Parallel Divide-Conquer-Combine Electronic-Structure Calculation: Data Structures

7/15/03

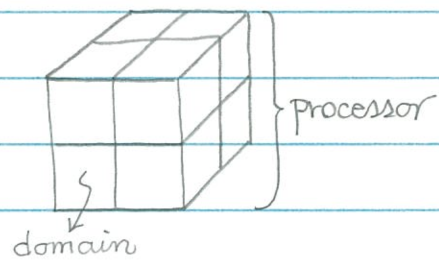
– Self-centric parallelization

$$\begin{cases} \text{Computation} = \sum_p \text{processor} & \sim \text{given neighbors} \\ \text{Physics} = \sum_\alpha \text{domain} \end{cases}$$

NDX, NDY, NDZ

– Processor (computational unit) / vs. domain (physical unit)

Each processor has $N_{dx} \times N_{dy} \times N_{dz}$ domains in the x, y, z directions, arranged in a 3D mesh.



$idz = 0$

idy \ idx	0	1	$2 = N_{dx}-1$
$N_{dy}-1 = 1$	2	5	9
0	0	4	8

$idz = 1 = N_{dz}-1$

3	7	11
1	6	10

(Domain ID)

id, idx, idy, idz

$$i_d = i_{dx}(N_{dy}N_{dz}) + i_{dy}N_{dz} + i_{dz}$$

or

$$\begin{cases} i_{dx} = \lfloor i_d / (N_{dy}N_{dz}) \rfloor \\ i_{dy} = \lfloor i_d / N_{dz} \rfloor \bmod N_{dy} \\ i_{dz} = i_d \bmod N_{dz} \end{cases}$$

NMSHX, NMSHY, NMSHZ ALX, ALY, ALZ

– Domain

Each domain core Ω_0 is a parallel-piped of size $L_x \times L_y \times L_z$, represented with a 3D mesh of size $N_{mshx} \times N_{mshy} \times N_{mshz}$. The mesh spacing is thus

$$\Delta_\mu = \frac{L_\mu}{N_{msh\mu}} \qquad (\mu = x, y, z)$$

DX, DY, DZ DXDYDZ $\equiv$ DVOL

(Example: domain = Wurtzite CdSe orthorhombic – 8 atom – cell)

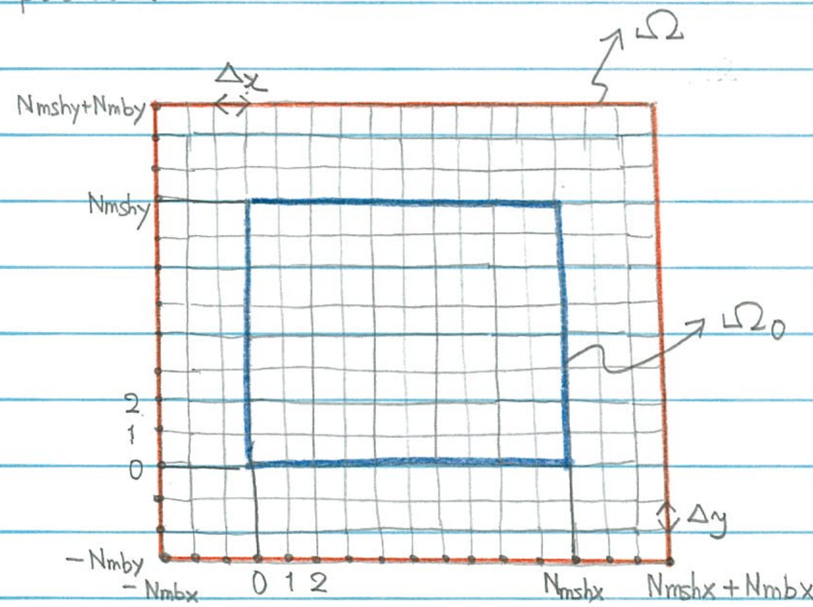
$(L_x, L_y, L_z) = (7.45018\,\text{Å},\ 4.30173\,\text{Å},\ 6.99865\,\text{Å})$

$(N_{mshx}, N_{mshy}, N_{mshz}) = (37, 21, 35)$

$(\Delta_x, \Delta_y, \Delta_z) = (0.201356\,\text{Å},\ 0.204844\,\text{Å},\ 0.199961\,\text{Å})$

(Augmented domain) NMBX, NMBY, NMBZ

Each domain is augmented with lower & upper buffer layers in the x, y, z directions, with depth $N_{mbx}, N_{mby}, N_{mbz}$ mesh points.



