**Bottomline:** Processor = domain equivalence.

1. The physical system is covered with nonoverlapping rectangular domains $\Omega_{0\alpha}$; $\Omega = \cup_{\alpha} \Omega_{0\alpha}$, $\Omega_{0\alpha} \cap \Omega_{0\beta} = \emptyset$.

2. Each domain is augmented with a buffer layer $\Gamma_{\alpha}$ of thickness $d_{buf}$, and the augmented, overlapping domain $\Omega_{\alpha}$ is defined as

$$\Omega_{\alpha} = \Omega_{0\alpha} \cup \Gamma_{\alpha}$$

(4)

3. The domains are sequentially indexed as $\alpha = 0, 1, ..., P-1$, where $P$ is the number of processors.

4. In this topology-preserving domain decomposition approach, the list $l_{NN}^{(i)} = (\alpha_1, \alpha_2, ..., \alpha_n)$ stores the ID of the nearest-neighbor domains, $\alpha_i \in \{0, 1, ..., P-1\} \cup \{\text{NIL}\}$ ($i=1(\text{x-low}), 2(\text{x-high}), 3(\text{y-low}), 4(\text{y-high}), 5(\text{z-low}), 6(\text{z-high})$), and NIL denotes that $\Omega_{\alpha}$ is at the edge of the physical system thus has no neighbor domain.

5. Periodic boundary condition is transparent in this "self-centric parallelization" scheme.
Overlapping domain-decomposition support function

\[
\left\{
\begin{array}{l}
P^{\alpha}(ir) = 1 \\
P^{\alpha}(ir) = 0 \quad (ir \notin \Omega_\alpha)
\end{array}
\right.
\]

Specifically, let's consider the rectangular domain core \( \Omega_\alpha \) with size \( L_x \times L_y \times L_z \). Then, let's define

\[
P_{0x}(\alpha) = \begin{cases} 
3 \left( \frac{t}{\text{dbuf}} + 1 \right)^2 - 2 \left( \frac{t}{\text{dbuf}} + 1 \right) & (-\text{dbuf} \leq t < 0) \\
1 & (0 \leq t \leq L_\mu) \\
3 \left( \frac{L_\mu + \text{dbuf} - t}{\text{dbuf}} \right)^2 - 2 \left( \frac{L_\mu + \text{dbuf} - t}{\text{dbuf}} \right) & (L_\mu \leq t \leq L_\mu + \text{dbuf})
\end{cases}
\]

(4)

\[
P_0(ir) = P_{0x}(x) \cdot P_{0y}(y) \cdot P_{0z}(z)
\]

(5)

\[
P^{\alpha}(ir) = P_0(ir - \Theta_\alpha)
\]

(6)

where \( \Theta_\alpha \) is the origin (low-x, low-y, low-z corner) of the domain core \( \Omega_{\alpha} \). Now the support function is

\[
P^{\alpha}(ir) = \frac{P^{\alpha}_0(ir)}{\sum_{\alpha=0}^{\alpha-1} P^{\alpha}_0(ir)}
\]

(7)

In the self-centric parallelization, \( P^{\alpha}(ir) \) can be constructed with up to 26 non-NIL neighbors' \( P^{\alpha}_0(ir) \). (Need NN caching.)
Density decomposition

\[ \rho(r) = \left( \sum_{\alpha} p(z^{(r)}) \right) \rho(r) = \sum_{\alpha} \rho_{\alpha}(r) \rho(r) = \sum_{\alpha} \rho_{\alpha}(r) \]  

(8)

This decomposition can be expressed "exactly" as

\[ \rho_{\alpha}(r) = \rho_{\alpha}(r) \langle r | \sum_{\beta} \frac{\exp[\beta(|r-R_{\beta}|)]}{\exp[\beta(|r-R_{\beta}|)] + 1} | r \rangle_{\beta \rightarrow 0} \]

(9)

one-electron Hamiltonian "global" chemical potential.

The one-electron Hamiltonian in the screened-pseudopotential case is

\[ \hat{H} = -\frac{1}{2} \nabla^2 + V_{\text{loc}}(r) \]  

(10)

\[ V_{\text{loc}}(r) = \sum_{I} V_{I}(|r-R_{I}|) \]  

(11)

where \( R_{I} \) is the position of the \( I \)th atom, and we use the atomic unit such that the length and energy units are

\[ \begin{align*}
\frac{a_0}{\alpha} &= \frac{\hbar}{m_e} \\
\frac{\hbar}{\alpha} &= \frac{\hbar}{m_e} \\
\frac{E_{\text{au}}}{\alpha} &= 2 \text{ Ry} = 27.2116 \text{ eV}
\end{align*} \]

