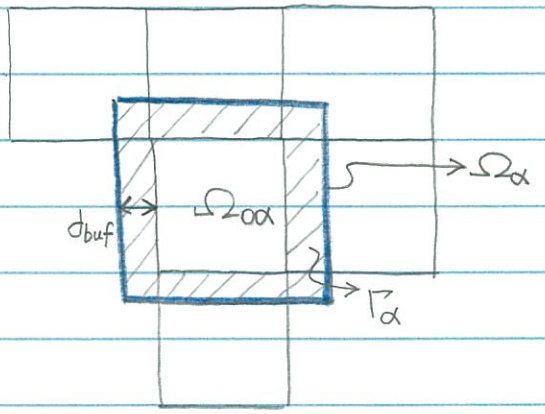
Divide-Conquer-Combine Electronic Structure Calculation

7/11/03

— Bottomline: Processor = domain equivalence.

1. The physical system is covered with nonoverlapping rectangular domains $\Omega_{0\alpha}$; $\Omega = \bigcup_\alpha \Omega_{0\alpha}$, $\Omega_\alpha \cap \Omega_{\alpha'} = \emptyset$.
2. Each domain is augmented with a buffer layer Γ_α of thickness d_{buf}, and the augmented, overlapping domain Ω_α is defined as

$$\Omega_\alpha = \Omega_{0\alpha} \cup \Gamma_\alpha \qquad (1)$$

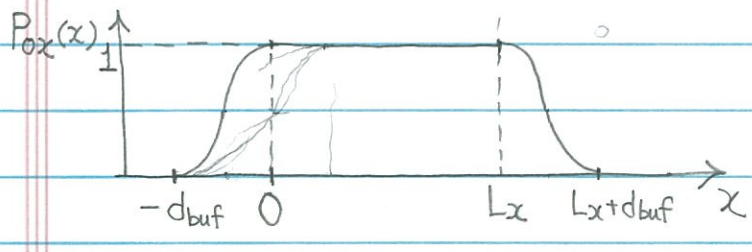


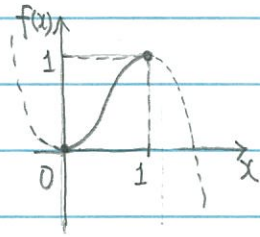
3. The domains are sequentially indexed as $\alpha = 0, 1, \ldots, P-1$, where P is the number of processors. ← my multiple domains / processor
4. In this topology-preserving domain decomposition approach, the list $l_{NN}^{(\alpha)} = (\alpha_1, \alpha_2, \ldots, \alpha_6)$ stores the ID of the nearest-neighbor domains, $\alpha_i \in \{0, 1, \ldots, P-1\} \cup \{\text{NIL}\}$ ($i = 1$ (x-low), 2 (x-high), 3 (y-low), 4 (y-high), 5 (z-low), 6 (z-high)), and NIL denotes that Ω_α is at the edge of the physical system thus has no neighbor domain. (↳ NN(6); ↳ -1)
5. Periodic boundary condition is transparent in this "self-centric parallelization" scheme.

— Overlapping domain-decomposition support function

$$\begin{cases} \sum_{\alpha=0}^{P-1} P^{\alpha}(\mathbf{r}) = 1 & (2) \\ P^{\alpha}(\mathbf{r}) = 0 \quad (\mathbf{r} \notin \Omega_{\alpha}) & (3) \end{cases}$$

Specifically, let's consider the rectanglar domain core Ω_α with size $L_x \times L_y \times L_z$. Then, let's define





$f(x) = 3x^2 - 2x^3 = x^2(3-2x)$

$f'(x) = 6x - 6x^2 = 6x(1-x)$

x	⋯	0	⋯	1	⋯
f'	−	0	+	0	−
f	↘	0	↗	1	↘

DBFX etc.

$$P_{0\mu}(t) = \begin{cases} 3\left(\frac{t}{d_{buf}}+1\right)^2 - 2\left(\frac{t}{d_{buf}}+1\right)^3 & (-d_{buf} \le t < 0) \\ 1 & (0 \le t < L_\mu) \\ 3\left(\frac{L_\mu + d_{buf} - t}{d_{buf}}\right)^2 - 2\left(\frac{L_\mu + d_{buf} - t}{d_{buf}}\right)^3 & (L_\mu \le t < L_\mu + d_{buf}) \end{cases} \quad (4)$$

