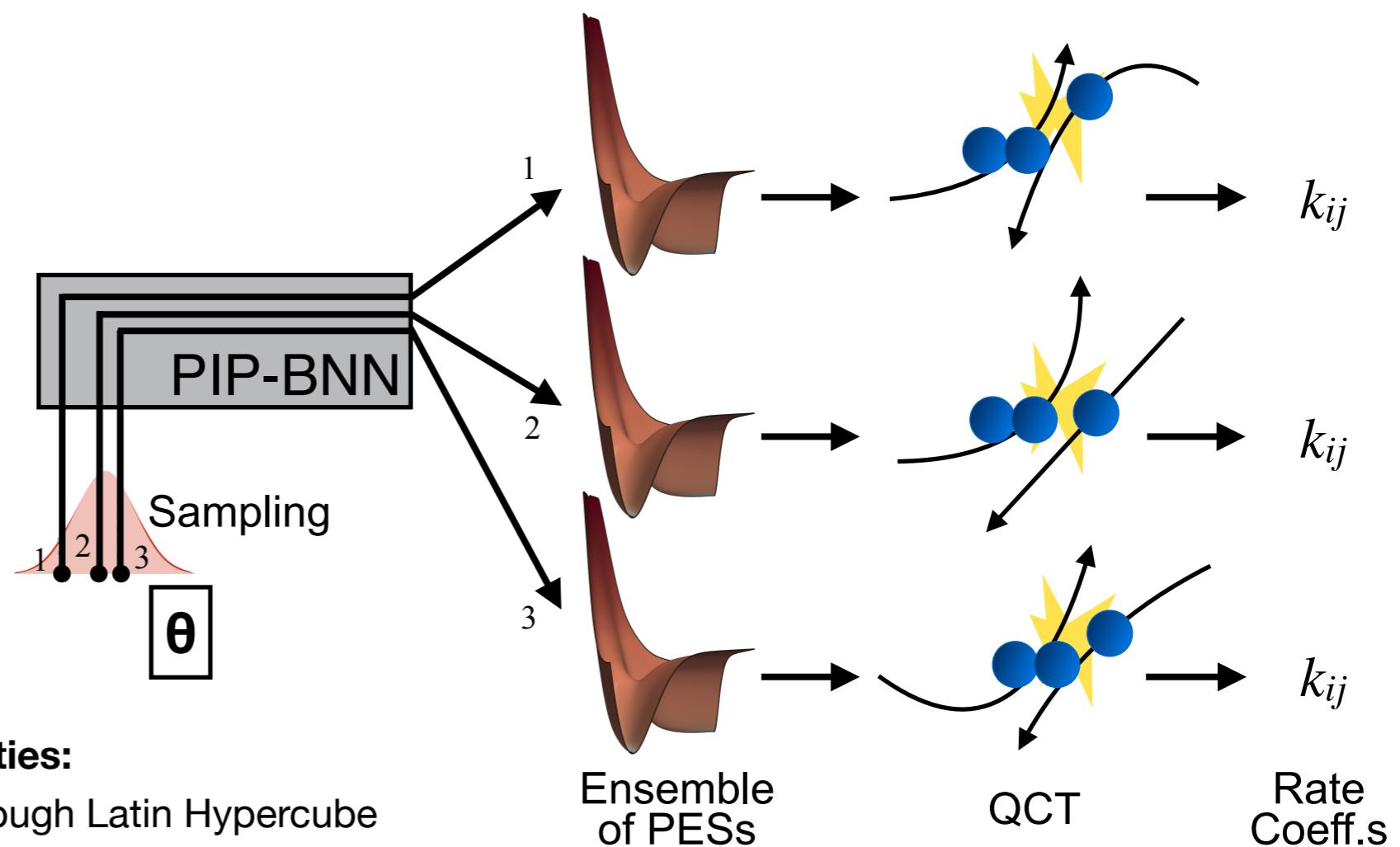
- ◆ Some noise superimposed to the functional form (model uncertainty).

PES UQ: Methodology



Solution of the inverse problem:

The optimal PDFs characterizing the PIP-BNN parameters are learnt through Bayesian variational inference from the ab initio data points.

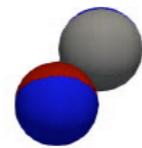
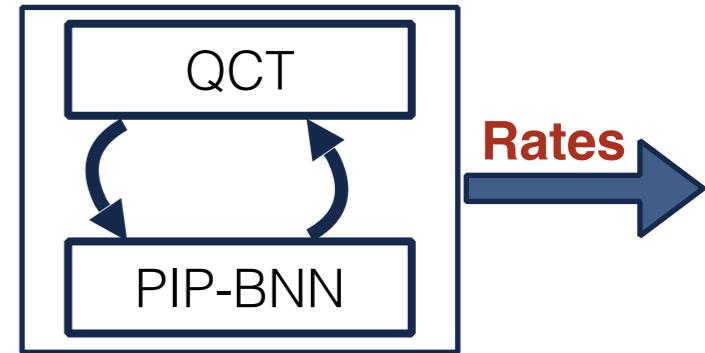


Forward propagation of the Uncertainties:

The posterior distribution is sampled through Latin Hypercube Sampling, an ensemble of PESs is computed through the PIP-BNN, and the surfaces are used for simulating collisions.

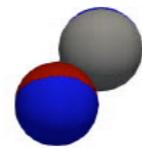
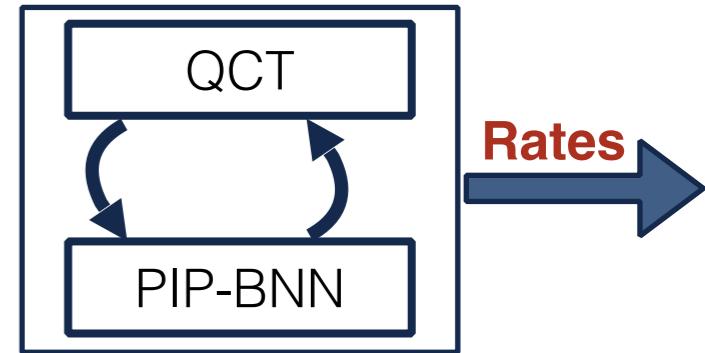
From Deterministic To Stochastic

The PIP-BNN Potential Energy Surface has been implemented in I-VVTC QCT Code.