For hexagonal CdSe,

\[ V_{I}(r) = \int \frac{d\mathbf{q}}{(2\pi)^3} \sum_{I} e^{i\mathbf{q} \cdot \mathbf{R}_{I}} \]

(12)

\[ V_{I}(\mathbf{q}) = \frac{a_{1I}(\mathbf{q})^2 - a_{2I}}{a_{3I} \exp(a_{4I} \mathbf{q}^2) + 1} \]

(13)

\[
\begin{array}{cccc}
\text{Cd} & a_1 \text{ (a.u.)} & a_2 \text{ (a.u.)} & a_3 \text{ (a.u.)} & a_4 \text{ (a.u.)} \\
0.193 & 0.936 & 0.196 & 1.68 \\
Se & 0.0291 & 4.40 & -1.20 & 0.318 \\
\end{array}
\]
1. We represent the screened local potentials on a one-dimensional numerical mesh with cut-off radius $r_{CI}$ (I=Cd or Se).

2. In the self-centric parallelization, the positions of atoms $\{R_I\}$ within a skin of depth $r_{CI}$ must be cached from the neighbor domains to calculate global $V_{loc}(r)$, which we will use. ($r_{CI}$ could be larger than $\Delta_{buf}$, i.e., $R_I \notin \Omega_a$.)

![Diagram showing the relationship between $r_{CI}$, $R_I$, and $\Omega_a$.]

The chemical potential in Eq. (9) is determined by solving

$$\mu_{el} = \int_{dir} \rho(r) = \int_{dir} \frac{2}{\exp(\beta(\hat{H} - \mu)) + 1} dr$$

(14)
— Crux of the linear-scaling "approximation"

The exact decomposed density \( \rho^\alpha(\mathbf{r}) \), Eq. (9), is now approximated as

\[
\rho^\alpha(\mathbf{r}) \equiv \rho^\alpha(\mathbf{r}) \left| \mathbf{r} \right| \frac{2}{\exp[\beta(\mathbf{A}-\mathbf{\mu})] + 1} \left| \mathbf{r} \right|
\]

\[
\rho^\alpha(\mathbf{r}) \left| \mathbf{r} \right| \frac{2}{\exp[\beta(\mathbf{A}^\alpha - \mathbf{\mu})] + 1} \left| \mathbf{r} \right|
\]

so that the eigenstates of \( \hat{\mathbf{A}}^\alpha \), thus \( \rho^\alpha(\mathbf{r}) \), can be computed locally on processor \( \alpha \).

Here the local Hamiltonian \( \hat{\mathbf{H}}^\alpha \) is defined with "global" potential (i.e., including \( V^\alpha(\mathbf{r}^\alpha - \mathbf{r}^\beta) \) from \( \mathbf{R}^\beta \notin \Omega^\alpha \)) but the basis restricted in \( \Omega^\alpha \).

\[
\hat{\mathbf{H}}^\alpha = \frac{1}{2} \sum_{\mathbf{R}^\beta \in \Omega} \left( \int_{\Omega^\alpha} \int_{\Omega^\alpha} \left( \frac{1}{2} \nabla^2 + \sum_{\mathbf{R}^\beta \in \Omega} V^\alpha(\mathbf{r}^\alpha - \mathbf{r}^\beta) \right) \right) \left| \mathbf{r}^\alpha \right| \left| \mathbf{r}^\beta \right|
\]
Divide-conquer-combine algorithm

1. Divide the space $\Omega$ into nonoverlapping domains $\Omega = \bigcup_{\alpha} \Omega_{\alpha}$, $\Omega_{\alpha} \cap \Omega_{\alpha'} = \emptyset$; augment each domain core $\Omega_{\alpha}$ with a buffer layer $\Omega_{\alpha} = \Omega_{\alpha} + \Gamma_{\alpha}$.

2. Conquer: Solve the sub-domain eigenvalue problems independently in each $\Omega_{\alpha}$

$$\hat{H}_{m^\alpha}^\alpha |m^\alpha\rangle = \varepsilon_{m^\alpha} |m^\alpha\rangle \quad (m = 1, \ldots, \text{Norbmax})$$

(16)

3. \[ \rho_{\alpha}(ir) = \sum_m \rho_{\alpha}(ir) \cdot \frac{2}{\exp[\beta(\varepsilon_{m^\alpha})] + 1} \cdot \left| \psi_{m^\alpha}^{\alpha}(ir) \right|^2 \leq \text{loop to be consistent} \]

(17)

4. Determine $\mu$ by solving

$$N_{\alpha} = \sum_{\text{dir}} \rho_{\alpha}(ir) \leq \text{consistent}$$

(18)

5. Combine: Use inner solutions $\{ \psi_{m^\alpha}^{\alpha}(ir) \in \Omega_{\alpha} \}$ of neighbor domains, $\alpha' \in \cup_{\text{NN}}^{(d)}$, as boundary conditions at the outer surface $S_\alpha$ of $\Omega_\alpha$ to perturb $|m^\alpha\rangle$.

