1 Gaussian functions per reference system

The Gaussian weighting for each reference system is given by:

$$W_A^r(CN_{cov}^A, CN_{cov}^{A,r}) = \sum_{j=1}^{N_{gauss}} \frac{1}{\mathcal{N}} \exp\left[-6j \cdot (CN_{cov}^A - CN_{cov}^{A,r})^2\right] \tag{1}$$

with

$$\sum_{r}^{N_{A,ref}} W_A^r(CN_{cov}^A, CN_{cov}^{A,r}) = 1 \tag{2}$$

$\mathcal{N}$ is a normalization constant.
The number of Gaussian functions per reference system N_{gauss} is mostly one, but equal to three for $CN_{cov}^{A,r} = 0$ and reference systems with similar coordination number.

QUESTION: How do we obtain the number of gaussian functions per reference system (N_{gauss})?

QUESTION: How or where do we get the normalization constant?

2 SAD - Superposition of Atomic Densities

The superposition of atomic densities(SAD) is an approach to obtain a good approximation of a collection of atoms, to be used as an initial guess for solving the self-consistent field(SCF) equation.

As originally implemented in DISCO, the molecular electron density can be obtained by adding the densities of all the constituting atoms.

This is how we get the density matrix for an isolated atom?

$$\rho_0 = \sum_A \rho_0^A \tag{3}$$

$$D_{ij} = \sum_a^{occ} c_{ia} c_{ja} \tag{4}$$

To get the coefficients we need to solve SCF for each atom. The SAD method is then the sum of all of these.

QUESTION: How can we get the initial guess for the Fock matrix and Coefficient matrices needed to run SCF on the individual atoms?

Direct SCF Approach

$$
\begin{aligned}
\Delta F_{ab} =& (c_{ia}c_{jb} + c_{ja}c_{ib}) \\
& \Delta F_{ij} + (c_{ia}c_{kb} + c_{ka}c_{ib}) \\
& \Delta F_{ik} + (c_{ia}c_{lb} + c_{la}c_{ib}) \\
& \Delta F_{il} + (c_{ja}c_{kb} + c_{ka}c_{jb}) \\
& \Delta F_{jk} + (c_{ja}c_{lb} + c_{la}c_{jb}) \\
& \Delta F_{jl} + (c_{ka}c_{lb} + c_{la}c_{kb}) \Delta F_{kl} \\
& = l_{ijkl}(4E^{ab}_{ij}D_{kl} + 4D_{ij}E^{ab}_{kl} - E^{ab}_{ik}D_{jl} - D_{ik}E^{ab}_{jl} - E^{ab}_{il}D_{jk} - D_{il}E^{ab}_{jk})
\end{aligned}
\tag{5}
$$

where

$$
E^{ab}_{ij} = c_{ia}c_{jb} + c_{ja}c_{ib} \tag{6}
$$

3 Questions for Albert

QUESTION: Does the xTB program compute the self-consistent field(SCF) or is that part of an external project?

QUESTION: How do you get your initial guess for the Fock matrix and Coefficient matrices needed to run SCF on the individual atoms?

QUESTION: Can you shed some light on where and how the xTB program computes the initial guess?

QUESTION: How and where is the overlap matrix computed? Which terms are needed?

QUESTION: For the dispersion term, how do we get $\overline{\alpha}_A$ and $\overline{\alpha}_{A,r}$?

QUESTION: For the dispersion term, how do we get the integration weights ω?

QUESTION: How do we get the atomic charges? Is it the mulliken charges?

QUESTION: How do we get the covalent coordination number $CN^A_{\mathbf{cov}}$ and $CN^{A,r}_{\mathbf{cov}}$ for an atom A?

QUESTION: What is $N_{A,\mathbf{ref}}$? The number of reference... orbitals? for an atom A?

θ_{ABC} is the angle between the two edges going from B to the other two atoms.
QUESTION: Is this definition correct? I assume we have the coordinates for each atom in (x,y,z)?