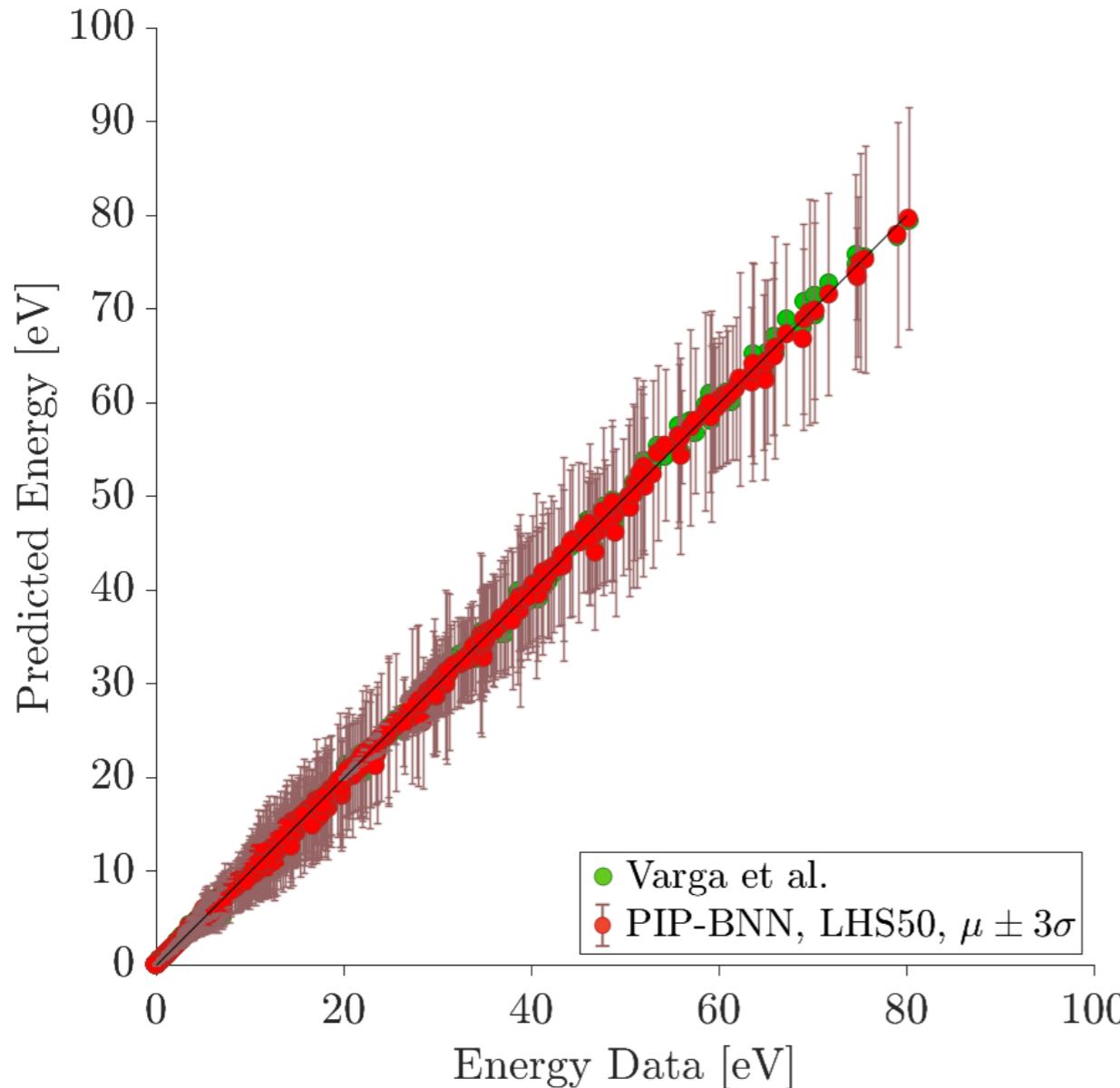
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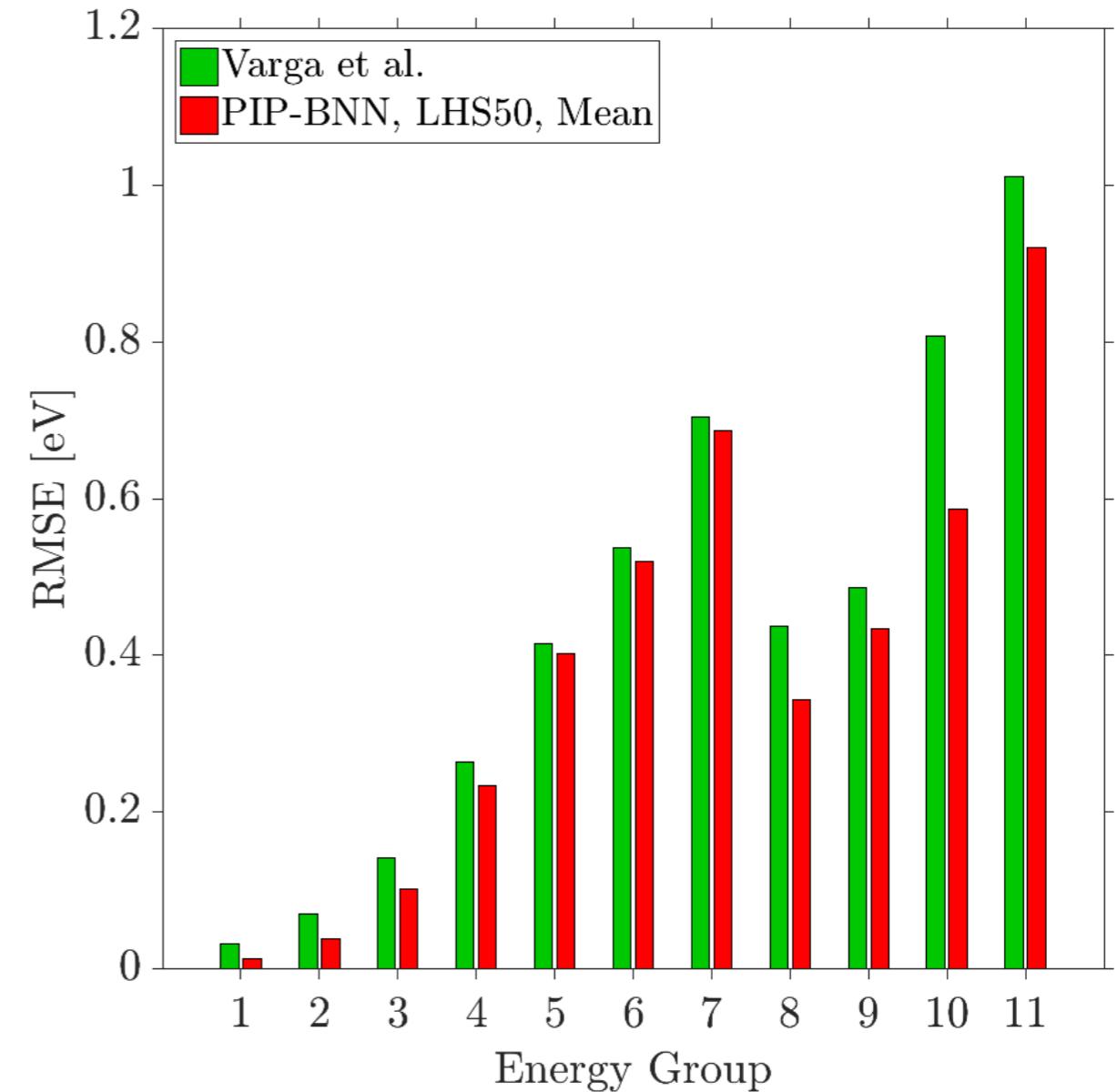