6. Compute

$$\rho(ir) = \sum_{\alpha} \rho_{\alpha}(ir)$$

etc.
Computation of physical quantities

(Density)

\[ \rho^{(ir)} = \sum_{\alpha} \rho^{\alpha}(ir) \] (19)

Note that

\[ \rho^{\alpha}(ir) \propto \frac{2}{m \exp[\beta (E_m^{\alpha} - \mu) + 1]} (\frac{\langle \psi_m^{\alpha} | P^{\alpha}(ir) | \psi_m^{\alpha} \rangle}{\Omega_{\alpha}})^2 \rho^{\alpha}(ir) \]

\[ \therefore \rho^{\alpha}(ir) \propto \frac{2}{m \exp[\beta (E_m^{\alpha} - \mu) + 1]} \langle \psi_m^{\alpha} | P^{\alpha}(ir) | \psi_m^{\alpha} \rangle \Omega_{\alpha} \] (20)

\( \rho^{\alpha}(ir) \) is computed locally on each \( \Omega_{\alpha} \); to compute \( \rho^{(ir)} \), neighbor \( \rho^{\alpha'}(ir) \) \((\alpha' \in \Omega_{\text{NN}})\) need be cached via 6-step copy operations.

(Energy)

\[ E = \text{tr} \frac{2}{\exp[\beta (H - \mu)] + 1} H \]

\[ = \sum_{\Omega} \sum_{\mbox{dir}} \frac{2}{\exp[\beta (E_m - \mu)] + 1} \langle m | H | ir \rangle \]

\[ = \sum_{\Omega} \sum_{\mbox{dir}} \frac{2}{\exp[\beta (E_m + \mu)] + 1} E_m | \psi_m^{(ir)} \rangle^2 \]

\[ = \sum_{\alpha} \sum_{\Omega} \sum_{\mbox{dir}} \frac{2}{\exp[\beta (E_m^{\alpha} - \mu)] + 1} E_m^{\alpha} | \psi_m^{\alpha}(ir) \rangle^2 \rho^{\alpha}(ir) \]

Thus in the divide-and-conquer approximation,

\[ E^{\alpha} = \sum_m \frac{2}{\exp[\beta (E_m^{\alpha} - \mu)] + 1} E_m^{\alpha} \frac{\langle \psi_m^{\alpha} | P^{\alpha}(ir) | \psi_m^{\alpha} \rangle}{\Omega_{\alpha}} \]

\[ E^{\alpha} \propto \sum_m \frac{2}{\exp[\beta (E_m^{\alpha} - \mu)] + 1} E_m^{\alpha} \frac{\langle \psi_m^{\alpha} | P^{\alpha}(ir) | \psi_m^{\alpha} \rangle}{\Omega_{\alpha}} \] (21)

\[ E = \sum_{\alpha} E^{\alpha} \] (22)
Solving local eigenvalue problems.

Solve
\[ \left[ \frac{1}{2} \nabla^2 + V_{\text{loc}}(r) \right] \psi_n^{\alpha}(r) = \varepsilon_n^{\alpha} \psi_n^{\alpha}(r) \quad (n=1, \ldots, N_{\text{orb max}}) \quad (23) \]

with orthonormal constraints
\[ \int_{\Omega_{\alpha}} \psi_m^{\alpha}(r)^* \psi_n^{\alpha}(r) = \delta_{mn} \quad (24) \]

(Boundary condition)

During the divide-$$\phi$$-conquer phase, we try two boundary conditions:

(I) Rigid-wall boundary condition
\[ \psi_m^{\alpha}(r) = 0 \quad (r \in S_\alpha) \quad (25) \]

(II) Wigner-Seitz boundary condition
\[ \frac{\partial \psi_m^{\alpha}}{\partial r_\nu} = 0 \quad (r \in S_\alpha) \quad (26) \]

In the combine phase, inner solutions from neighbor domains will be cached and used to specify the boundary condition
\[ \psi_m^{\alpha}(r) = \left[ \sum_{n} \left( \varepsilon_m^{\alpha} - \varepsilon_n^{\alpha} \right)^{-\frac{3}{2}} \left| \psi_n^{\alpha}(r) \right|^2 \right]^{1/2} \quad (r \in S_\alpha \cap \Omega_{\phi}) \quad (27) \]