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Supplementary Information for Size-Sieving Separation of Hard-Sphere Gases at Low Concentrations through Cylindrically Porous Membranes

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This material elaborates the analytical theory of the collision dynamics between hard spheres and cylindrically porous membranes, as well as the computer algorithms to implement it in event-driven molecular dynamics simulations.

1. THEORY

There are three possibilities on how a particle collides with a cylindrical pore with a circular opening: it can hit a non-porous area (case 1), or hit and bounce off the edge of the pore (case 2), or directly collide with the inner wall of the pore (case 3) as shown in Fig. S1.

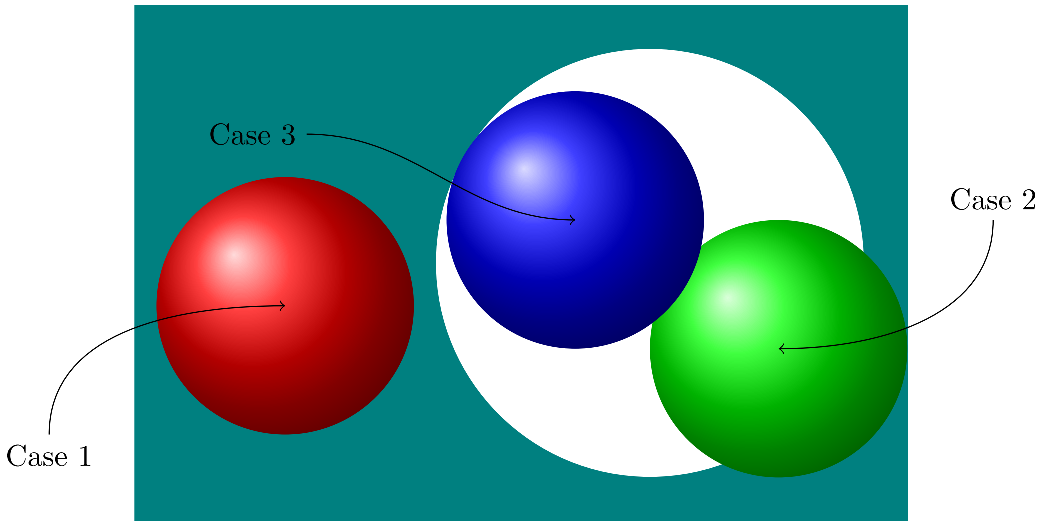

FIG. S1: Three cases of particle-pore collision.

Below we first calculate the time it takes for a particle outside the pore to reach the membrane in one of the three cases. Then we provide the dynamical details about the velocity vectors during the collision between the particle and the pore.

1.1. Collision time

In case 1, the time till colliding with the membrane t_M is simply the particle's z-direction distance to the membrane it flies toward divided by its z velocity, i.e.

$$t_M = \left| \frac{z - z_M}{v_z} \right| \tag{1}$$

where z_M is the z-position of the membrane in question. For the next two cases, the particle would be flying towards a certain pore. We will denote its position as that of its geometric center, $\overrightarrow{\mathbf{r}}_M = (x_M, y_M, z_M)$. Its diameter we denote as d. The particle originally at position $\overrightarrow{\mathbf{r}}$ collides with the membrane when its position becomes $\overrightarrow{\mathbf{r}}'$.

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In case 2, by the time the collision occurs, in other words, when $\vec{\mathbf{r}}$ becomes $\vec{\mathbf{r}}' = \vec{\mathbf{r}} + t_M\vec{\mathbf{v}}$, as shown in Fig. S2. It shows specifically the case where the particle is flying towards the pore from a non-membrane space. However, in terms of physics, all arguments are valid in the case that the particle is inside the membrane:

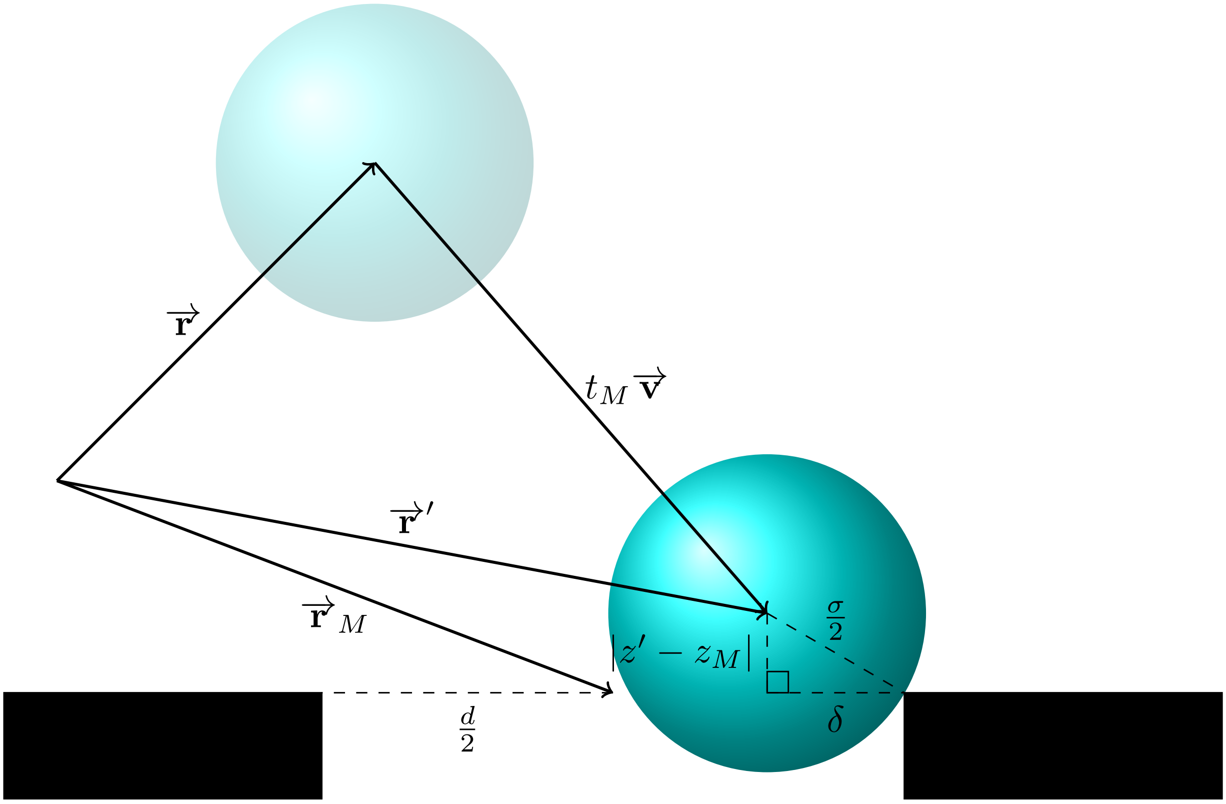

FIG. S2: Case 2 collision process

The way to determine t_M lies in the right triangle with dashed edges, formed from the particle's geometric/mass center, its vertical projection onto the plane of the pore, and the particle-pore contact point. In the pore's plane, parallel to the xy-plane, the distance from the particle center to the pore center would be:

$$\delta' = \sqrt{(x + v_x t_M - x_M)^2 + (y + v_y t_M - y_M)^2} \tag{2}$$

And the difference between it and the pore radius is:

$$\delta = \frac{d}{2} - \delta' \tag{3}$$

Finally, by the Pythagorean theorem:

$$\left(\frac{\sigma}{2}\right)^2 = (z + v_z t_M - z_M)^2 + \delta^2 \tag{4}$$

Now we have an equation with t_M as the only unknown. To solve it, we must first expand it into a polynomial form. For simplicity, let us define:

$$\begin{aligned} v^2 &= v_x^2 + v_y^2 + v_z^2 \\ r_v &= (x - x_M)v_x + (y - y_M)v_y + (z - z_M)v_z \\ \Delta r &= \sqrt{(x - x_M)^2 + (y - y_M)^2 + (z - z_M)^2} \end{aligned} \tag{5}$$

Then through algebraic manipulation, we convert Eq.(4) into the following 4th-order polynomial with normalized highest-order coefficient

$$t_M^4 + at_M^3 + bt_M^2 + ct_M + d = 0 \tag{6}$$

where

$$
\begin{aligned}
a &= \tfrac{4r_v}{v^2} \\
b &= \tfrac{4r_v^2 - d^2(v_x^2+v_y^2)}{v^4} + \tfrac{2(\Delta r)^2 + \frac{d^2-\sigma^2}{2}}{v^2} \\
c &= \tfrac{2d^2(z-z_M)v_z + r_v[4(\Delta r)^2 - d^2 - \sigma^2]}{v^4} \\
d &= \tfrac{\left[(\Delta r)^2 + \frac{d^2-\sigma^2}{4}\right] - d^2[(x-x_M)^2+(y-y_M)^2]}{v^4}
\end{aligned} \tag{7}
$$

To solve this equation, the first step is to define

$$
s = t_M + \frac{a}{4} \tag{8}
$$

Substituting t_M for s in Eq.(6), we get

$$
s^4 + ps^2 + qs + w = 0 \tag{9}
$$

where

$$
\begin{aligned}
p &= b - \tfrac{3}{8}a^2 \\
q &= \tfrac{a^3}{8} - \tfrac{ab}{2} + c \\
w &= -\tfrac{3}{256}a^4 + \tfrac{a^2 b}{16} - \tfrac{ac}{4} + d
\end{aligned} \tag{10}
$$

