CP2K User Meeting 2015
— HowTo: Filter Matrix Diagonalisation

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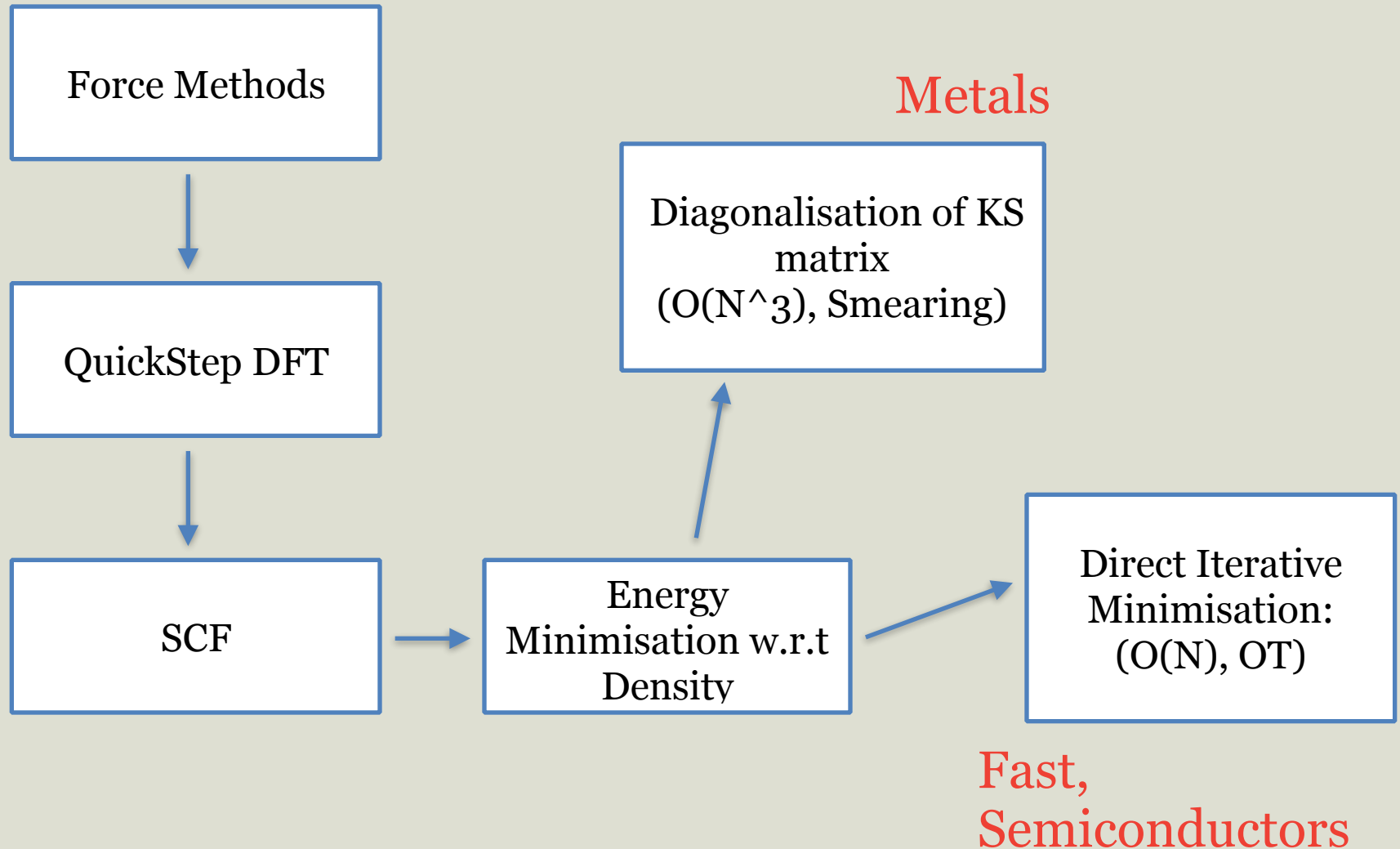
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The Problem:

