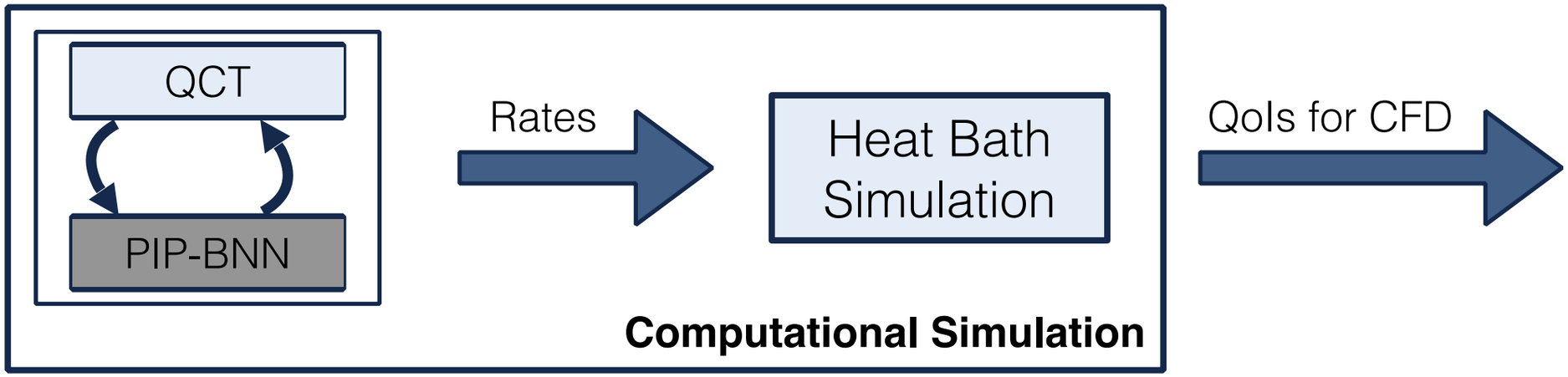
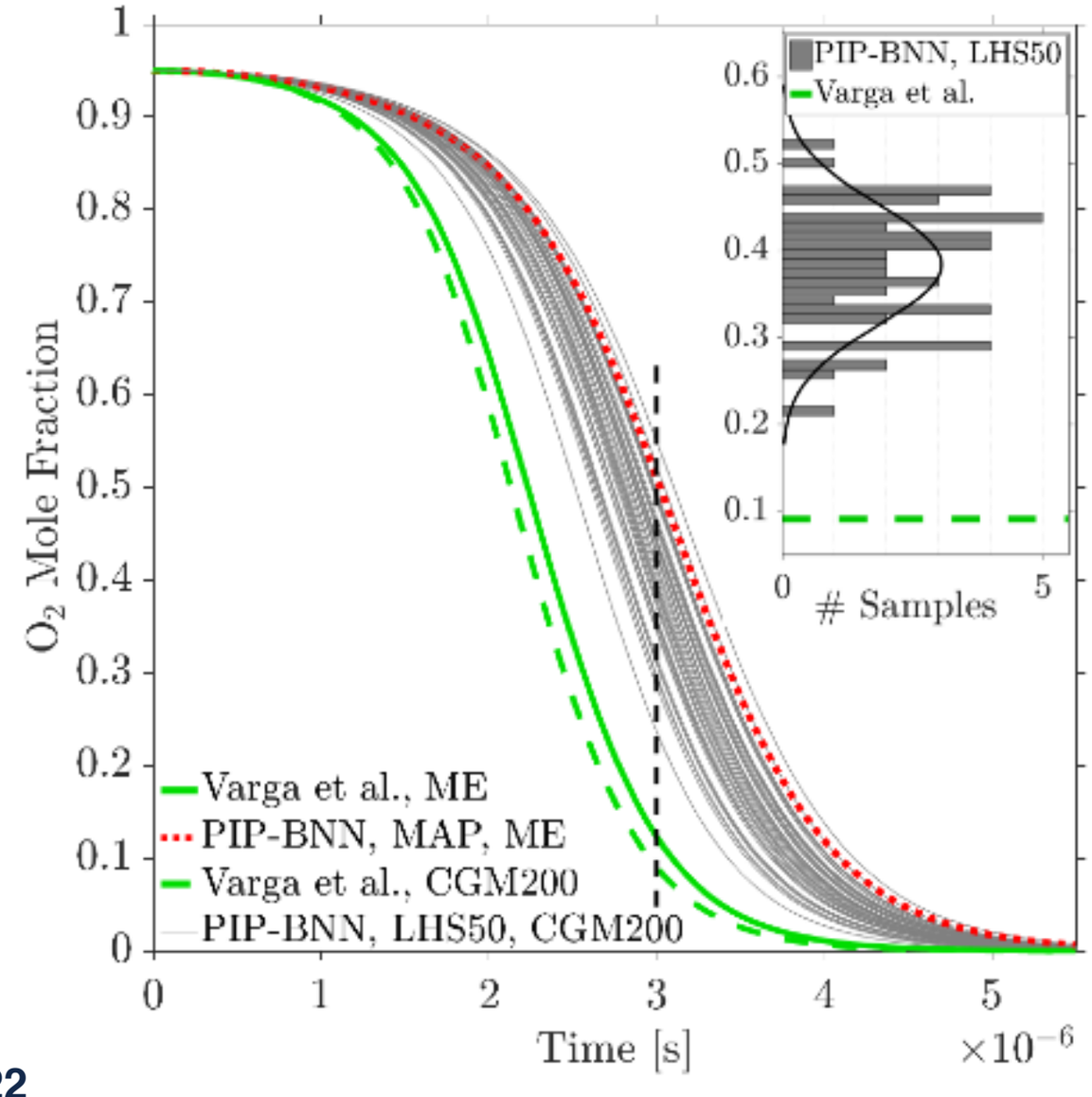
Results

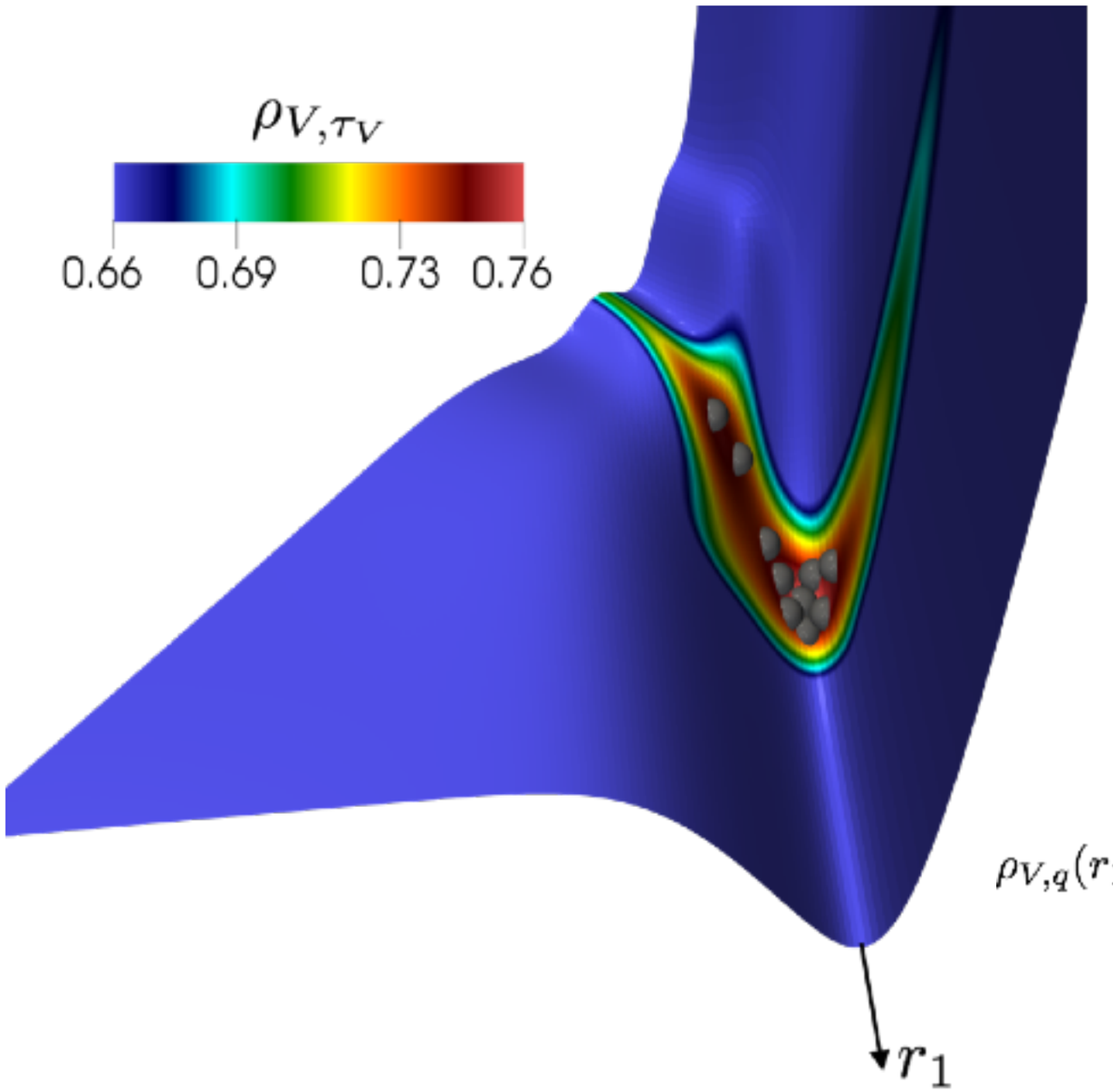