Eq.(9) has a systemic solution set. To solve for it, we must first obtain the solution for this cubic equation of u

$$
u^3 - \frac{p}{2}u^2 - wu + \frac{4wp - q^2}{8} = 0. \tag{11}
$$

Such an equation has at least one solutioion and at most three, u_i $(i = 0, 1, 2)$. Now, the determinant Δ for any cubic equation or the form $x^3 + Ax^2 + Bx + C = 0$ is

$$
\begin{aligned}
\Delta &= \left(\tfrac{P}{3}\right)^3 + \left(\tfrac{Q}{2}\right)^2 \\
P &= B - \tfrac{A^2}{3} \\
Q &= \tfrac{2}{27}A - \tfrac{AB}{3} + C
\end{aligned} \tag{12}
$$

Once we plug in $A = -\frac{p}{2}$, $B = -w$, $C = \frac{4wp-q^2}{8}$, there are three different scenarios

$$
\begin{cases}
\Delta > 0 : u_0 = u_1 = u_2 = \sqrt[3]{\sqrt{\Delta} - \frac{Q}{2}} - \sqrt[3]{\sqrt{\Delta} + \frac{Q}{2}} - \frac{A}{3} \\
\Delta = 0 \begin{cases} u_0 = -2\sqrt[3]{\frac{Q}{2}} - \frac{A}{3} \\ u_1 = u_2 = \sqrt[3]{\frac{Q}{2}} - \frac{A}{3} \end{cases} \\
\Delta < 0 \begin{cases} u_0 = 2\sqrt{-\frac{P}{3}}\cos\theta - \frac{A}{3} \\ u_1 = 2\sqrt{-\frac{P}{3}}\cos\left(\theta + \frac{2\pi}{3}\right) - \frac{A}{3} \quad \theta = \frac{1}{3}\arccos\left(\frac{-Q/2}{\sqrt{-(P/3)^3}}\right) \\ u_2 = 2\sqrt{-\frac{P}{3}}\cos\left(\theta - \frac{2\pi}{3}\right) - \frac{A}{3} \end{cases}
\end{cases} \tag{13}
$$

For any u_i, if $q \geq 0$, then to get real solutions of s, and thus of t_M, we need to solve

$$
\begin{aligned}
s^2 + s\sqrt{2u - p} + u - \sqrt{u^2 - w} &= 0 \\
s^2 - s\sqrt{2u - p} + u + \sqrt{u^2 - w} &= 0
\end{aligned} \tag{14}
$$

On the other hand, if $q < 0$, the equations become:

$$
\begin{aligned}
s^2 + s\sqrt{2u - p} + u + \sqrt{u^2 - w} &= 0 \\
s^2 - s\sqrt{2u - p} + u - \sqrt{u^2 - w} &= 0
\end{aligned} \tag{15}
$$

For any solution of t_M solved, the least positive value is the answer we search for.

Finally, in case 3, which only happens when $\sigma < d$, we again taking the case where the particle starts in a non-membrane space. For this type of collision, the z-direction: does not matter, therefore we need only care about the motion parallel to the xy-plane:

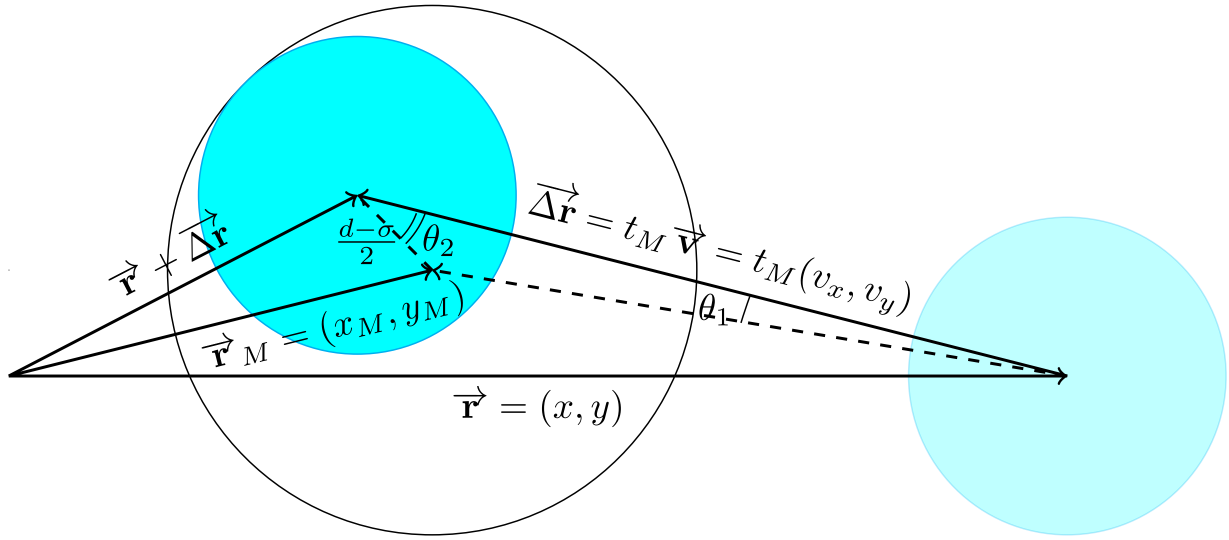

FIG. S3: Case 3 collision process in the xy-plane

In the Fig. S3, only the x and y coordinates and components are considered. t_M could be calculated as

$$t_M = \frac{||\overrightarrow{\Delta \mathbf{r}}||}{||\overrightarrow{\mathbf{v}}||} = \frac{||\overrightarrow{\Delta \mathbf{r}}||}{\sqrt{v_x^2 + v_y^2}} \tag{16}$$

To calculate $||\overrightarrow{\Delta \mathbf{r}}||$, we rely on a trigonometric relation. The angle θ_1 could be calculated using the inner product between $\overrightarrow{\mathbf{v}}$ and the difference vector between $\overrightarrow{\mathbf{r}}_M$ and $\overrightarrow{\mathbf{r}}$

$$\cos\theta_1 = \frac{\overrightarrow{\mathbf{v}} \cdot (\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}})}{||\overrightarrow{\mathbf{v}}|| \cdot ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||} \tag{17}$$

And by the law of sines, we get that

$$\sin\theta_2 = \frac{||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||}{(d-\sigma)/2} \sin\theta_1 = \frac{||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||}{(d-\sigma)/2} \sqrt{1 - \cos^2\theta_1} \tag{18}$$

Now, θ_2 solved this way would have two possble solutions, but we only take $\theta_2 \leq 90°$, which makes physical sense. In this case, $\cos\theta_2 \geq 0$. We finalize our calculation with using the law of cosines to solve for $||\overrightarrow{\Delta \mathbf{r}}||$ using this relation:

$$\begin{aligned} ||\overrightarrow{\Delta \mathbf{r}}||^2 &= ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||^2 + \left(\frac{d-\sigma}{2}\right)^2 - 2||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}|| \cdot \frac{d-\sigma}{2} \cdot \cos(\pi - \theta_1 - \theta_2) \\ &= ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||^2 + \left(\frac{d-\sigma}{2}\right)^2 + ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}|| \cdot (d-\sigma) \cdot \cos(\theta_1 + \theta_2) \\ &= ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}||^2 + \left(\frac{d-\sigma}{2}\right)^2 \\ &+ ||\overrightarrow{\mathbf{r}}_M - \overrightarrow{\mathbf{r}}|| \cdot (d-\sigma) \cdot (\cos\theta_1 \sqrt{1 - \sin^2\theta_2} - \sqrt{1 - \cos^2\theta_1} \sin\theta_2) \end{aligned} \tag{19}$$

Solving $||\overrightarrow{\Delta \mathbf{r}}||$ this way and replugging it into (16) will get us the value of t_M.

1.2. Collision dynamics

In case 1, the only change to that particle's velocity is that v_z reverses sign

$$v_z \leftarrow -v_z \tag{20}$$

In case 2, the dynamics is equivalent to a sphere elastically colliding with a tangential plane passing through the particle-pore contact point. Therefore, what would happen is that the component of the initial velocity vector parallel to this plane's normal line, $\vec{\mathbf{v}}_\parallel$, would change sign. Meanwhile, the corresponding normal vector $\vec{\mathbf{n}} = (n_x, n_y, n_z)$ to the plane is along the line segment that connects the particle's contact point to the pore edge and its center. The physical process could be understood using the figure below, where the red and blue vectors denotes the velocity before and after collision respectively, along with their components with respect to $\vec{\mathbf{n}}$

