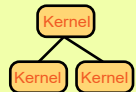


for developers

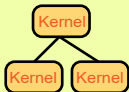


$$\text{Tr}_e \left[|n\rangle\langle m| e^{i\hat{H}t} |k\rangle\langle l| e^{-i\hat{H}t} \right] \mapsto \left(\bar{C}_{nm,kl}(t) \right)^{-1} \int w(\gamma) d\gamma \int_{\mathcal{S}(\mathbf{x}_0, \mathbf{p}_0, \Gamma_0; \gamma)} F d\mathbf{x}_0 d\mathbf{p}_0 d\Gamma_0 \bar{\mathcal{Q}}_{nm,kl}$$

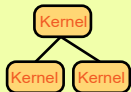
$$\mathbf{f}_{\text{NaF}}(\mathbf{R}) = -\nabla_{\mathbf{R}} E_{j_{\text{occ}}(t)} - \sum_{k \neq l} \left[(E_k(\mathbf{R}) - E_l(\mathbf{R})) \mathbf{d}_{lk}(\mathbf{R}) \right] \tilde{\rho}_{kl}(\mathbf{R})$$



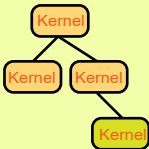
appendChild



insertAt



removeAt



updateAt



Build Solver

Set Inputs

for users

Dynamics Steps

Dump Data & DataFrame

Sample & Save to Files

Others

Build Data Structure

Analysis / Application