Results

As test cases, we selected 2 of the 9 O₂+O PESs developed by Varga et al. We used their same data points (~ 1600 configurations and ab initio energies), and we solved the Inverse problem. Plotted here are the results for one of the quintet PESs (with degeneracy 5/27).



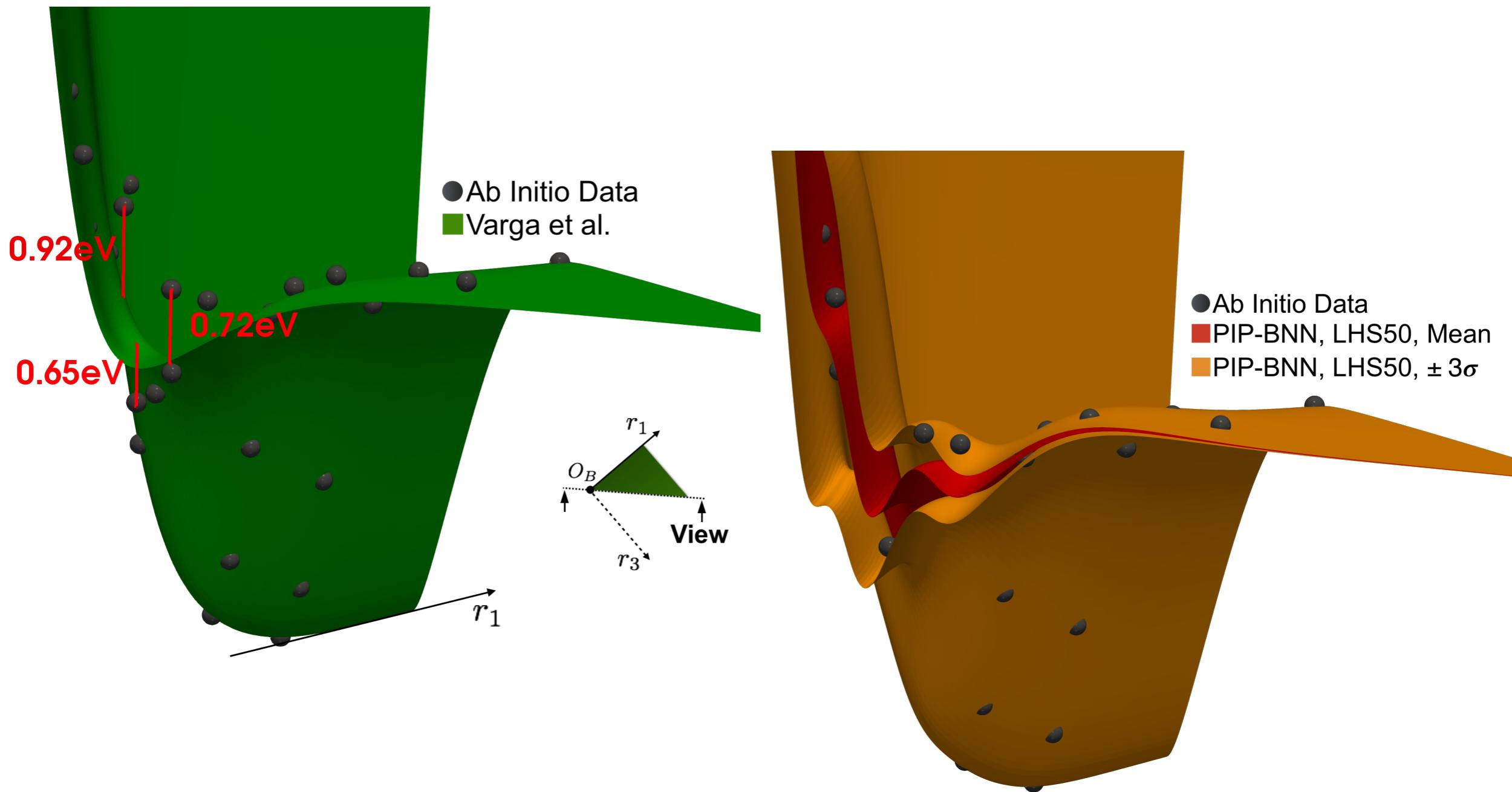
Means (red dots) and three-sigma confidence intervals (red lines) of the potential energies computed at the 1617 data points using the 50 PIP-BNN samples, compared to the energies resulting from Varga et al.'s fits (green dots).



