An Introduction to Uncertainty Quantification for Predictive Science Part II

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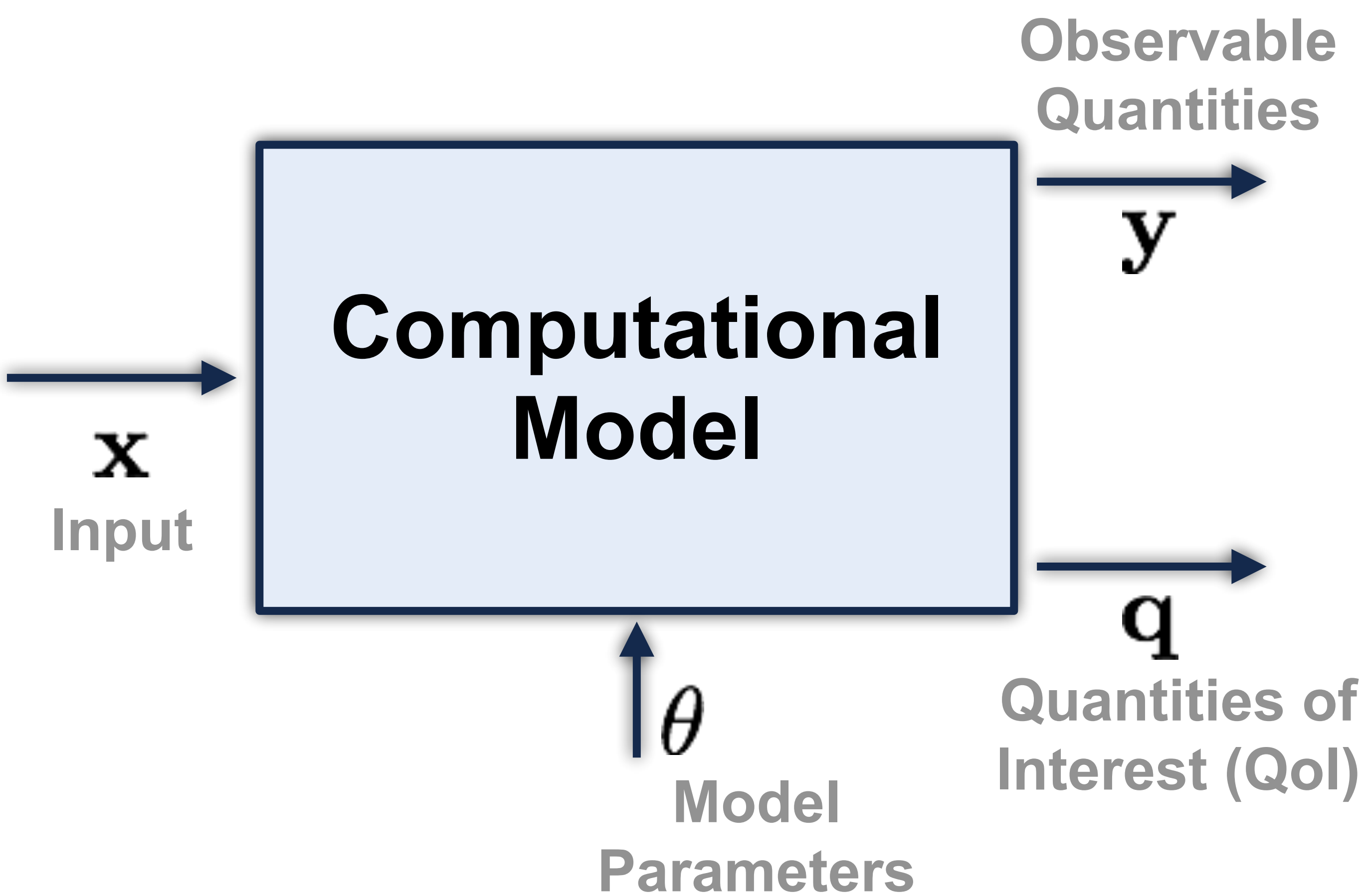
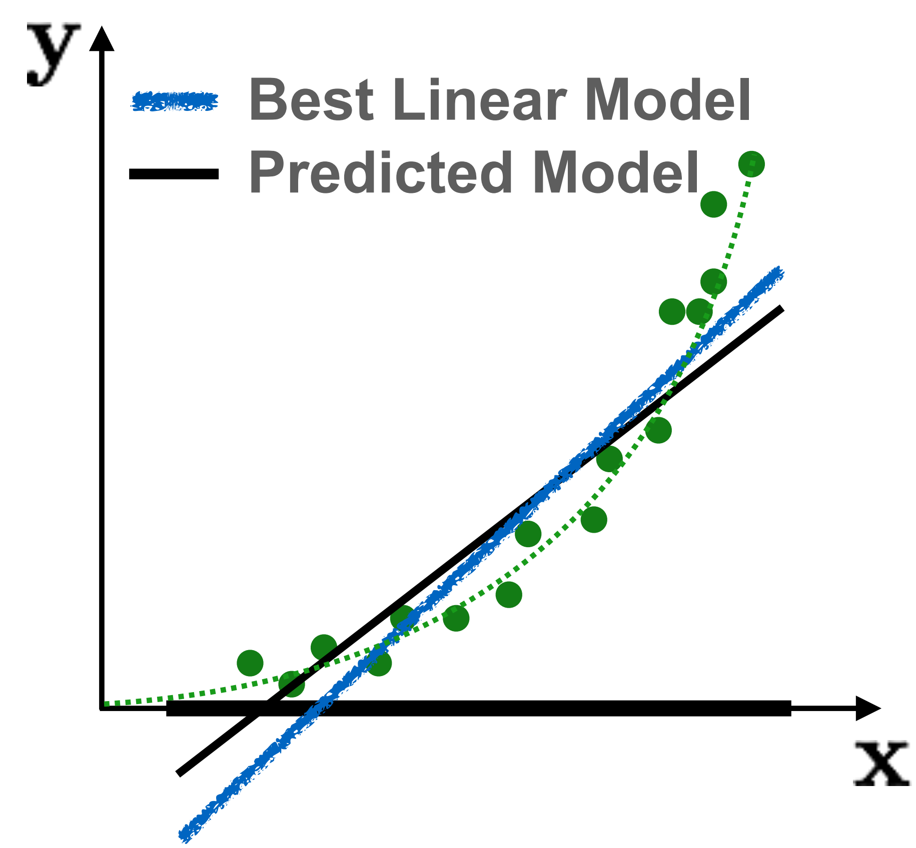
Prof. Panesi's UQ Class, Fall 2019
September, 6th

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

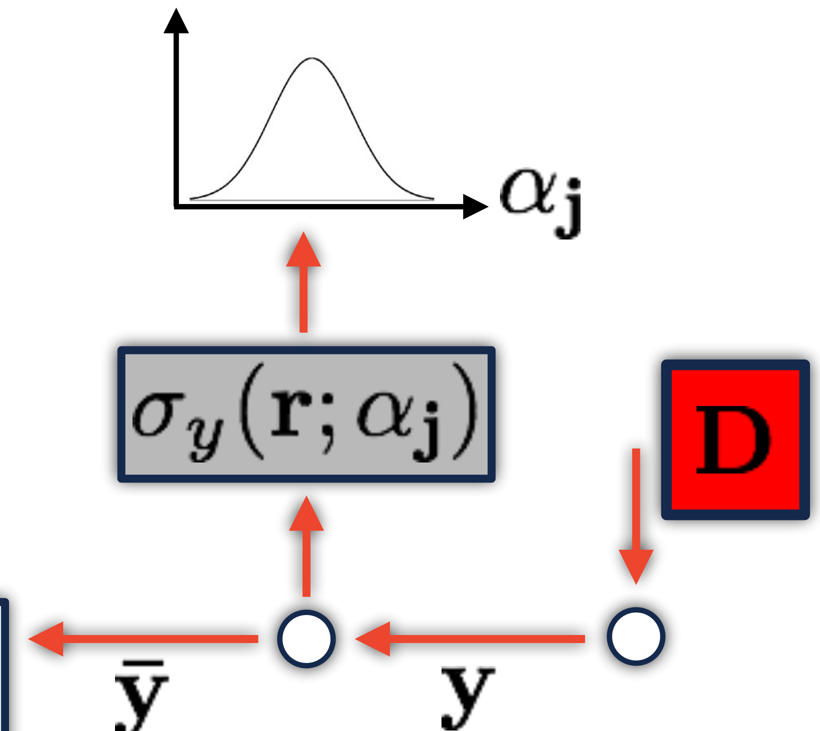
Due to Embedded Model!

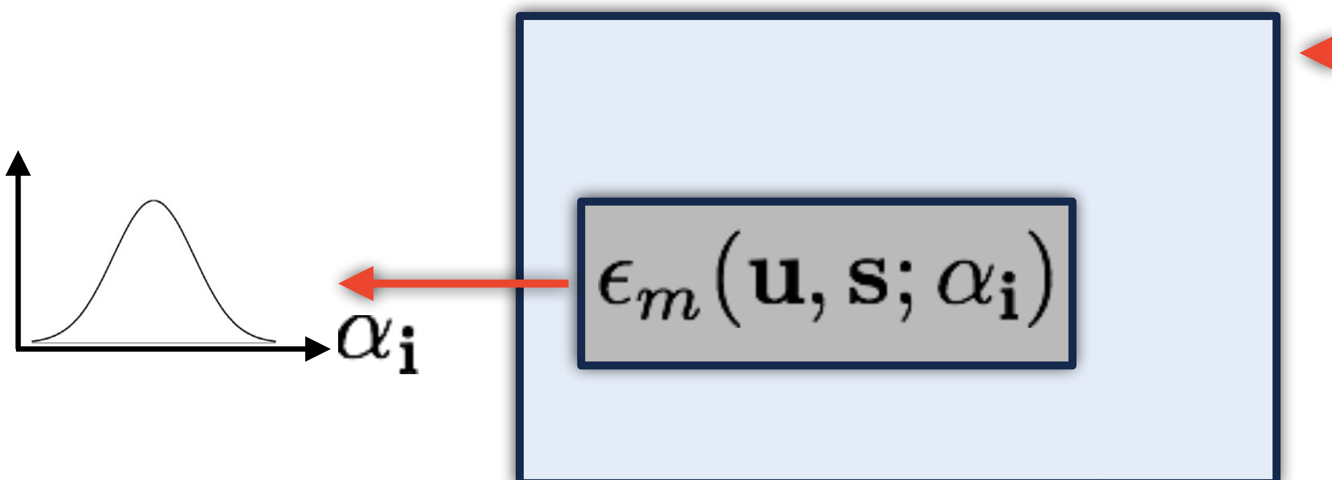
[1] Oliver et al., "*Validating Predictions of Unobserved Quantities*", Computer Methods in Applied Mechanics and Engineering, Vol. 283, 2015.

Last Class …

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

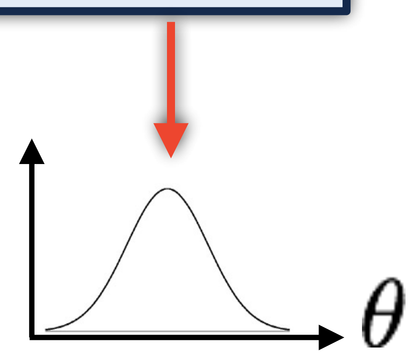
The model is **informed by data.** Parameter values and their uncertainties are inferred from available observations by **solving an inverse problem.**





~ Information

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



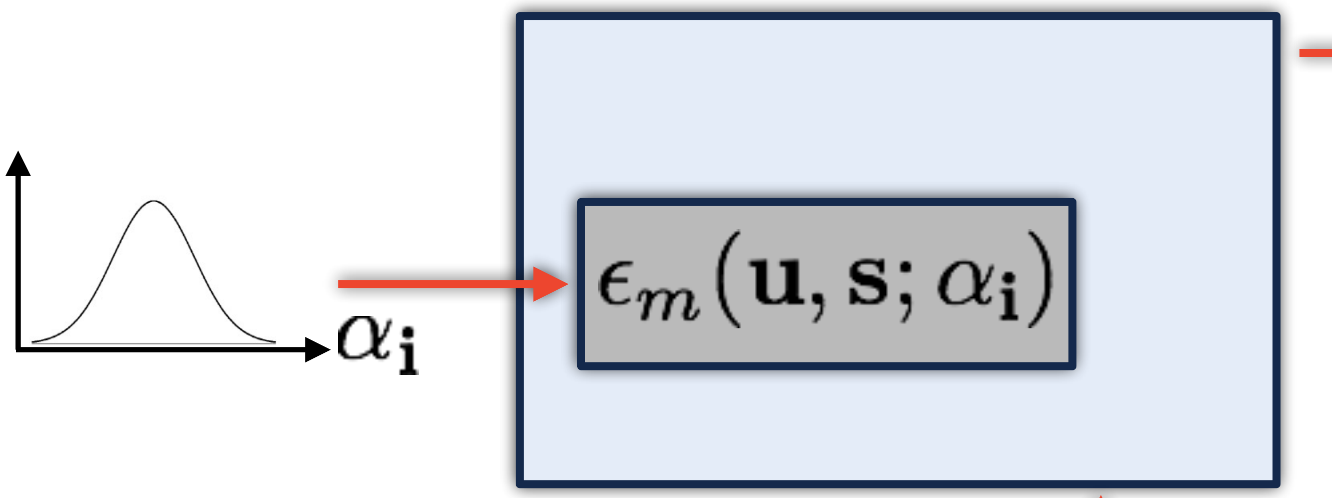
Posterior, Likelihood, Prior

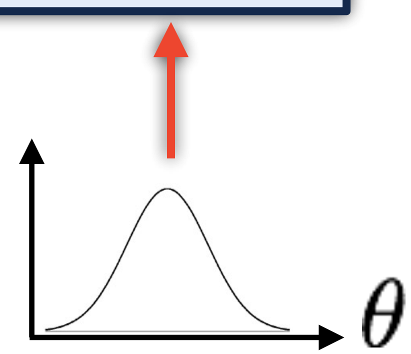
$$p(\theta,\alpha|\mathbf{D},\mathcal{M}) = \frac{\mathcal{L}(\theta,\alpha;\mathbf{D},\mathcal{M})\ \mathbf{p}(\theta,\alpha|\mathcal{M})}{\int \mathcal{L}(\theta,\alpha;\mathbf{D},\mathcal{M})\ \mathbf{p}(\theta,\alpha|\mathcal{M})\ \mathbf{d}\theta\mathbf{d}\alpha}$$

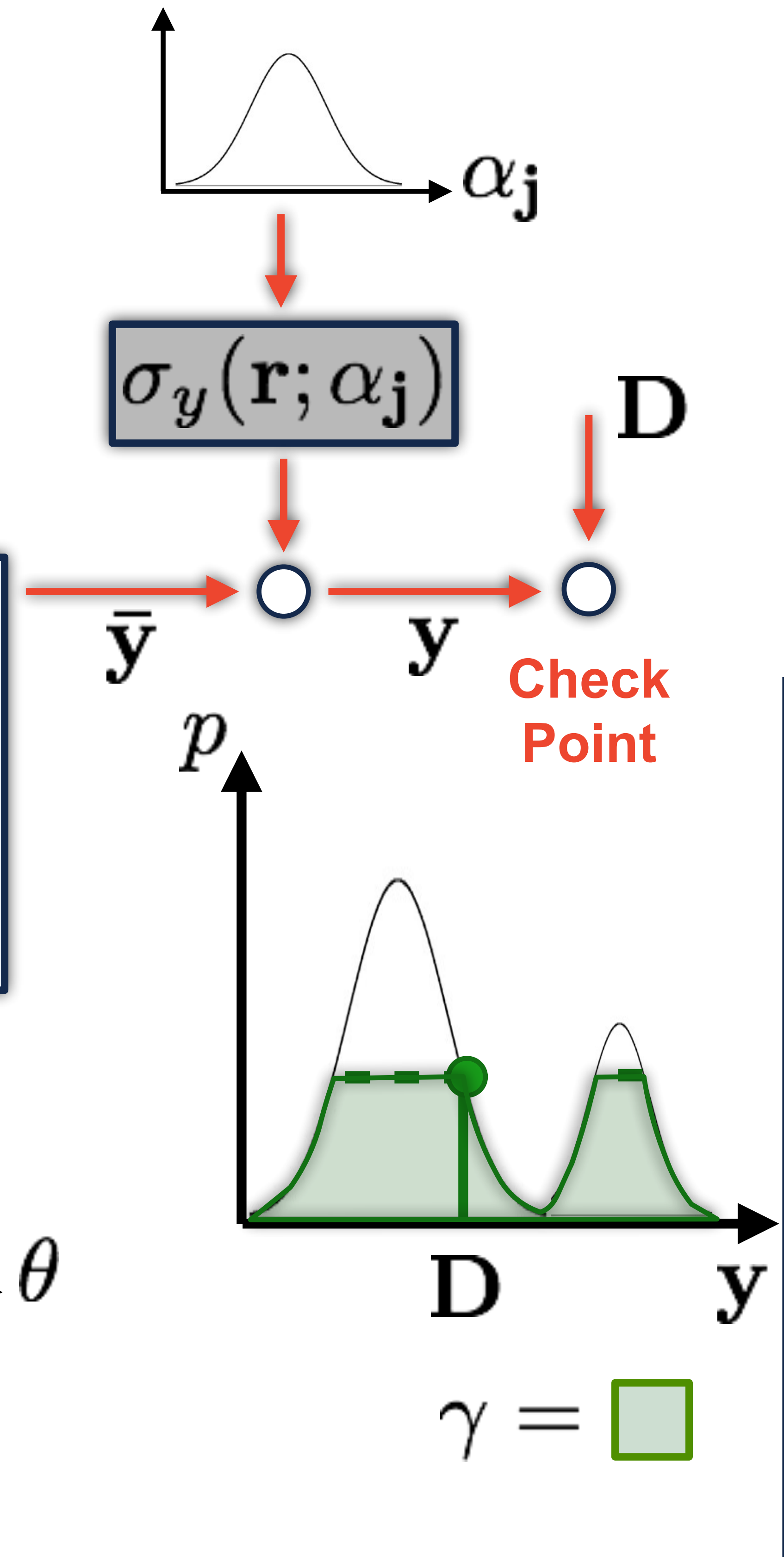
Last Class ...

- Calibration
- <u>Validation</u>
- 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**
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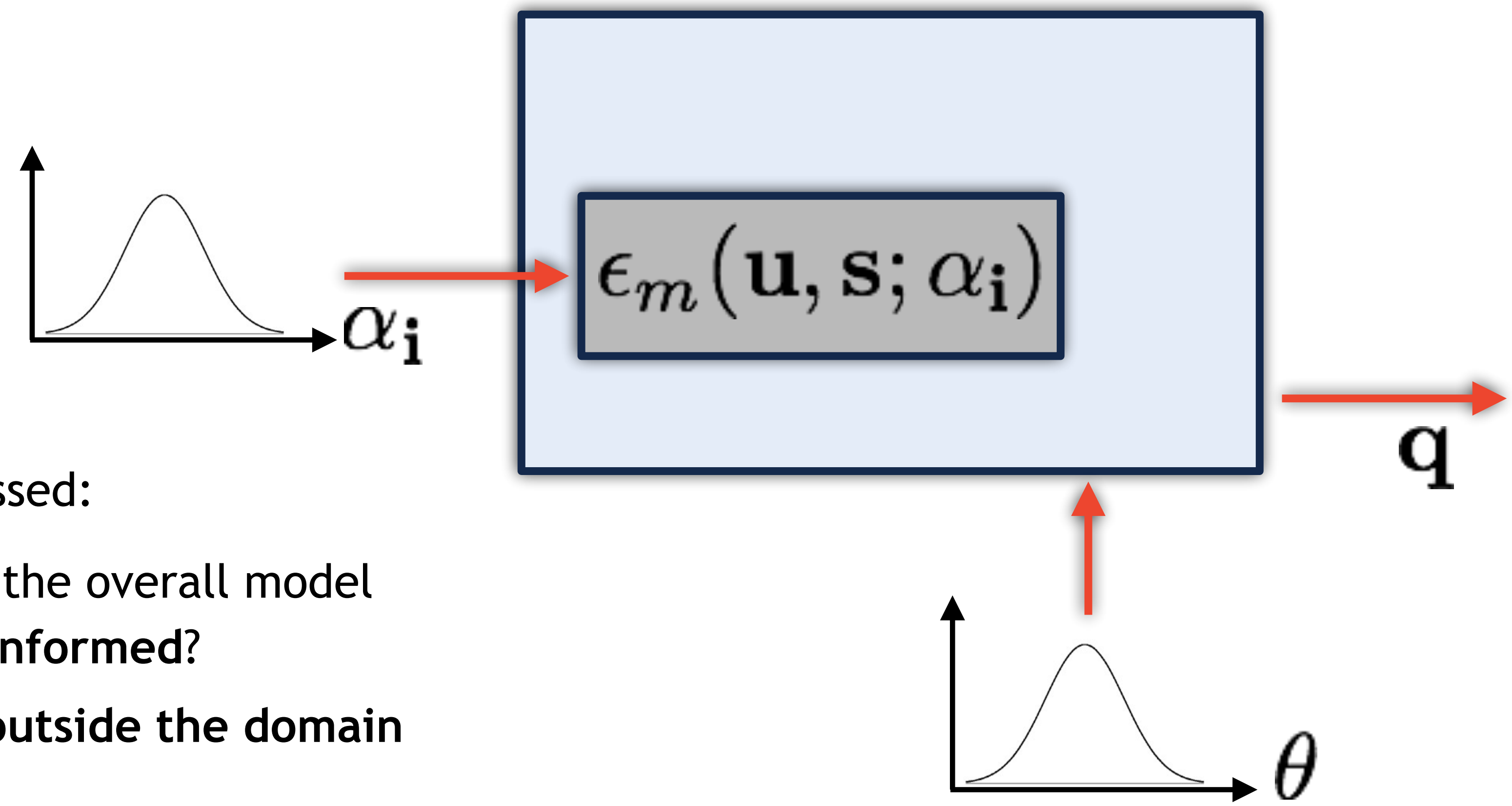
Determines whether the calibration and validation phases were sufficiently informative and challenging to provide confidence in the reliability of the predictions of the QoIs.



