Preconditioned Conjugate Gradient Iteration for Kohn-Sham Orbitals

9/28/03

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

normalize : $|\psi_n\rangle \leftarrow |\psi_n\rangle / \sqrt{\langle\psi_n|\psi_n\rangle}$

initial gradient : $R(\mathbf{r}) \leftarrow -\hat{h}\,\psi_n(\mathbf{r}) + \underbrace{\overset{\text{HPP}}{\langle\psi_n|\hat{h}|\psi_n\rangle}}_{\equiv h_{pp}} \psi_n(\mathbf{r})$

do $i_{cg} = 1, \; I_{cgmax}$

preconditioning : solve $[-\frac{1}{2}\nabla^2 + v(\mathbf{r})]\, Z(\mathbf{r}) = R(\mathbf{r})$

$\overset{\text{GAMMA1}}{\gamma_1} = \langle R|Z\rangle$

if $i_{cg} = 1$

$Y(\mathbf{r}) = Z(\mathbf{r})$

else

$Y(\mathbf{r}) \leftarrow Z(\mathbf{r}) + \frac{\overset{\text{GAMMA1}}{\gamma_1}}{\gamma_0} Y(\mathbf{r})$

endif

Gram-Schmidt : $|Y\rangle \leftarrow |Y\rangle - \sum_{m=1}^{n} |\psi_m\rangle\langle\psi_m|Y\rangle$

normalize : $|Y\rangle \leftarrow |Y\rangle / \sqrt{\langle Y|Y\rangle}$

calculate $\overset{\text{HPY}}{h_{py}} = 2\underbrace{\langle\psi_n|\hat{h}|Y\rangle}_{\text{HPSI}}$ $\quad \overset{\text{HYY}}{h_{yy}} = \langle Y|\hat{h}|Y\rangle$

$$\cos 2\theta_{min} = -\frac{h_{pp}-h_{yy}}{\underbrace{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}}_{\text{ANORM}}} \; ; \; \sin 2\theta_{min} = -\frac{h_{py}}{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}}$$

$$\cos\theta_{min} = \sqrt{\frac{1+\cos 2\theta_{min}}{2}} \; ; \; \sin\theta_{min} = \frac{\sin 2\theta_{min}}{2\cos\theta_{min}}$$

$$E_{min} = \frac{h_{pp}+h_{yy}}{2} - \frac{\sqrt{(h_{pp}-h_{yy})^2 + h_{py}^2}}{2}$$

$$\overset{\text{DELE}}{\Delta} = (E_{min} - h_{pp}) / |h_{pp}|$$

if $\Delta > 0$

  exit // discard the attempt, keep the old ψ_n & h_{pp}

else // accept the attempt, update ψ_n & h_{pp}

  $\psi_n(\mathbb{r}) \leftarrow \cos\theta_{min}\, \psi_n(\mathbb{r}) + \sin\theta_{min}\, \Upsilon(\mathbb{r})$

  $R(\mathbb{r}) \leftarrow -\hat{h}(\mathbb{r})\, \psi_n(\mathbb{r}) + \underbrace{\langle \psi_n | \hat{h} | \psi_n \rangle}_{\to HPP} \psi_n(\mathbb{r})$

  if $|\Delta| < \epsilon$ exit

endif

$\gamma_0 \leftarrow \gamma_1$

enddo

$\epsilon_n \leftarrow h_{pp}$

$residue_n \leftarrow \langle R | R \rangle$

Multigrid Preconditioning

9/30/03

- Error vector

$$[-\tfrac{1}{2}\nabla^2 + v(\mathbf{r})]\,\psi(\mathbf{r}) - \underbrace{\langle\psi|\overset{-\frac{1}{2}\nabla^2+v(\mathbf{r})}{h}|\psi\rangle}_{\epsilon}\psi(\mathbf{r}) = -g(\mathbf{r}) \quad (1)$$

$$[-\tfrac{1}{2}\nabla^2 + v(\mathbf{r})]\,\psi^*(\mathbf{r}) - \underbrace{\langle\psi^*|h|\psi^*\rangle}_{\epsilon^*}\psi^*(\mathbf{r}) = 0 \quad (2)$$

