Nonlocal Correction Revisited: nlp-prop() and calc_energy()

6/25/22

— Goal: Design band-blocking algorithm for $O(N^3)$ nonlocal correction to improve data locality. [7/28/21].

— Time propagation: nlp-prop()

$$\underset{\substack{\downarrow \\ \text{psi[]}}}{|\psi_n\rangle} \mathrel{-}= \underbrace{\frac{i\Delta_{sci}\Delta_{QD}}{2}}_{\text{cfac}} \sum_{m=nlumo}^{Norb-1} \underset{\substack{\downarrow \\ \text{psio[]}}}{|m\rangle} \langle m|\psi_n\rangle \quad (n \in [0, nhomo]) \tag{1}$$

$$|\psi_n\rangle \longleftarrow \frac{1}{\sqrt{\langle\psi_n|\psi_n\rangle}} |\psi_n\rangle \tag{2}$$

Note

$$\langle m|\psi_n\rangle = \underbrace{\Delta_x\Delta_y\Delta_z}_{\text{Dvol}} \sum_{ijk} \psi_{ijk}^{(m)*}(t=0)\, \psi_{ijk}^{(n)}(t) \tag{3}$$

- Current algorithm

```
for n
    for m
        complex ovlp_m ← 0
        for (i,j,k)
            ovlp_m += ψ_ijk^(m)*(0) ψ_ijk^(n)(t)
        ovlp_m *= cfac · Dvol
        for (i,j,k)
            ψ_ijk^(n)(t) -= ovlp_m · ψ_ijk^(m)(0)
    norm_factor ← 0
    for (i,j,k)
        norm_factor += ||ψ_ijk^(n)(t)||^2
    norm_factor *= Dvol          // <ψ_n|ψ_n>
    norm_factor = 1 / √norm_factor
    for (i,j,k)
        ψ_ijk^(n)(t) *= norm_factor
```

- Energy correction : calc_energy()

$$\epsilon_{pot} \mathrel{+}= \Delta_{sci} \sum_{n=0}^{nhomo} \underbrace{f_n}_{occ[n]=2} \sum_{m=n_{LUMO}}^{Norb-1} |\langle \underbrace{m}_{psi0[\,]} | \underbrace{\psi_n}_{psi[\,]} \rangle|^2 \qquad (4)$$

- Current algorithm

for n

  fext $\leftarrow 0$

  for m

    complex ovlp_val $\leftarrow 0$

    for (i,j,k)

      ovlp_val += $\psi_{ijk}^{(m)*}(t=0)\, \psi_{ijk}^{(n)}(t)$

    fext += $\| \text{Dvol} \cdot \text{ovlp\_val} \|^2$

  $\epsilon_{pot} \mathrel{+}= \underbrace{\Delta_{sci}}_{\text{Dscissor}} \cdot f_n \cdot \text{fext}$

— Matrix-multiplication analogy

$$|\psi_n\rangle = \underbrace{\frac{i\Delta_{sci}\Delta_{QD}}{2}}_{\lambda} \sum_m |m\rangle\langle m|\psi_n\rangle \tag{5}$$

Let the serialized mesh index be

$$\kappa = i \cdot \text{Xstride\_wf} + j \cdot \text{Ystride\_wf} + k \cdot \text{Zstride\_wf} \tag{6}$$

then

$$\underbrace{\psi_{\kappa n}}_{\psi_{ijk}^{(n)}(t)} = \lambda \sum_m \underbrace{\psi^0_{\kappa m}}_{\psi_{ijk}^{(m)}(t=0)} \cdot \Delta_{vol} \sum_{\kappa'} \psi^{0*}_{\kappa' m} \psi_{\kappa' n} \tag{7}$$

Hermitian conjugate

$$\therefore \psi_{\kappa n} = \lambda \Delta_{vol} \underbrace{\sum_m \psi^0_{\kappa m} \underbrace{\sum_{\kappa'} [\psi^{0\dagger}]_{m\kappa'} \psi_{\kappa' n}}_{[\psi^{0\dagger}\psi]_{mn}}}_{[\psi^0\psi^{0\dagger}\psi]_{\kappa n}} \tag{8}$$

cf. If needed, datamode_switch() switches between band-first & band-last modes for psi[].