Mean squared displacement is the usual definition:

$$\mathrm{MSD}(\tau) = \langle |\mathbf{r}(\tau) - \mathbf{r}(0)|^2 \rangle$$

The average, written explicitly, is done over windows of span τ that can be constructed in the interval $[w_f \dots w_t]$. To reduce computation, this average will be done with a stride of w_s (i.e. only one window every w_s will be considered):

$$\mathrm{MSD}(\tau) = \underbrace{\frac{w_s}{w_t - w_f - \tau} \sum_{t_0 = w_f \text{ every } w_s}^{w_t - \tau - 1}}_{\text{Average over intervals of span } \tau} \underbrace{\frac{1}{N} \sum_{i=1}^{N} \left(\mathbf{r}_i(t_0 + \tau) - \mathbf{r}_i(t_0)\right)^2}_{\text{Average over selected atoms}}$$

When the center of mass drift subtraction is enabled, the following replacement is applied to the above formula:

$$\mathbf{r}(t) \to \mathbf{r}(t) - \mathbf{r}_0(t)$$

where $\mathbf{r}_0(t)$ is the position of the center of mass of the selected atoms at time t:

$$\mathbf{r}_0(t) = \sum_{i=1}^{N} \mathbf{r}_i(t)/N$$