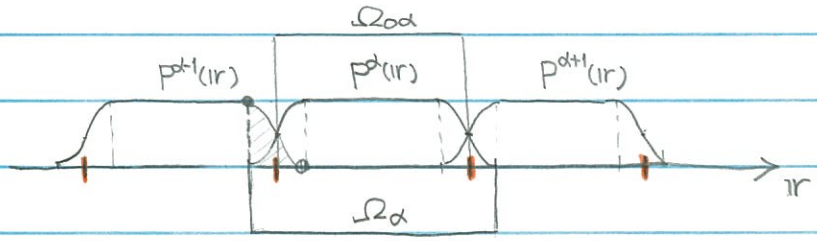
$(\mu = x, y, z)$

$$P_0(\mathbf{r}) = P_{0x}(x)\, P_{0y}(y)\, P_{0z}(z) \quad (5)$$

$$P_0^{\alpha}(\mathbf{r}) = P_0(\mathbf{r} - \Phi_\alpha) \quad (6)$$

where Φ_α is the origin (low-x, low-y, low-z corner) of the domain core $\Omega_{0\alpha}$. Now the support function is

$$P^{\alpha}(\mathbf{r}) = \frac{P_0^{\alpha}(\mathbf{r})}{\sum_{\alpha'=0}^{P-1} P_0^{\alpha'}(\mathbf{r})} \quad (7)$$



In the self-centric parallelization, $P^{\alpha}(\mathbf{r})$ can be constructed with up to 26 non-NIL neighbors' $P_0^{\alpha'}(\mathbf{r})$. (Need NN caching.)

— Density decomposition

$$\rho(\mathbf{r}) = \underbrace{\left(\sum_\alpha \rho^\alpha(\mathbf{r})\right)}_{1} \rho(\mathbf{r}) = \sum_\alpha \underbrace{\rho^\alpha(\mathbf{r})\rho(\mathbf{r})}_{\equiv \rho^\alpha(\mathbf{r})} = \sum_\alpha \rho^\alpha(\mathbf{r}) \tag{8}$$

This decomposition can be expressed "exactly" as

$$\rho^\alpha(\mathbf{r}) = \rho^\alpha(\mathbf{r}) \left\langle \mathbf{r} \left| \frac{\Sigma}{\exp[\beta(\hat{H}-\mu)]+1} \right| \mathbf{r} \right\rangle \Big|_{\beta\to 0} \tag{9}$$

($\hat{H}$: one-electron Hamiltonian; μ: "global" chemical potential.)

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

$$\hat{H} = -\frac{1}{2}\nabla^2 + V_{loc}(\mathbf{r}) \tag{10}$$

$$V_{loc}(\mathbf{r}) = \sum_I v_I(|\mathbf{r}-\mathbf{R}_I|) \tag{11}$$

where $\mathbf{R}_I$ is the position of the Ith atom, and we use the atomic unit such that the length and energy units are

$\begin{cases} \text{length}: a_B = \hbar^2/me^2 = 0.5291772\ \text{Å} \\ \text{energy}: E_{au} = me^4/\hbar^2 = 27.2116\ \text{eV} \quad (= 2\text{Ry}) \end{cases}$

$\frac{e^2}{a} = \frac{\hbar^2}{ma^2}$

$\frac{e^2}{a} = e^2 \cdot \frac{me^2}{\hbar^2}$

For hexagonal CdSe,

$$v_I(r) = \int \frac{d\mathbf{q}}{(2\pi)^3} v_I(q)\, e^{i\mathbf{q}\cdot\mathbf{r}} \tag{12}$$

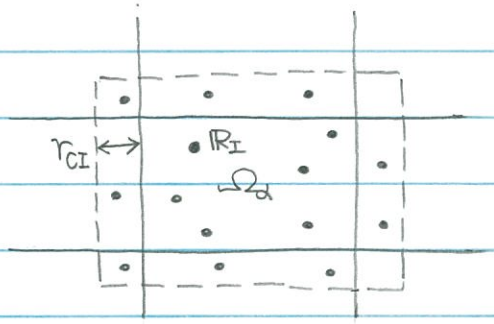
$$v_I(q) = \frac{a_{1I}(q^2 - a_{2I})}{a_{3I}\exp(a_{4I}q^2) + 1} \tag{13}$$

APP1(4)

I	a_1 (a.u.)	a_2 (a.u.)	a_3 (a.u.)	a_4 (a.u.)
Cd	.193	.936	.196	1.68
Se	−.0291	4.40	−1.20	.318

APP2(4)

1. We represent the radial values of 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 $\{\mathbb{R}_I\}$ within a skin of depth r_{cI} must be cached from the neighbor domains to calculate global $V_{loc}(\mathbb{r})$, which we will use. (r_{cI} could be larger than d_{buf}, i.e., $\exists \mathbb{R}_I \notin \Omega_\alpha$.)



