What is the charge flipping algorithm?

The charge flipping algorithm makes it possible to solve crystal structures from experimental intensity measurements. Let us recall that to solve a structure, we need both the **amplitudes** and the **phases** of the structure factor and **only the amplitudes** of the structure factors can be obtained in a diffraction experiment.

As indicated in the figure below, the process of charge flipping is iterative.

$$\begin{array}{ccccc} & & \rho(\mathbf{r}) & \xrightarrow{\text{step } 2} & g(\mathbf{r}) \\ & & \text{step } 1 \uparrow & & \downarrow \text{step } 3 \\ |F(\mathbf{h})| & \xrightarrow{\text{step } 0} & F(\mathbf{h}) & \xleftarrow{\text{step } 4} & G(\mathbf{h}) \end{array}$$

It consists of one initial step (0) followed by iterations consisting of four steps (1-4).

Step 0

We assign random phases (or zero phases) to each structure factor.

Step 1

From the structure factor with phases (that are arbitrary in the first iteration process) and amplitudes, we can calculate the electron density of the unit cell.

Step 2

The electron density will not be positive everywhere, which it should be if the phases were correct. Keeping the positive densities, we transform all the negative densities into positive ones. Following this step, we end up with positive densities everywhere.

Step 3

From the new electron densities $g(\mathbf{r})$, we can calculate the new structure factors $G(\mathbf{h})$ with their amplitudes and phases.

Step 4

Keeping the phases, we replace the amplitudes of $G(\mathbf{h})$ with the experimental values, thereby ending up with a new structure factor $F(\mathbf{h})$. The process is repeated for tens or hundreds of cycles until we reach convergence for the final structure.

The iteration terminates when the electron density is not changing anymore. At this point, the electron density yields the correct structure which can be further optimised using a structure model.