Mshlb Mshub

(Data structures)

NORBMAX

Wave functions : $\{\psi_n^\alpha(\mathbf{r}) \mid n=1,2,\ldots,N_{orbmax} ; \alpha=0,\ldots,N_{dx}N_{dy}N_{dz}-1\}$

$$\mathrm{PSI}(\underbrace{-N_{mbx}^{f}}_{\text{Mshlb}} : \underbrace{N_{mshx}+N_{mbx}^{f}}_{\text{Mshub}},\ -N_{mby}^{f} : N_{mshy}+N_{mby}^{f},\ -N_{mbz}^{f} : N_{mshz}+N_{mbz}^{f},$$

$$N_{orbmax},\ 0 : \underbrace{N_{dx}N_{dy}N_{dz}}_{\text{NDXYZ}}-1)$$

$$\mathrm{PSI}(\underbrace{i_x, i_y, i_z}_{\text{mesh}} ; \underbrace{n}_{\text{orbital}} ; i_d)$$

$$= \psi_n^{(i_d)}(i_x\Delta x, i_y\Delta y, i_z\Delta z)$$

※ The surface planes, $i_\mu = -N_{mb\mu}^{f}$ & $N_{msh\mu}+N_{mb\mu}^{f}$ $(\mu = x, y, z)$, are used to hold the boundary conditions and the wave functions on these mesh points are not dynamic variables (e.g., they are Ø in the rigid-wall boundary condition).

Eigenenergies : $\{\epsilon_n^\alpha \mid n=1,2,\ldots,N_{orbmax} ; \alpha=0,\ldots,N_{dx}N_{dy}N_{dz}-1\}$

$\mathrm{EORB}(N_{orbmax}, 0 : N_{dx}N_{dy}N_{dz}-1)$

Occupation number : $\{f_n^\alpha \in [0,2] \mid n=1,2,\ldots,N_{orbmax} ; \alpha=0,\ldots,N_{dx}N_{dy}N_{dz}-1\}$

$\mathrm{OCC}(N_{orbmax}, 0 : N_{dx}N_{dy}N_{dz}-1)$

$$f_n^\alpha = \frac{2}{\exp[\beta(\epsilon_n^\alpha - \underbrace{\mu}_{\text{CHEMP}})]+1}$$

Screened local pseudopotential: $v_{loc}^{\alpha}(\mathbf{r})$

Use 1 VLOC per processor see 7/30/03

$$VLOC(-N_{mbx} : N_{mshx} + N_{mbx}^{f}, -N_{mby}^{f} : N_{mshy} + N_{mby}^{f}, -N_{mbz}^{f} : N_{mshz} + N_{mbz}^{f}, 0 : N_{dx} N_{dy} N_{dz} - 1)$$

$$v_{loc}^{\alpha}(\mathbf{r}) = \sum_{\|\mathbf{R}_I - \Omega_\alpha\| < r_c^I} v_{loc}^{I}(|\mathbf{r} - \mathbf{R}_I|)$$

↳ atomic-species-dep cut-off

Domain support function: $P^{\alpha}(\mathbf{r})$

$$DSF(-N_{mbx}^{f} : N_{mshx} + N_{mbx}^{f}, -N_{mby}^{f} : N_{mshy} + N_{mby}^{f}, -N_{mbz}^{f} : N_{mshz} + N_{mbz}^{f}, 0 : N_{dx} N_{dy} N_{dz} - 1)$$

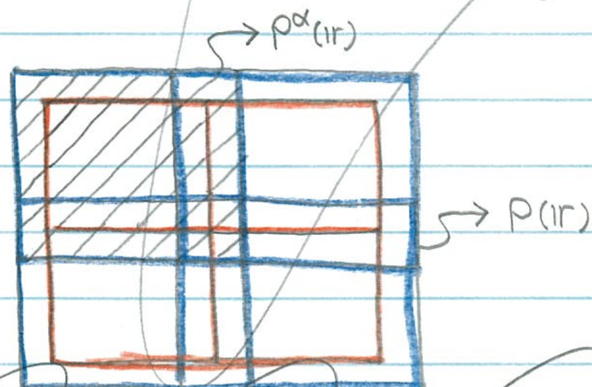
Local density : $\rho^{\alpha}(\mathbf{r})$

$$RHOL(-N_{mbx}^{f} : N_{mshx} + N_{mbx}^{f}, -N_{mby}^{f} : N_{mshy} + N_{mby}^{f}, -N_{mbz}^{f} : N_{mshz} + N_{mbz}^{f}, 0 : N_{dx} N_{dy} N_{dz} - 1)$$