−)

$$[-\tfrac{1}{2}\nabla^2 + v(\mathbf{r})][\psi^*(\mathbf{r}) - \psi(\mathbf{r})] - \underbrace{\epsilon^*\psi^*(\mathbf{r}) + \epsilon\psi(\mathbf{r})}_{\simeq\,\epsilon[\psi^*(\mathbf{r}) - \psi(\mathbf{r})]} = g(\mathbf{r}) \quad (3)$$

$$[-\tfrac{1}{2}\nabla^2 + v(\mathbf{r}) - \epsilon][\psi^*(\mathbf{r}) - \psi(\mathbf{r})] = g(\mathbf{r}) \quad (4)$$

$$\therefore\ \psi(\mathbf{r}) \leftarrow \psi(\mathbf{r}) + z(\mathbf{r}) \quad (5)$$

where the error vector $z(\mathbf{r})$ is

$$[-\tfrac{1}{2}\nabla^2 + v(\mathbf{r}) - \underbrace{\langle\psi|h|\psi\rangle}_{\text{HPP}}]\,\underbrace{z(\mathbf{r})}_{\text{ZV}} = \underbrace{g(\mathbf{r})}_{\text{RV}} \quad (6)$$

- Relaxation

$$\frac{\partial z(\mathbf{r})}{\partial t} = -[-\tfrac{1}{2}\nabla^2 + v_{mg}(\mathbf{r})]\,z(\mathbf{r}) + g(\mathbf{r}) \quad (7)$$

Let's discretize

$$z(\mathbf{r}) \longrightarrow z(i\overset{\text{DX}}{\Delta_x},\ j\overset{\text{DY}}{\Delta_y},\ z\overset{\text{DZ}}{\Delta_z})$$

Equation (7) becomes

$$\frac{z_{ijk}^{new} - z_{ijk}}{\Delta t}$$

$$= \frac{1}{2}\left[\frac{z_{i-1jk} - 2z_{ijk} + z_{i+1jk}}{\Delta_x^2} + \frac{z_{ij-1k} - 2z_{ijk} + z_{ij+1k}}{\Delta_y^2} + \frac{z_{ijk-1} - 2z_{ijk} + z_{ijk+1}}{\Delta_z^2}\right]$$

$$- v_{ijk}^{mg} z_{ijk} + g_{ijk}$$

$$\boxed{\begin{aligned} z_{ijk} \leftarrow z_{ijk} &+ \overbrace{\frac{\Delta t}{2\Delta_x^2}}^{DTKX}(z_{i-1jk} - 2z_{ijk} + z_{i+1jk}) \\ &+ \overbrace{\frac{\Delta t}{2\Delta_y^2}}^{DTKY}(z_{ij-1k} - 2z_{ijk} + z_{ij+1k}) \\ &+ \overbrace{\frac{\Delta t}{2\Delta_z^2}}^{DTKZ}(z_{ijk-1} - 2z_{ijk} + z_{ijk+1}) \\ &- \underbrace{\Delta t\, v_{ijk}^{mg}}_{VDT(MSHSZ,MSHSZ,MSHSZ)} z_{ijk} + \Delta t\, g_{ijk} \qquad (8) \end{aligned}}$$

Use

$$\underbrace{\Delta t = \frac{\overset{ALMG}{\alpha}}{\cancel{4}\; 3} \min(\Delta_x^2, \Delta_y^2, \Delta_z^2)}_{DTMG} \qquad (9)$$

(see p.6)

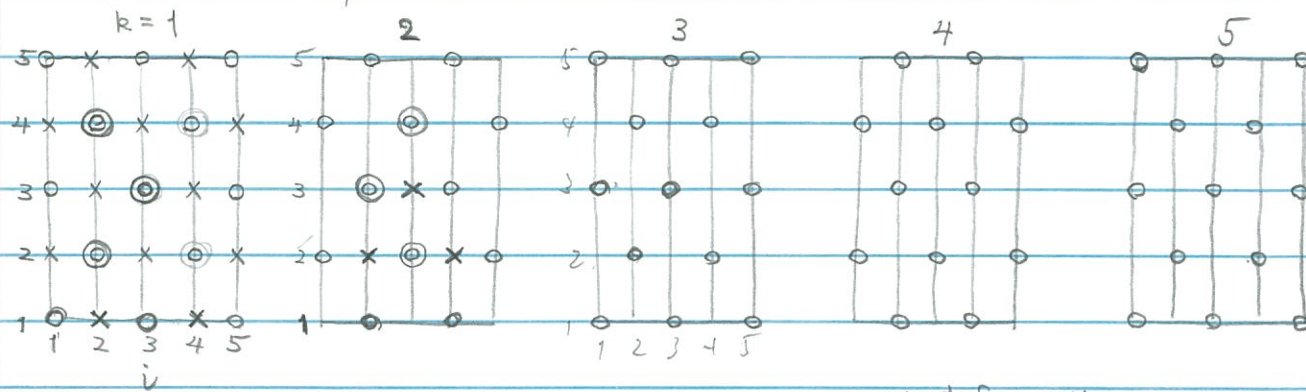
~~Δt very big~~ on coarse grid?