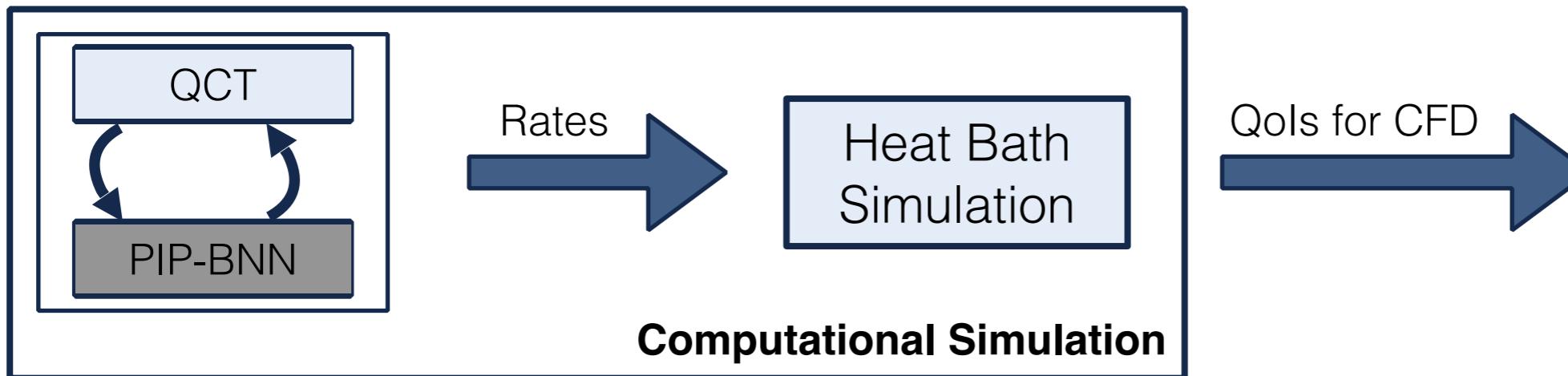
In green, the errors produced by Varga et al.'s fits; in red, the ones generated by the means of 50 PIP-BNN samples. Upper bounds of the groups: VMax = {2:0; 4:0; 6:0; 8:0; 10:0; 15:0; 20:0; 25:0; 30:0; 50:0; 100:0} eV.

Results

3D views of the PESs at $O_AO_BO_C = 50^\circ$ for $r_1 > r_3$, compared to the correspondent ab initio data points (black dots). The green surface represents the original fit, the red one identifies the mean of the 50 PIP-BNN samples, while the orange ones correspond to the bounds of the 3-sigma confidence intervals generated by such samples.

