# 1 Infinite Boundaries

We start with

$$d^2 = \sum_{\langle i,j \rangle} \left(\vec{r}_{ij} - \vec{s}_{ij}\right)^2$$

Where $\vec{r}_{ij}$ is the distance between particles $i$ and $j$ in packing 1, and $\vec{s}_{ij}$ is the particle distance between particles $i$ and $j$ in packing 2.

Then

$$\begin{aligned}
d^2 &= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{r}_{ij} - \vec{s}_{ij}\right)^2 \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{r}_i - \vec{r}_j - \vec{s}_i + \vec{s}_j\right)^2 \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\left(\vec{r}_i - \vec{s}_i\right) - \left(\vec{r}_j - \vec{s}_j\right)\right)^2 \\
&\equiv \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{\delta}_i - \vec{\delta}_j\right)^2 \\
&= \frac{N}{2}\sum_{i=1}^{N}\vec{\delta}_i^2 + \frac{N}{2}\sum_{j=1}^{N}\vec{\delta}_j^2 + \sum_{i=1}^{N}\vec{\delta}_i \cdot \sum_{j=1}^{N}\vec{\delta}_j \\
&= N\sum_{i=1}^{N}\vec{\delta}_i^2 + \left(\sum_{i=1}^{N}\vec{r}_i - \sum_{i=1}^{N}\vec{s}_i\right) \cdot \left(\sum_{j=1}^{N}\vec{r}_j - \sum_{j=1}^{N}\vec{s}_j\right)
\end{aligned}$$

Where $\vec{\delta}_i$ and $\vec{\delta}_j$ are defined as $\left(\vec{r}_i - \vec{s}_i\right), \left(\vec{r}_j - \vec{s}_j\right)$ to make that work.

Now let's imagine that I've chosen the origin of $\vec{r}_i$ so that $\sum \vec{r}_i = 0$, and I have chosen the origin $\vec{\Delta}_s$ of $\vec{s}_i$ so that they minimize $\sum_i \left(\vec{r}_i - \vec{s}_i\right)^2$. The derivative of $\sum_i (\vec{r}_i - \vec{s}_i)^2$ with respect to that origin is therefore 0, so

$$\begin{aligned}
\vec{\nabla}_{\vec{\Delta}_s} \sum_i (\vec{r}_i - \vec{s}_i)^2 &= 0 \\
\vec{\nabla}_{\vec{\Delta}_s} \sum_i \left(\vec{r}_i - \left(\vec{s}'_i - \vec{\Delta}_s\right)\right)^2 &= 0 \\
\vec{\nabla}_{\vec{\Delta}_s} \sum_i \left[(\vec{r}_i - \vec{s}'_i)^2 + 2(\vec{r}_i - \vec{s}'_i) \cdot \vec{\Delta}_s + \vec{\Delta}_s^2\right] &= 0 \\
\sum_i \left[2(\vec{r}_i - \vec{s}'_i) + 2\vec{\Delta}_s\right] &= 0 \\
\vec{\Delta}_s = -\frac{1}{N} \sum_i (\vec{r}_i - \vec{s}'_i) \\
= \frac{1}{N} \sum_i \vec{s}'_i
\end{aligned}$$

So therefore if $\vec{s}_i$ are the coordinates with the new origin $\vec{\Delta}_s$, then $\vec{s}_i = \vec{s}'_i - \vec{\Delta}_s$, and $\sum_i \vec{s}_i = (\sum_i \vec{s}'_i) - N\vec{\Delta}_s = 0$.

This choice yields $\sum_i \vec{s}_i = 0$, which then means

$$\begin{aligned}
d^2 &= N \sum_{i=1}^{N} \vec{\delta}_i^2 \\
\frac{d^2}{N} &= \sum_{i=1}^{N} (\vec{r}_i - \vec{s}_i)^2
\end{aligned}$$

## 2 Periodic Boundaries

**Problem.** I expanded $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, and I can't choose an origin so that $\vec{r}_{ij}$ is always the minimal periodic distance vector.