Diagonalisation

$$\hat{H}|\psi_n\rangle = \epsilon_n|\psi_n\rangle$$

$$\mathbb{1} \qquad \mathbb{1}$$

$$\sum_{j\beta}\langle\phi_{i\alpha}|\hat{H}|\phi_{j\beta}\rangle\langle\phi_{j\beta}|\psi_n\rangle = \epsilon_n\sum_{j\beta}\langle\phi_{i\alpha}|\phi_{j\beta}\rangle\langle\phi_{j\beta}|\psi_n\rangle$$

atom   shell

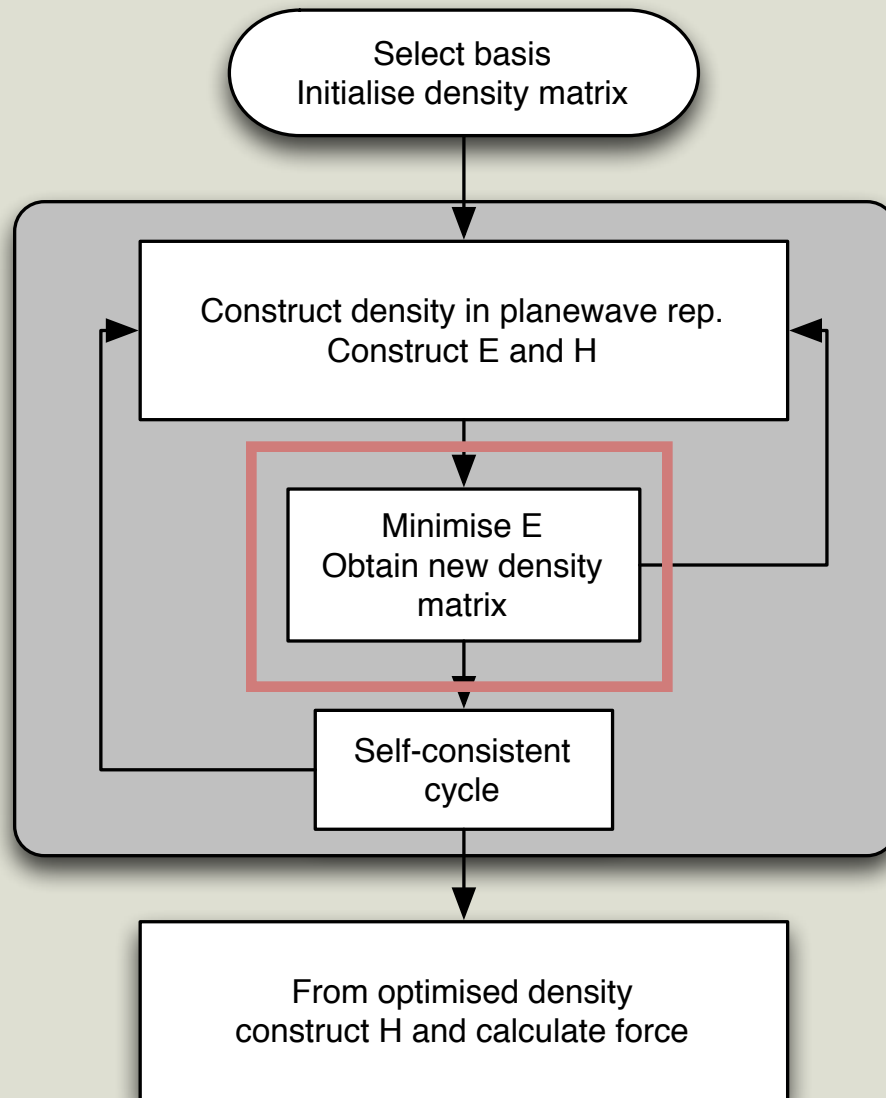$$H_{i\alpha,j\beta} \qquad\qquad S_{i\alpha,j\beta} \qquad \psi_{j\beta,n}$$

Functional of the density

$$\hat{P} = \sum_n f_n|\psi_n\rangle\langle\psi_n| \qquad\qquad \rho(\mathbf{r}) = \langle\mathbf{r}|\hat{P}|\mathbf{r}\rangle$$

Self-Consistent Field Calculation

Select basis
Initialise density matrix

Construct density in planewave rep.
Construct E and H

Minimise E
Obtain new density
matrix

Self-consistent
cycle

From optimised density
construct H and calculate force

Standard Diagonalisation Problem:

- ~ 100 to 1000 atoms, or even more

- Pseudopotential and DZVP basis set: Double ζ for occupied orbitals, plus a set of polarisation/unoccupied orbitals.

