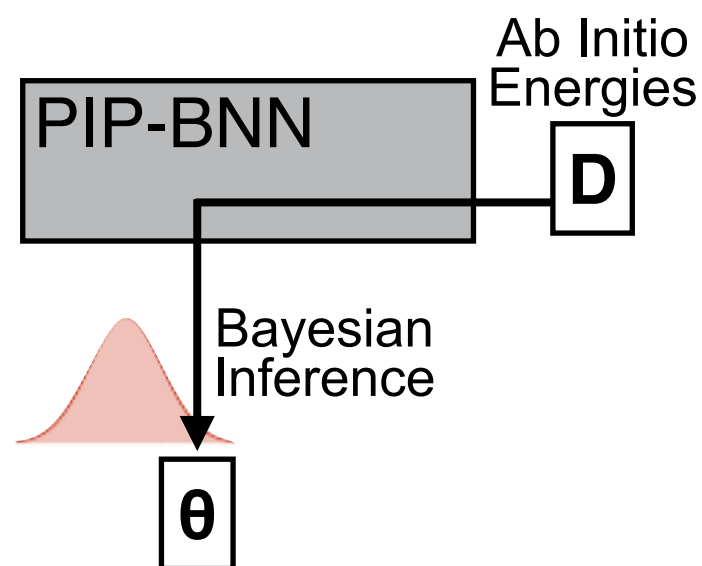
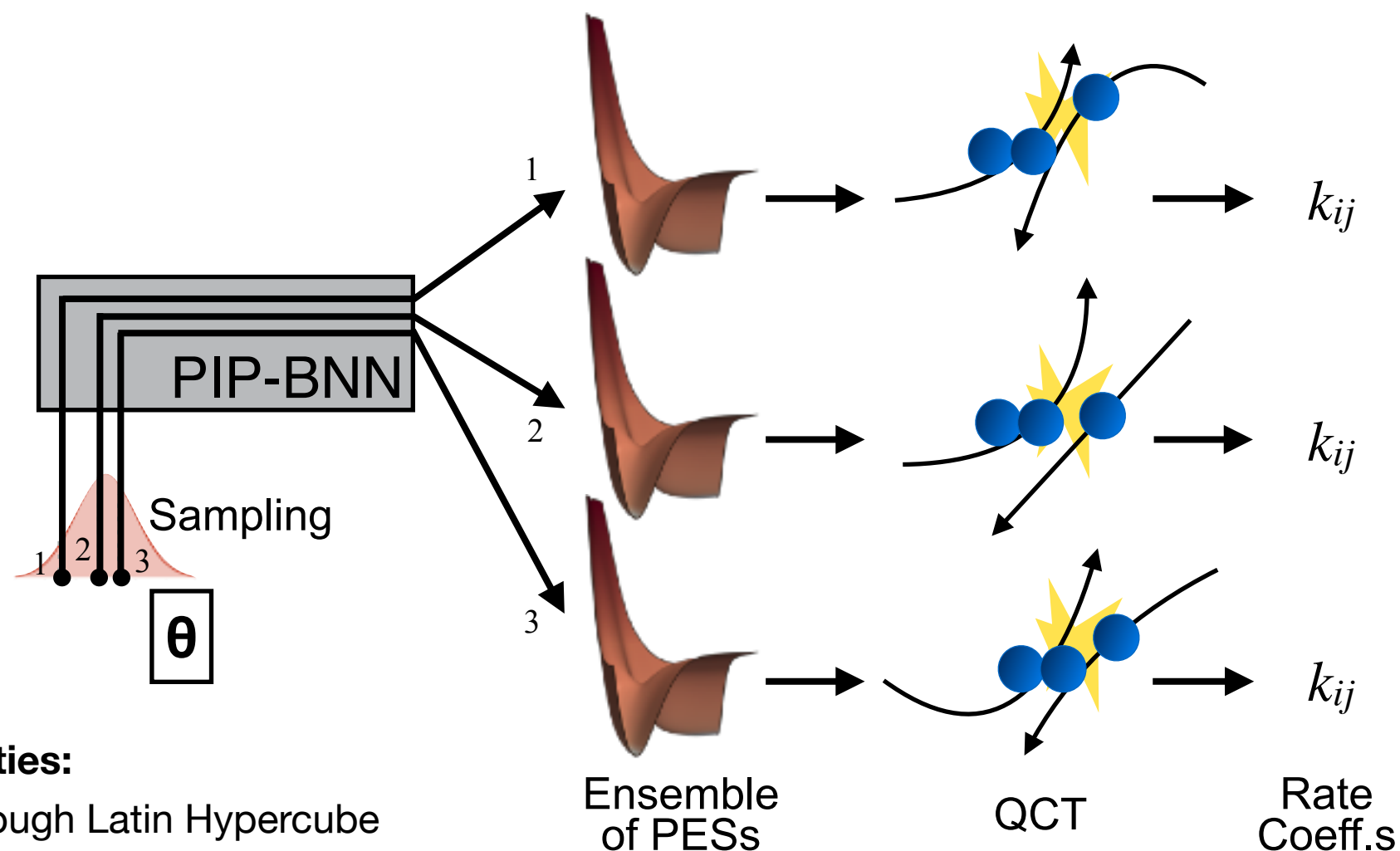


PES UQ: Methodology



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.

