Suppose we transform the wrapped coordinates x_i from cartesian space, where we assume the coordinates have the origin at one corner of the periodic box, to reduced coordinates y_i by transforming x_i by the inverse box transform. Mathematically, this would be represented by

$$y_i = L_i^{-1} x_i \tag{1}$$

In this setup, $0 \leq y_i < 1$. In this new coordinate space, we can define quantities analogous to those specific to orthonormal periodic cells.

$$d = y_{i+1}^u - y_i^u \tag{2}$$

$$y_i^u = y_i^w - m \tag{3}$$

$$y_{i+1}^u = y_{i+1}^w - n \tag{4}$$

With some rearrangement, we obtain the following:

$$d = y_{i+1}^w - y_i^w - n + m \tag{5}$$

Since y_i and y_{i+1} are bounded, $|y_{i+1}^w - y_i^w| < 1$. If $d < \frac{1}{2}$, indicating that the atom in question did not move more than half a box length, then $|n - m| <= 1$, since n and m are both integers. The $n - m$ term can be computed from the floor function of the wrapped displacement, yielding the displacement scheme equation in this new coordinate space.

$$y_{i+1}^u = y_i^u + y_{i+1}^w - y_i^w - \left\lfloor y_{i+1}^w - y_i^w + \frac{1}{2} \right\rfloor \tag{6}$$

However, this equation is only valid in the reduced coordinate space. To unwrap into cartesian coordinates, we take Eq. 6 and apply the box transform L_{i+1}, and substitute in the definition for y_i from Eq. 1, yielding:

$$L_{i+1}\left(L_{i+1}^{-1} x_{i+1}^u\right) = L_{i+1}\left(L_i^{-1} x_i^u + L_{i+1}^{-1} x_{i+1}^w - L_i^{-1} x_i^w\right) - L_{i+1}\left\lfloor L_{i+1}^{-1} x_{i+1}^w - L_i^{-1} x_i^w + \frac{1}{2} \right\rfloor \tag{7}$$

Recalling that box transformations and inverse box transformations yield the identity matrix, $L_i L_i^{-1} = I$, and defining that $L_{i+1} L_i^{-1} = \alpha$, the above expression further simplifies to:

$$x_{i+1}^u = \alpha x_i^u + x_{i+1}^w - \alpha x_i^w - L_{i+1}\left\lfloor L_{i+1}^{-1} x_{i+1}^w - L_i^{-1} x_i^w + \frac{1}{2} \right\rfloor \tag{8}$$

The advantage to Eq. 8 is that it lends itself well to solution by linear algebra methods. For triclinic boxes, L_i^{-1} is readily accessible via matrix inversion, and calculating α is a straightforward matrix multiplication. From there, the unwrapped coordinates for frame $i + 1$ is calculated as the sum of multiple vectors, some of which are derived from matrix-vector products.