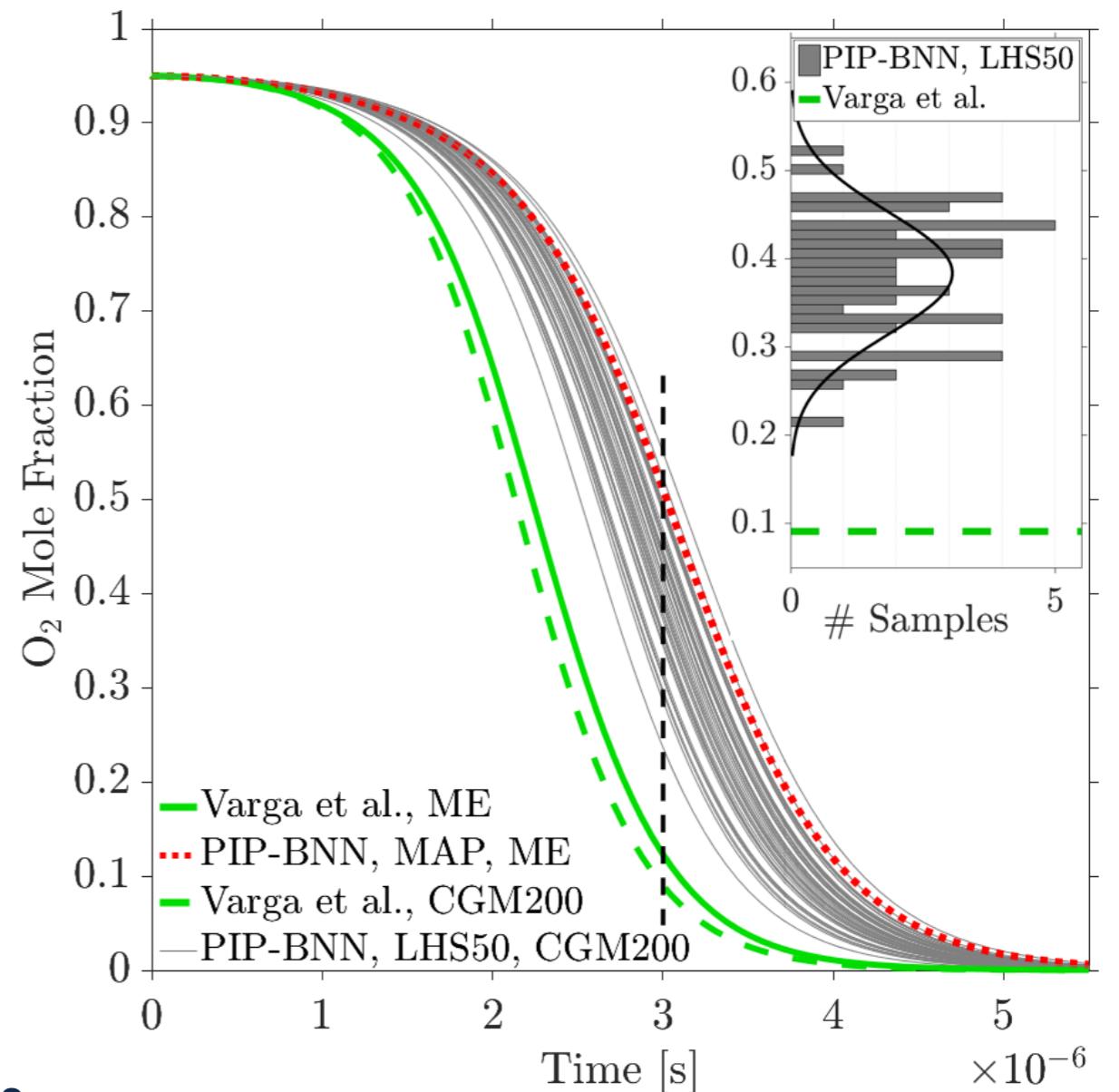


Results

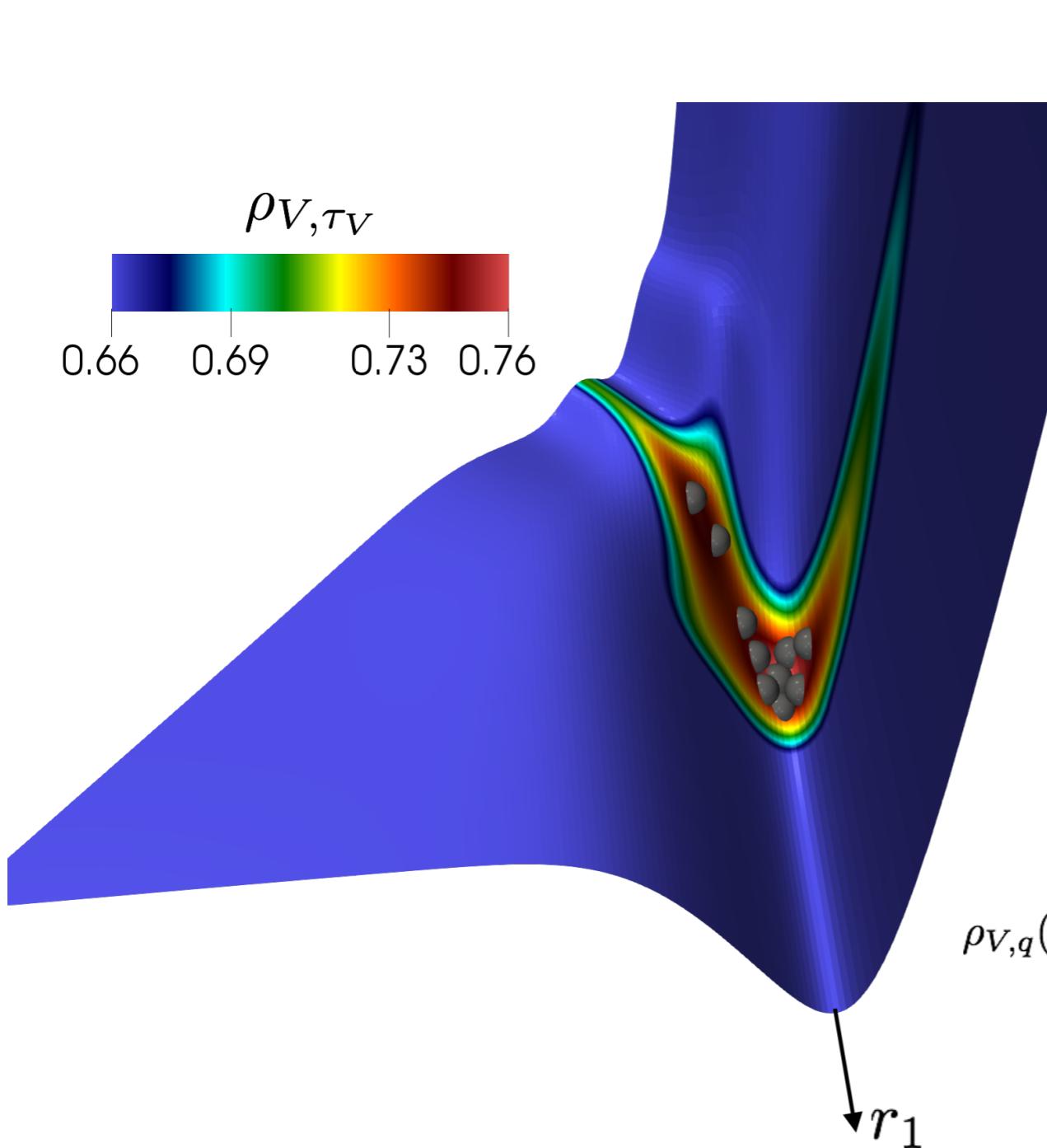


The PESs have been used for computing rates, that have then been employed in a Master Equation study of heat baths at fixed translational temperatures (for the plot on the right, $T_{\text{Tran}} = 10,000\text{K}$).

The PIP-BNN 99.99% confidence interval spans an interval of $\pm 45\%$ the expected value, and it does not contain the predictions from the original fit

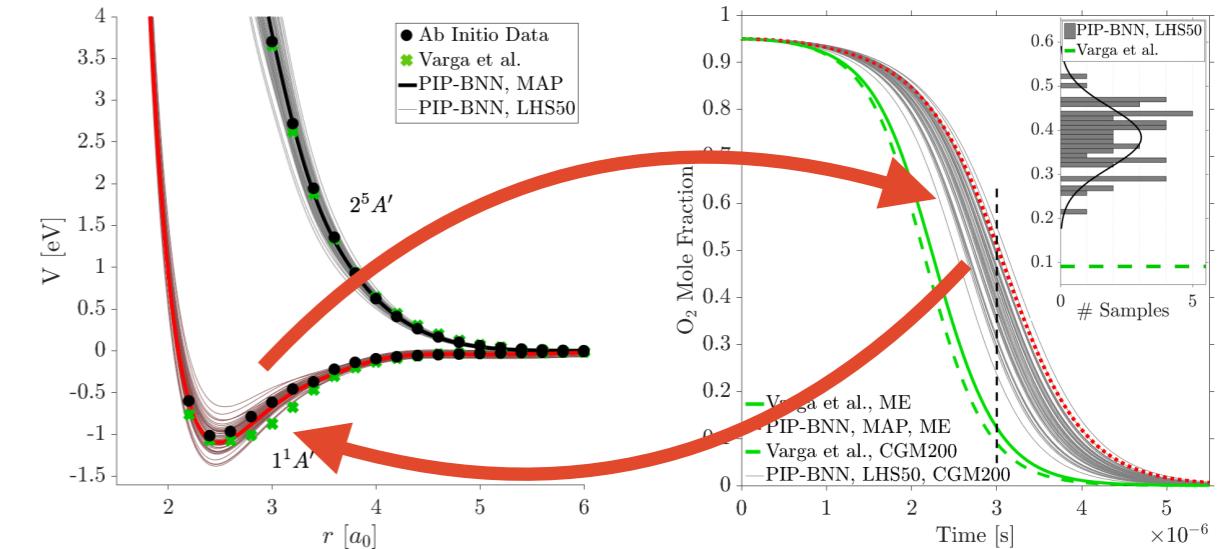


Results



By **correlating** the PES to the QoI, we can understand in **what areas the uncertainties on the surface** affect the most the accuracy of our prediction.