(Coarsest solution)

$$-\left(\frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2} + \frac{1}{\Delta_z^2}\right) z_{222} - v_{222}^{mg} z_{222} + g_{222} = 0$$

$$z_{222} = \frac{g_{222}}{\underbrace{\frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2} + \frac{1}{\Delta_z^2}}_{2\sum_{\alpha=1}^{3} dk(\alpha, maxdpth)} + \underbrace{v_{222}^{mg}}_{z(iv(maxdpth)) - eshft}}$$

– Red-black Gauß-Seidel iteration



start from x to propagate rigid wall boundary.

Red : o $\quad i+j+k = \text{odd}$ $\qquad$ Black : x $\quad i+j+k = \text{even}$

```
do k = 2, Nz - 1
   do j = 2, Ny - 1
      if (k+j) mod 2 = 0            if (k+j) mod 2 = 0
         ibgn = 3                      ibgn = 2
         iend = Nx - 2                 iend = Nx - 1
      else                          else
         ibgn = 2                      ibgn = 3
         iend = Nx - 1                 iend = Nx - 2
      endif                         endif
         do i = ibgn, iend step 2
            update Zijk
         enddo_i
   enddo_j
enddo_k
```

– Multigrid V cycle

$$\overset{\text{Hamiltonian at depth } d}{H_d}\, Z_d - g_d \equiv -\overset{\text{defect}}{\delta_d} \qquad (10)$$

$$-)\ \ H_d Z_d^* - g_d = 0 \qquad (11)$$

$$H_d \underbrace{(Z_d^* - Z_d)}_{u_d} = \delta_d$$

$$\therefore\ Z_d^* \leftarrow Z_d + \overset{\text{error}}{u_d} \qquad (12)$$

where

$$H_d u_d = \delta_d$$

(Single V cycle)

Relax $H_d Z_d = g_d$

Compute residual $\delta_d = -H_d Z_d + g_d$

Restrict $\delta_d \rightarrow \delta_{d+1}$

Solve $H_{d+1} u_{d+1} = \delta_{d+1}$

Interpolate $u_{d+1} \rightarrow u_d$

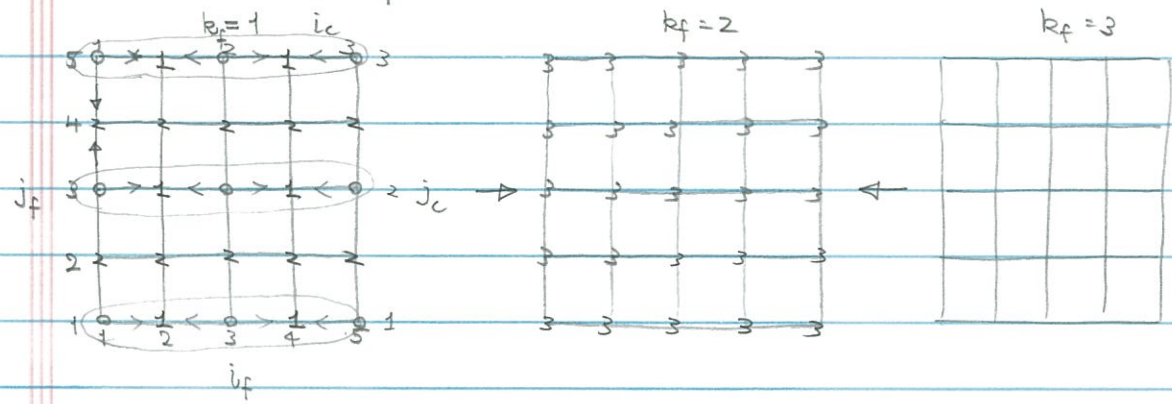
$Z_d \leftarrow Z_d + u_d$

Relax $H_d Z_d = g_d$

$$\delta_{ijk} = +\left[+\frac{Z_{i-1jk} - 2Z_{ijk} + Z_{i+1jk}}{\overset{\text{DKX}}{2\Delta_x^2}} + \frac{Z_{ij-1k} - 2Z_{ijk} + Z_{ij+1k}}{\overset{\text{DKY}}{2\Delta_y^2}} + \frac{Z_{ijk-1} - 2Z_{ijk} + Z_{ijk+1}}{\overset{\text{DKZ}}{2\Delta_z^2}} \right]$$