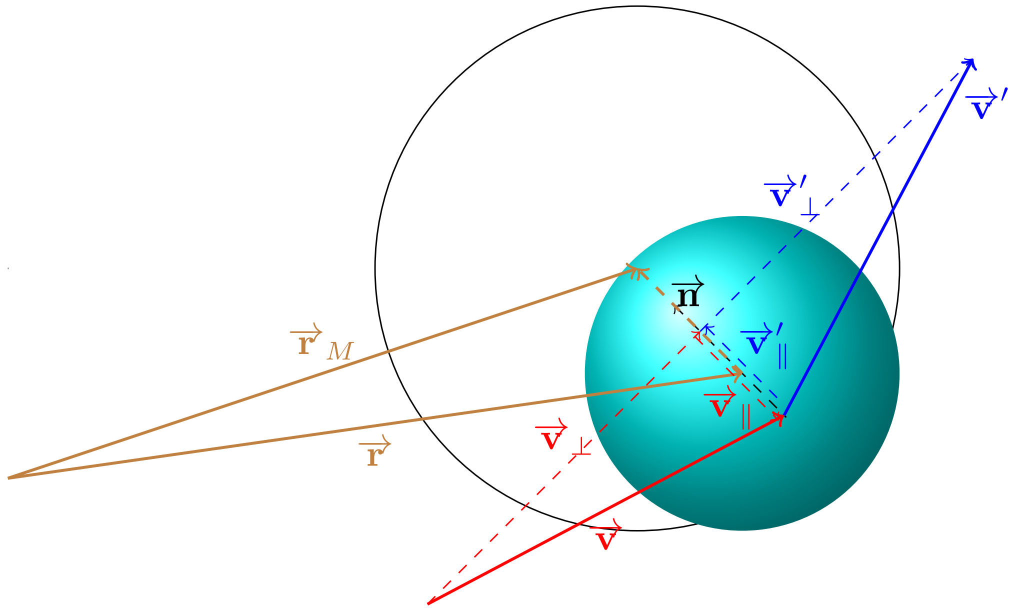

FIG. S4: Dynamics of case 2

By the above reasoning, $\vec{\mathbf{n}}$ can be chosen to be the vector starting from the particle-pore contact point to the particle center. If we refer back to Fig. S2 and equations (2) and (3), taking account that here $t_M = 0$

$$\begin{aligned} \sqrt{n_x^2 + n_y^2} &= \delta' = \tfrac{d}{2} - \sqrt{(x_M - x)^2 + (y_M - y)^2} \\ n_z &= z - z_M \end{aligned} \tag{21}$$

In the xy-plane, (n_x, n_y) should follow the direction from the particle center to the pore center, therefore

$$\begin{aligned} n_x &= \delta' \cdot \frac{x_M - x}{\sqrt{(x_M - x)^2 + (y_M - y)^2}} = \left[\frac{d/2}{\sqrt{(x_M - x)^2 + (y_M - y)^2}} - 1 \right] (x_M - x) \\ n_y &= \delta' \cdot \frac{y_M - y}{\sqrt{(x_M - x)^2 + (y_M - y)^2}} = \left[\frac{d/2}{\sqrt{(x_M - x)^2 + (y_M - y)^2}} - 1 \right] (y_M - y) \end{aligned} \tag{22}$$

So

$$\vec{\mathbf{v}}_\parallel = \frac{\vec{\mathbf{v}} \cdot \vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} \vec{\mathbf{n}} = \frac{v_x n_x + v_y n_y + v_z n_z}{n_x^2 + n_y^2 + n_z^2} (n_x, n_y, n_z) \tag{23}$$

Meanwhile

$$\begin{aligned} \vec{\mathbf{v}}'_\parallel &= -\vec{\mathbf{v}}_\parallel \\ \vec{\mathbf{v}}'_\perp &= \vec{\mathbf{v}}_\perp \end{aligned} \tag{24}$$

By combining (23) and (24), we get

$$\vec{\mathbf{v}}' = \vec{\mathbf{v}}'_{\perp} + \vec{\mathbf{v}}'_{\parallel} = \vec{\mathbf{v}}_{\perp} - \vec{\mathbf{v}}_{\parallel} = (\vec{\mathbf{v}}_{\perp} + \vec{\mathbf{v}}_{\parallel}) - 2\vec{\mathbf{v}}_{\parallel} = \vec{\mathbf{v}} - 2\vec{\mathbf{v}}_{\parallel} = \vec{\mathbf{v}} - 2(\vec{\mathbf{v}} \cdot \vec{\mathbf{n}})\vec{\mathbf{n}} \tag{25}$$

Or in terms of vector components

$$\begin{cases} v'_x = v_x - 2\frac{\vec{\mathbf{v}}\cdot\vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} n_x \\ v'_y = v_y - 2\frac{\vec{\mathbf{v}}\cdot\vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} n_y \\ v'_z = v_z - 2\frac{\vec{\mathbf{v}}\cdot\vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} n_z \end{cases} \tag{26}$$

