

Review:

$$\rho_a = \sum_b m_b W_{ab}$$

$$\dot{V}_a = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \nabla_a W_{ab} \right) \nabla_a W_{ab}$$

This must also be accounted for in the energy equation.

$$\dot{e}_a = \left(\frac{P_a}{\rho_a^2} \right) \sum_b m_b (V_a - V_b) \cdot \nabla_a W_{ab}$$

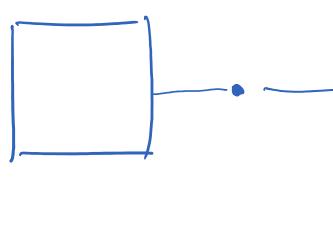
$$\dot{e}_a = \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \nabla_a W_{ab} \right) (V_a - V_b) \cdot \nabla_a W_{ab}$$

$$\dot{e}_a = \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \nabla_a W_{ab} \right) (V_a - V_b) \cdot \nabla_a W_{ab}$$

$$\dot{e}_b = - \sum_a m_a \left(\frac{P_b}{\rho_b^2} + \nabla_b W_{ab} \right) (V_b - V_a) \cdot \nabla_b W_{ab}$$

Periodic Boundary Conditions:

Method 1: Modify the Ball-Box intersection Test



distance to the image

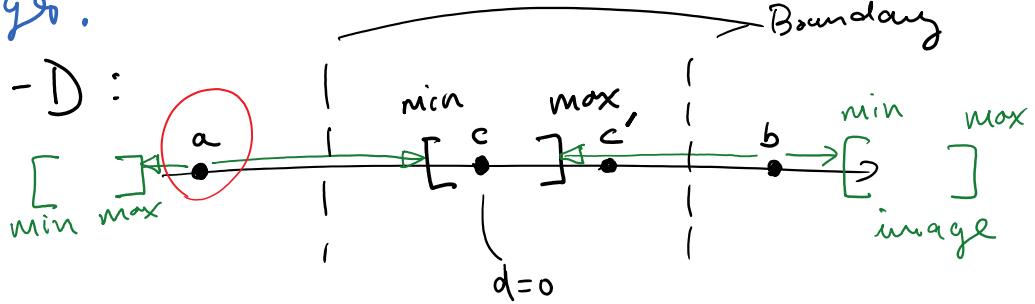
Take the shortest distance to any image

Every Cell will have 1 unique distance, which is the shortest over all periodic images.

Boundary

images.

In 1-D:



def ! \rightarrow $fDist2 = 0$
 $fDist2Periodic(cell, l, in_r, out_r) :$

$$dx = cell.min - in_r$$

$$dx1 = in_r - cell.max$$

true : we are
doing case a)

do
this for
components
 x_1, x_2
 x_3, x_4
 x_5, x_6

```

if ( $dx[0] > 0$ )
     $dx1[0] += l[0]$ 
    if ( $dx1[0] < dx[0]$ )
         $fDist2 += dx1[0] * dx1[0]$ 
         $out\_r[0] = in\_r[0] + l[0]$ 
    else
         $fDist2 += dx[0] * dx[0]$ 
         $out\_r[0] = in\_r[0]$ 
    else if ( $dx1[0] > 0$ ) { case c)
         $dx[0] += l[0]$ 
        if ( $dx[0] < dx1[0]$ )
             $fDist2 += dx[0] * dx[0]$ 
             $out\_r[0] = in\_r[0] - l[0]$ 
        else
             $fDist2 += dx1[0] * dx1[0]$ 
             $out\_r[0] = in\_r[0]$ 
    else case c)
         $out\_r[0] = in\_r[0]$ 
    return fDist2

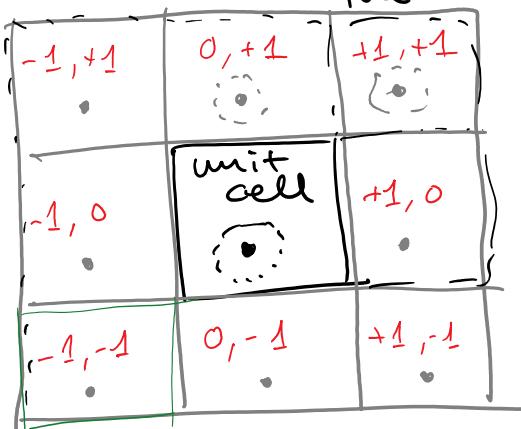
```

..... couch ball

Works as long as your search box is less than $\frac{1}{2}|\ell|$! Careful

We only consider 1 image (as closest) in the particle-cell distance test.

Method 2: Must walk each of the images of the unit cell (root of the tree).



NN-walk($c, pq, \underline{r_s}$)

$$\underline{r_s} = \underline{r} + \underline{r_{Offset}}$$

However: make sure we walk the closest image first, since \underline{r} is inside the unit cell, choosing to walk the unit cell first is the best strategy.

$$\underline{r_{Offset}} = \langle 0, 0, 0 \rangle$$

NN-walk(c, pq, \underline{r})

for all images ($\underline{r_{Offset}} \neq \langle 0, 0, 0 \rangle$)

$$\underline{r_s} = \underline{r} + \underline{r_{Offset}}$$

NN-walk($c, pq, \underline{r_s}$)

will shrink the search radius substantially, so that usually there is almost no work to be

done for the images!