- Typical: Si atom (2*s, 2*p, d): 4 X 2 + 5 = 13 orbitals

- 1000 atom Si lattice: 13000 X 13000 matrix

- Minimum basis (s, p): include only one copy of occupied orbitals per atom

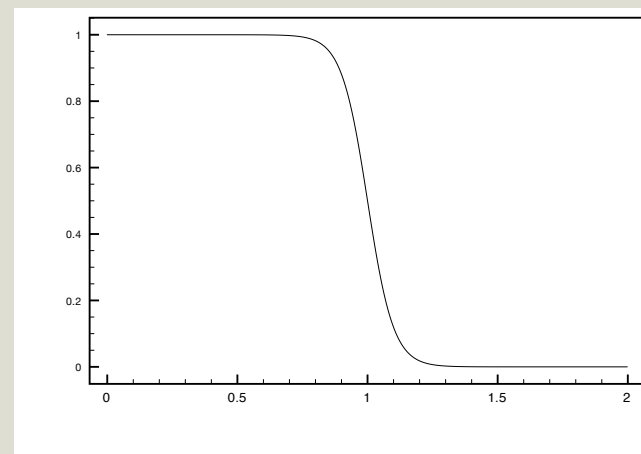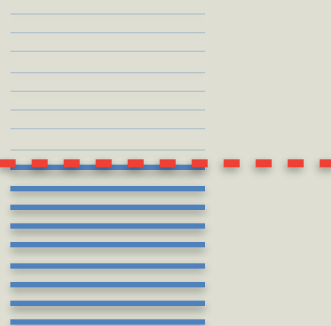- 1000 Si atoms: 4 orbitals per atom, leading to 4000 X 4000 matrix

34 times cheaper

Density Matrix is a Projection Operator

Scalar

$$\sum_n f_n |\psi_n\rangle\langle\psi_n|v\rangle = \sum_{n,i\alpha} f_n \psi^*_{i\alpha,n} v_{i\alpha} |\psi_n\rangle$$
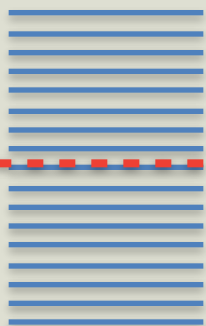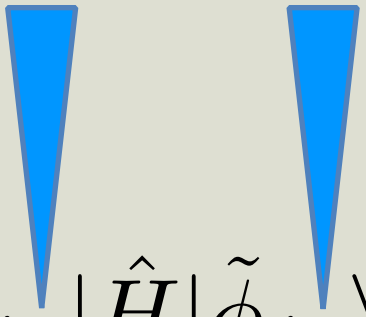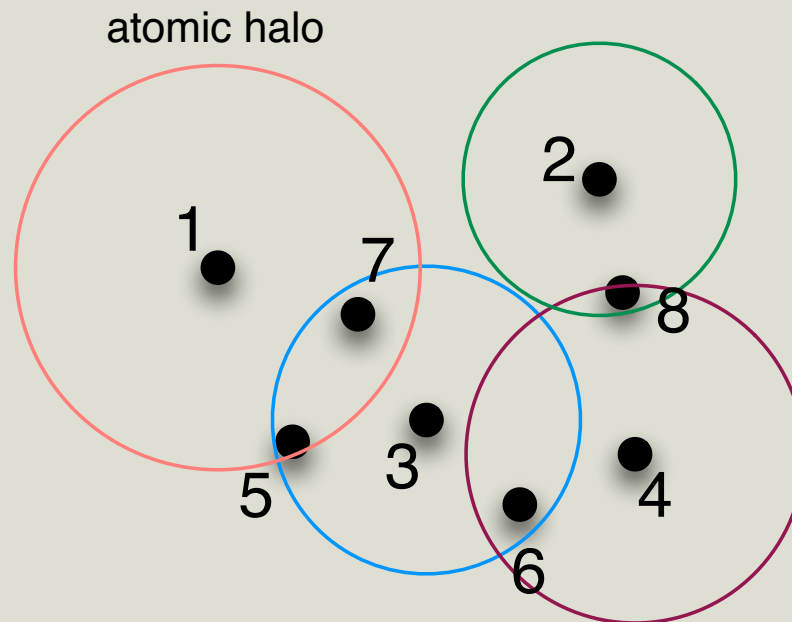
$$\rho = \sum_n f_n \Psi_n \Psi^*_n$$

$$E = E[\rho]$$

- The density matrix projects any state into a space spanned by the lower energy eigenstates

- The smaller set of lower energy eigenstates give exact ground state energy (i.e. a smaller basis set)

We do not know Molecular Orbitals...