In case 3, which is specific to when a particle has a diameter smaller than the pore it enters, the collision can also considered to be equivalent to that between a sphere and a tangential plane passing the particle-pore contact point. The main difference between this case and the previous is that v_z remains unchanged. Any change in velocity happens in the xy-plane. Hence, we have the following figure to depict this process with only the xy dimension:

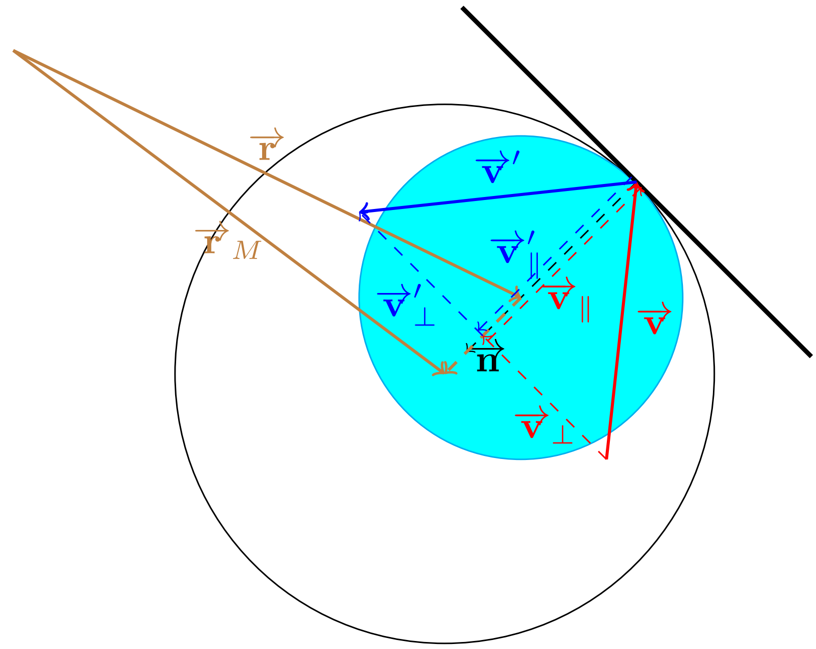

FIG. S5: Dynamics of case 3 in xy-plane

Per the same logic in case 2, what we have is that $\vec{v}_{\parallel}$ reverses direction, only now it is limited to considering inside the xy plane. Here, $\vec{\mathbf{n}}$ is parallel to $\vec{\mathbf{r}}_M - \vec{\mathbf{r}}$, so we can choose to make them equal, in other words

$$\vec{\mathbf{n}} = (n_x, n_y) = \frac{\sigma}{\sqrt{(x_M - x)^2 + (y_M - y)^2}}(x_M - x, y_M - y) = \frac{\sigma}{d - \sigma}(x_M - x, y_M - y) \tag{27}$$

In this way

$$\vec{\mathbf{v}}_{\parallel} = \frac{\vec{\mathbf{v}} \cdot \vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2}\vec{\mathbf{n}} = \frac{v_x n_x + v_y n_y}{||\vec{\mathbf{n}}||^2}\vec{\mathbf{n}} \tag{28}$$

The rest follows similar logic to the case 2 dynamics, and we would get:

$$\begin{cases} v'_x = v_x - 2\frac{\vec{\mathbf{v}}\cdot\vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} n_x \\ v'_y = v_y - 2\frac{\vec{\mathbf{v}}\cdot\vec{\mathbf{n}}}{||\vec{\mathbf{n}}||^2} n_y \end{cases} \tag{29}$$

2. ALGORITHM

This session provides sample algorithms to implement above theoretical results for particle-pore collision dynamics.

2.1. Collision time

Before getting to the algorithm for computing t_M, we should first write down the solution for the case 2 equation for t_M in code. To start, the solutions to (11) should be

---

Algorithm 1 Cubic equation solutions

Require: A, B, C

$P \leftarrow B - \frac{A^2}{3}, Q \leftarrow \frac{2A^3}{27} - \frac{AB}{3} + C$

if $\left(\frac{P}{3}\right)^3 + \left(\frac{Q}{2}\right)^2 > 0$ **then**

$\quad u_1 = u_2 = u_3 \leftarrow \sqrt[3]{\sqrt{\left(\frac{P}{3}\right)^3 + \left(\frac{Q}{2}\right)^2} - \frac{Q}{2}} - \sqrt[3]{\sqrt{\left(\frac{P}{3}\right)^3 + \left(\frac{Q}{2}\right)^2} + \frac{Q}{2}} - \frac{A}{3}$

else if $\left(\frac{P}{3}\right)^3 + \left(\frac{Q}{2}\right)^2 == 0$ **then**

$\quad u_1 \leftarrow 2\sqrt[3]{-\frac{Q}{2}} - \frac{A}{3}$

$\quad u_2 = u_3 \leftarrow -\sqrt[3]{-\frac{Q}{2}} - \frac{A}{3}$

else

$\quad \theta \leftarrow \frac{1}{3}\arccos\left(\frac{-Q/2}{\sqrt{-(P/3)^3}}\right)$

