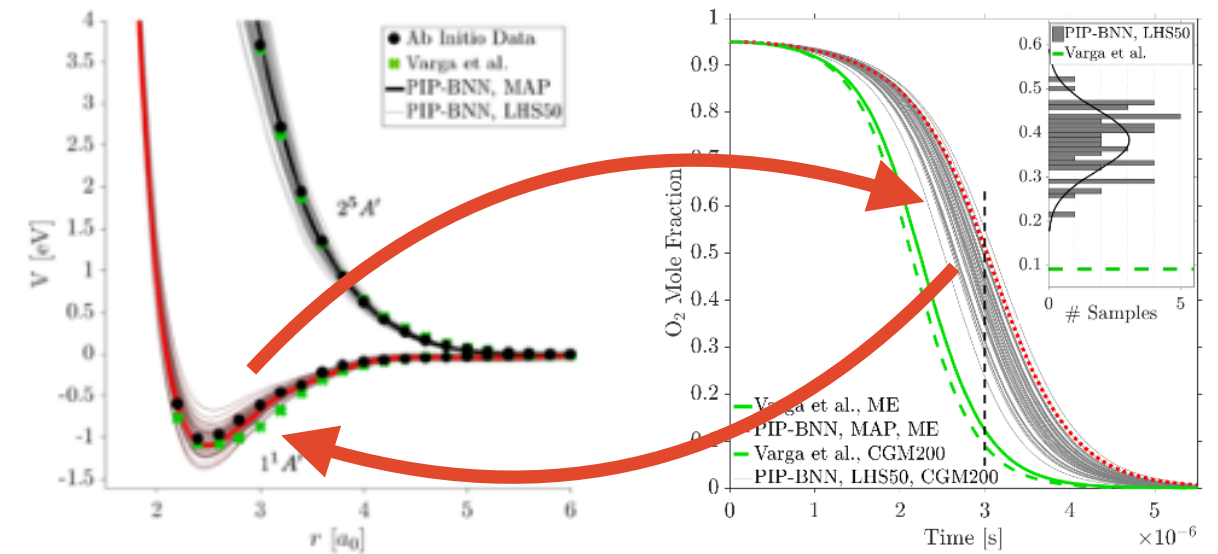
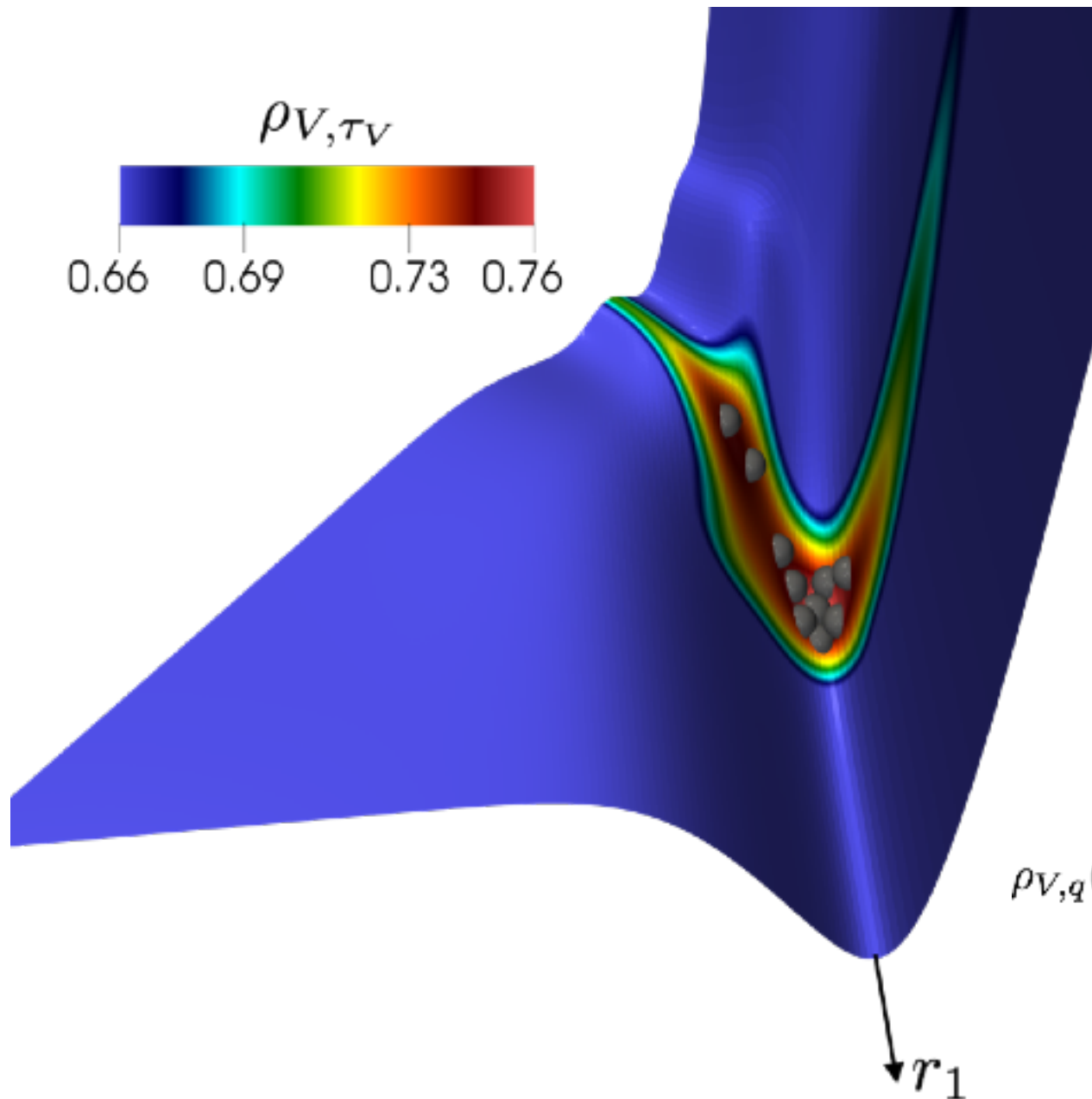


Results



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 **relevant** 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)**;
- **Forward propagating** of the (approximated) posterior distribution;
- **Analyzing the Qols' sensitivity**;
- Conducting **predictive assessment**;
- **Proposing improvements.**