Two primary questions need to be addressed:

- Are **QoIs 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 …

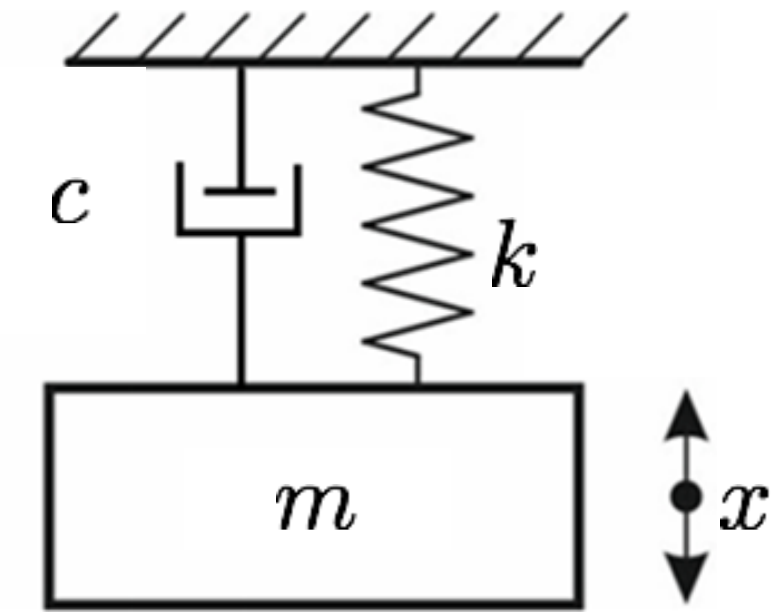
Example: Mass-Spring-Damper, Real World System

Reliable Physical Theory

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

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

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



Real World Embedded Model

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

$$\boxed{\begin{aligned} k &= \text{const} \\ c(T) &= \exp\left(\frac{T_0}{T} - 1\right) \\ \dot{T} &= c(T)\dot{x}^2 - \frac{T - T_0}{t_T} \end{aligned}}$$

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

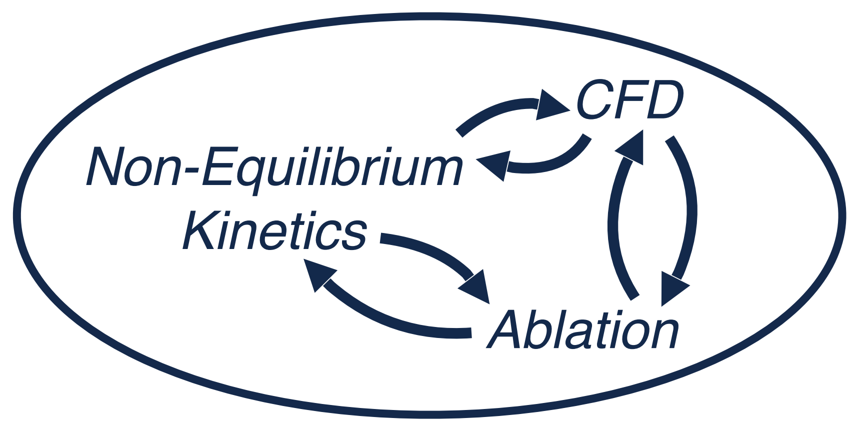
$$\boxed{\begin{aligned} \mathbf{y} &= x \\ \mathbf{q} &= \max(\dot{x}) \end{aligned}}$$

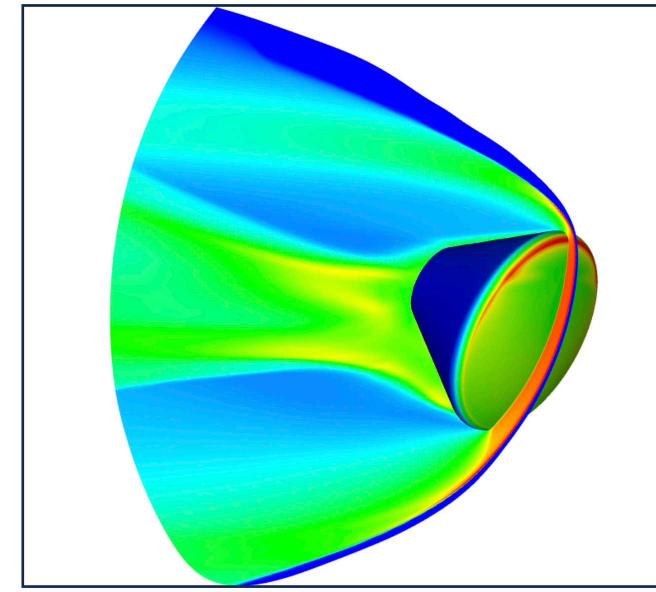
A Bayesian Neural Network Approach to the Quantification of Uncertainties on Ab Initio Potential Energy Surfaces

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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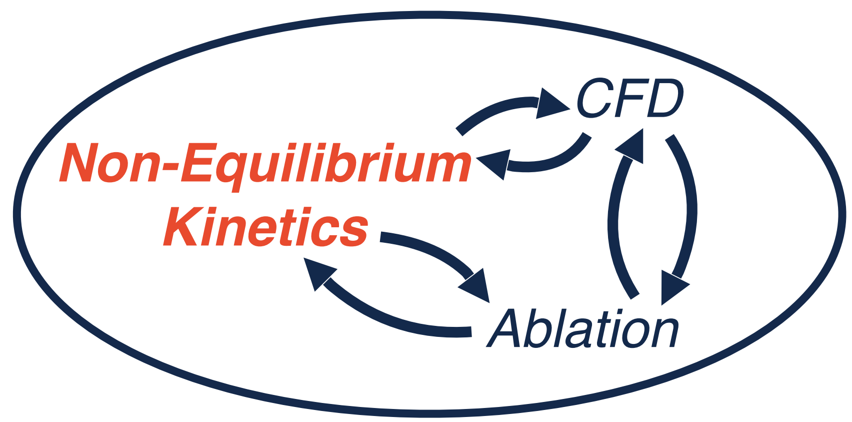

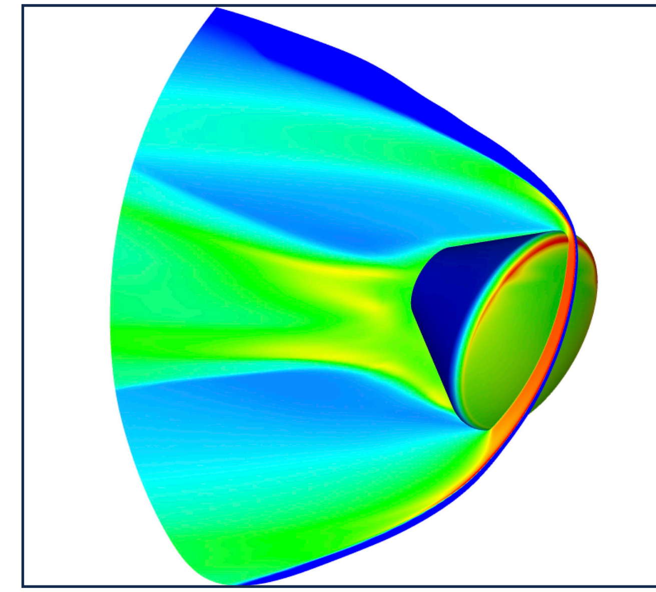

Courtesy of NASA

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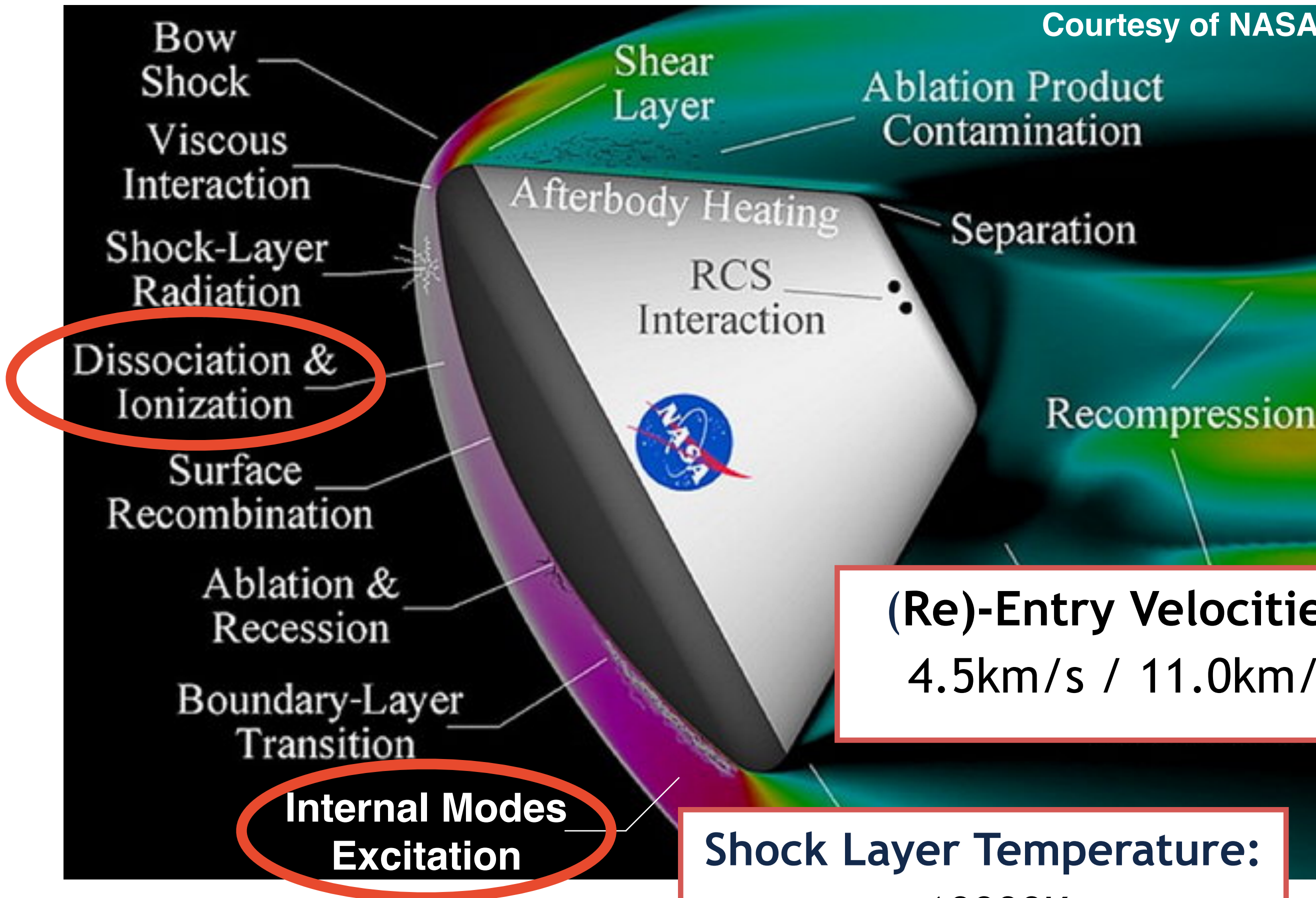
Motivation: Non-Equilibrium Flows



(Re)-Entry Velocities:
4.5km/s / 11.0km/s

Shock Layer Temperature:
~10000K

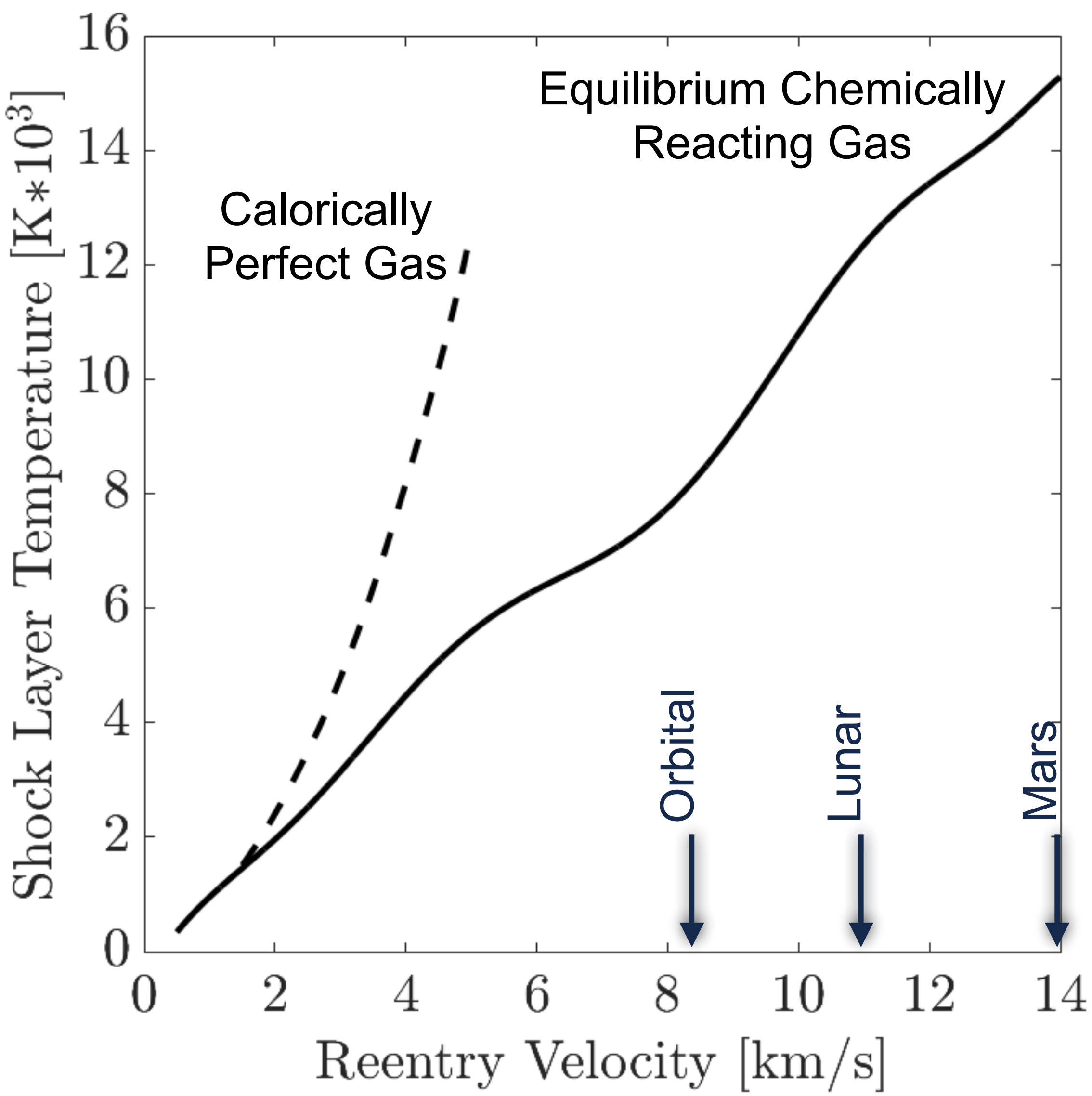
- The mixture is **thermally and chemically reacting**, and the fluid in the shock layer cannot be modeled as a perfect gas.
- It is necessary to understand how the energy of the flow is stored in its internal modes and is affected by the chemistry.
- A resolution up to the atomic and molecular scale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

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

Molecular Collisions $\xrightarrow{\text{Rates}}$ CFD $\xrightarrow{\text{Heat Fluxes}}$

Computational Simulation

Motivation: Non-Equilibrium Flows



From J. D. Anderson, "*Hypersonic and High-temperature Gas Dynamics*", American Institute of Aeronautics and Astronautics, 2006.

Low accuracy on the non-ideal (+ non equilibrium) gas behavior in Computational Hypersonics

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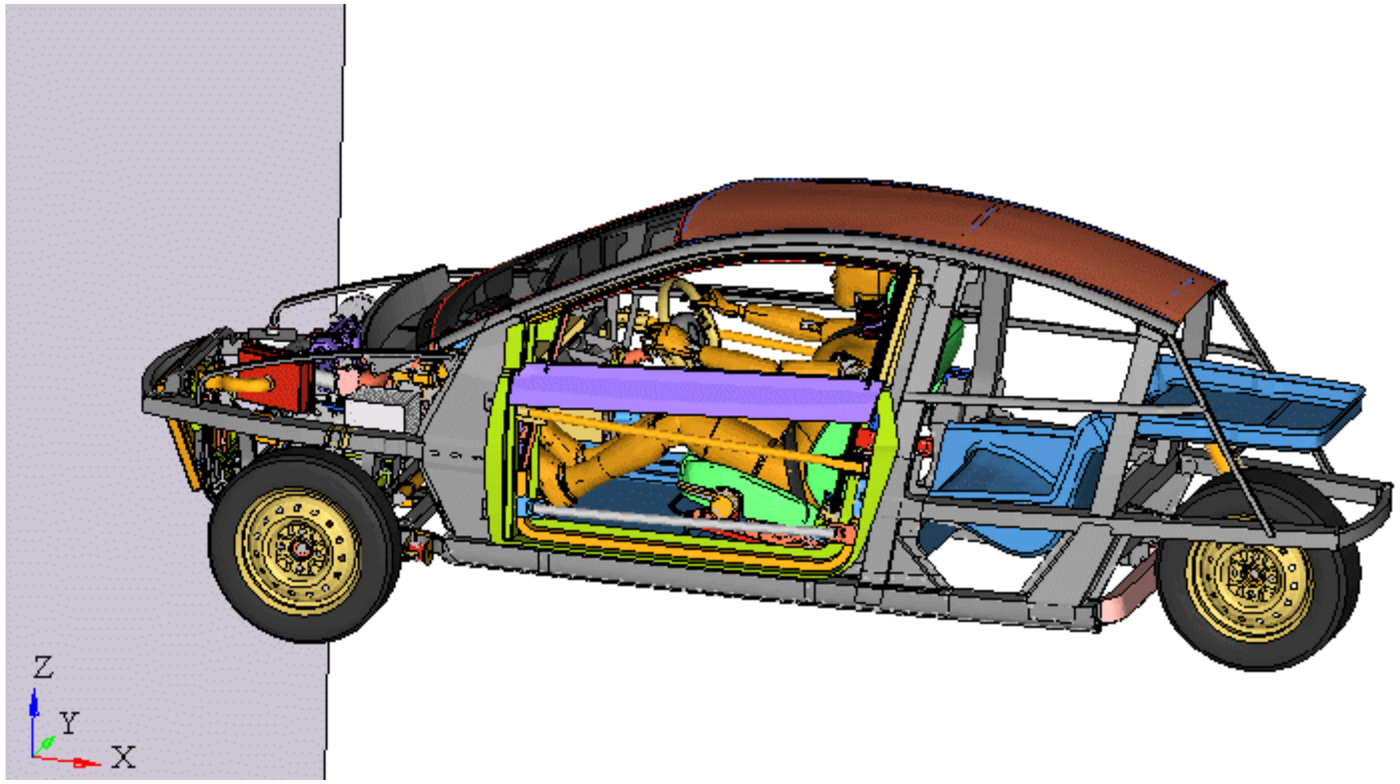
Low accuracy on deformations in a crash test Computational Simulation