We can **sample points** from those regions, and generate new ab initio data for improving the accuracy of the PES.



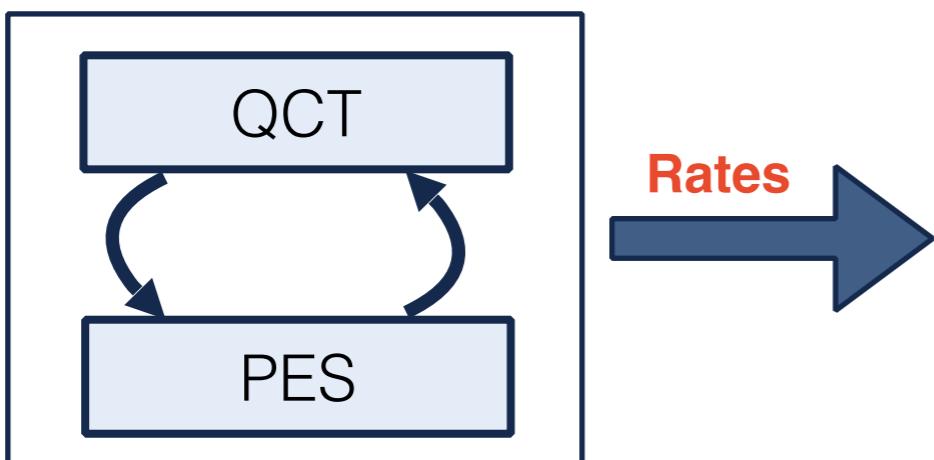
Pearson Correlation Coefficient:

$$\rho_{V,q}(r_1, r_2, r_3) = \frac{\sum_{j=1}^{N_{LHS}} (V_{LHS}^j - \bar{V}_{LHS})(q^j - \bar{q})}{\sqrt{\sum_{j=1}^{N_{LHS}} (V_{LHS}^j - \bar{V}_{LHS})^2 \sum_{j=1}^{N_{LHS}} (q^j - \bar{q})^2}}$$

Conclusions

Main steps:

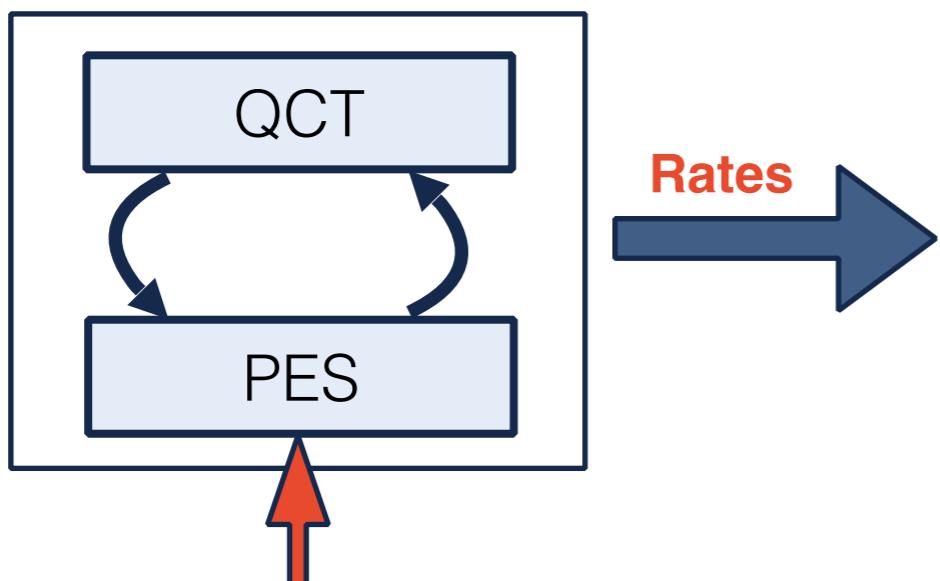
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- [Constructing surrogate models];
- **Calibrating** Parameters and hyperparameters;
- Performing the **reductions** of the downstream **models (when possible)**;
- **Forward propagating** of the (approximated) posterior distribution;
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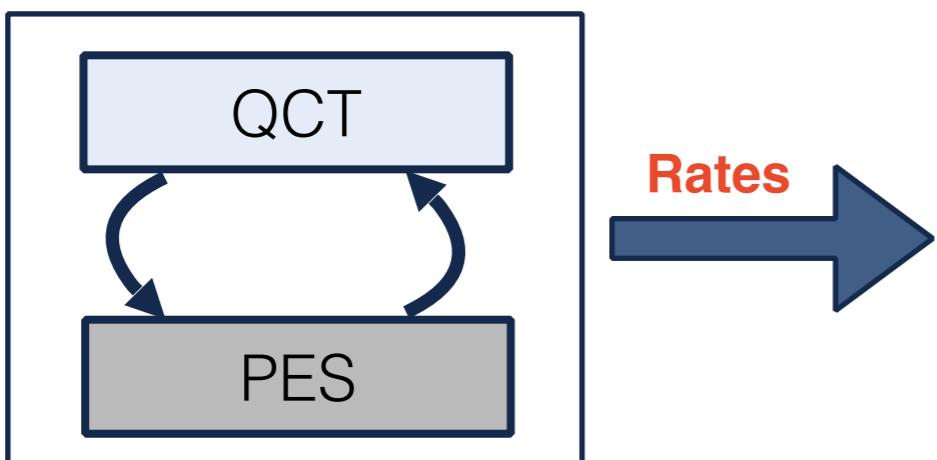
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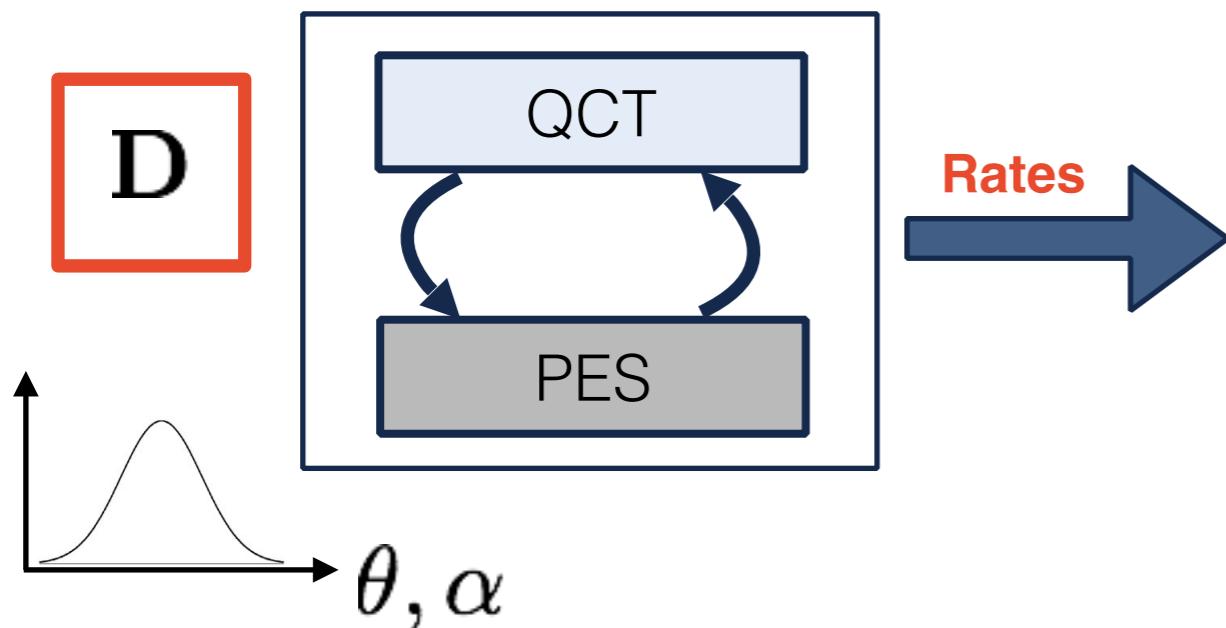
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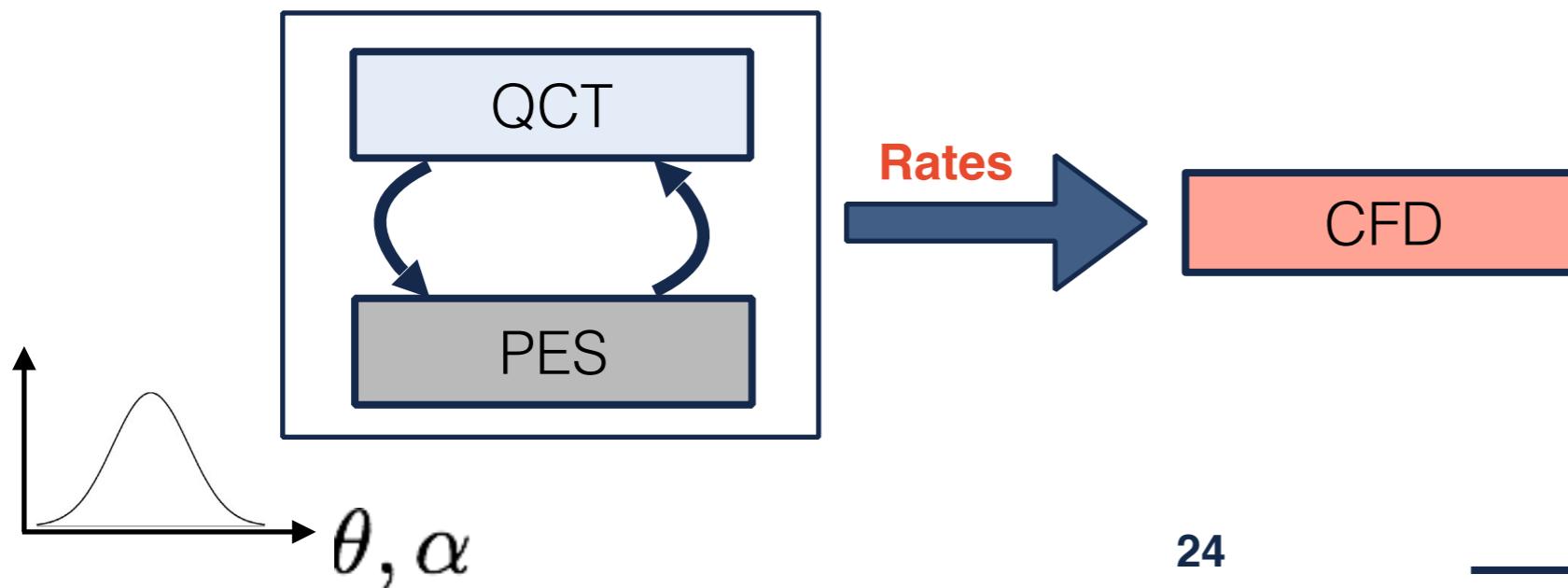
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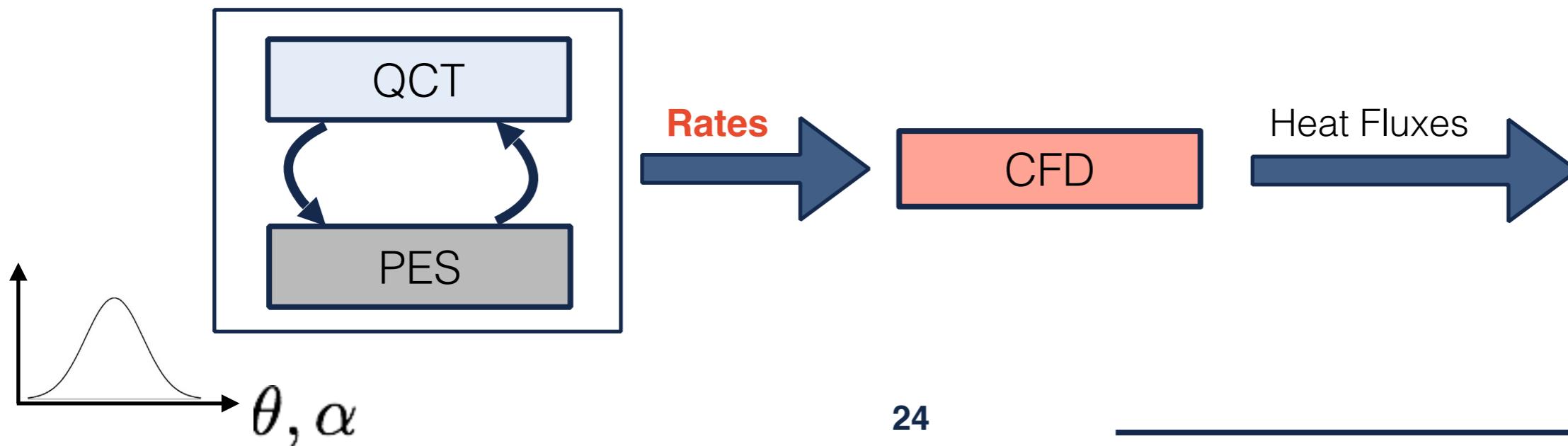