If we know the molecular orbitals then we already know the answer to our problem.

atomic halo

$$\langle \phi_{i\alpha} | \hat{H} | \phi_{j\beta} \rangle$$

$$\langle \tilde{\phi}_{i\mu} | \hat{H} | \tilde{\phi}_{j\nu} \rangle$$

So we try to construct a new basis set, still centred on each atom, but with fewer shells, while still give good ground state energy.

- Rayson and Briddon, Phys. Rev. B 80, 205104 (2009)

It may be better to do the shrinking dynamically...

- More basis functions generally gives more accurate results
  - Goal: From a given set of basis functions, try to find an optimal subspace, which minimises energy
- Approaches:
  - Optimise a reduced basis set before calculation starts, based on sample calculations on atoms or sub-systems/molecules, then carry out the calculation using the optimised basis set
  - Optimise a reduced basis set dynamically during a calculation, based on changes in charge density and ionic positions — Filter Matrix Diagonalisation Method
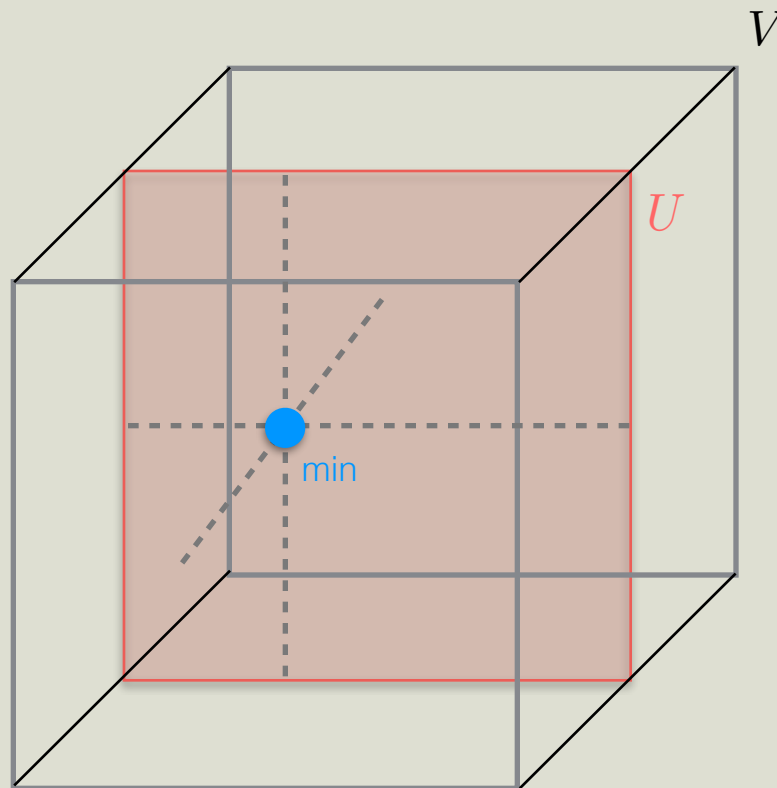
Interactions are important
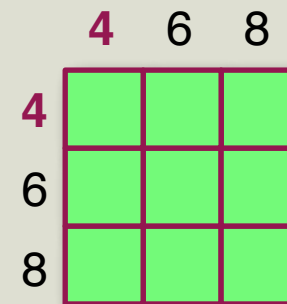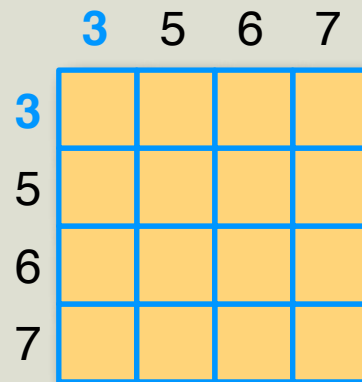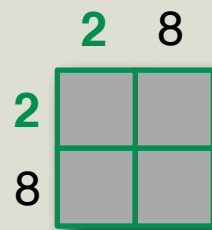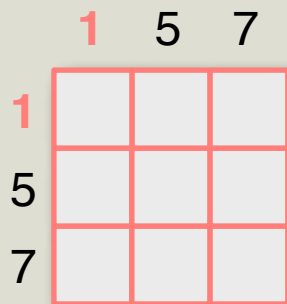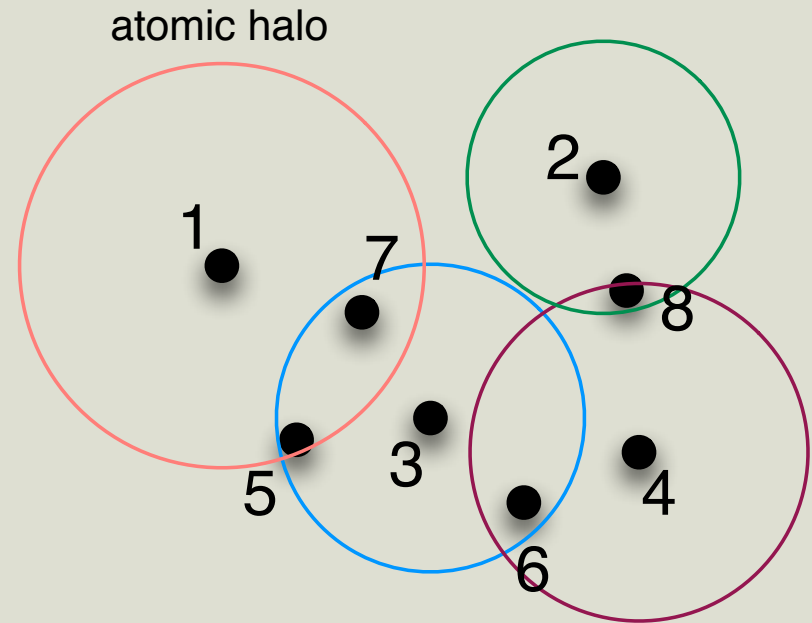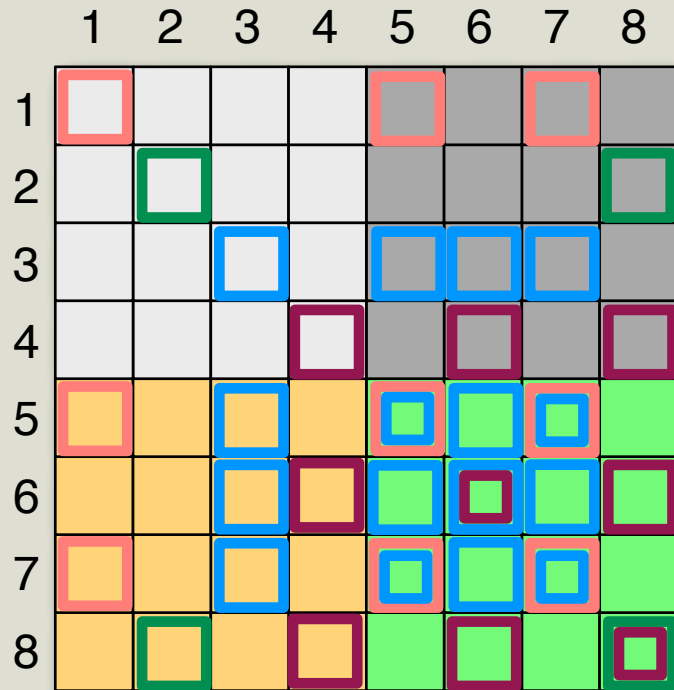
Atomic Density Matrices: Projectors for our new basis

$$\tilde{P} = \sum_n F_n |\tilde{\psi}_n\rangle\langle\tilde{\psi}_n|$$

$$\tilde{H}_i$$
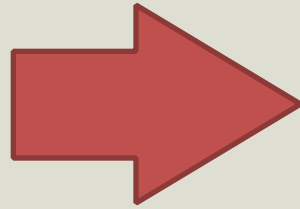
A high temperature Fermi-Dirac function to include more higher energy orbitals, as we are in an interactive environment

$$|\tilde{\phi}_{i\mu}\rangle = \tilde{P}|t_{i\mu}\rangle = \sum_n F_n |\tilde{\psi}_n\rangle\langle\tilde{\psi}_n|t_{i\mu}\rangle$$

