

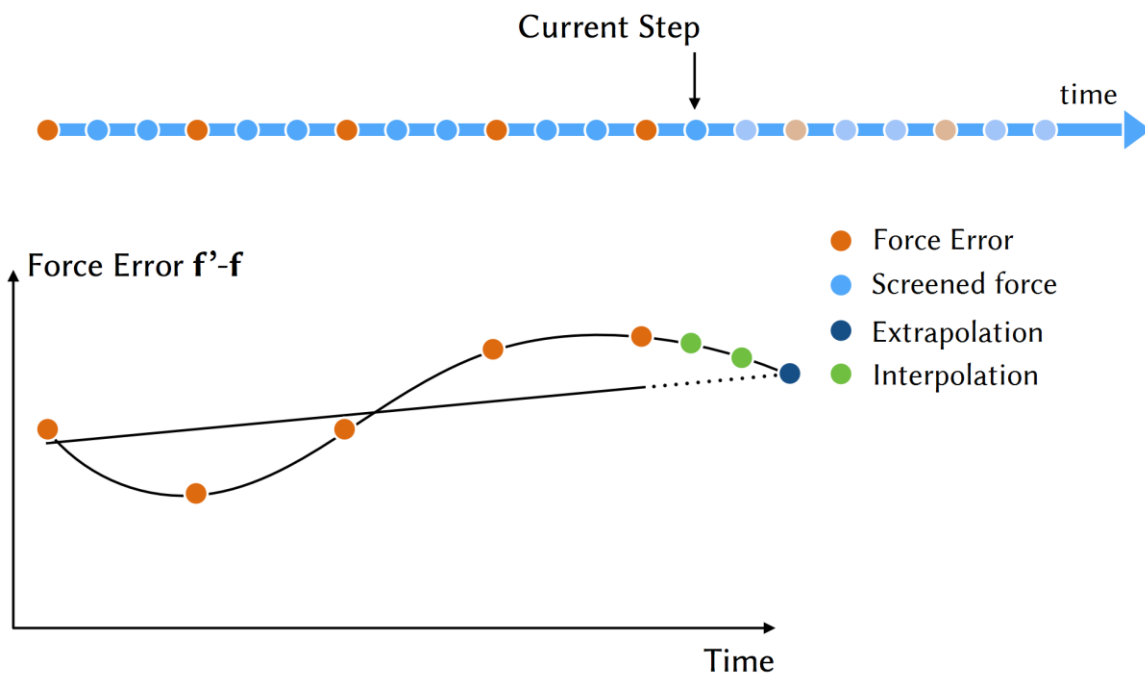
Faster HFX forces in MD runs

$$E_X^{\text{HF}} = -\frac{1}{2} \sum_{\lambda\sigma\mu\nu} \left[\sum_i C_{\mu i} C_{\sigma i} \right] \left[\sum_j C_{\nu j} C_{\lambda j} \right] \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{\phi_\mu(\mathbf{r}_1) \phi_\nu(\mathbf{r}_1) \cdot \phi_\lambda(\mathbf{r}_2) \phi_\sigma(\mathbf{r}_2)}{|\mathbf{r}_2 - \mathbf{r}_1|}$$

Density Matrix Components
Atomic Orbital Basis
Electron-repulsion integrals (ERI)

$|\mathbf{F}| > 10^{-3}$: 10^2 per atom

$|\mathbf{F}| < 10^{-9}$: 10^6 per atom



Speed-up:

CoO: 3.0x

FeO: 2.4x