Implementation

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Outline

- 3D distribution
- k point parallelism
- SCF loop
    - Initialization
    - iterative diagonalization
    - sum
    - mixing

FFT grids (one dimension)

- The real space grid: $x_i = \frac{i}{N} L \quad \text{with} \quad i = 0, 1, 2 \ldots, N-1$
- The reciprocal space grid: $G_i = i \frac{2\pi}{L}$

  $\text{with} \quad i = -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \ldots, 0, 1, \ldots, \frac{N}{2}$

$$n_{max} \frac{2\pi}{L} < 2G_{cut}$$

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In 3 dimensions

- Bravais and reciprocal lattices:

$$\mathbf{a_1}\,,\mathbf{a_2}\,,\mathbf{a_3} \qquad \mathbf{b_i} = \frac{2\pi}{\Omega}\sum_{ijk}\epsilon_{ijk}\mathbf{a_j}\wedge\mathbf{a_k}$$

- real space grid: $\mathbf{r_n} = \sum_{i=1}^{3}\frac{n_i}{N_i}\mathbf{a}_i \quad with \;\; n_i = 0, 1, 2, \ldots, N_i - 1$

- reciprocal space: $\mathbf{G_m} = \sum_{i=1}^{3} m_i\mathbf{b}_i \quad \text{with} \quad m_i = -\frac{N_i+1}{2}, \ldots, 0, \ldots, \frac{N_i}{2}$

$$m_i^{max}\,|\mathbf{b}_i| < 2\sqrt{E_{cut}}$$

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Gamma Trick

- Doing large calculations one uses only the gamma point k=(0,0,0)
- wave functions may be evaluated as real in this case for the Fourier trasforms holds the equality

$$c_{-\mathbf{G}} + c^*_{\mathbf{G}}$$

This allows to store only one half of the components for each wave function.

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$$\mathcal{F}_{\mathbf{G_i}}\left\{\sum_j F(\mathbf{r_i}-\mathbf{r_j})G(\mathbf{r_j})\right\} = F(\mathbf{G_i})G(\mathbf{G_j})$$

Fourier Transform

- If one has a quantity defined in a grid in real space its FT is:

$$F(\mathbf{G}) = \sum_i F(\mathbf{r_i})e^{-i\mathbf{G}\cdot\mathbf{r_i}}$$

- The inverse transform is:

$$F(\mathbf{r_i}) = \frac{1}{N_1 N_2 N_3}\sum_j F(\mathbf{G_j})e^{-i\mathbf{r_i}\cdot\mathbf{G_j}}$$

- Convolution

$$\mathcal{F}_{\mathbf{G_i}}\left\{\sum_j F(\mathbf{r_i}-\mathbf{r_j})G(\mathbf{r_j})\right\} = F(\mathbf{G_i})G(\mathbf{G_i}) \text{ and vice versa}$$

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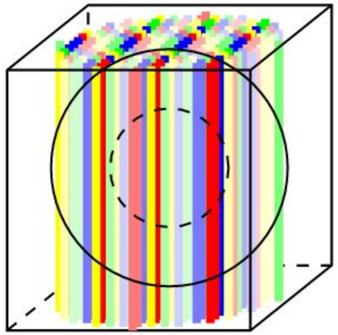
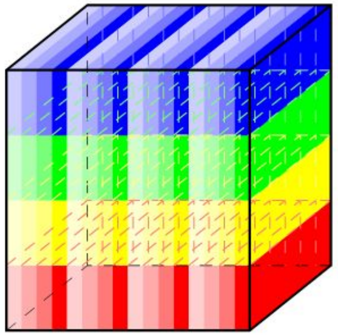
Data distribution

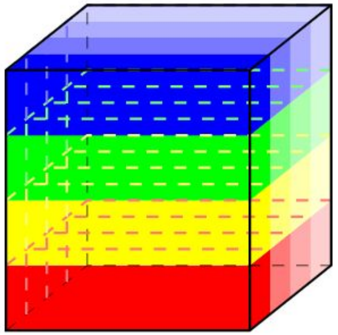
- Data in G space are distributed as sticks in the z directions
- Data in R spase are distributed as z plane slices in the y direction
- At any moment a whole 1 dimensional FFT may be done in each process.



