Parallel DCC Algorithm

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set up parallel environment, l_{NN} & $\mathbb{R}_{org}$

$\forall\alpha = 0, \ldots, N_{dx}N_{dy}N_{dz}-1$ set up domain supports $p^\alpha(\mathbb{r})$

set up initial ionic positions $\{\mathbb{R}_I \mid I = 1, \ldots, N_{ion}\}$

could depend on $\mathbb{R}_I$'s

$\forall\alpha = 0, \ldots, N_{dx}N_{dy}N_{dz}-1$ set up initial wave functions $\{\psi_n^\alpha(\mathbb{r}) \mid n = 1, \ldots, N_{orbmax}\}$
(random + Gram-Schmidt orthonormalization)

cache boundary ions $\{\mathbb{R}_I \mid I = N_{ion}+1, \ldots, N_{ion}+N_{bion}\}$

(set up initial $\rho(\mathbb{r}) \neq \sum_n |\psi_n(\mathbb{r})|^2$ for DFT)

for $i_{sc} = 1, I_{scmax}$

just to repeat subspace diagonalization

$\forall\alpha = 0, \ldots, N_{dx}N_{dy}N_{dz}-1$ compute $v_{loc}^\alpha(\mathbb{r})$; $h^\alpha(\mathbb{r}) = -\frac{1}{2}\nabla^2 + v_{loc}^\alpha(\mathbb{r})$

$\forall\alpha$ subspace diagonalization of $\langle\psi_m^\alpha|h^\alpha|\psi_n^\alpha\rangle$ to get $\{\epsilon_n^\alpha\}$
(order the orbitals in increasing order of ϵ_n^α)

$\forall\alpha$ conjugate-gradient relaxation of $\{\psi_n^\alpha \mid n = 1, \ldots, N_{orbmax}\}$

$occ(N_{orbmax}) \in [0,2]$

compute density $\rho(\mathbb{r})$

Determine μ self-consistently

1. $\forall\alpha$ compute local density $\rho^\alpha(\mathbb{r}) = \sum_{n=1}^{N_{orbmax}} f_n |\psi_n^\alpha(\mathbb{r})|^2 p^\alpha(\mathbb{r})$
2. compute global $\rho(\mathbb{r}) = \sum_\alpha \rho^\alpha(\mathbb{r})$; local sum $\rightarrow$ cache

$N_{el} = \sum_\alpha \sum_n f_n(\underline{\mu}) \underbrace{\langle\psi_n^\alpha|p^\alpha|\psi_n^\alpha\rangle}_{\text{compute once}}$

compute energy E_{new}

1. $\forall\alpha$ compute local energy $E^\alpha = \sum_{n=1}^{N_{orbmax}} f_n \epsilon_n^\alpha \int d\mathbb{r} |\psi_n^\alpha(\mathbb{r})|^2 p^\alpha(\mathbb{r})$
2. global sum $E_{new} = \sum_\alpha E^\alpha$

ETOTTH

if ($i_{sc} \neq 1$ & $|E_{new} - E_{old}| \leq E_{th}$) break

$E_{old} \leftarrow E_{new}$

endfor i_{sc} (self-consistent equation)

– Band-by-band conjugate gradient minimization

for $\alpha = 0, N_{dx}N_{dy}N_{dz} - 1$

  for $n = 1, \ldots, N_{orbmax}$

  Gram-Schmidt: $\psi_n^\alpha(\mathbf{r}) \leftarrow \psi_n^\alpha(\mathbf{r}) - \sum_{m=1}^{n-1} \psi_m^\alpha(\mathbf{r}) \langle \psi_m^\alpha | \psi_n^\alpha \rangle$

    $\overset{\to \text{RV}}{R}(\mathbf{r}) \leftarrow \underbrace{- h^\alpha(\mathbf{r}) \psi_n^\alpha(\mathbf{r})} + \langle \psi_n^\alpha | \underbrace{h^\alpha | \psi_n^\alpha}\rangle^{\to h_{pp}} \psi_n^\alpha(\mathbf{r})$

    $\overset{\to \text{GAMMA}\emptyset}{\gamma_0} \leftarrow \langle R | R \rangle$

    Gram-Schmidt $R(\mathbf{r}) \leftarrow R(\mathbf{r}) - \sum_{m=1}^{n} \psi_m^\alpha(\mathbf{r}) \langle \psi_m^\alpha | R \rangle$

    Normalize $\langle R | R \rangle = 1$

    $Y(\mathbf{r}) \leftarrow R(\mathbf{r})$

    for $i_{CG} = 1, \ldots, I_{CGmax}$

      compute $2\overset{\to h_{yp}}{h_Y \psi_n^\alpha}, \overset{\to h_{yy}}{h_{YY}}$

      $\cos 2\theta_{min} = - \dfrac{h_{pp} - h_{yy}}{\sqrt{(h_{pp} - h_{yy})^2 + h_{yp}^2}}^{\to \text{ANORM}}, \quad \sin 2\theta_{min} = - \dfrac{h_{yp}}{\sqrt{(h_{pp} - h_{yp})^2 + h_{yp}^2}}$

      $\cos \theta_{min} = \sqrt{\dfrac{1 + \cos 2\theta_{min}}{2}}, \quad \sin \theta_{min} = \dfrac{\sin 2\theta_{min}}{2 \cos \theta_{min}}$

      Line minimize $\psi_n^\alpha(\mathbf{r}) \leftarrow \cos\theta_{min} \psi_n^\alpha(\mathbf{r}) + \sin\theta_{min} Y(\mathbf{r})$

      $\epsilon_{min} \leftarrow \dfrac{h_{pp} + h_{yy}}{2} - \dfrac{\sqrt{(h_{pp} - h_{yy})^2 + h_{yp}^2}}{2}$

      if $(| \epsilon_{min} - h_{pp} | < \overset{\to \text{EORBTH}}{\epsilon_{th}})$ break

      $h_{pp} \leftarrow \epsilon_{min}$

      $R(\mathbf{r}) \leftarrow - h^\alpha(\mathbf{r}) \psi_n^\alpha(\mathbf{r}) + h_{pp} \psi_n^\alpha(\mathbf{r})$

      $\gamma_1 \leftarrow \langle R | R \rangle$

      $Y(\mathbf{r}) \leftarrow R(\mathbf{r}) + \dfrac{\gamma_1}{\gamma_0} Y(\mathbf{r})$ (overwrite)

      Gram-Schmidt $Y(\mathbf{r}) \leftarrow Y(\mathbf{r}) - \sum_{m=1}^{n} \psi_m^\alpha(\mathbf{r}) \langle \psi_m^\alpha | Y \rangle$

      normalize $\langle Y | Y \rangle = 1$

      $\gamma_0 \leftarrow \gamma_1$

  endfor n (band)

endfor α (domain)