Optimised for the atom within its environment

$$|\tilde{\psi}_n\rangle = \sum_{j\beta} C_{j\beta,n}|\phi_{j\beta}\rangle, \qquad \|\mathbf{R}_i - \mathbf{R_j}\| < r_{\text{cut}}(i)$$

Still localised around position of atom i

Meaning of Basis Transformation Matrix

$$|\tilde{\phi}_{i\mu}\rangle = \sum_{j\beta} K_{j\beta,i\mu}|\phi_{j\beta}\rangle$$

The $i\mu$-th column in the basis transformation matrix $\mathbf{K}$ is exactly the coefficients of the new basis function $|\tilde{\phi}_{i\mu}\rangle$ in the original basis

$$|\tilde{\phi}_{i\mu}\rangle = \tilde{P}_i|t_{i\mu}\rangle = \sum_{j\beta}\sum_{k\gamma}(\tilde{P}_i)_{j\beta,k\gamma}|\phi_{j\beta}\rangle(t_{i\mu})_{k\gamma}$$

$$\sum_{k\gamma}(\tilde{P}_i)_{j\beta,k\gamma}(t_{i\mu})_{k\gamma} = K_{j\beta,i\mu}$$

Contributes to $i\mu$-th column of $\mathbf{K}$

Overall Scheme Of SCF Calculation
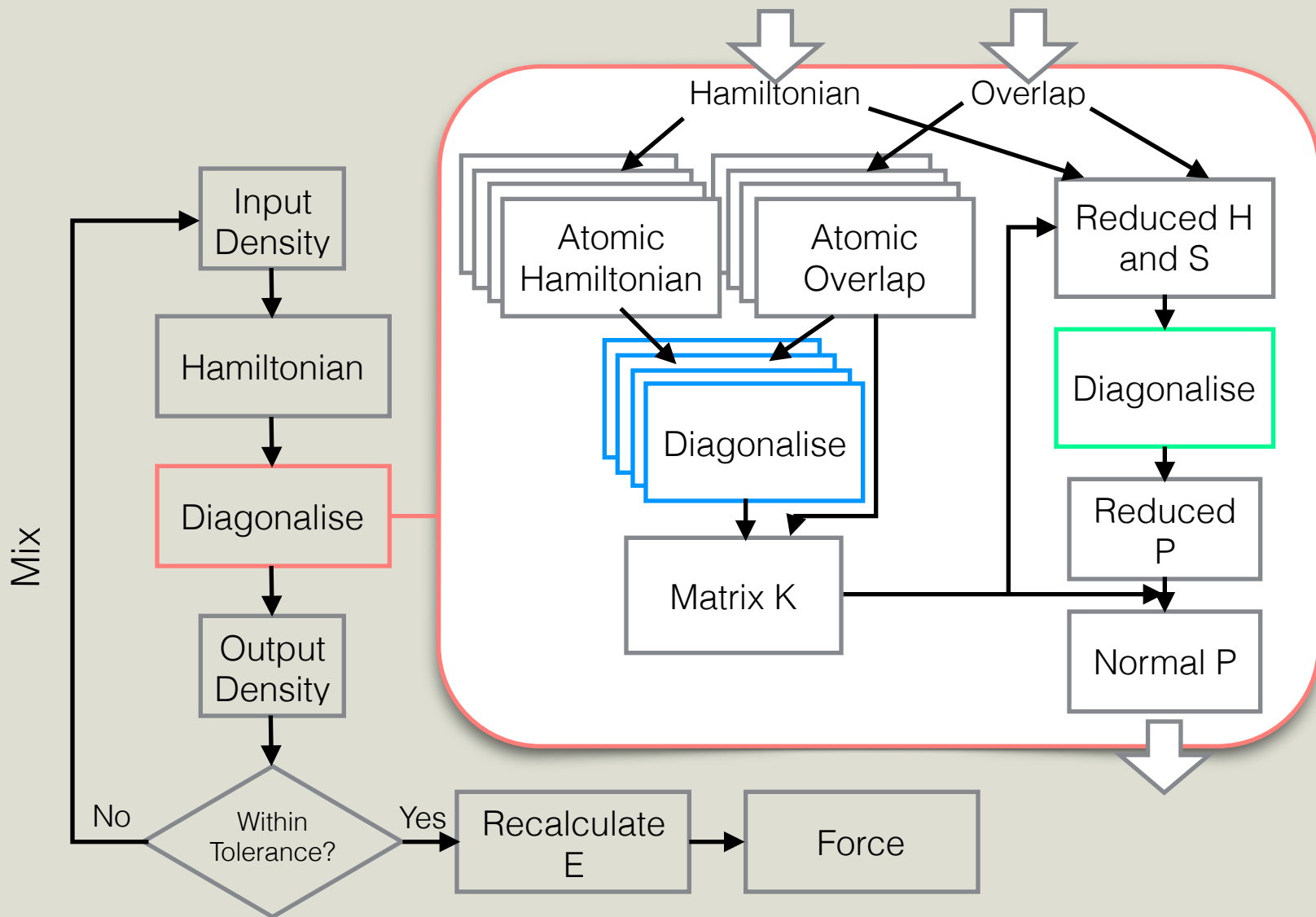
Expected Speed Up