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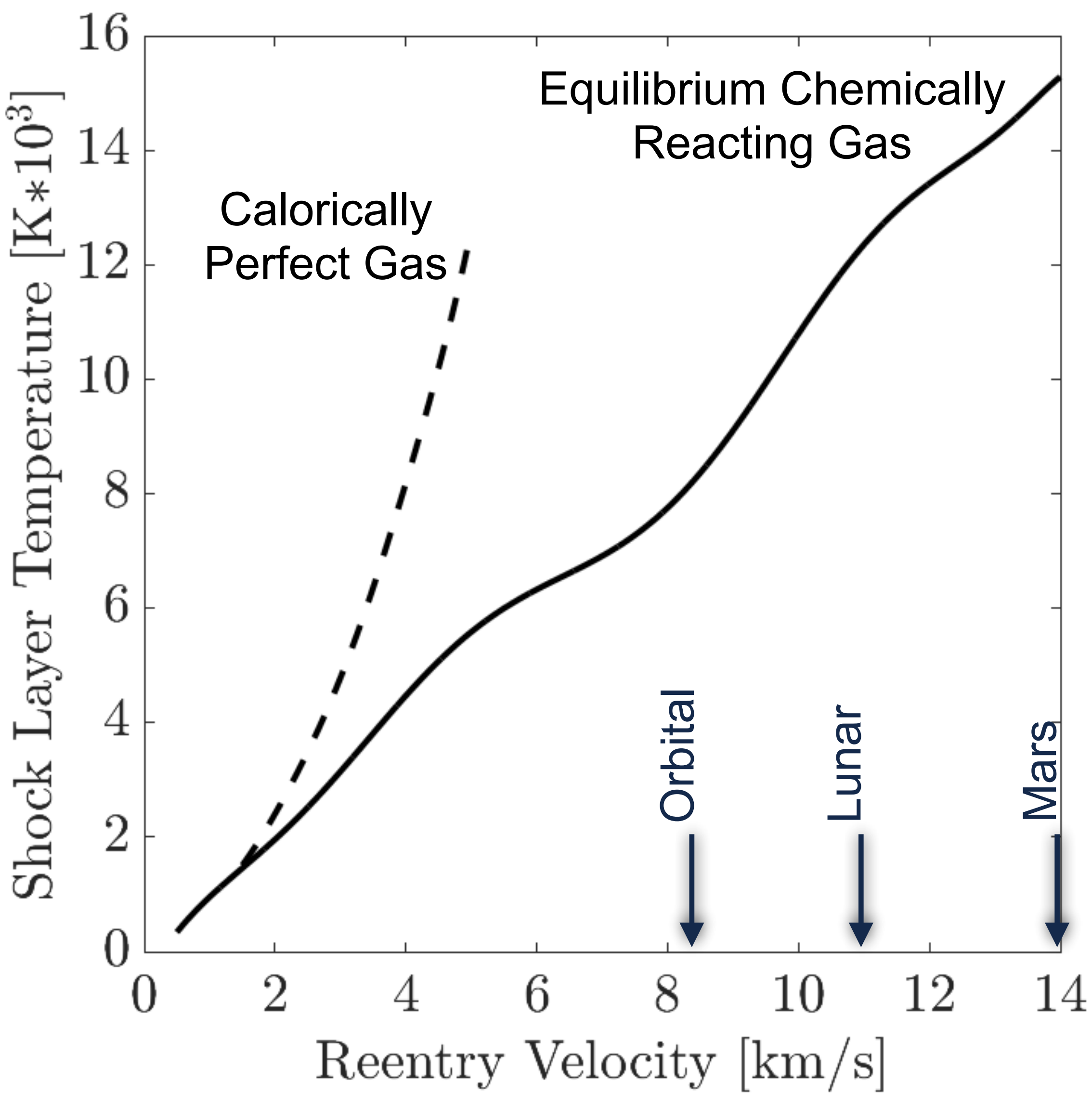

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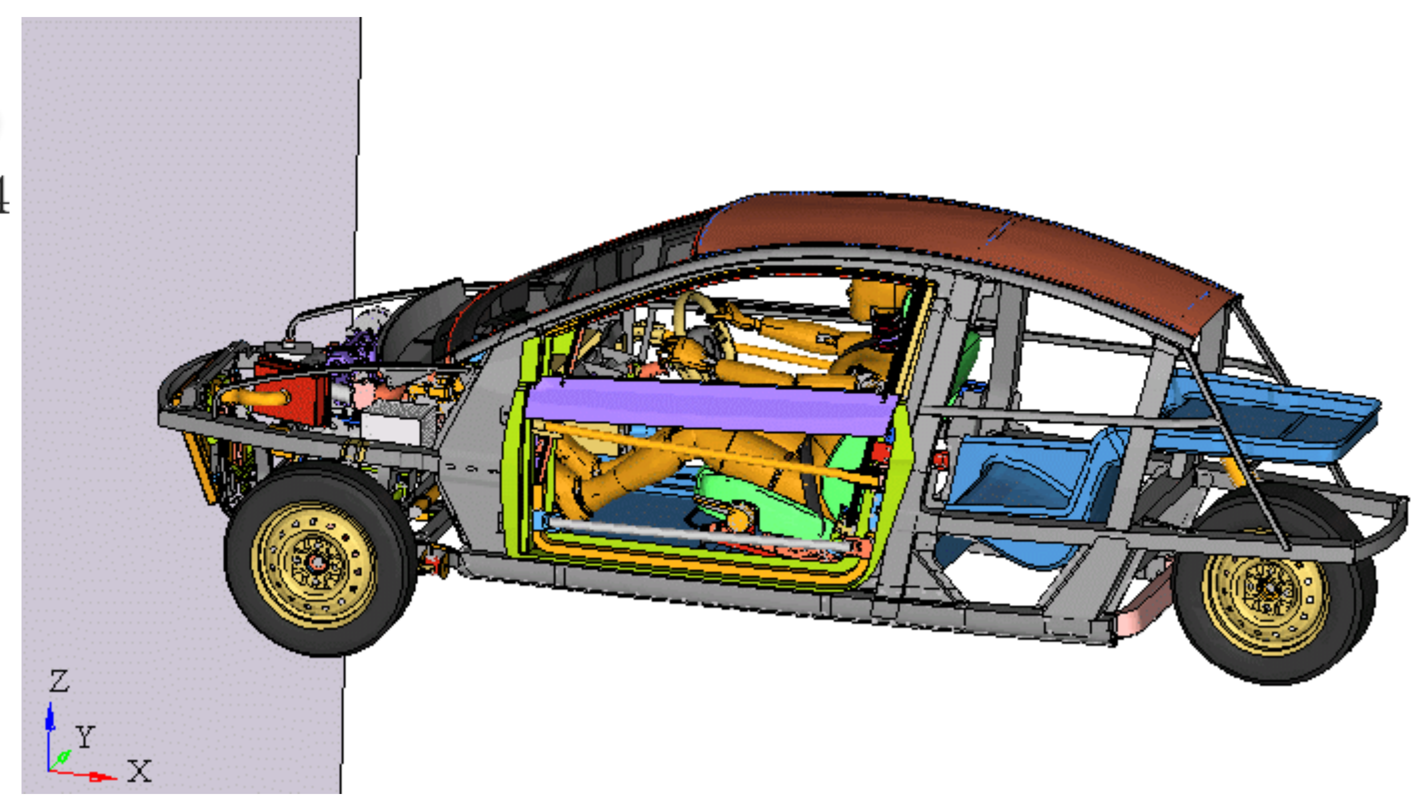

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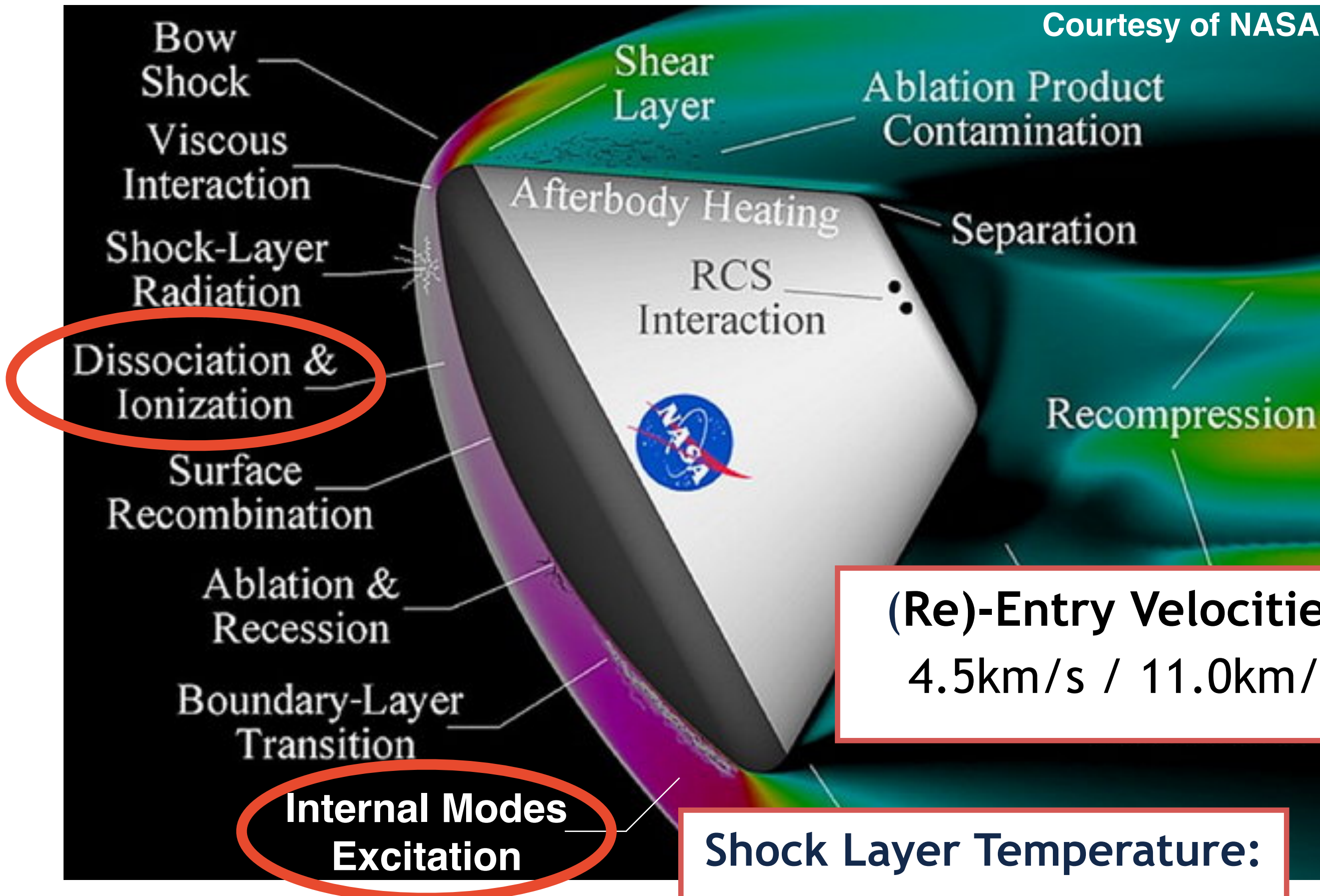

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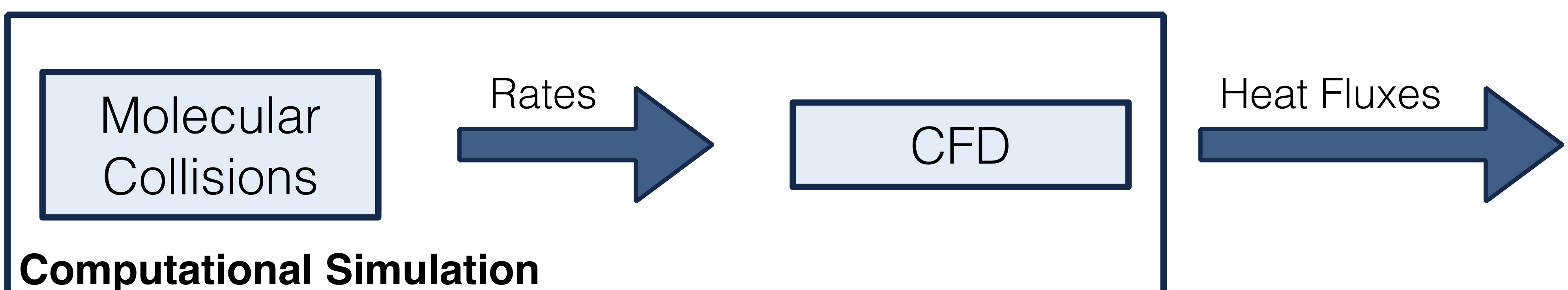
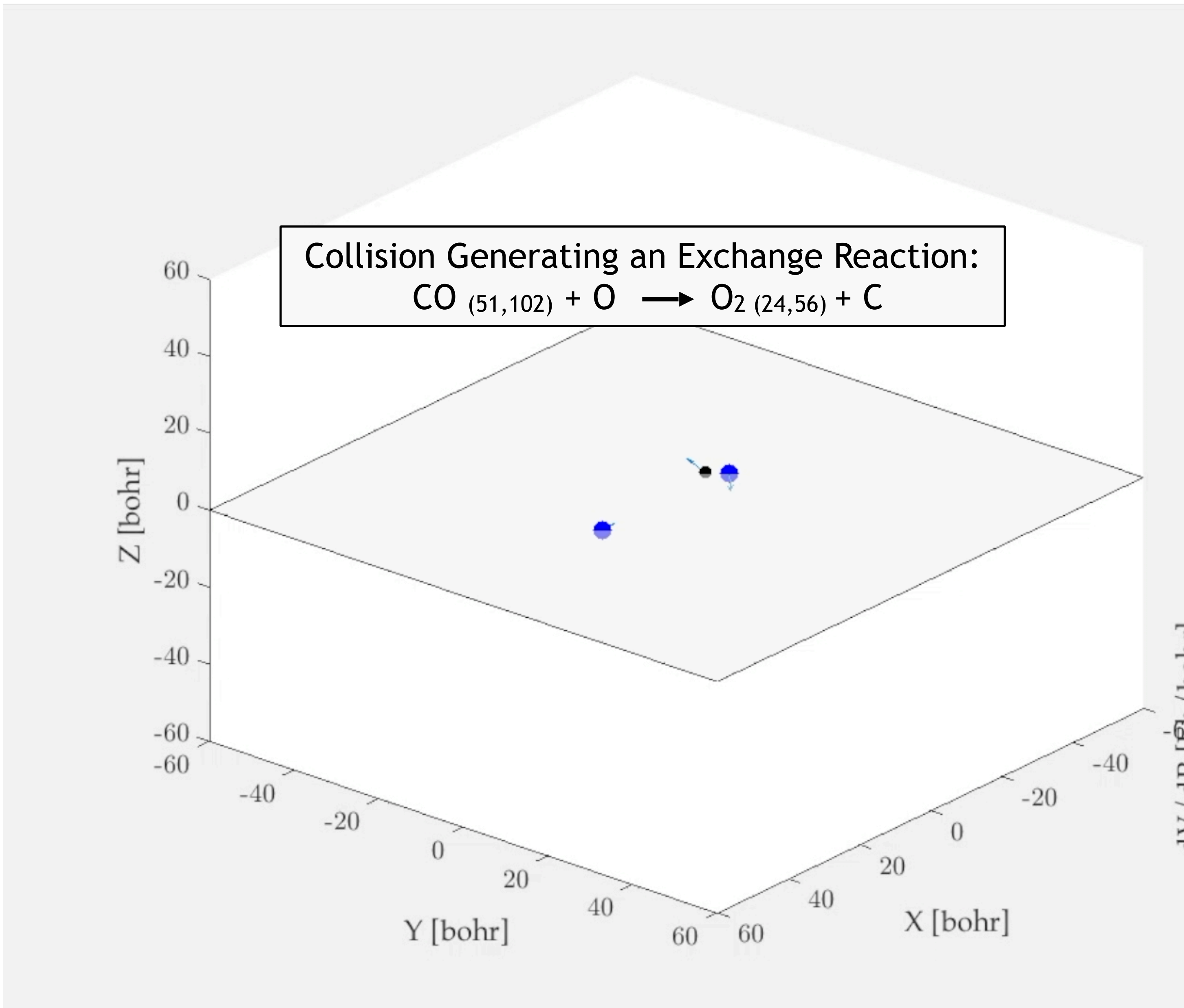
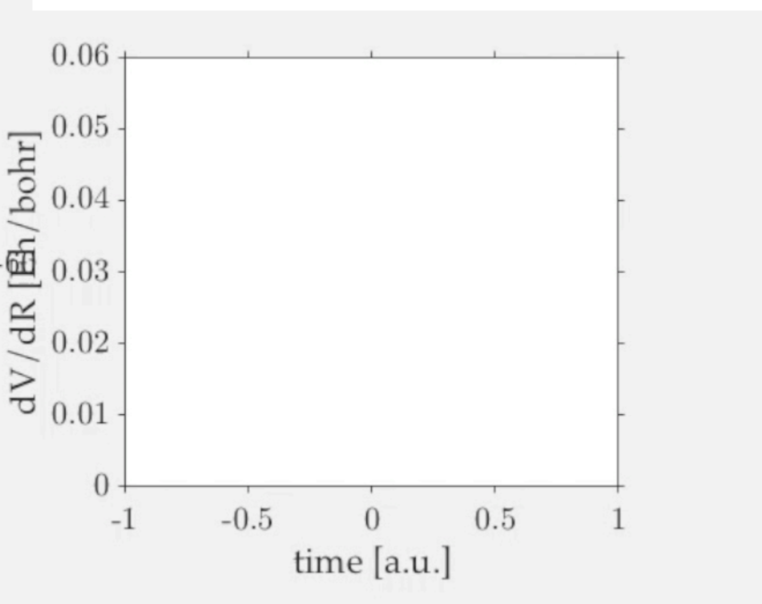
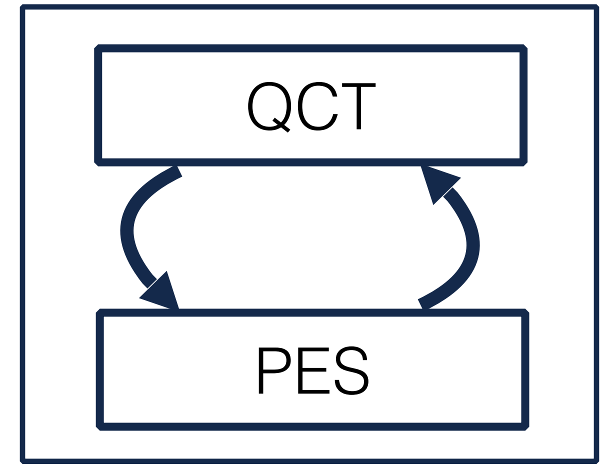


Motivation: PES-to-Rate Coeff.s Approach







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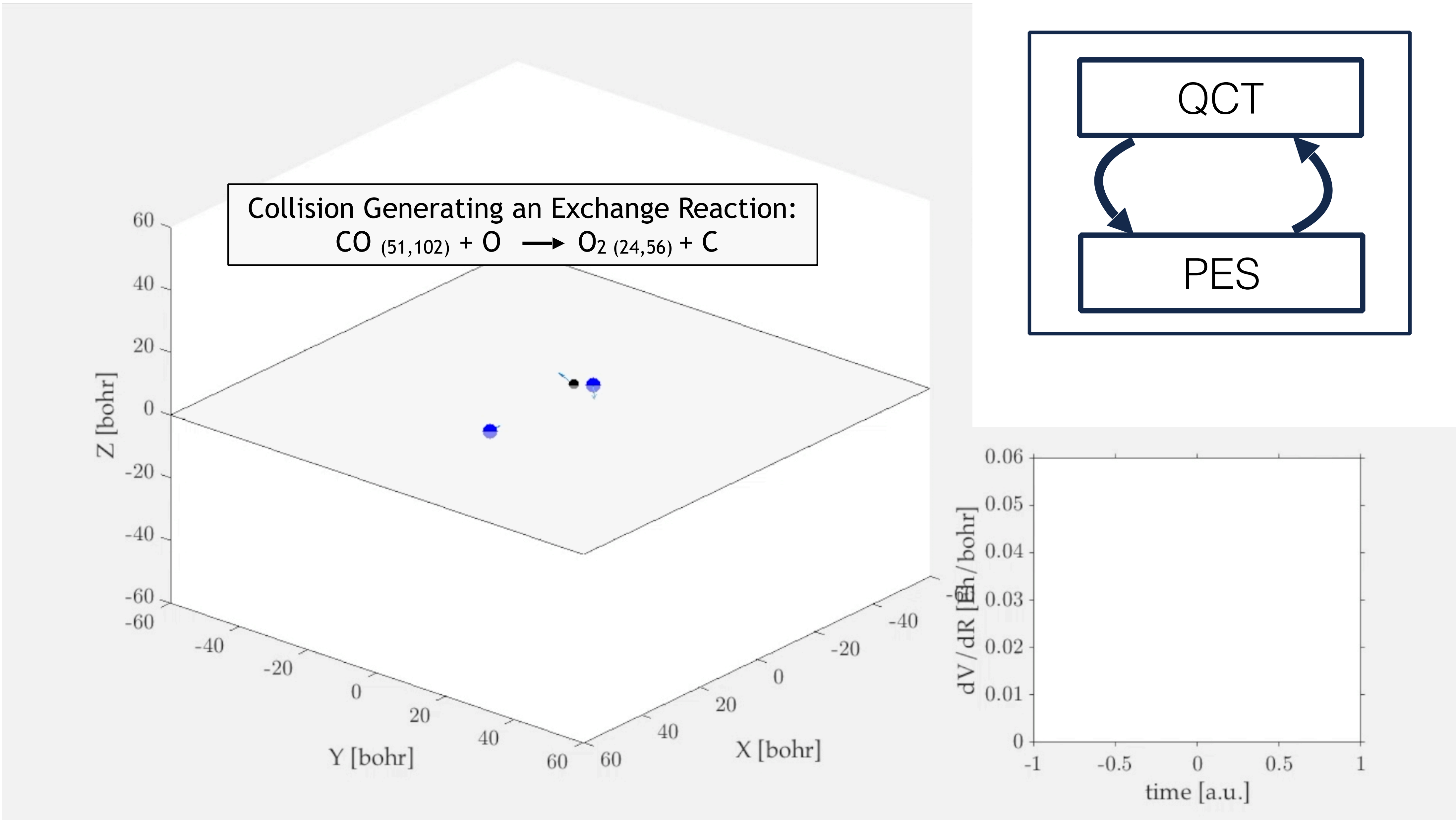