Global density : $\rho(\mathbf{r})$

Use this! see 7/30/03

$$RHO(\overbrace{-N_{mbx}^{f}}^{Mshpl} : \overbrace{N_{mshx} N_{dx} + N_{mbx}^{f}}^{Mshpu}, -N_{mby}^{f} : N_{mshy} N_{dy} + N_{mby}^{f}, -N_{mbz}^{f} : N_{mshz} N_{dz} + N_{mbz}^{f})$$



Use the same support as ρ^{α}

$$RHO(-N_{mbfx} : N_{mshx} + N_{mbfx}, -N_{mbfy} : N_{mshy} + N_{mbfy}, -N_{mbfz} : N_{mshz} + N_{mbfz}, 0 : N_{dx} N_{dy} N_{dz} - 1)$$

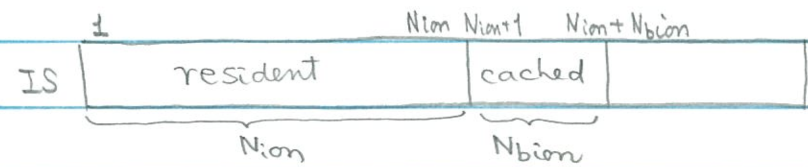
Atomic data are handled by per-processor basis.

NION : N_{ion} = the number of resident ions in this
($L_x N_{dx}$, $L_y N_{dy}$, $L_z N_{dz}$) subspace

NBION: Number of cached boundary ions, $\mathbb{R}_I \notin \bigcup_{\alpha \in P} \Omega_{0\alpha}$
$\wedge \; \| \mathbb{R}_I - \Omega_\alpha \| < r_c^I$

(Note the skin is $N_{mb\mu}^{f} \Delta_\mu + r_c^I$, $I = Cd, Se$, $\mu = x, y, z$)

IS(NEMAX) : Species (1=Cd, 2=Se) of the ith ion



X(3NEMAX): $\{\mathbb{R}_I \mid I = 1, \ldots, N_{ion}\}$, X(3I-2|3I-1|3I) is the
x|y|z coordinates (a.u.) of the Ith ion

— Processor

Each processor (a parallel piped with size $L_x N_{dx} \times L_y N_{dy} \times L_z N_{dz}$) is fully identified by:

~~① Origin of its lower x, y, z corner,~~

~~$\mathbb{R}_{org} = (X_{org}, Y_{org}, Z_{org})$ → XORG, YORG, ZORG~~

② Neighbor processor list

$$l_{NN} = (P_1, P_2, \ldots, P_6) \rightarrow \text{NN}(6)$$

$$P_\mu \in \{0, 1, 2, \ldots, \underset{\text{NPROC}}{P}-1\} \cup \{\underset{\substack{\text{constant} \\ \text{NIL} \equiv -1}}{\text{NIL}}\} \quad (\mu = 1 \text{ (x-low)}, 2 \text{ (x-high)}, 3 \text{ (y-low)}, 4 \text{ (y-high)}, 5 \text{ (z-low)}, 6 \text{ (z-high)})$$

where the processors are numbered sequentially from 0 to P−1, and NIL stands for no neighbor in that direction.

①' Use $\mathbb{S}_V(k)$ for the relative coordinate of neighbor processor k

$$SV(6) = \begin{array}{ll} (-L_x N_{dx}, 0, 0)\ (1) & (L_x N_{dx}, 0, 0)\ (2) \\ (0, -L_y N_{dy}, 0)\ (3) & (0, L_y N_{dy}, 0)\ (4) \\ (0, 0, -L_z N_{dz})\ (5) & (0, 0, L_z N_{dz})\ (6) \end{array}$$

(Global 3D mesh topology)

The neighbor processor list l_{NN} and the shift vectors $\mathbb{S}_v(1), \ldots, \mathbb{S}_v(6)$ completely specify the processor topology, in the local-topology-preserving, self-centric parallelization.

In our initial implementation, we preserve global 3D mesh topology (as a special case) in addition to the (general) local 3D mesh topology.

NP NPX|Y|Z

The processors are organized in $N_p = N_{px} \times N_{py} \times N_{pz}$ mesh of processors. The sequential & vector processor ID's are defined as

MYID

$$P = P_x (N_{py} N_{pz}) + P_y \cdot N_{pz} + P_z$$

$$\begin{cases} P_x = \lfloor P / N_{py} N_{pz} \rfloor \\ P_y = \lfloor P / N_{pz} \rfloor \bmod N_{py} \\ P_z = P \bmod N_{pz} \end{cases}$$

MYX|Y|Z.