N = number of atoms in system

T = cost of diagonalising one atomic block

n_μ = number of reduced basis orbitals per atom

n_α = number of original basis orbitals per atom

m = number of atoms within interaction range of one atom

$$(mn_\alpha)^3 NT + N^3 \left(\frac{n_\mu}{n_\alpha}\right)^3 T \qquad\qquad N^3 n_\alpha^3 T$$

atomic diagonalisation   main diagonalisation $\div$ main diagonalisation

$$\frac{(mn_\alpha)^3}{N^2} + \frac{n_\mu^3}{n_\alpha^6} \rightarrow \frac{n_\mu^3}{n_\alpha^6} < 1, \text{ as } N \rightarrow \infty$$

Cost Ratio

Expected Speed Up

$$N^3 n_\alpha^3 T$$

$$(mn_\alpha)^3 NT + N^3 \left(\frac{n_\mu}{n_\alpha}\right)^3 T$$
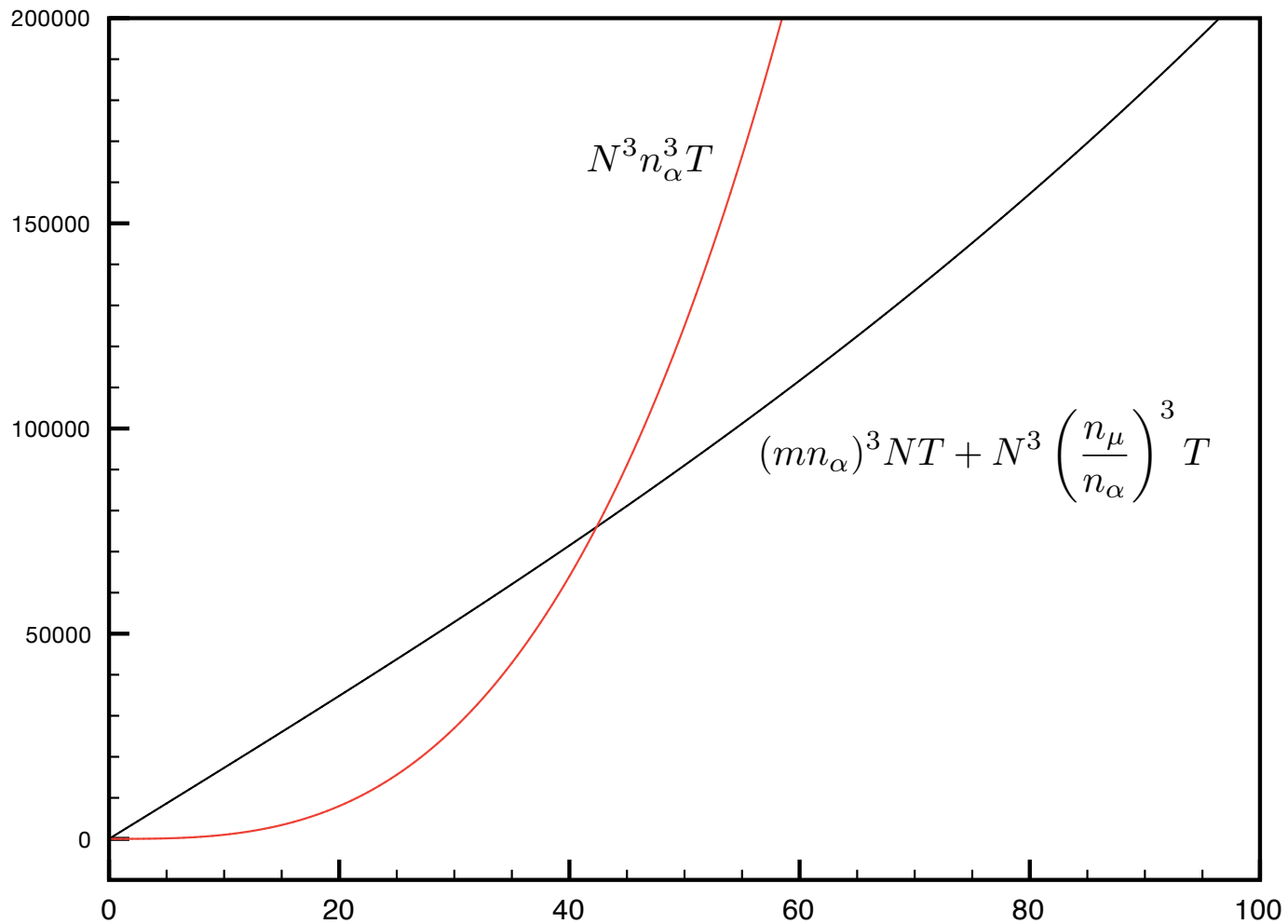
Input

```
&FORCE_EVAL
  METHOD Quickstep
  &DFT
    BASIS_SET_FILE_NAME  BASIS_SET
    POTENTIAL_FILE_NAME  GTH_POTENTIALS
    &MGRID
      CUTOFF 300
    &END MGRID
    &QS
      EPS_DEFAULT 1.0E-12
    &END QS
    &SCF
      SCF_GUESS ATOMIC
      EPS_SCF 1.0E-6
      MAX_SCF 100
      ADDED_MOS 16
      MAX_DIIS 100
      &SMEAR ON
        METHOD FERMI_DIRAC
        ELECTRONIC_TEMPERATURE [K] 300
      &END SMEAR
      &DIAGONALIZATION
        # ALGORITHM STANDARD
        ALGORITHM FILTER_MATRIX
        &FILTER_MATRIX
          # FILTER_TEMPERATURE 400000
          FILTER_TEMPERATURE [au_temp] 0.1
          AUTO_CUTOFF_SCALE 1.0
        &END FILTER_MATRIX