$\quad u_1 \leftarrow 2\sqrt{-\frac{P}{3}}\cos\theta - \frac{A}{3}$

$\quad u_2 \leftarrow 2\sqrt{-\frac{P}{3}}\cos\left(\theta + \frac{2\pi}{3}\right) - \frac{A}{3}$

$\quad u_3 \leftarrow 2\sqrt{-\frac{P}{3}}\cos\left(\theta - \frac{2\pi}{3}\right) - \frac{A}{3}$

end if

With Algorithm 1, we can define a function for solving t_M under case 2, inputing the positions and diameters of both particle and pore, plus the particle's velocity components.

Algorithm 2 Quartic equation solutions

Require: $d, x, v_x, x_M, y, v_y, y_M, z, v_z, z_M, \sigma$

$t_M \leftarrow +\infty$
$r_v \leftarrow (x - x_M)v_x + (y - y_M)v_y + (z - z_M)v_z$
$(\Delta r)^2 \leftarrow (x - x_M)^2 + (y - y_M)^2 + (z - z_M)^2$
$v^2 \leftarrow v_x^2 + v_y^2 + v_z^2$

$a \leftarrow \frac{4r_v}{v^2}$
$b \leftarrow \frac{4r_v^2 - d^2(v_x^2+v_y^2)}{v^4} + \frac{2(\Delta r)^2 + \frac{d^2-\sigma^2}{2}}{v^2}$
$c \leftarrow \frac{2d^2(z-z_M)v_z + r_v[4(\Delta r)^2 - d^2 - \sigma^2]}{v^4}$
$d \leftarrow \frac{\left[(\Delta r)^2 + \frac{d^2-\sigma^2}{4}\right] - d^2[(x-x_M)^2+(y-y_M)^2]}{v^4}$

$p \leftarrow b - \frac{3}{8}a^2$
$q \leftarrow \frac{a^3}{8} - \frac{ab}{2} + c$
$w \leftarrow -\frac{3a^4}{256} + \frac{a^2 b}{16} - \frac{ac}{4} + d$
Cubic equation solutions$\left(A = -\frac{p}{2}, B = -w, C = \frac{wp}{2} - \frac{q^2}{8}\right)$

for $i = 0;\ i < 3;\ i++$ **do**
  if $q \geq 0$ **then**
    if $2u_i - p \geq 0$ **and** $u_i^2 - w \geq 0$ **and** $4\sqrt{u_i^2 - w} - 2u_i - p \geq 0$ **then**
      $t \leftarrow \frac{1}{2}(-\sqrt{2u_i - p} + \sqrt{4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$

      $t \leftarrow \frac{1}{2}(-\sqrt{2u_i - p} - \sqrt{4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$
    end if
    if $2u_i - p \geq 0$ **and** $u_i^2 - w \geq 0$ **and** $-4\sqrt{u_i^2 - w} - 2u_i - p \geq 0$ **then**
      $t \leftarrow \frac{1}{2}(\sqrt{2u_i - p} + \sqrt{-4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$

      $t \leftarrow \frac{1}{2}(\sqrt{2u_i - p} - \sqrt{-4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$
    end if
  else
    if $2u_i - p \geq 0$ **and** $u_i^2 - w \geq 0$ **and** $4\sqrt{u_i^2 - w} - 2u_i - p \geq 0$ **then**
      $t \leftarrow \frac{1}{2}(\sqrt{2u_i - p} + \sqrt{4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$

      $t \leftarrow \frac{1}{2}(\sqrt{2u_i - p} - \sqrt{4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$
    end if
    if $2u_i - p \geq 0$ **and** $u_i^2 - w \geq 0$ **and** $-4\sqrt{u_i^2 - w} - 2u_i - p \geq 0$ **then**
      $t \leftarrow \frac{1}{2}(-\sqrt{2u_i - p} + \sqrt{-4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$

      $t \leftarrow \frac{1}{2}(-\sqrt{2u_i - p} - \sqrt{-4\sqrt{u_i^2 - w} - 2u_i - p}) - \frac{r_v}{v^2}$
      $t_M \leftarrow t > 10^{-10}\ ?\ \min(t_M, t)\ :\ t_M$
    end if
  end if
end for
return t_M

In theory, we should test for $t > 0$. But numerical computation comes with a finite precision, therefore a calculation that should yield 0 might give some value extremely close but nonzero. In our program, we chose $\epsilon = 10^{-10}$ as our tolerance.