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

$$N_{el} = \int d\mathbb{r}\, \rho(\mathbb{r}) = \int d\mathbb{r}\, \langle \mathbb{r}| \frac{2}{\exp[\beta(\hat{H}-\mu)]+1} |\mathbb{r}\rangle \qquad (14)$$

— Crux of the linear-scaling "approximation"

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

$$\rho^\alpha(\mathbf{r}) \equiv \rho^\alpha(\mathbf{r}) \langle \mathbf{r}| \frac{2}{\exp[\beta(\hat{H}-\mu)]+1} |\mathbf{r}\rangle$$

$$\tilde{=} \rho^\alpha(\mathbf{r}) \langle \mathbf{r}| \frac{2}{\exp[\beta(\hat{H}^\alpha-\mu)]+1} |\mathbf{r}\rangle \quad (14)$$

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

Here the local Hamiltonian $\hat{H}^\alpha$ is defined with "global" potential (i.e., including $v_I(|\mathbf{r}-\mathbf{R}_I|)$ from $\mathbf{R}_I \notin \Omega_\alpha$) but the basis restricted in Ω_α.

$$\hat{H}^\alpha \equiv \int_{\Omega_\alpha} d\mathbf{r} \int_{\Omega_\alpha} d\mathbf{r}' |\mathbf{r}\rangle \left(-\frac{1}{2}\nabla_{\mathbf{r}}^2 + \sum_{\mathbf{R}_I \in \Omega} v_I(|\mathbf{r}'-\mathbf{R}_I|) \right) \langle \mathbf{r}'| \quad (15)$$

— Divide-conquer-combine algorithm

1. Divide the space Ω into nonoverlapping domains $\Omega = \bigcup_\alpha \Omega_{0\alpha}$ $\Omega_{0\alpha} \cap \Omega_{0\alpha'} = \emptyset$; augment each domain core $\Omega_{0\alpha}$ with a buffer layer $\Omega_\alpha = \Omega_{0\alpha} + \Gamma_\alpha$.

2. Conquer: Solve the sub-domain eigenvalue problems independently in each Ω_α

$$\hat{H}^\alpha |m^\alpha\rangle = \epsilon_m^\alpha |m^\alpha\rangle \quad (m = 1, \cdots, N_{orbmax}) \tag{16}$$

3. $$\rho^\alpha(\mathbf{r}) = \sum_m p^\alpha(\mathbf{r}) \frac{2}{\exp[\beta(\epsilon_m^\alpha - \mu)] + 1} |\psi_m^\alpha(\mathbf{r})|^2 \tag{17}$$

4. Determine μ by solving

$$N_{el} = \sum_\alpha \int d\mathbf{r}\, \rho^\alpha(\mathbf{r}) \tag{18}$$

loop to be consistent

5. Combine: Use inner solutions $\{\psi_n^{\alpha'}(\mathbf{r}) \in \Omega_{0\alpha'}\}$ of neighbor domains, $\alpha' \in l_{NN}^{(\alpha)}$, as boundary conditions at the outer surface S_α of Ω_α to perturb $|m^\alpha\rangle$.

6. Compute

$$\rho(\mathbf{r}) = \sum_\alpha \rho^\alpha(\mathbf{r})$$

etc.