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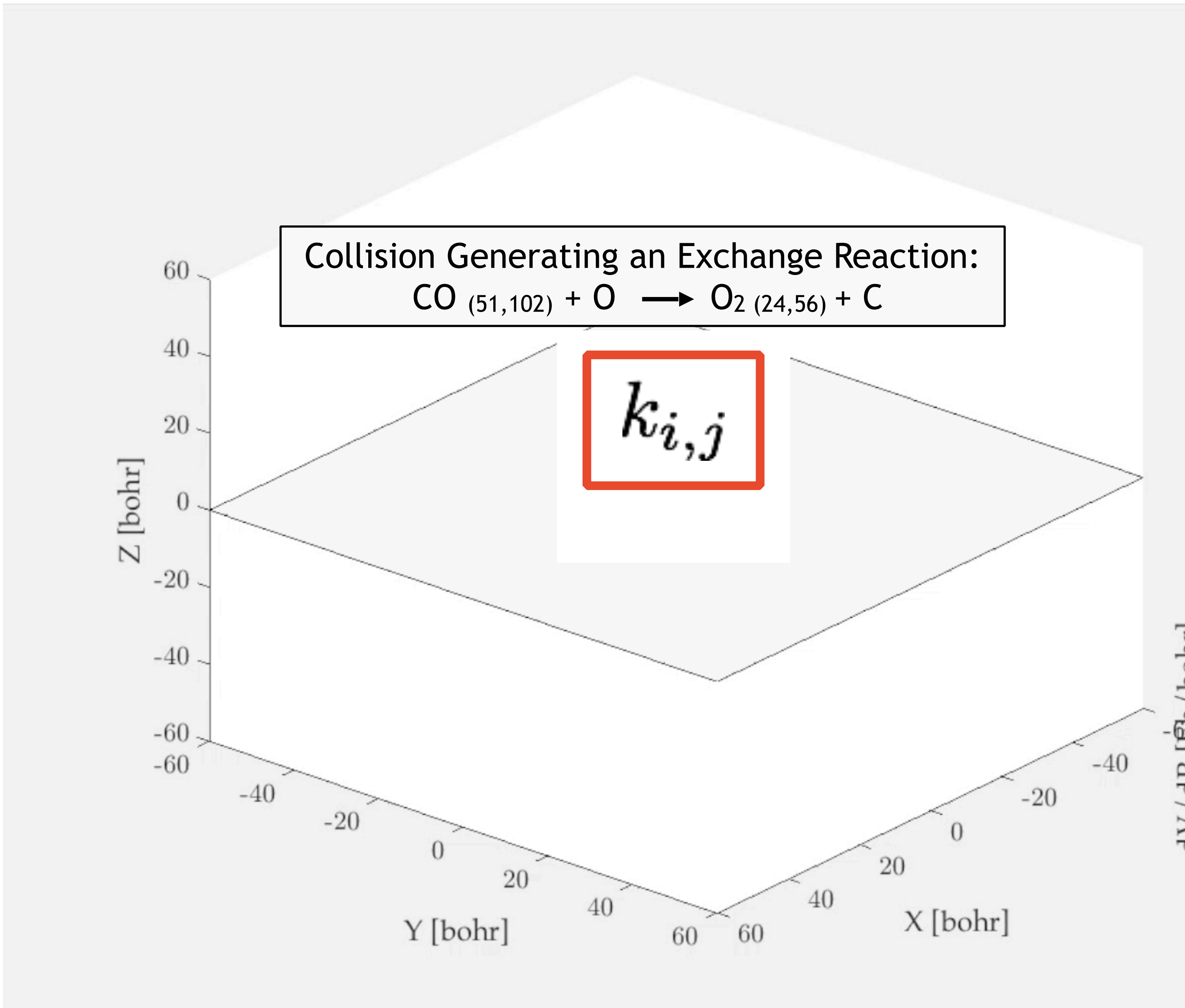

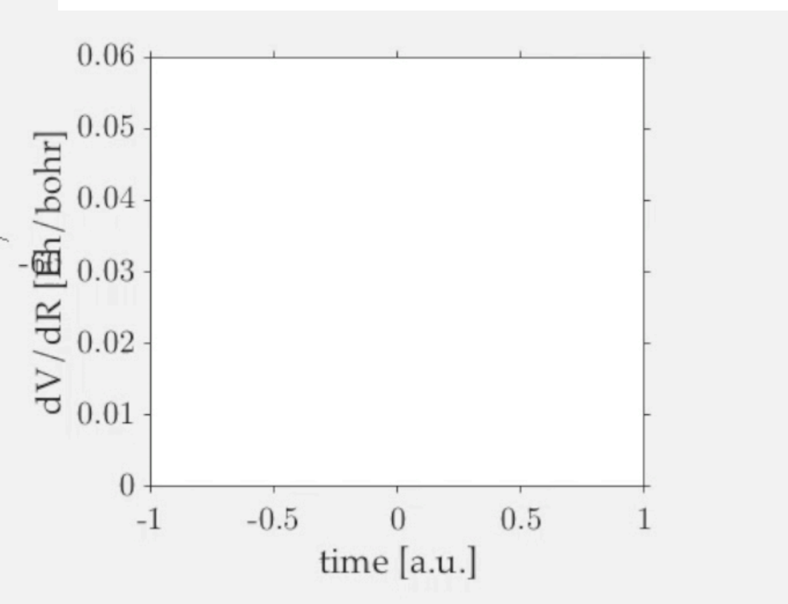

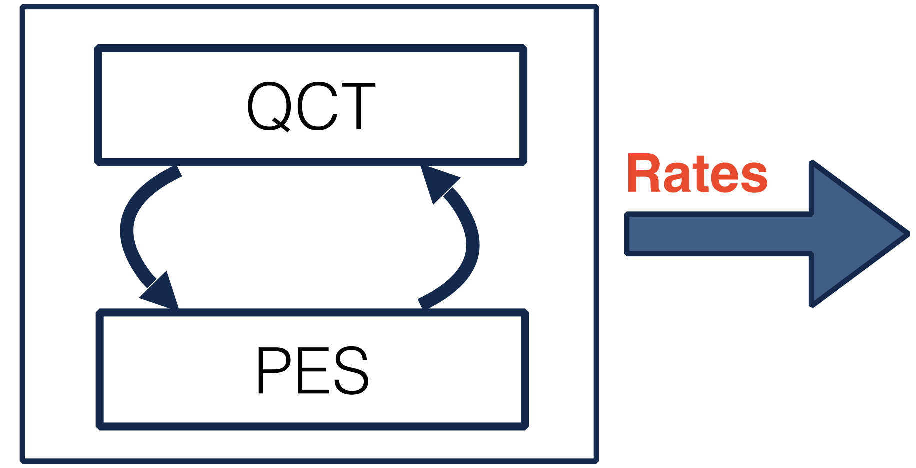

1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as **source terms of the Hamiltonian Eq.s** for the calculation of atom trajectories;

2. Rate Coefficients are finally obtained **by integrating over Maxwellian distributions** of collisional energies.

PESs drive the collision dynamics, and govern the values of rate coefficients

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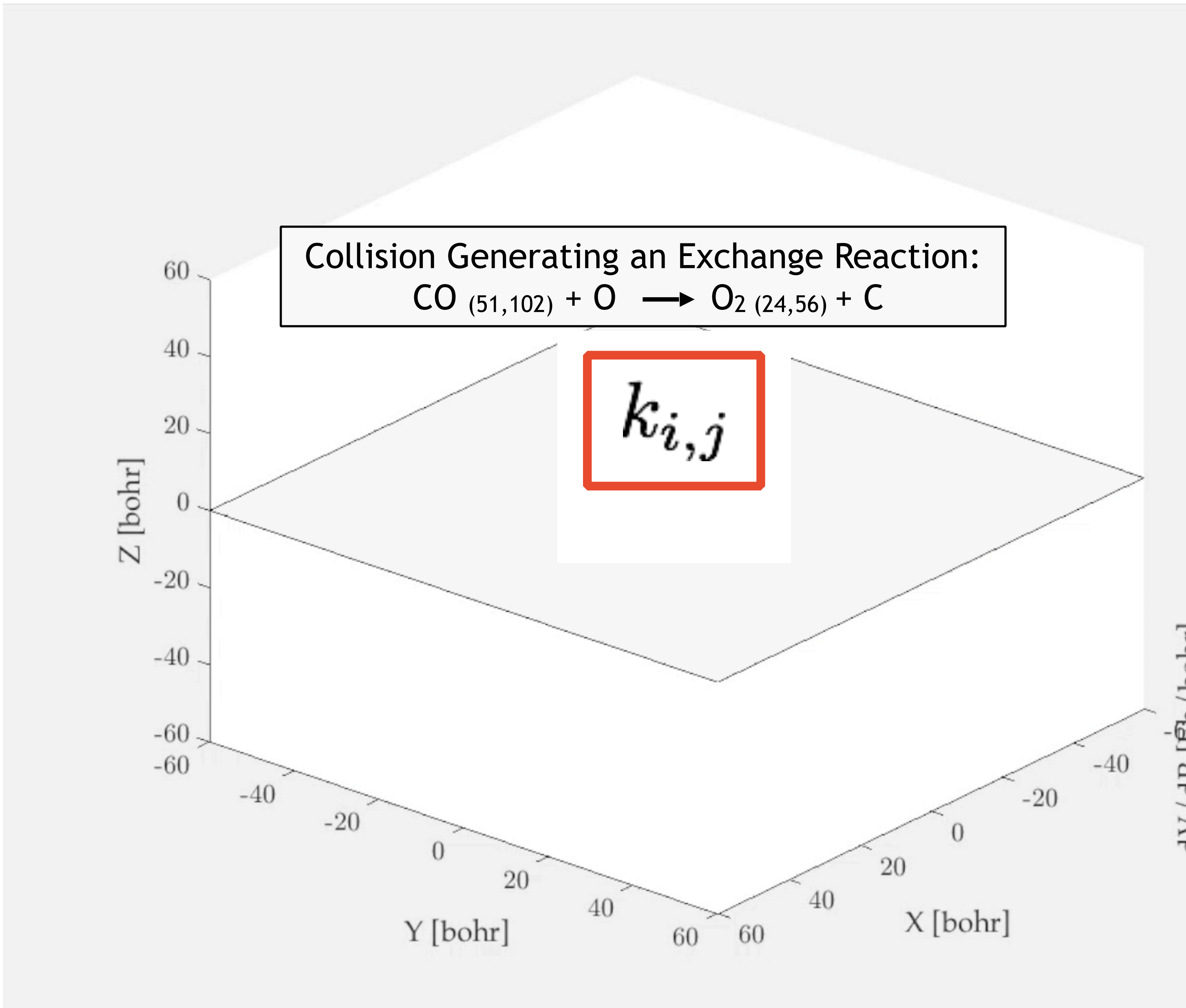

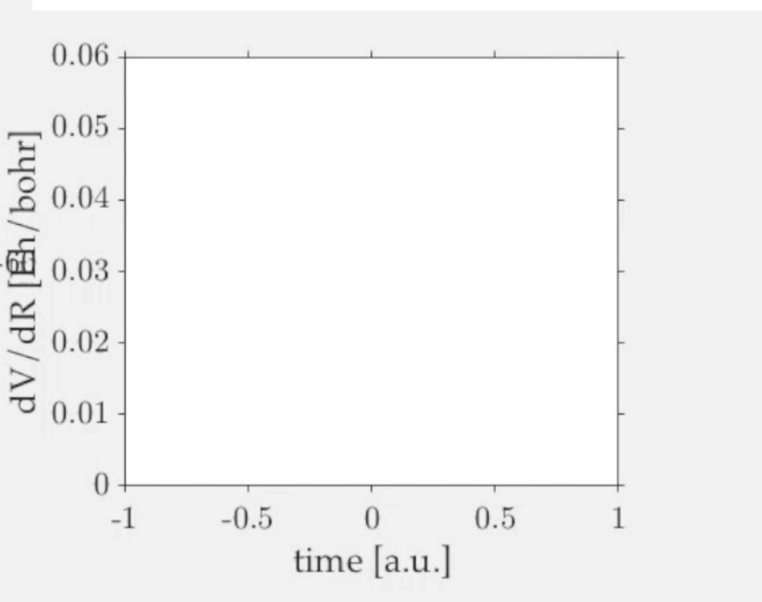

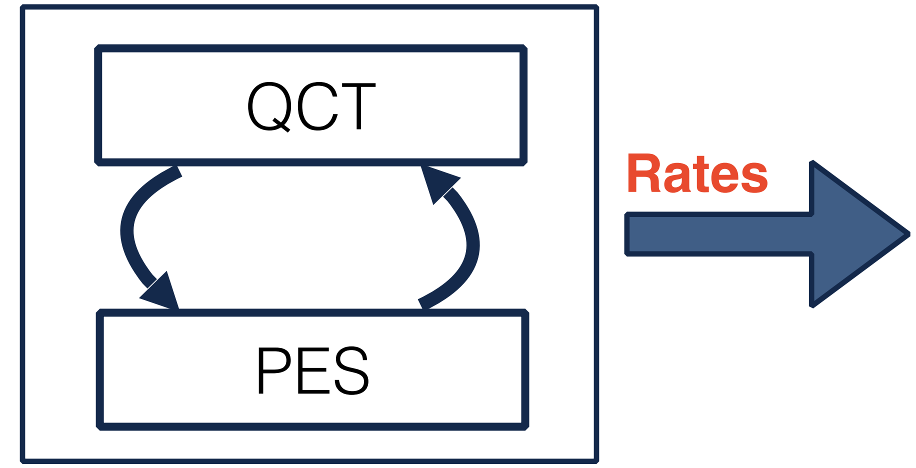

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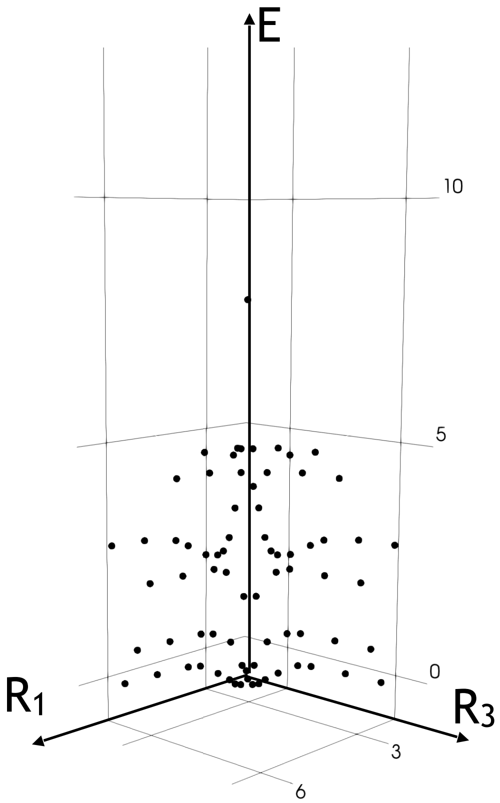
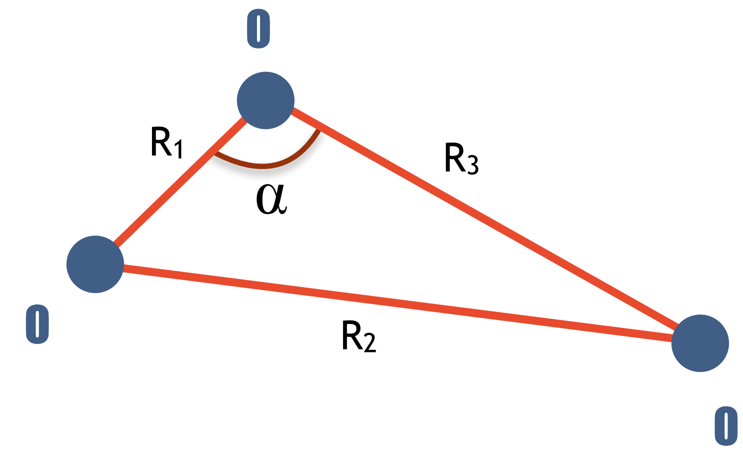
Motivation: PES

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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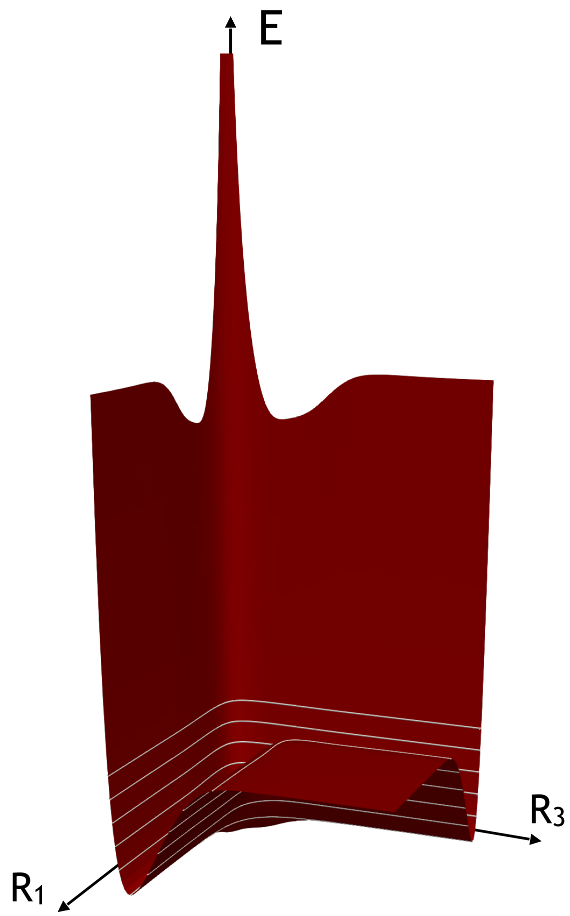

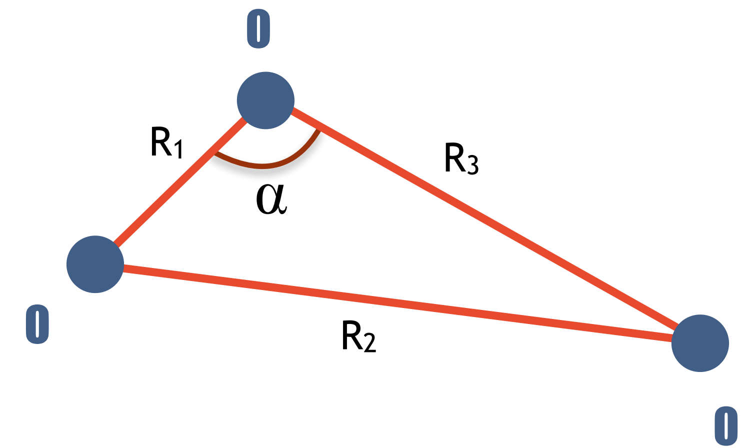

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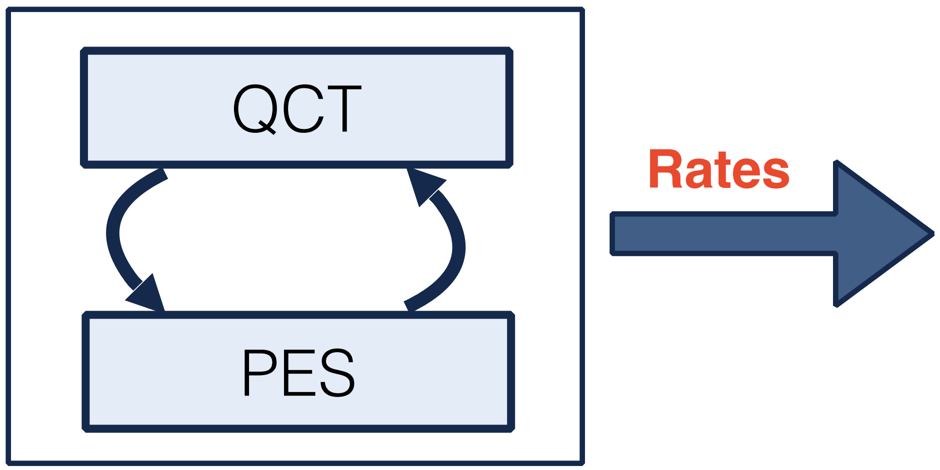
Each research group typically has its distinctive protocols to PES generations.
The result is that the surfaces for a given collisional system are diverse from one laboratory to the other.