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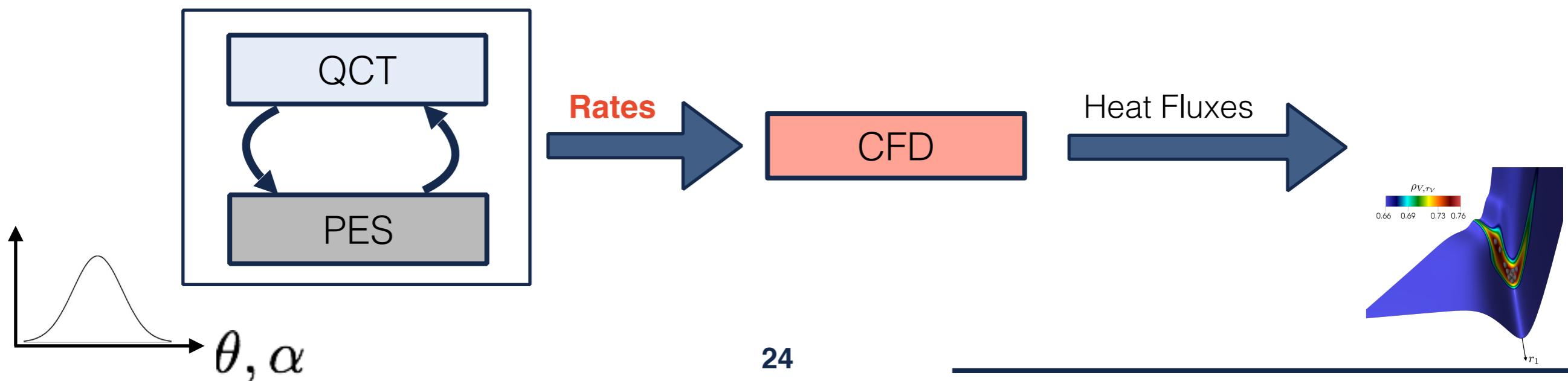
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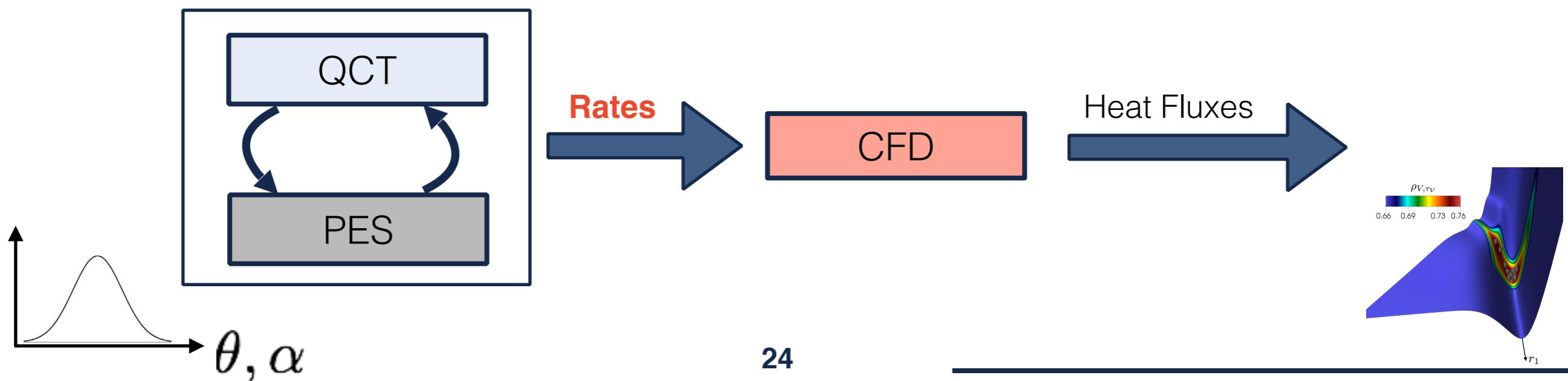
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Conclusions

- The big picture stands out (System Engineering Point of View)

- The black boxes must be opened (Scientific Understanding)

Choices need to be made for:

- Priors
 - Inadequacy Models
 - Domains of Applicability
 - Unknown Unknowns?
 - When to Ask for more Data, and What to Ask
- ...

- The curse of dimensionality is not an enemy (Recall to Efficiency)

- Sensitivity Analysis
 - Code Optimization
 - Model Reduction
- ...

Questions?

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