$F(G_x,G_y,G_z)$
$F(G_x,G_y,R_z)$



$F(G_x,G_y,G_z)$
$F(G_x,R_y,R_z)$



$F(G_x,G_y,G_z)$
$F(R_x,R_y,R_z)$

K point parallelism

- Each k point has its own block of Hamiltonian restricted to the space spanned by the |k+G> vectors. Each block may be diagonalized autonomously
- It is possible to parallelize the diagonalization so that a pool of processors diagonalizes a set of k-points
- the k point parallelism is selected using the option -nk = <number of pools>
- How to chose an optimal value for nk?
  - Each pool need to have a sufficient number of processors to perform the FFTs efficiently
  - k parallelism increases the required memory
  - k parallelism is linear so the more pools the faster
  - obviously you can’t use more pools than the number of k-points

SCF loop: initialization

- Generates the **G** vectors and sets up the k-point mesh
- Read the pseudopotentials and initializes $V_{loc}(\mathbf{r})$ and V_{nonloc} in G space (V_{nonloc} is made by separable Kleinmann-Bylander projectors)
- Generates (or read from file) initial wave functions and charge density

SCF loop: iterative diagonalization

- The KS Hamiltonian in plane waves basis is too large to be memorized and diagonalized directly.
- It is just and operator made by:
    - Kinetic energy (in G space)
    - V_{loc} in R space
    - V_{nonloc} in G space (sometimes in real space)
- To compute the eigenfunctions and the eigenvalues we keep in memory only the trial wave functions and their image through H

$$\{|\psi_i\rangle, \hat{H}\psi_i\rangle\}$$

SCF: loop diagonalization

- Davidson diagonalization
- We have an initial base of trial wfc and compute the matrix of H in this space

$$H_{ij}^{dav} = \langle\psi_i|H|\psi_j\rangle$$

- We diagonalize it and compute the residuals:

$$H^{dav}|\phi_i^{dav}\rangle = \epsilon_i^{dav}|\phi_i^{dav}\rangle \qquad |\Delta_i\rangle = (H - \epsilon_i^{dav})|\phi_i^{dav}\rangle$$

- We now expand our trial basis adding the residuals

SCF loop: davidson diagonalization

- Compute the new ϵ_i^{dav} , ϕ_i^{dav} and Δ_i
- reiterate the procedure until $|\Delta_i|^2 < threshold$ for all the eigenfunctions
- the final values of ϵ_i^{dav} and ϕ_i^{dav} are our calculated eigenvalues and eigenfunctions
- This procedure involves the diagonalization of a matrix which can become very large. For systems with many bands one need to use parallel linear algebra routines
- the parallelism for diagonalization is controlled in pw with the flag `-nd` or `-ndiag`, as it uses scalapack ndiag must be set to some perfect square integer lower than the number of processors.

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SCF loop: sum

- Now we compute the new charge density and augmentation charges (if you using USPP or PAW)

$$n_v(\mathbf{r}) = \sum_{n,\mathbf{k}} \phi^*_{n,\mathbf{k}} \phi_{n,\mathbf{k}} + \sum_{ij} \rho_{ij} Q_{ij}(\mathbf{r}) \qquad \rho_{ij} = \sum_{n,\mathbf{k}} \langle \phi_{n,\mathbf{k}} | \beta_i \rangle \langle \beta_j | \phi_{n,\mathbf{k}} \rangle$$

- This is done with a sum on the k points, if symmetry is used each k points contributes also for its symmetry equivalent points, these quantities must also be symmetrized.

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SCF loop: mixing

- The new charge is mixed with the old one:
    - Broyden method is based on Quasi Newton optimization, it can be less or more aggressive it is regulate by the Beta mixing_beta parameter
    - Thomas Fermi uses the dielectric permittivity to compute the new charge density

References

- Picket “Pseudopotentials methods in condensed matter applications” Computer Physics Reports 9 (1989) 115-198
- Payne, Teter, Allan et al. “ıterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients” Rev. Mod. Phys. **64**, 1045