- **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

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



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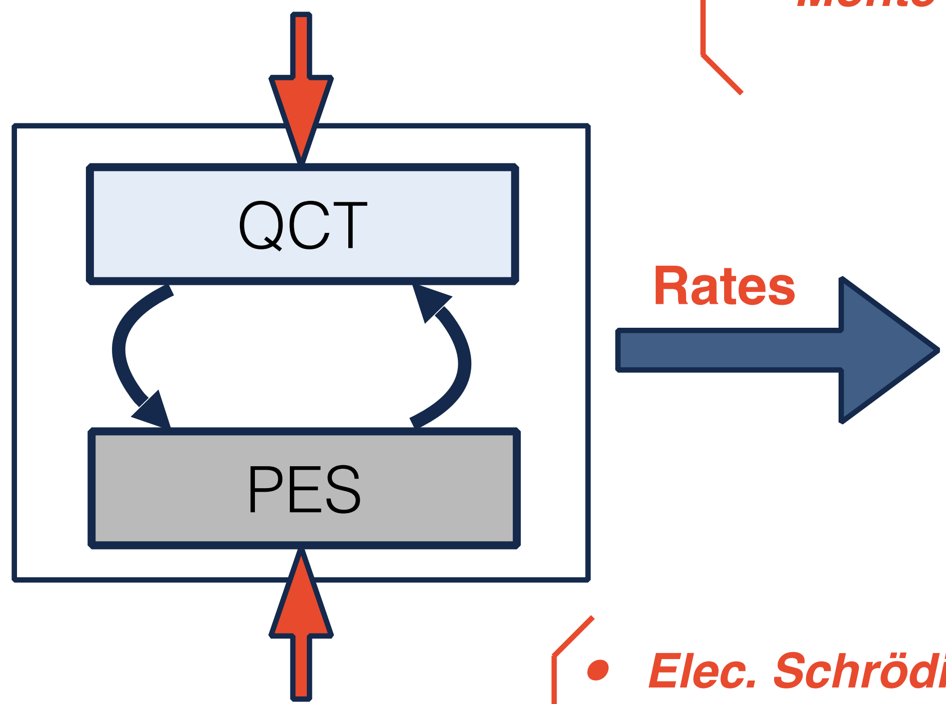
Collisional Dynamics Uncertainty

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



PES Uncertainty

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

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Collisional Dynamics Uncertainty

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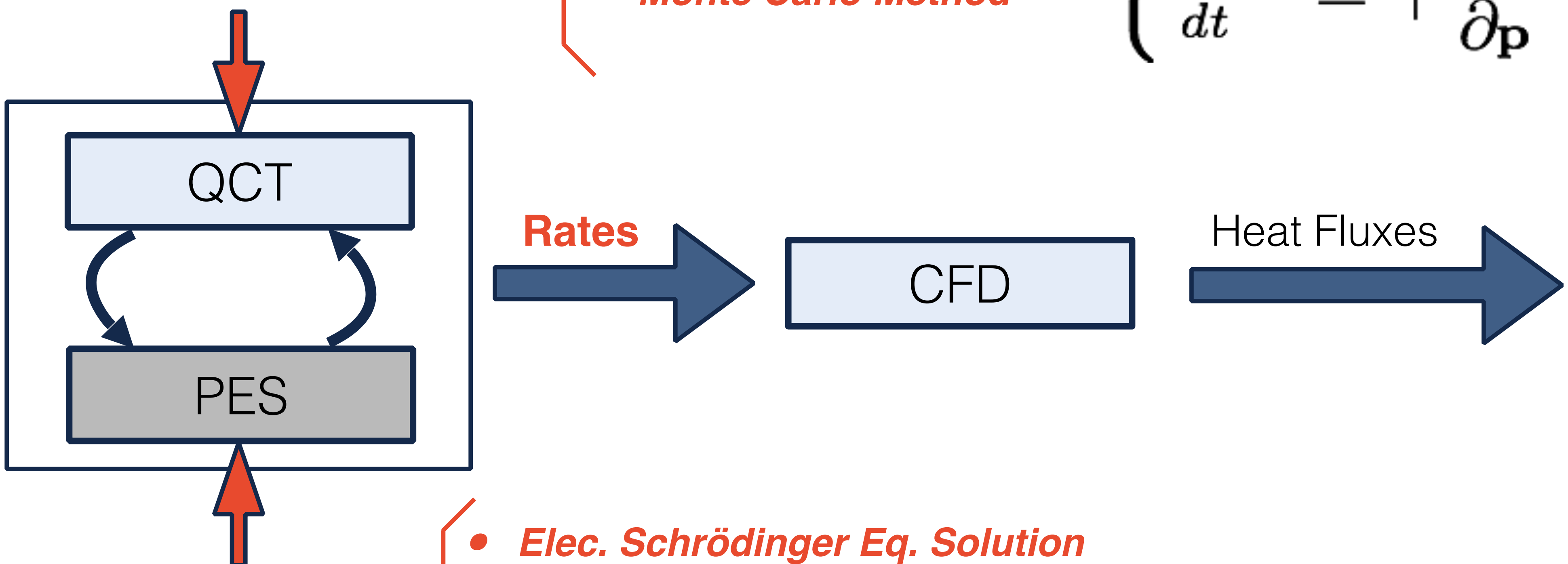

PES Uncertainty

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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

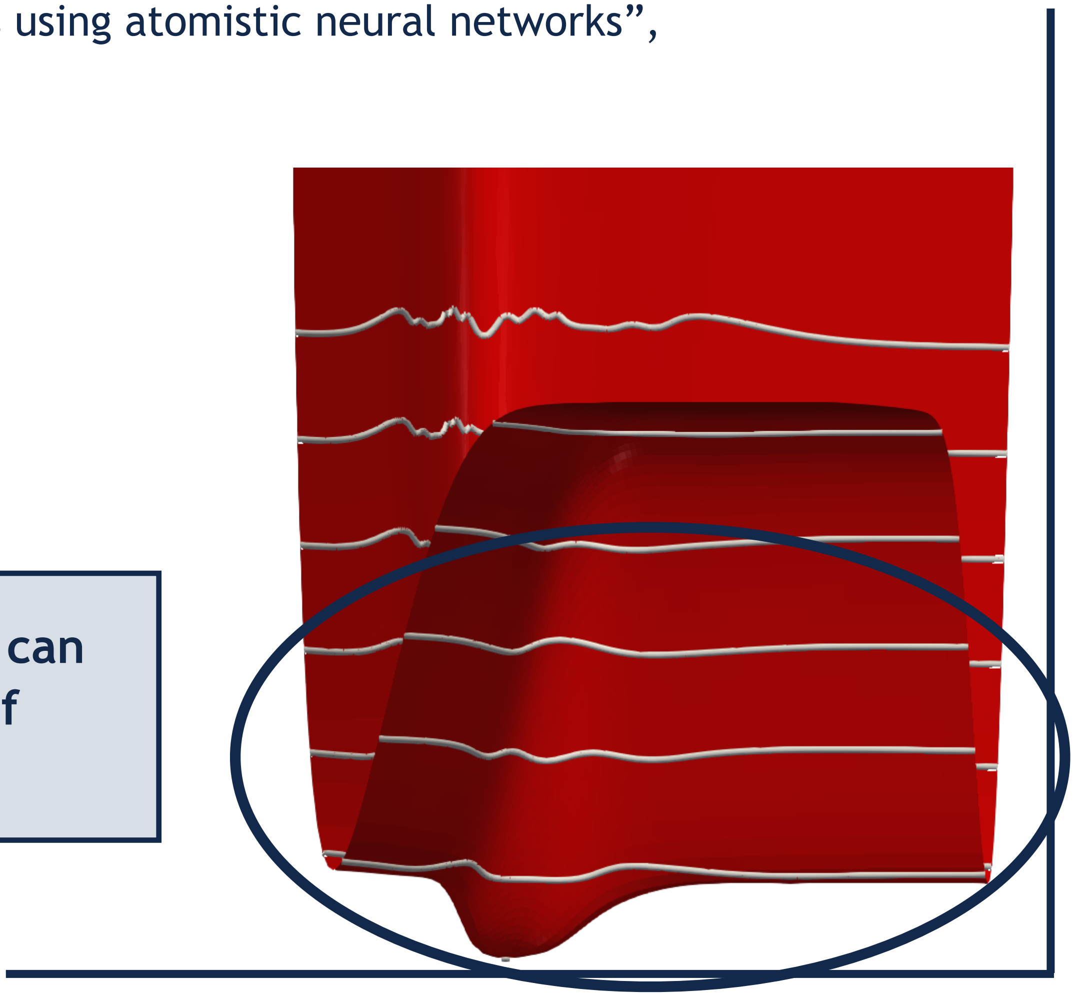
In the last decade there has been an increasing effort in taking advantage of Machine Learning for constructing Potential Energy Surfaces. In particular, using:

- ✦ **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.



ANN for PESs: Methodology

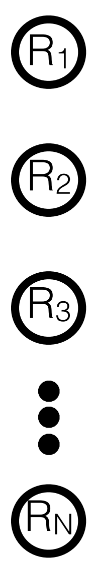
Multi-layer feed-forward Neural Networks (NN) have been adopted **as fitting functional**:

- ✦ 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

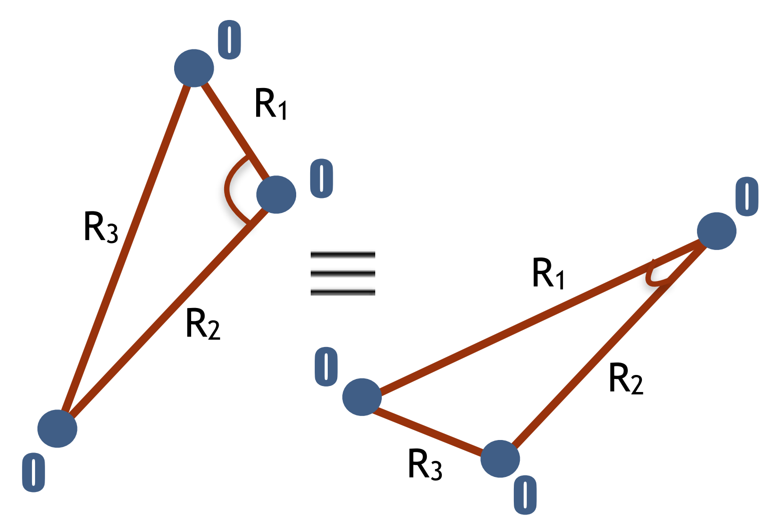
Lasagne



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.



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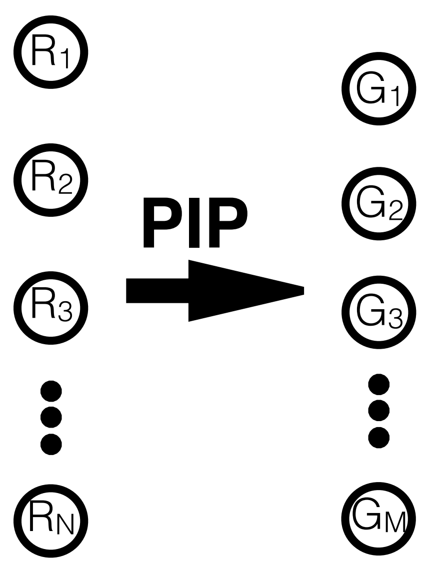

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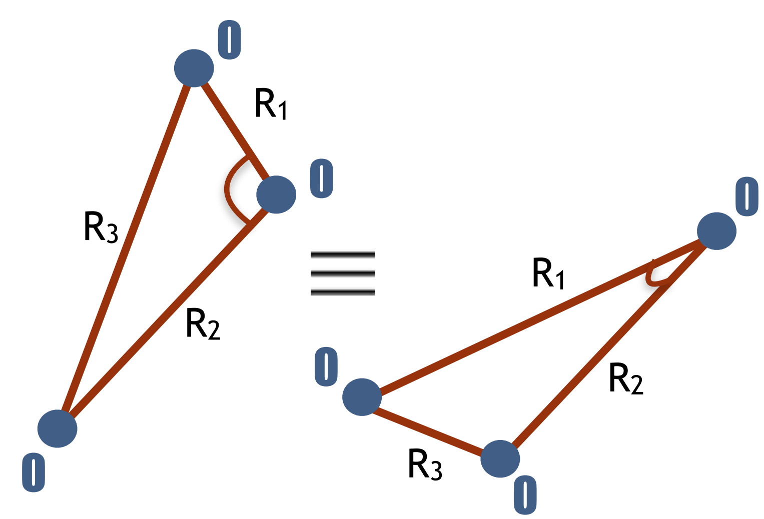
$$G_3 = p_1p_2p_3$$

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



ANN for PESs: Methodology

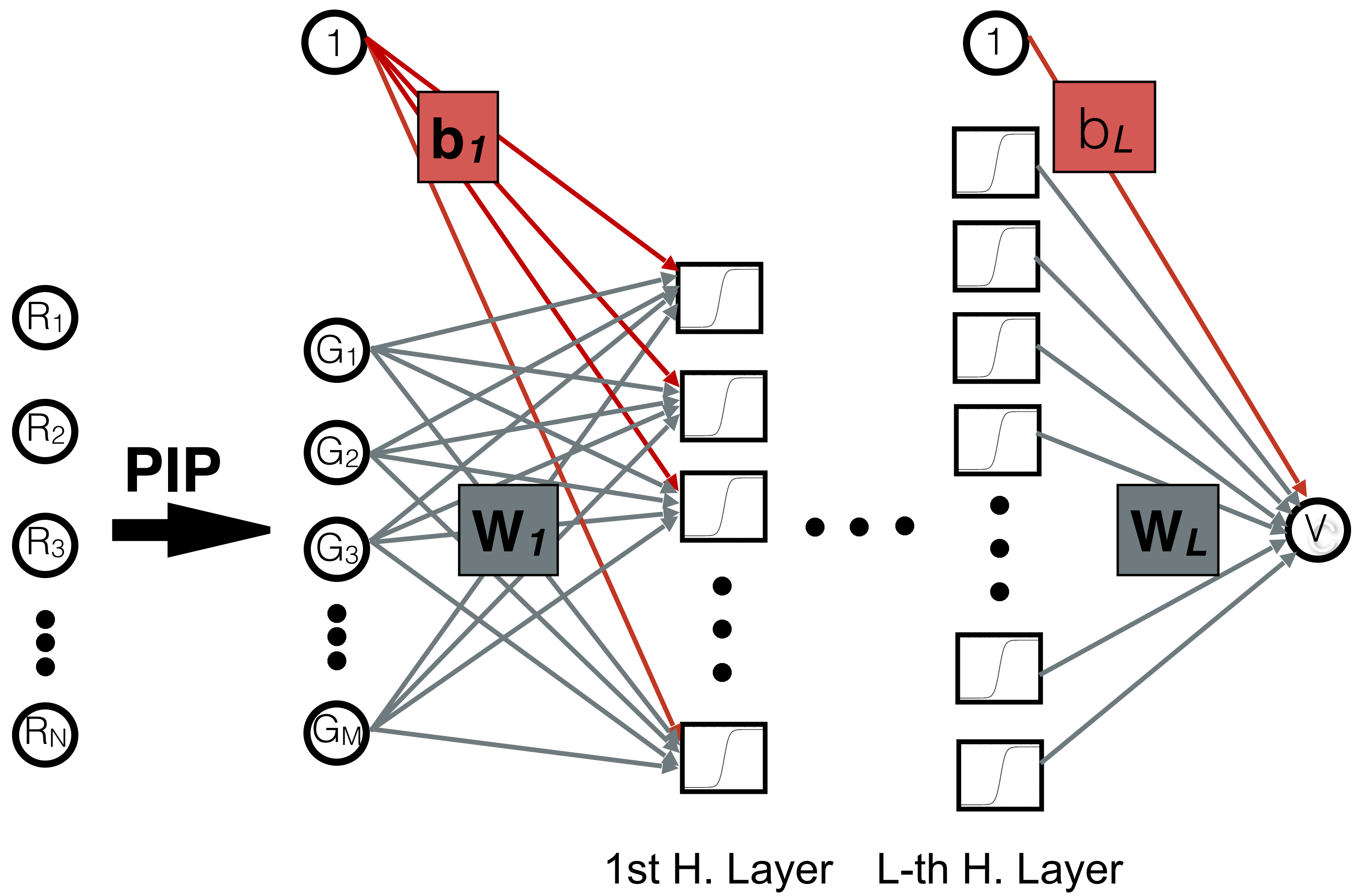
Multi-layer feed-forward Neural Networks (NN) have been adopted **as fitting functional**:

- 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



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

Output from the k-th Neuron of the i-th Layer

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

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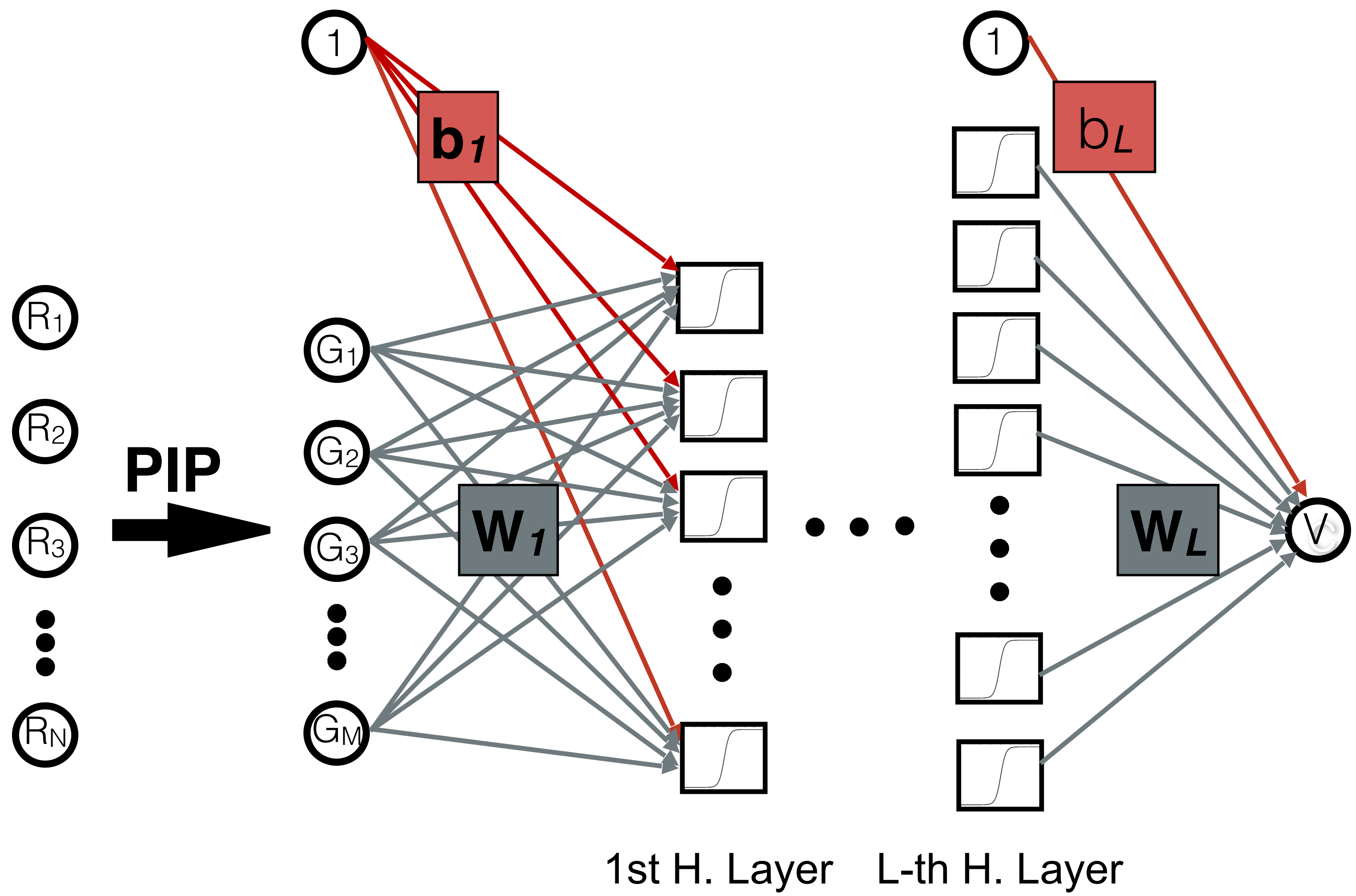