$$- (v_{ijk} - \epsilon) Z_{ijk} + g_{ijk}$$

— Bilinear interpolation



— Gauß-Seidel for $\Delta_x = \Delta_y = \Delta_z = \Delta$, $\alpha = 1$

$$\cancel{z_{ijk}} \leftarrow \cancel{z_{ijk}} + \frac{1}{6}(z_{i-1} - \cancel{2z} + z_{i+1}) + \frac{1}{6}(z_{j-1} - \cancel{2z} + z_{j+1}) + \frac{1}{6}(z_{k-1} - \cancel{2z} + z_{k+1})$$

$$- \frac{\Delta^2}{3}(v - e)\, z + \frac{\Delta^2}{3} g$$

$$\therefore z_{ijk} \leftarrow \frac{1}{6}(z_{i-1jk} + z_{i+1jk} + z_{ij-1k} + z_{ij+1k} + z_{ijk-1} + z_{ijk+1})$$

$$- \frac{\Delta^2}{3}(v_{ijk} - h_{pp}) + \frac{\Delta^2}{3} g_{ijk}$$

Presmoothening start with $z_{ijk} \leftarrow 0$

$$\therefore z_{ijk} = - \frac{\Delta^2}{3}(v_{jik} - h_{pp}) + \frac{\Delta^2}{3} g_{ijk}$$

– MG array size

For res, rhs, u, v.

$$\underbrace{M}_{\text{MEMLEN}} = 4 \sum_{l=1}^{L} \Big[\underbrace{(2^l+1)^3}_{\text{array size}} + \underbrace{1}_{\text{size info}} \Big]$$

$$= 4 \sum_{l=1}^{L} \left(8^l + 3 \cdot 4^l + 3 \cdot 2^l + 1 + 1 \right)$$

$$= 4 \left[\frac{8(8^L - 1)}{8-1} + \cancel{3} \cdot \frac{4(4^L-1)}{\cancel{4-1}} + 3 \cdot \frac{2(2^L-1)}{\cancel{2-1}} + 2L \right]$$

$$= 4 \left[\frac{8}{7}(8^{\overset{\to NG}{L}}-1) + 4(4^L-1) + 6(2^L-1) + 2L \right]$$

- Note on Δt for relaxation

For coarser levels, $\min(\Delta_x^2, \Delta_y^2, \Delta_z^2)$ is large, and $\Delta t(v_{ijk} - h_{pp})$ may become to large!

Experiment on 10/1/03 shows $\alpha = 10^{-2}$ & NPRE=NPOST=1000 very quickly converges to the answer!

(Recipe)

$$\Delta t = \alpha \min\left(\frac{1}{3} \min(\Delta_x^2, \Delta_y^2, \Delta_z^2),\ \frac{1}{\max|v_{ijk} \cancel{- h_{pp}}|} \right)$$

compute in mginit

Trace of mglin (slvsml ~~res~~ → rhs corrected) 12/30/03

$N_x = N_y = N_z = 17$

dpth	mesh
0	$17 = 2^4+1$
1	$9 = 2^3+1$
2	$5 = 2^2+1$
maxdpth = 3	$3 = 2+1$

0 copy rhs_0 <- u
0 u_0 <- 0
0 relax u_0 <- u_0 & rhs_0 & v_0
0 resid res_0 <- u_0 & rhs_0 & v_0

1 rstrct rhs_1 <- res_0(j-1)
1 u_1 <- 0
1 relax u_1 <- u_1 & rhs_1 & v_1
1 resid res_1 <- u_1 & rhs_1 & v_1

2 rstrct rhs_2 <- res_1(j-1)
2 u_2 <- 0
2 relax u_2 <- u_2 & rhs_2 & v_2
2 resid res_2 <- u_2 & rhs_2 & v_2

3 rstrct rhs_3 <- res_2(j-1)
3 slvsml u_3 <- rhs_3 & v_3

2 addint u_2 <- u_2 + interp u_3(j+1)
2 relax u_2 <- u_2 & rhs_2 & v_2

1 addint u_1 <- u_1 + interp u_2(j+1)
1 relax u_1 <- u_1 & rhs_1 & v_1

0 addint u_0 <- u_0 + interp u_1(j+1)
0 relax u_0 <- u_0 & rhs_0 & v_0