**Fix.** We include an $L_{ij}$, $M_{ij}$, and $N_{ij}$ term, where $\vec{L}_{ij}, \vec{M}_{ij}, \vec{N}_{ij}$ are vectors like $(n_1 L, n_2 L)$. If we work backwards, starting with no assumptions about which translation or periodic image we are taking:

$$
\begin{aligned}
d^2 &= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{r}_{ij}-\vec{s}_{ij}-\vec{N}_{ij}\right)^2 \qquad (1)\\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{r}_i-\vec{r}_j-\vec{L}_{ij}+\vec{s}_i-\vec{s}_j-\vec{M}_{ij}-\vec{N}_{ij}\right)^2\\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left((\vec{r}_i-\vec{s}_i)-(\vec{r}_j-\vec{s}_j)-\left(\vec{L}_{ij}-\vec{M}_{ij}-\vec{N}_{ij}\right)\right)^2\\
&\equiv \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\vec{\delta}_i-\vec{\delta}_j-\vec{\Delta}_{ij}\right)^2\\
&= \frac{N}{2}\sum_{i=1}^{N}\vec{\delta}_i^2+\frac{N}{2}\sum_{j=1}^{N}\vec{\delta}_j^2+\sum_{i=1}^{N}\vec{\delta}_i\cdot\sum_{j=1}^{N}\vec{\delta}_j-\sum_{i=1}^{N}\vec{\delta}_i\cdot\sum_{j=1}^{N}\vec{\Delta}_{ij}-\sum_{j=1}^{N}\vec{\delta}_j\cdot\sum_{i=1}^{N}\vec{\Delta}_{ij}+\sum_{i=1}^{N}\sum_{j=1}^{N}\vec{\Delta}_{ij}^2\\
&= N\sum_{i=1}^{N}\vec{\delta}_i^2+\left(\sum_{i=1}^{N}(\vec{r}_i-\vec{s}_i)\right)\cdot\left(\sum_{j=1}^{N}(\vec{r}_j-\vec{s}_j)\right)-2\left(\sum_{i=1}^{N}(\vec{r}_i-\vec{s}_i)\right)\cdot\sum_{j=1}^{N}\vec{\Delta}_{ij}+\sum_{i=1}^{N}\sum_{j=1}^{N}\vec{\Delta}_{ij}^2
\end{aligned}
$$

Now if we make the same choice of origins as above, we get

$$
d^2 = N\sum_{i=1}^{N}(\vec{r}_i-\vec{s}_i)^2+\sum_{i=1}^{N}\sum_{j=1}^{N}\vec{\Delta}_{ij}^2 \qquad (2)
$$

Where $\vec{\Delta}_{ij} = \vec{L}_{ij}-\vec{M}_{ij}-\vec{N}_{ij}$, and $\vec{L}_{ij}$ are vectors of box-lengths that minimize $\left(\vec{r}_i-\vec{r}_j-\vec{L}_{ij}\right)^2$, $\vec{M}_{ij}$ minimizes $\left(\vec{s}_i-\vec{s}_j-\vec{M}_{ij}\right)^2$, and $\vec{N}_{ij}$ minimizes $\left(\vec{r}_{ij}-\vec{s}_{ij}-\vec{N}_{ij}\right)^2$.

Now we can choose which mirror image of $\vec{r}_i$ and $\vec{s}_i$ we want, which translation of $\vec{r}_i$ and/or $\vec{s}_i$ we want, and also choose each $\vec{N}_{ij}$ as we wish, as long as the $\vec{N}_{ij}$ coordinates are box-length.

If we make these choices so as to minimize $d^2$, then clearly for equation 2 we get the minimal distance squared between the two sets. For equation 1, then clearly the choice that minimizes $d^2$ is one in which $\left(\vec{r}_{ij}-\vec{s}_{ij}-\vec{\Delta}_{ij}\right)$ is as short as possible, e.g., the box-wrapped shortest distance vector from $\vec{r}_{ij}$ to $\vec{s}_{ij}$. These two equations are equivalent, so the choice to minimize Eq. 1 is the same as the choice to minimize Eq. 2. Therefore, if we simply calculate $d^2 = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\vec{r}_{ij}\ominus\vec{s}_{ij})^2$ (where $\vec{r}\ominus\vec{s}$ is the box-wrapped distance vector between them), we have the minimal value of $d^2$:

$$
d^2 = \frac{1}{N}\sum_{\langle i,j\rangle}(\vec{r}_{ij}\ominus\vec{s}_{ij})^2 = \min_{\vec{\delta}}\sum_{i=1}^{N}\left(\vec{r}_i\ominus\left(\vec{s}_i-\vec{\delta}\right)\right)^2
$$

Note that we still need to try all 8 rotoflips, as $\vec{r}_{ij}$ depends on those.