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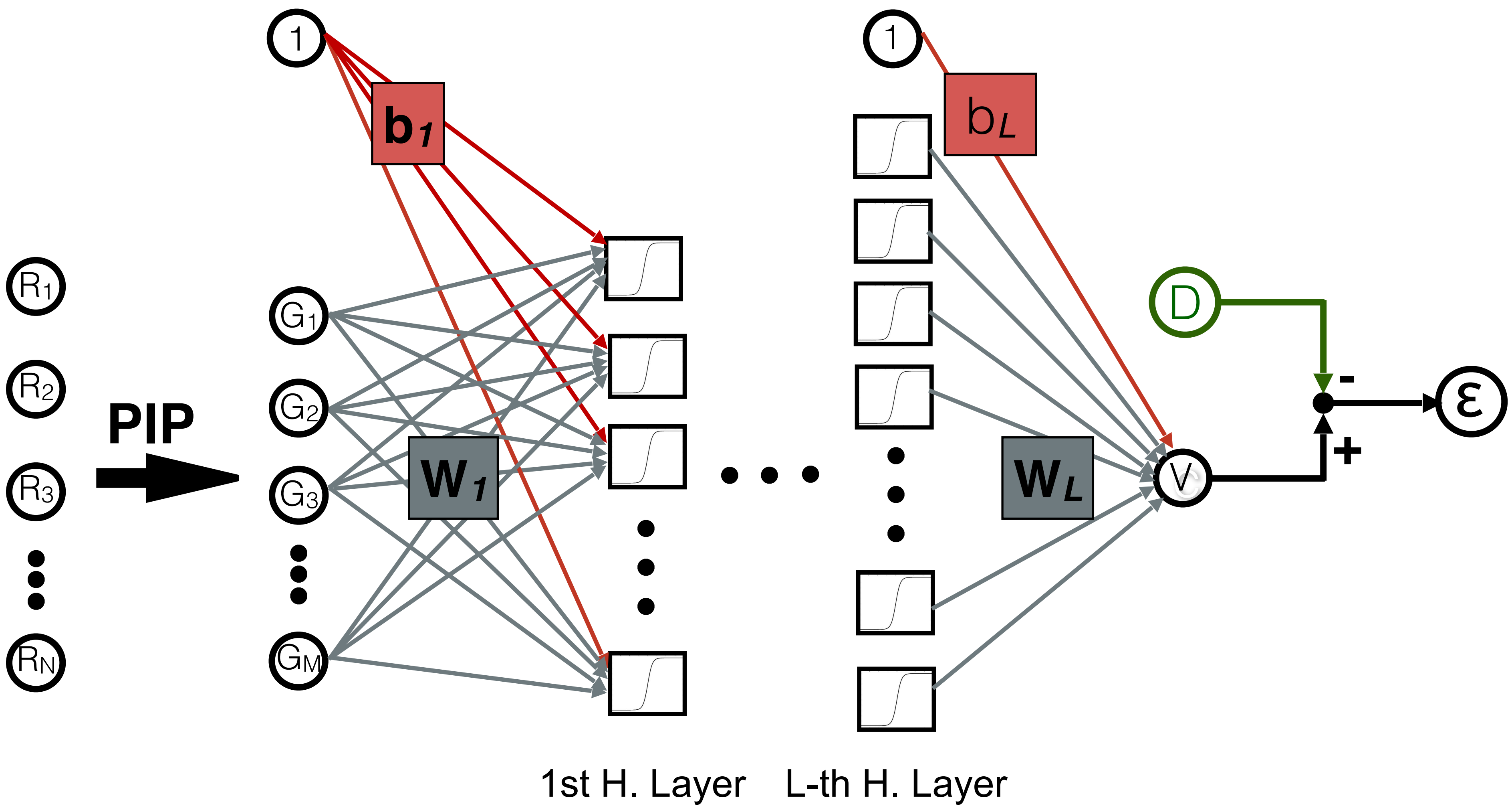


3. E is compared with some ab-initio data (D), in order to estimate the error in the prediction (ε). The values of $\mathbf{W}_i$ and $\mathbf{b}_i$ are then **learnt through an optimization algorithm** (e.g., adadelta, rmsprop, …), which minimizes a loss function by cycles of forward propagations, error 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	⟨10 NN⟩	1 GP	⟨10 GP⟩
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

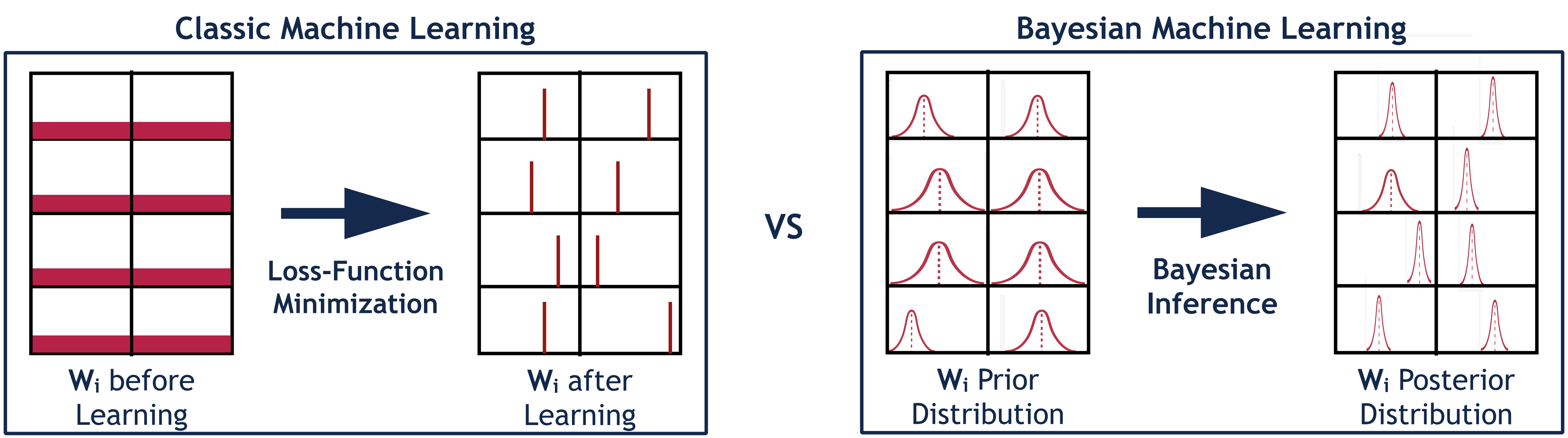
From Deterministic To Stochastic

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:

$$\underbrace{p(\mathbf{W_i}, \mathbf{b_i}|D, M)}_{\text{Posterior}} \propto \underbrace{p(D|\mathbf{W_i}, \mathbf{b_i}, M)}_{\text{Likelihood}} \underbrace{p(\mathbf{W_i}, \mathbf{b_i}|M)}_{\text{Prior}}$$

Prior: $p(\mathbf{W_i}, \mathbf{b_i}|\mathbf{M}) \sim \mathcal{N}(\mu = ..., \sigma = ...)$

Likelihood: $p(\mathbf{D}|\mathbf{W_i}, \mathbf{b_i}, \mathbf{M}) = \frac{1}{\sqrt{2\pi\sigma_L^2}} \exp\left(\sum_{j}^{N_D} \frac{(\log(\mathbf{V_j}) - \log(\mathbf{D_j}))^2}{2\sigma_L}\right)$

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

PyMC3

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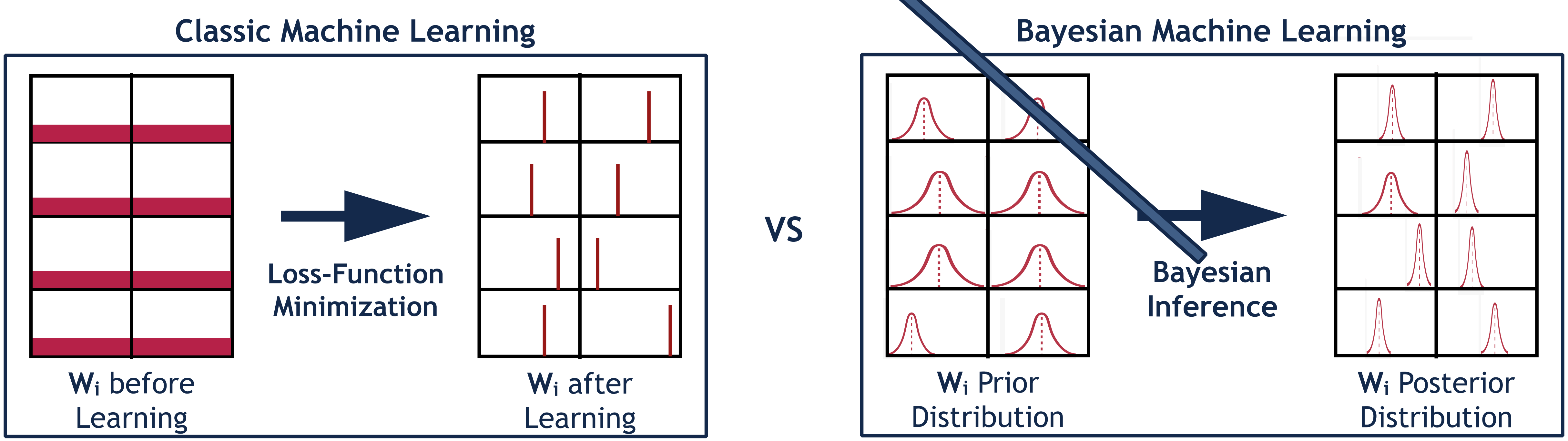
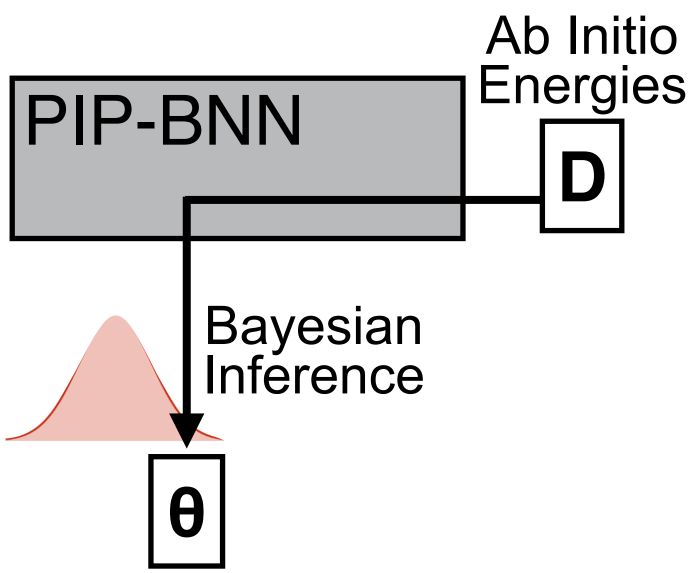
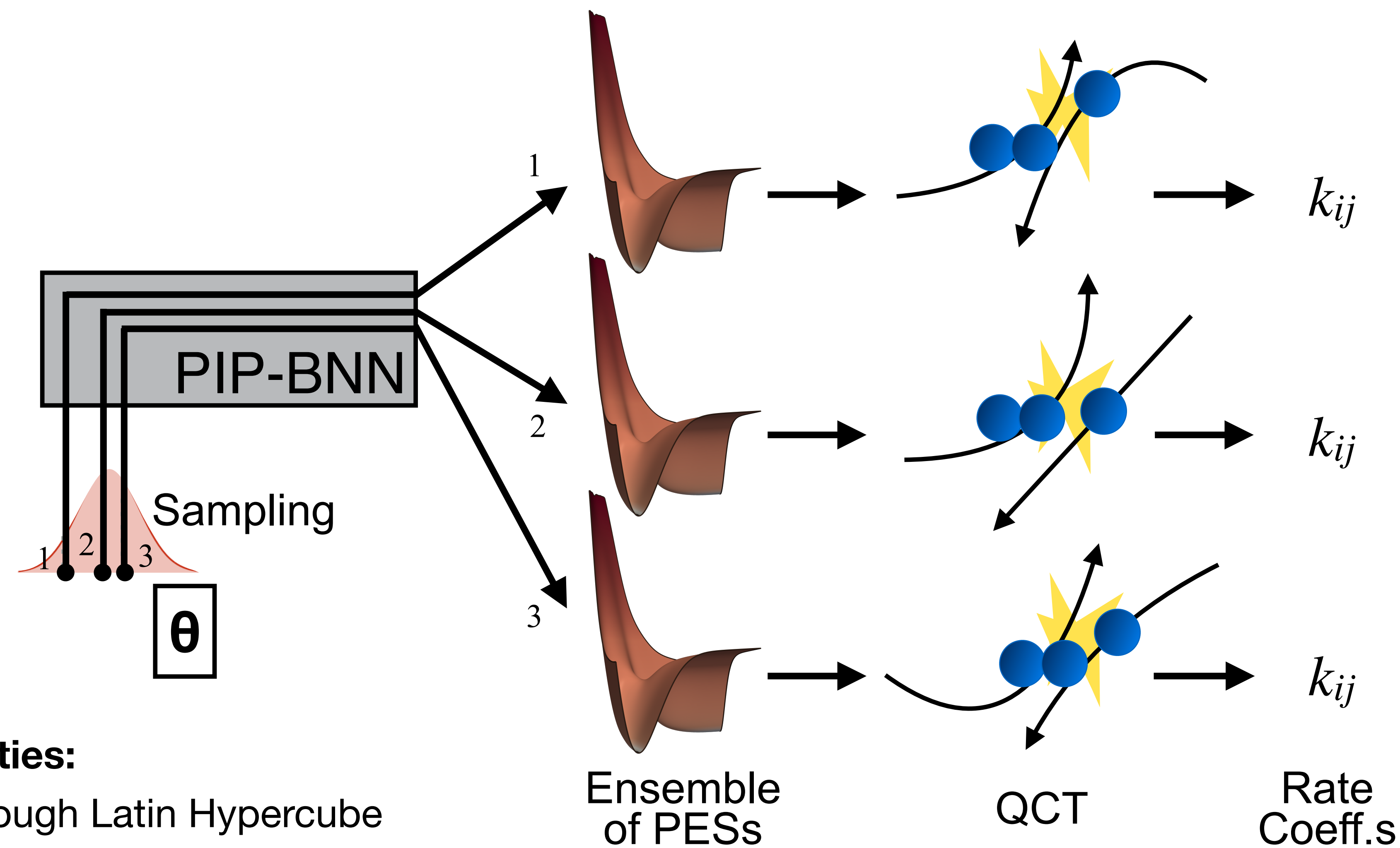


- Some **noise superimposed** to the functional form (model uncertainty).

PES UQ: Methodology



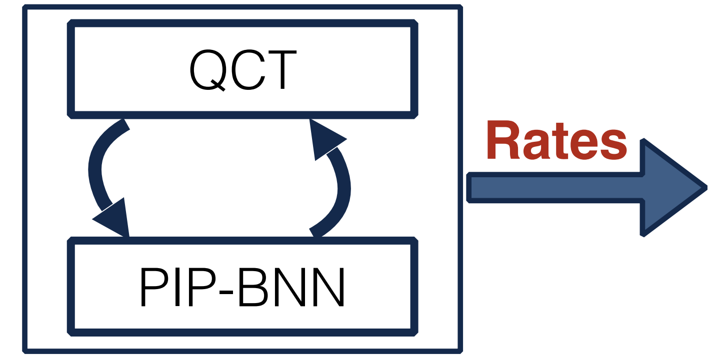
Solution of the inverse problem:
The optimal PDFs characterizing the PIP-BNN parameters are learnt through Bayesian variational inference from the ab initio data points.

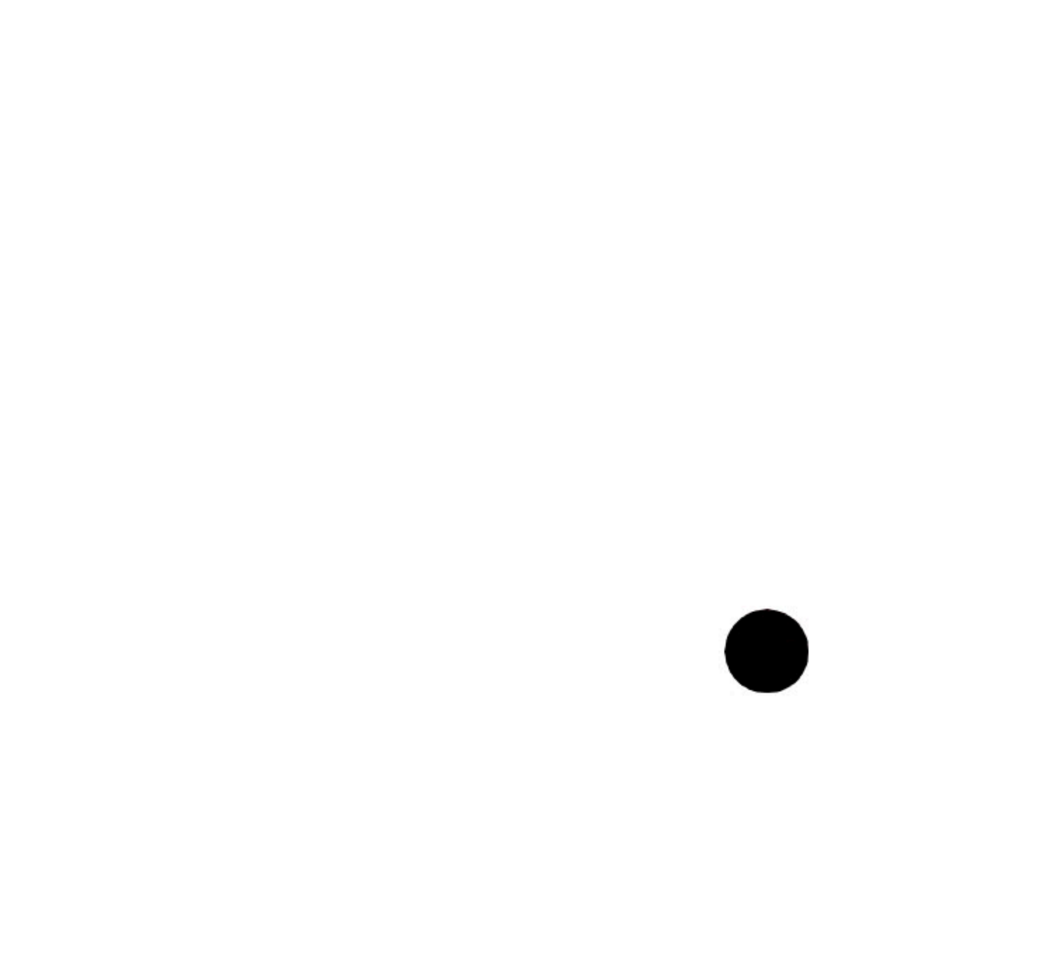


Forward propagation of the Uncertainties:
The posterior distribution is sampled through Latin Hypercube Sampling, an ensemble of PESs is computed through the PIP-BNN, and the surfaces are used for simulating collisions.