– Computation of physical quantities

(Density)

$$\rho(\mathbf{r}) = \sum_{\alpha} \rho^{\alpha}(\mathbf{r}) \tag{19}$$

Note that

$$\rho^{\alpha}(\mathbf{r}) \simeq \sum_{m} \frac{2}{\exp[\beta(\epsilon_m^{\alpha}-\mu)]+1} \underbrace{|\psi_m^{\alpha}(\mathbf{r})|^2 \cdot p^{\alpha}(\mathbf{r})}$$

$$\therefore \rho^{\alpha}(\mathbf{r}) \simeq \sum_{m} \frac{2}{\exp[\beta(\epsilon_m^{\alpha}-\mu)]+1} \langle \psi_m^{\alpha} | p^{\alpha}(\mathbf{r}) | \psi_m^{\alpha} \rangle_{\Omega_\alpha} \tag{20}$$

$\rho^{\alpha}(\mathbf{r})$ is computed locally on each Ω_α; to compute $\rho(\mathbf{r})$, neighbor $\rho^{\alpha'}(\mathbf{r})$ ($\alpha' \in l_{NN}^{(\alpha)}$) need be cached via 6-step copy operations.

(Energy)

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

$$= \int_{\Omega} d\mathbf{r} \sum_{m} \langle \mathbf{r}|m\rangle \frac{2}{\exp[\beta(\epsilon_m-\mu)]+1} \epsilon_m \langle m|\mathbf{r}\rangle$$

$$= \int_{\Omega} d\mathbf{r} \sum_{m} \frac{2}{\exp[\beta(\epsilon_m-\mu)]+1} \epsilon_m |\psi_m(\mathbf{r})|^2$$

($\because \sum_{\alpha} p^{\alpha}(\mathbf{r}) = 1$)

$$= \sum_{\alpha} \int_{\Omega} d\mathbf{r} \sum_{m} \frac{2}{\exp[\beta(\epsilon_m-\mu)]+1} \epsilon_m |\psi_m(\mathbf{r})|^2 p^{\alpha}(\mathbf{r})$$

$$\simeq \sum_{\alpha} \int_{\Omega_\alpha} d\mathbf{r} \sum_{m} \frac{2}{\exp[\beta(\epsilon_m^{\alpha}-\mu)]+1} \epsilon_m^{\alpha} |\psi_m^{\alpha}(\mathbf{r})|^2 p^{\alpha}(\mathbf{r})$$

Thus in the divide-&-conquer approximation,

$$E = \sum_{\alpha} E^{\alpha} \tag{21}$$

$$E^{\alpha} \simeq \sum_{m} \overbrace{\frac{2}{\exp[\beta(\epsilon_m^{\alpha}-\mu)]+1}}^{\mathrm{occ}(m,\alpha)} \overbrace{\epsilon_m^{\alpha}}^{\mathrm{eorb}(m,\alpha)} \overbrace{\langle \psi_m^{\alpha} | p^{\alpha}(\mathbf{r}) | \psi_m^{\alpha} \rangle_{\Omega_\alpha}}^{\mathrm{dnorb}(m,\alpha)} \tag{22}$$

— Solving local eigenvalue problems

Solve

$$\left[-\frac{1}{2}\nabla^2 + V_{loc}(\mathbf{r})\right]\psi_n^\alpha(\mathbf{r}) = \varepsilon_n^\alpha \psi_n^\alpha(\mathbf{r}) \quad (n=1,\dots,N_{orbmax}) \tag{23}$$

with orthonormal constraints

$$\int_{\Omega_\alpha} d\mathbf{r}\, \psi_m^{\alpha *}(\mathbf{r})\, \psi_n^\alpha(\mathbf{r}) = \delta_{mn} \tag{24}$$

(Boundary condition)

During the divide-&-conquer phase, we try two boundary conditions:

(I) Rigid-wall boundary condition

$$\psi_m^\alpha(\mathbf{r}) = 0 \quad (\mathbf{r} \in S_\alpha) \tag{25}$$

(II) Wigner-Seitz boundary condition

$$\partial\psi_m^\alpha/\partial n_S = 0 \quad (\mathbf{r} \in S_\alpha) \tag{26}$$

In the combine phase, inner solutions from neighbor domains will be cached and used to specify the boundary condition

$$\psi_m^\alpha(\mathbf{r}) = \left[\sum_n \frac{|\epsilon_m^\alpha - \epsilon_n^\beta|^{-\xi}}{\sum_{m'} |\epsilon_{m'}^\alpha - \epsilon_n^\beta|^{-\xi}} |\psi_n^\beta(\mathbf{r})|^2\right]^{1/2} \quad (\mathbf{r} \in \underbrace{S_\alpha \cap \Omega_{o\beta}}_{\| \; S_{o\beta}}) \tag{27}$$