

Minimization stage

$$\min_{\mathcal{N}} \max_f \int_{\Gamma} \overbrace{\| -\nabla_{\mathbf{z}} A_{\mathcal{N}}(\mathbf{z}) - \mathbf{F}(\mathbf{z}) \|^2}_{\mathcal{L}_{\mathcal{N}}} f(\mathbf{z}) d\mathbf{z}$$

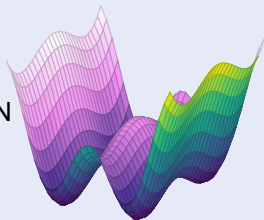
$\mathbf{F}(\mathbf{z})$: Force calculated from full MD

$f(\mathbf{z})$: Sampling Distribution

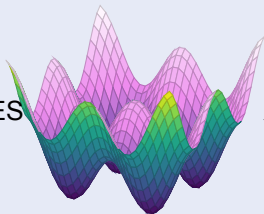
Enhance Sampling

Maximization stage

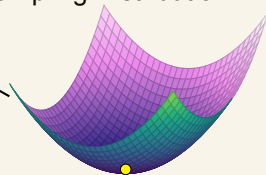
inferred DNN



reference FES



Quadritical Approximation



Posterior Error

