

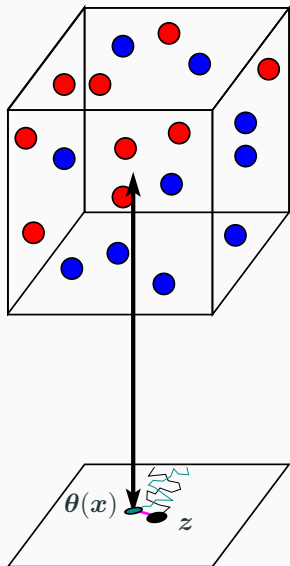
Recent simulation methods for resolving molecular details in thermodynamics and kinetics

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Heterogeneous Multiscale Molecular Dynamics (HMMD)



$$m_i \ddot{x}_i = -\nabla_i V(\mathbf{x}) - \sum_{j=1}^M \kappa[\theta_j(\mathbf{x}) - z_j] \frac{\partial \theta_j}{\partial x_i} + \text{e.f.}$$

Forces link \mathbf{x} and \mathbf{z}

Bias on \mathbf{z} : Enhanced sampling of feature space

$$\bar{m}_j \ddot{z}_j = \sum_{k=1}^M \mathcal{M}_{jk} \kappa[\theta_k(\mathbf{x}) - z_k] + \text{e.f.}$$