1 q_l

A proper definition of q_l [1] is:

$$q_l' = \sqrt{\frac{4\pi}{2l+1}\sum_{m=-l}^{l}|\sum_{f\in\mathfrak{F}(a)}\frac{A(f)}{A}Y_l^m(\theta_f,\psi_f)|^2} \tag{1}$$

and the symmetry properties of Y_{lm}:

$$\begin{aligned} Y_l^{m*}(\theta,\psi) &= (-1)^m Y_l^{-m}(\theta,\psi) \\ Y_l^m(-\mathbf{r}) &= (-1)^l Y_l^m(\mathbf{r}) \end{aligned}$$

thus leading a shorter version of q_l:

$$q_l' = \sqrt{\frac{4\pi}{(2l+1)A^2}\{|\sum_{f\in\mathfrak{F}(a)}A(f)Y_l^0(\theta_f,\psi_f)|^2 + \sum_{m=1}^{l}2|\sum_{f\in\mathfrak{F}(a)}A(f)Y_l^m(\theta_f,\psi_f)|^2\}} \tag{2}$$

Using voro++[2] we can build a specific $q6$ algorithm. Noting that directly using hardcoded Y_{lm} is faster than using recursion version. The algorithm can be formulated as follow:

Algorithm 1 specific q6

```
iteration on all particle
for all neighbors of particle do
  if neighbor_id > particle_id then
    q6list ← Y60
    for i = 1 → 6 do
      q6list ← Y6i
    end for
  end if
  for i = 0 to particle_number do
    q6 ← Σ|q6list|^2
  end for
end for
```

Noting that periodic boundary condition is used so that distance between particle is changed. Also notice that the id from xyz file is useless in calculating single frame quantities. Using that will cause more trouble. Q_4 is done in a similar way.

2 w_l

The definition of w_l [3] is:

$$w_l = \sum_{\substack{m_1,m_2,m_3 \\ m_1+m_2+m_3=0}} \begin{pmatrix} l & l & l \\ m_1 & m_2 & m_3 \end{pmatrix} \times q_{lm_1}q_{lm_2}q_{lm_3}$$

where

$$q_{lm} = \frac{A(f)}{A} Y_l^m(\theta_f, \psi_f)$$

and

$$\hat{w}_l = w_l / [\sum_{m=-l}^{l} |q_{lm}|^2]^{3/2}$$

so that the calculated q_l can be used and we only need to calculate half of the $q_6 list$:

$$\hat{w}_l = (\frac{4\pi}{2l+1})^{3/2} w_l / q_l^3$$

w_l is real so that imaginary part can be throw away in calculation.

References

[1] Walter Mickel, Sebastian C. Kapfer, Gerd E. Schröder-Turk, and Klaus Mecke. Shortcomings of the bond orientational order parameters for the analysis of disordered particulate matter. 138(4):044501.

[2] Chris H. Rycroft. VORO++: A three-dimensional Voronoi cell library in C++. 19(4):041111.

[3] Paul J. Steinhardt, David R. Nelson, and Marco Ronchetti. Bond-orientational order in liquids and glasses. 28(2):784–805.