From Deterministic To Stochastic

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





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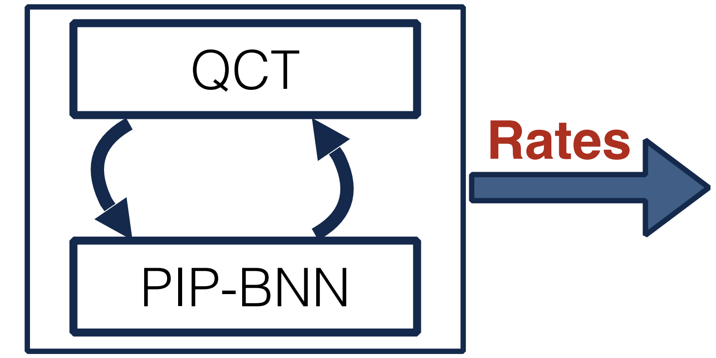
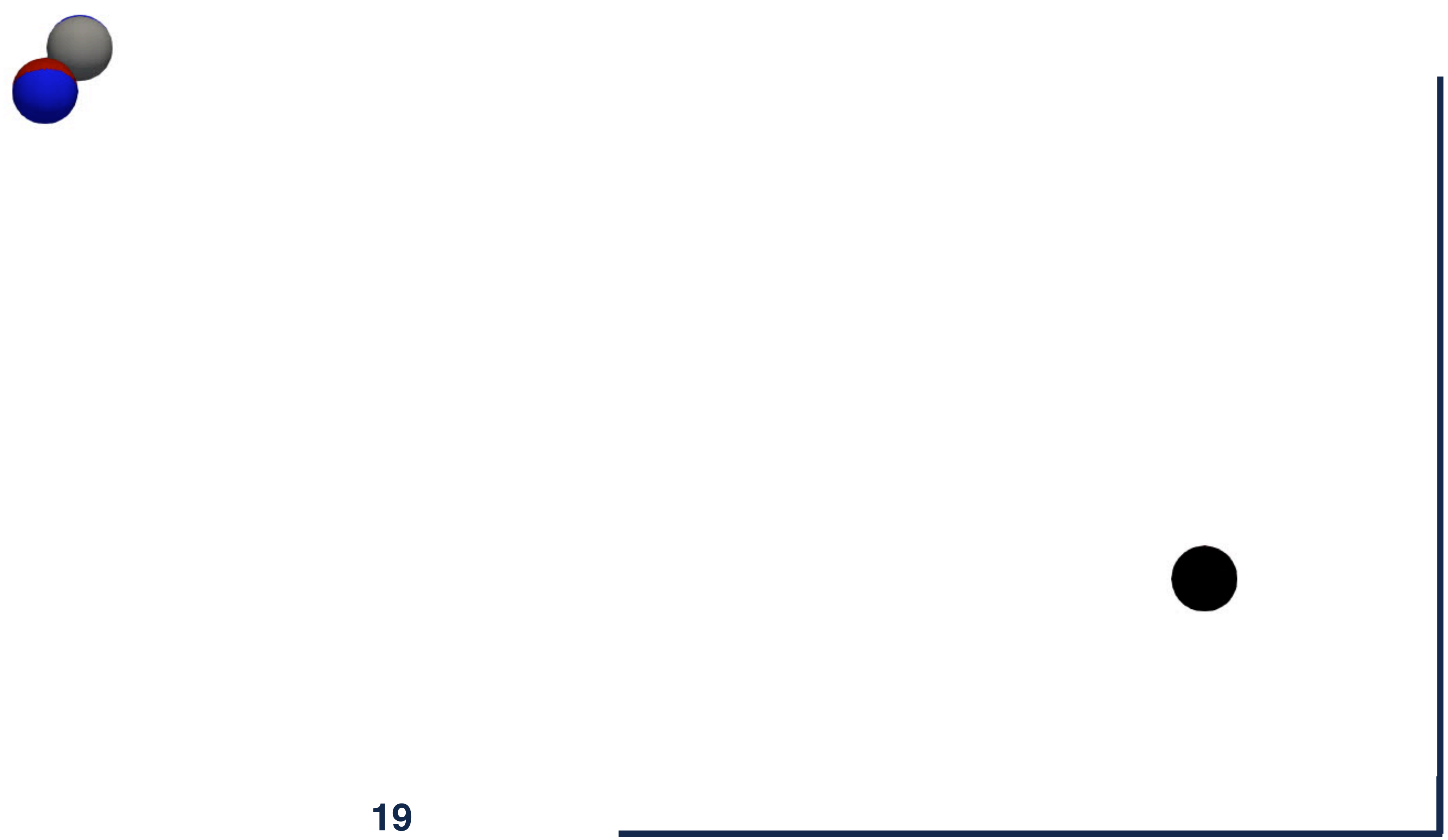
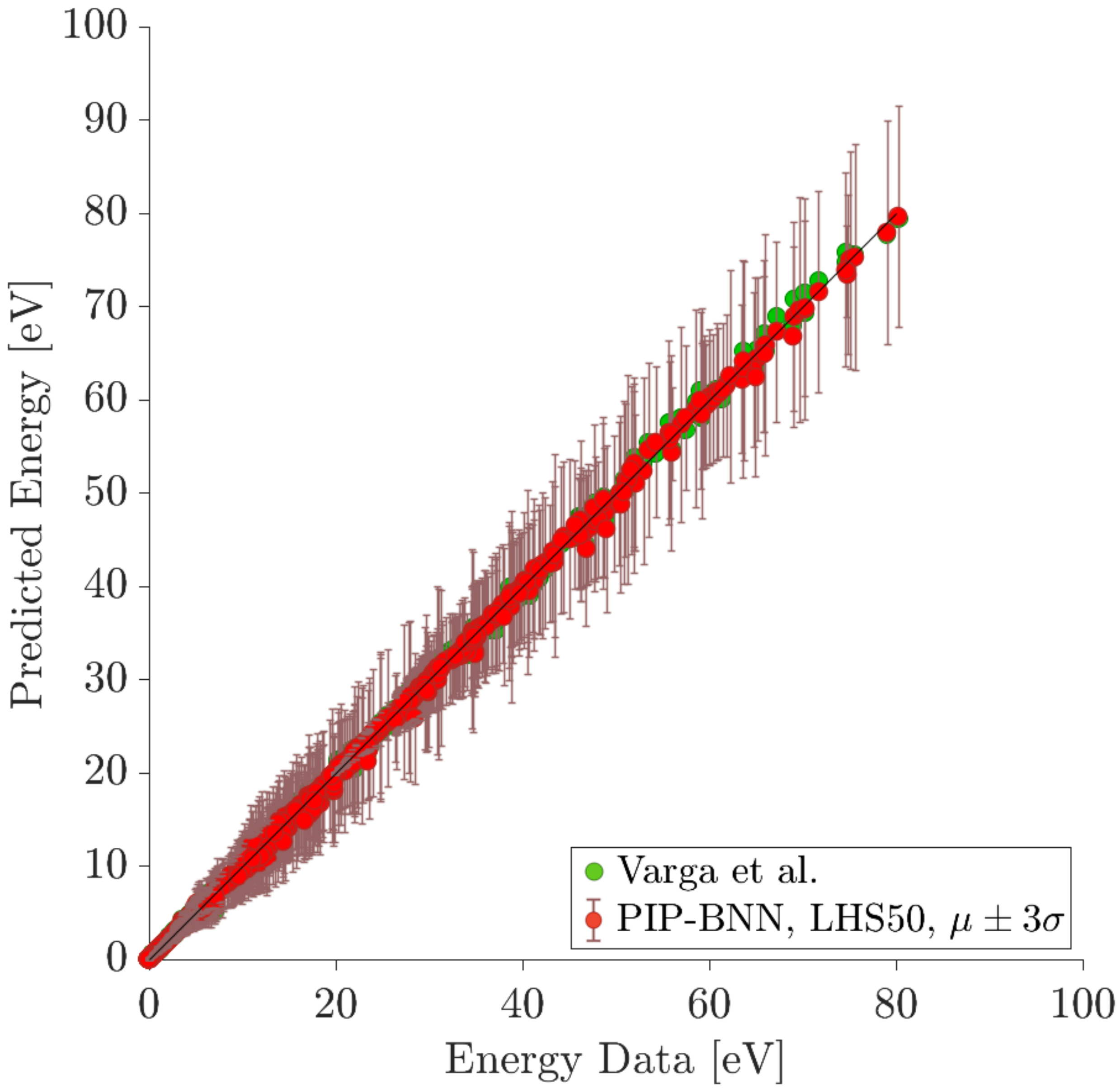


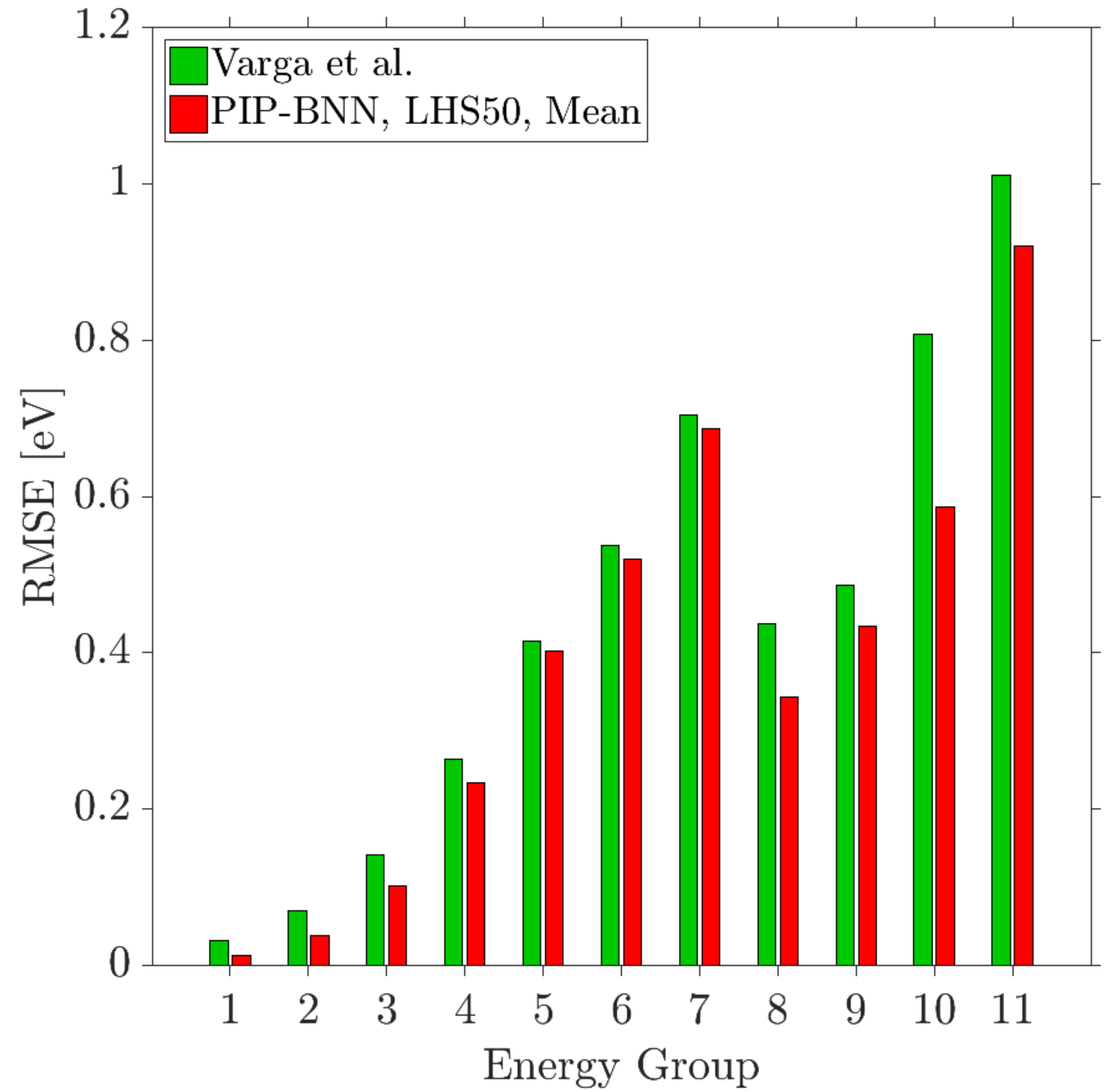


Results

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).



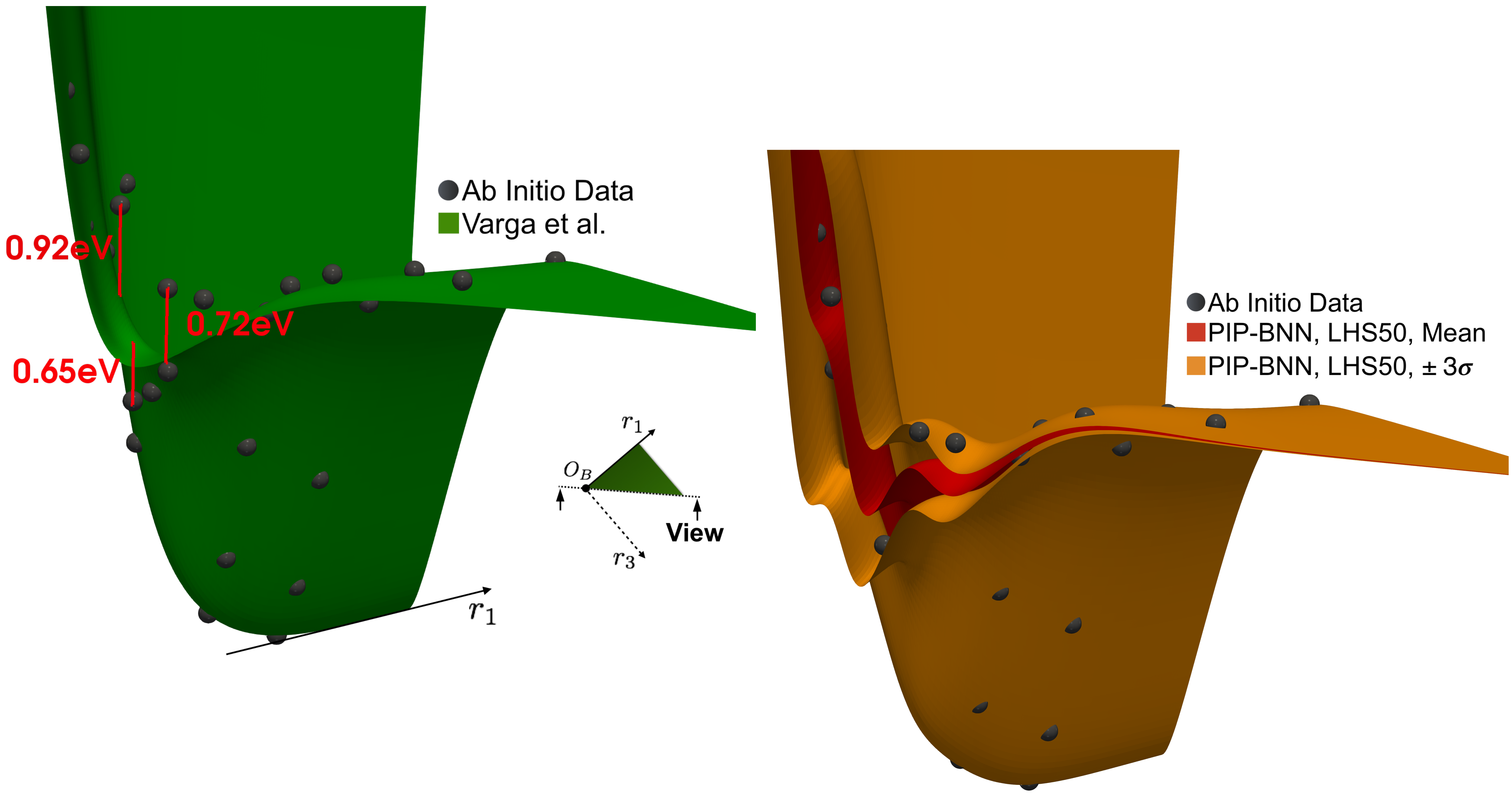
Means (red dots) and three-sigma confidence intervals (red lines) of the potential energies computed at the 1617 data points using the 50 PIP-BNN samples, compared to the energies resulting from Varga et al.'s fits (green dots).



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.

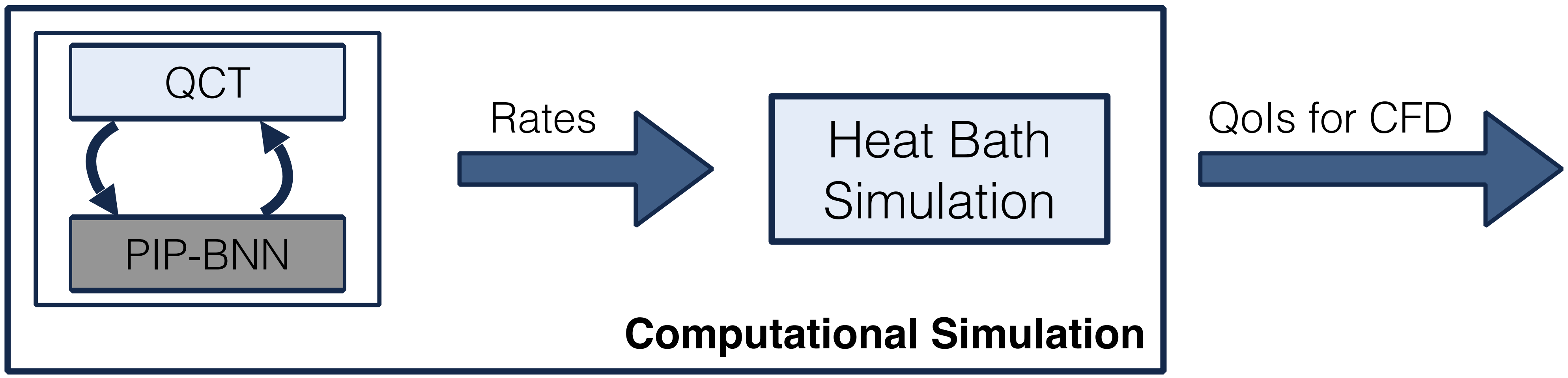
Results

3D views of the PESs at $O_AO_BO_C = 50°$ 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.

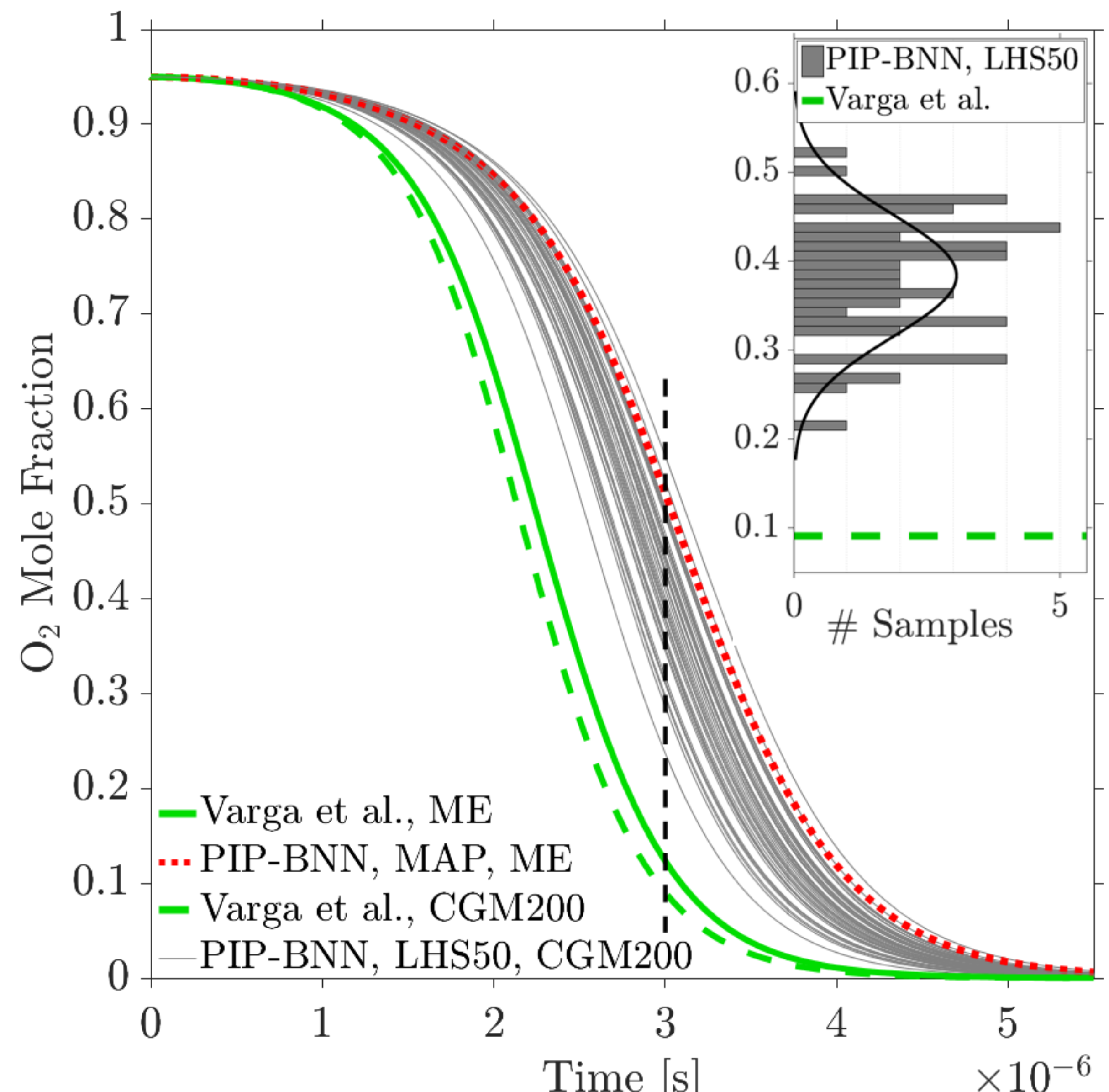


Significant discrepancies in the exchange regions and in the repulsive wall.