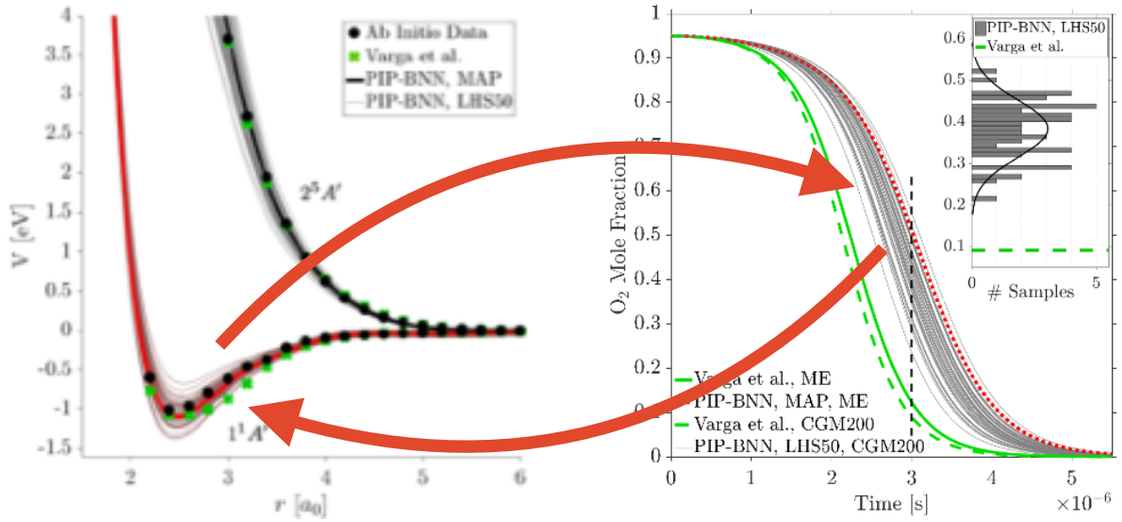
The PESs have been used for computing rates, that have then been employed in a Master Equation study of heat baths at fixed translational temperatures (for the plot on the right, T_{Tran} = 10,000K).



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.