      &END DIAGONALIZATION
      &MIXING
        # METHOD BROYDEN_MIXING
        METHOD PULAY_MIXING
        ALPHA 0.2
        BETA 0.2
        NBUFFER 8
      &END MIXING
      &OUTER_SCF
        EPS_SCF 1.0E-6
        MAX_SCF 0
      &END OUTER_SCF
      &PRINT
        &FILTER_MATRIX ON
        &END FILTER_MATRIX
      &END PRINT
      &END SCF
```

```
&SCF
  &DIAGONALIZATION
    ALGORITHM FILTER_MATRIX
    &FILTER_MATRIX
      FILTER_TEMPERATURE 300000
      AUTO_CUTOFF_SCALE  1.0
    &END FILTER_MATRIX
  &END DIAGONALIZATION
  &PRINT
    &FILTER_MATRIX  ON
    &END FILTER_MATRIX
  &END PRINT
&END SCF
```

Accuracy and Speed w.r.t. Cutoff Radius

Atomic Cutoff (au)	Time / SCF Step (s)	Err in SCF Energy (au)	Err in Lattice Const (au)
Standard DZP	1.4000	0.0000000	0.000000
Standard SZ	0.7442	1.7138000	0.305077
3.0428	0.8891	0.2907160	—
4.5642	1.3608	0.0719113	0.00568571
7.6070	5.1726	0.0028373	0.00392925
8.3677	5.0489	0.0028373	0.00392925
9.1284	4.8699	0.0003192	0.00403831
12.1712	4.8811	0.0003192	0.00403831
15.2140	4.9502	0.0003192	0.00403831
18.2568	4.8746	0.0003192	0.00403831

Bulk Si with 64 atom unit cell (LDA); running on 32 MPI processes. SCF Energy + Cell Optimisation calculations. Tor = 1E-06 a.u. for Energy, 1E-04 a.u. for forces and pressure in cell.

Cost of 1 SCF Iteration

Bulk Si (LDA); running on 32 MPI processes. Single SCF step.