Results

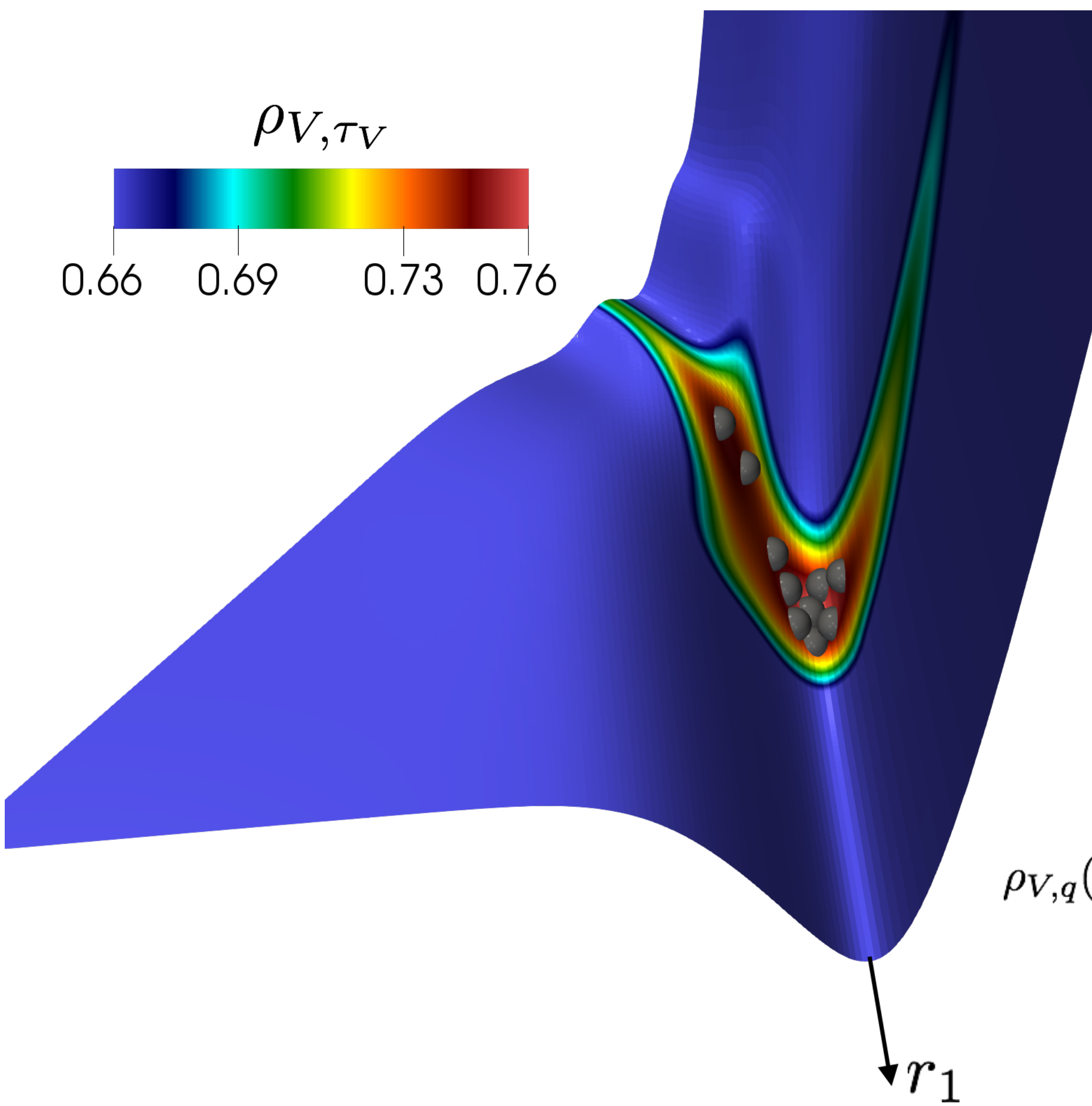


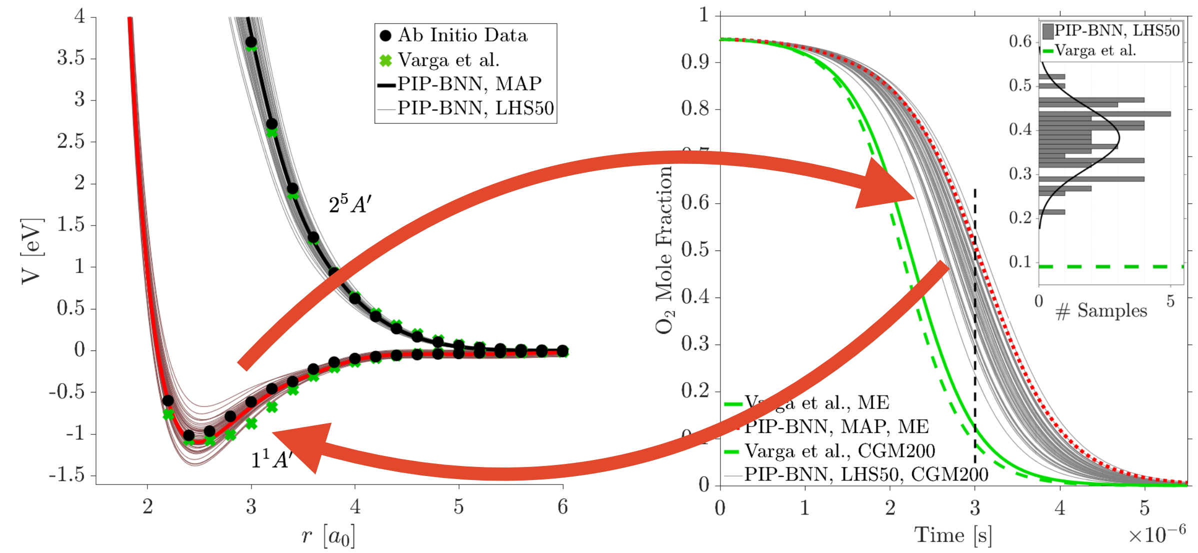
The PESs have been used for computing rates, that have then been employed in a Master Equation study of heat baths at fixed translational temperatures (for the plot on the right, T_{Tran} = 10,000K).



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

Results





Pearson Correlation Coefficient:

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

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.

Conclusions

Main steps:

- Identifying the **<u>relevant</u>** sources of uncertainty;
- [Performing (Local (i.e., around nominal values) or Global) Sensitivity Analysis for Parameter Selection];
- Creating a **physics-based non-deterministic** characterization of inadequacies;
- [Constructing surrogate models]**;**
- **Calibrating** Parameters and hyperparameters**;**
- Performing the **reductions** of the downstream **models (when possible);**
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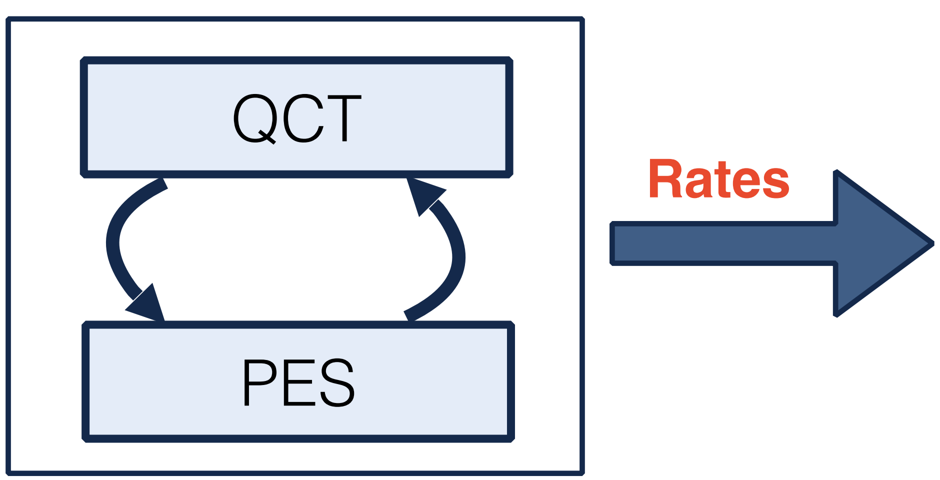

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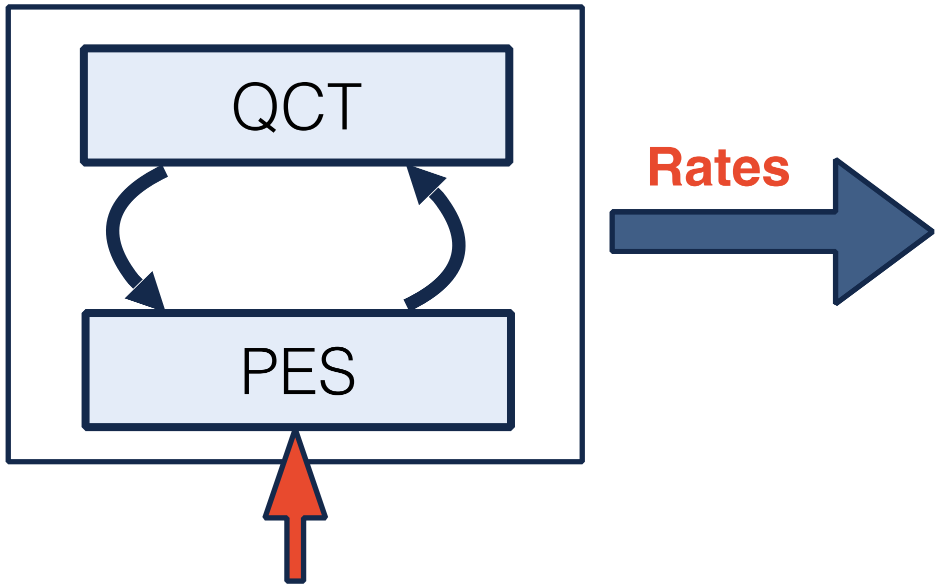

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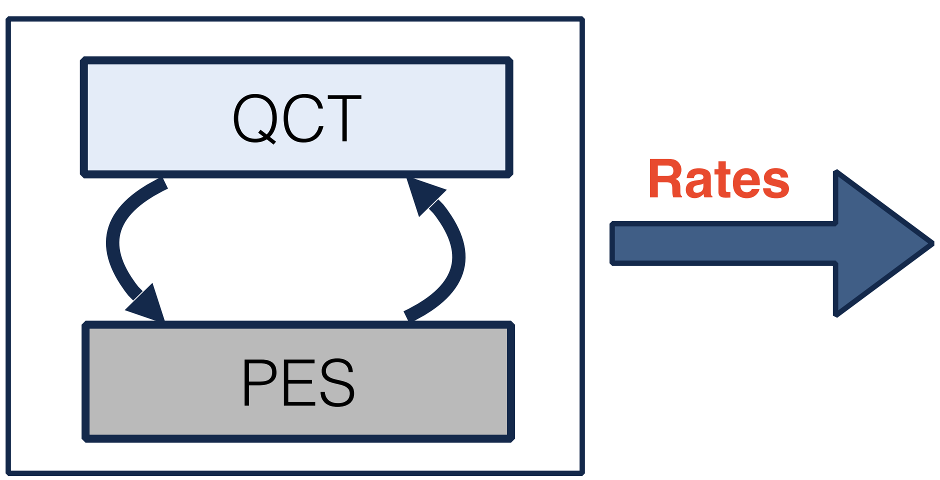

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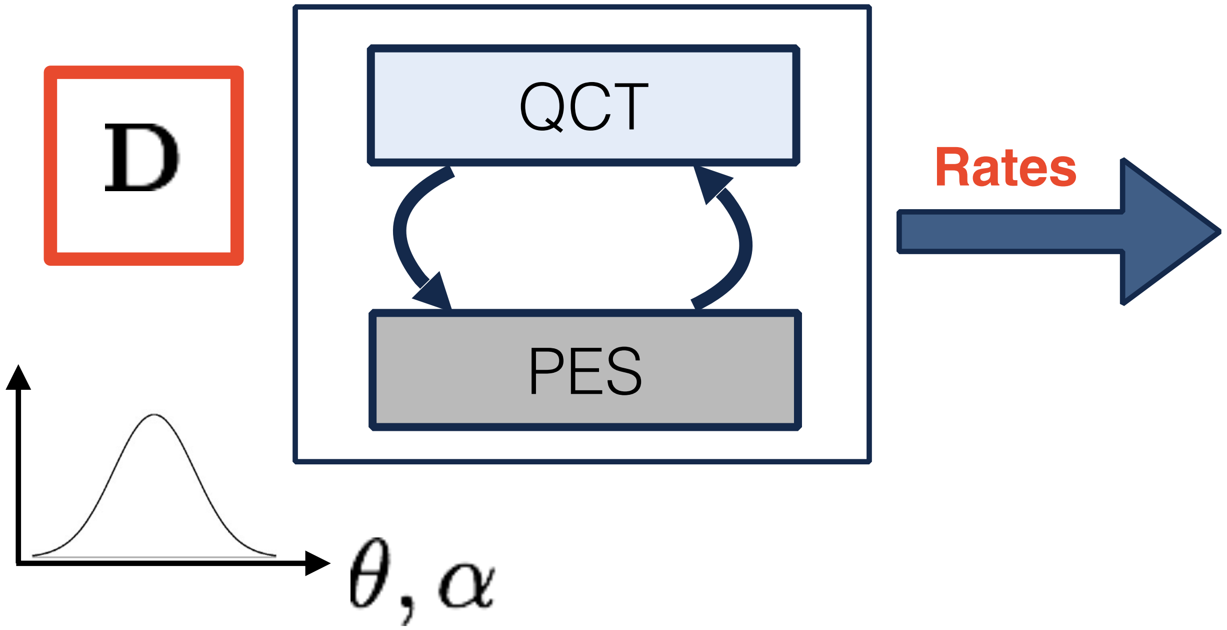

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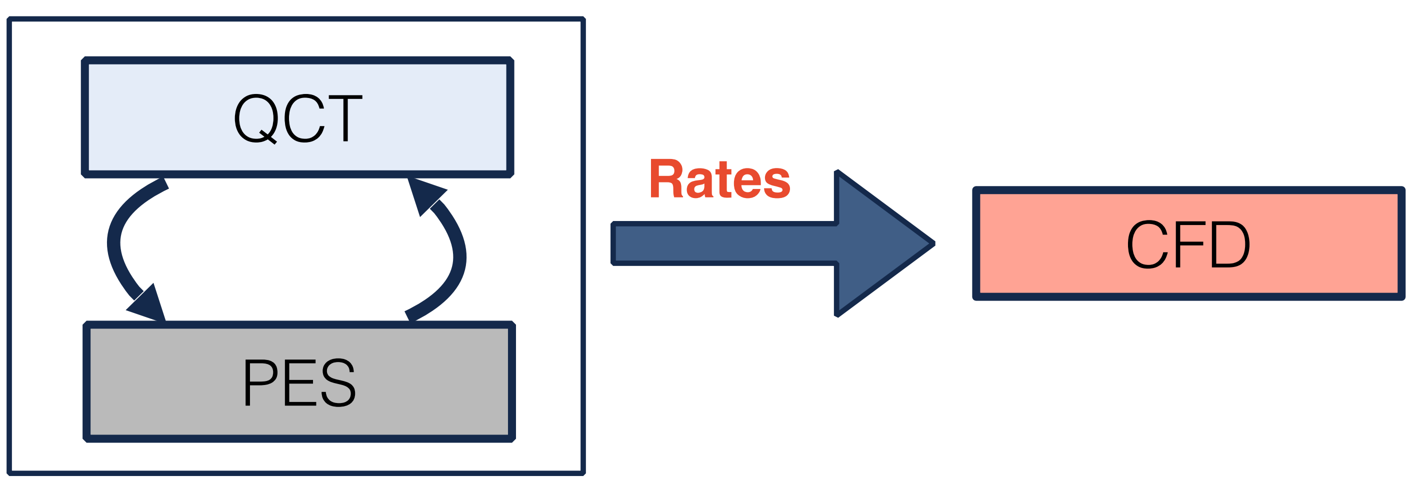

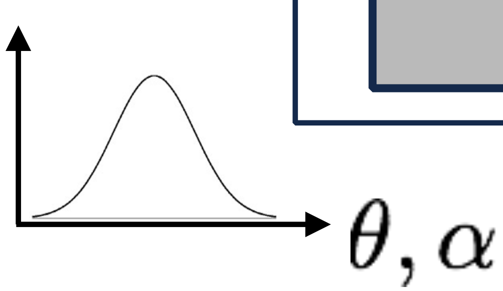

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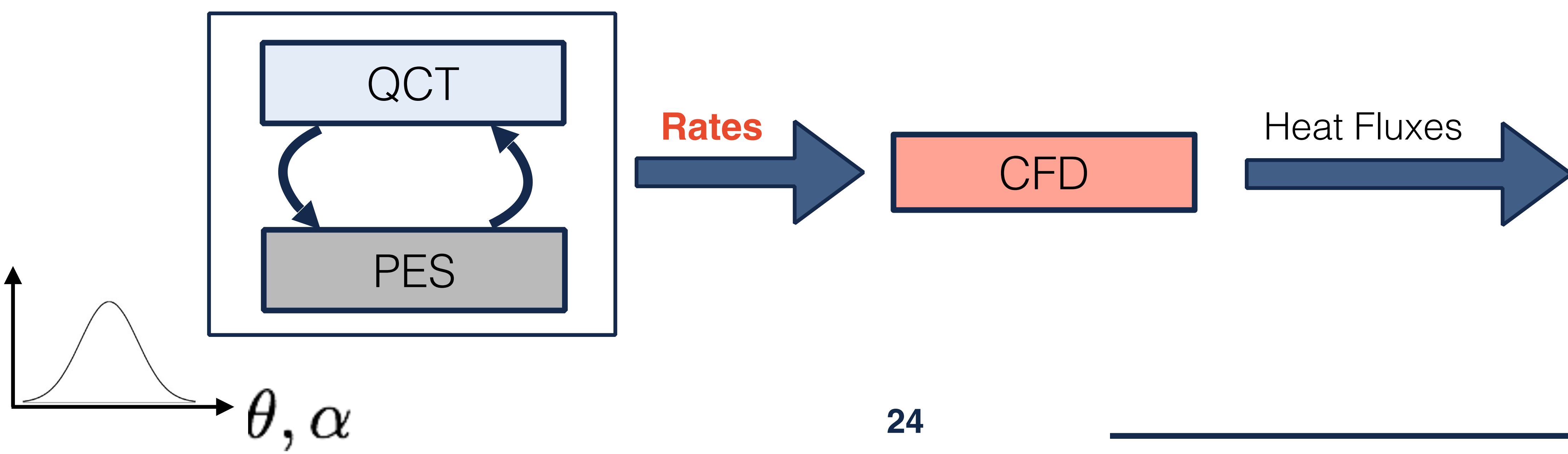

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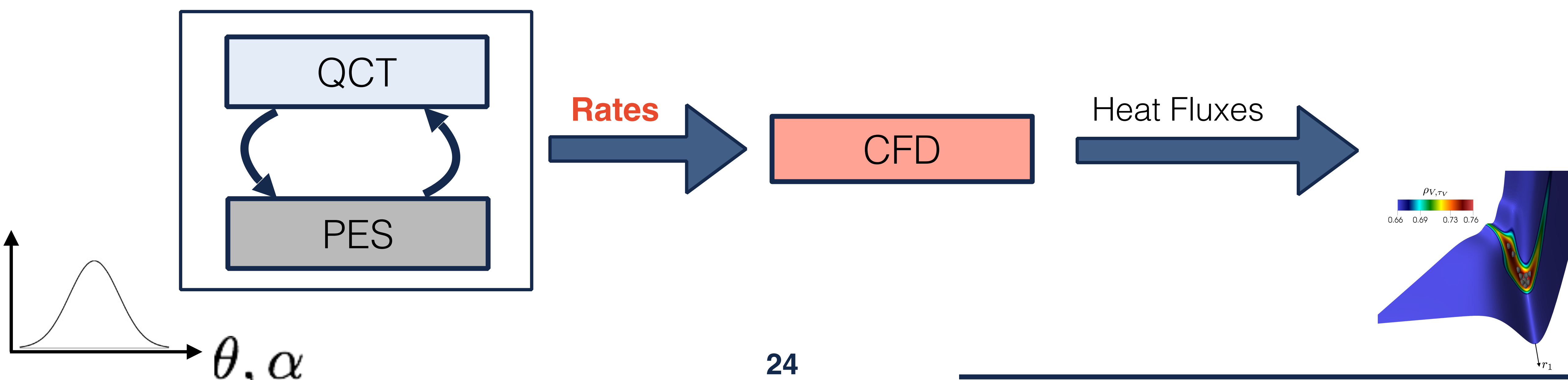

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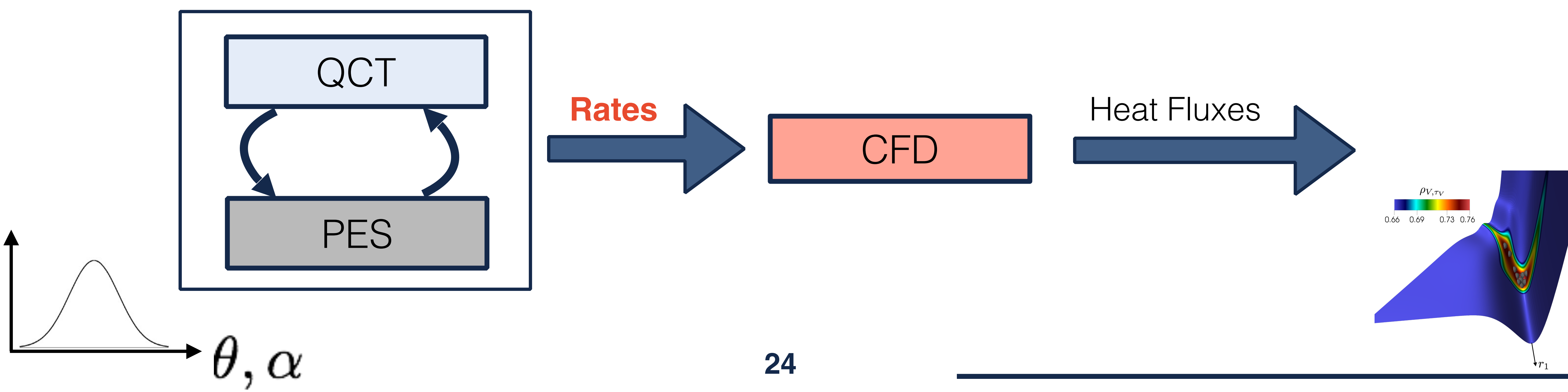

Conclusions

- **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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