Before we try to compute t_M, we have to determine which of the three cases we are in. To do this, we must first determine if the particle is completely outside the membrane area, partly embedded in a pore, or completely inside one. After that is determined, we should assign to that particle the parameters of the pore it flies toward, $(x_{Mi}, y_{Mi}, z_{Mi}, d_i)$, assuming such a pore exists. Shown below is the algorithm to do this, with the particle's label number i as input.

Algorithm 3 Assigning pore parameters

```
Require: i
  if (z_i ≥ σ_i/2 and z_i ≤ Z_1 − σ_i/2) or (z_i ≥ Z_2 + σ_i/2 and z_i ≤ L_z − σ_i/2) then
      x_Mi ← 0
      y_Mi ← 0
      d_i ← 0
      z_Mi ← v_iz > 0 ? (Z_1 − σ_i/2 ≥ z_i ? Z_1 : Z_3) : (Z_2 + σ_i/2 ≤ z_i ? Z_2 : 0)
      t ← v_iz > 0 ? (z_Mi − σ_i/2 − z_i)/v_iz : (z_Mi + σ_i/2 − z_i)/v_iz

      PosX ← x_i + v_ix t          ▷ x-position of particle when it just reaches membrane
      PosY ← y_i + v_iy t          ▷ y-position of particle when it just reaches membrane
      for j = 0; j < Number of pores; j++ do
          if (PosX − x_j)^2 + (PosY − y_j)^2 < (d_j/2)^2 then   ▷ If (PosX,PosY) is within the radial range of any pore
              x_Mi ← x_j
              y_Mi ← y_j
              d_i ← d_j
          end if
      end for
  else
      for j = 0; j < Number of pores; j++ do
          if (x_i − x_j)^2 + (y_i − y_j)^2 < (d_j/2)^2 then
              x_Mi ← x_j
              y_Mi ← y_j
              d_i ← d_j
          end if
      end for
  end if
```

Should the 2-dimensional point (PosX, PosY) be within the radial range of a pore, that pore is the one with which the particle would interact, leading to either case 2 or 3. Otherwise, we have case 1. After finishing the assignment, it would be convenient to define a function telling the z-coordinate of the pore on the other side of z_{Mi}.

Algorithm 4 Determining other side

```
Require: z
  if z == 0 then
      return Z_3 − L_z
  else if z == Z_1 then
      return Z_2
  else if z == Z_2 then
      return Z_1
  else if z == Z_3 then
      return L_z
  else
      return Z_3
  end if
```

We can now calculate t_M. First, there is the scenario that it is completely in one of the two chambers and has positive z-velocity.

Algorithm 5 Computing t_M, first scenario

if $v_{iz} > 0$ **and** $((z_i \geq \frac{\sigma_i}{2}$ **and** $z_i \leq Z_1 - \frac{\sigma_i}{2})$ **or** $(z_i \geq Z_2 + \frac{\sigma_i}{2}$ **and** $z_i \leq L_z - \frac{\sigma_i}{2}))$ **then** ▷ Judgement criteria, likewise for the rest
  if $d_i == 0$ **then** ▷ Case 1
    $t_M \leftarrow \frac{z_{Mi}-\sigma_i/2-z_i}{v_{iz}}$
  else if $\sigma_i > d_i$ **then** ▷ Particle larger than pore, only case 2 possible
    $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, z_{Mi}, σ_i)
  else
    $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, z_{Mi}, σ_i)
    if $t_M == \infty$ **or** $z_i + v_{zi}t_M > z_{Mi}$ **then** ▷ If no solution in previous step or solution non-physical
      $\cos\theta_1 \leftarrow \frac{(x_{Mi}-x_i)v_{xi}+(y_{Mi}-y_i)v_{yi}}{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\sqrt{v_{xi}^2+v_{yi}^2}}$
      $\sin\theta_2 \leftarrow \sqrt{1-\cos^2\theta_1}\cdot\frac{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}}{(d_i-\sigma_i)/2}$
      $t^2 \leftarrow (x_{Mi}-x_i)^2 + (y_{Mi}-y_i)^2 + \left(\frac{d_i-\sigma_i}{2}\right)^2 + (d_i-\sigma_i)\cdot\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\left(\cos\theta_1\sqrt{1-\sin^2\theta_2}-\sqrt{1-\cos^2\theta_1}\sin\theta_2\right)$
      if $z_i + v_{zi}t \leq$ Determining other side(z_{Mi}) **then**
        $t_M \leftarrow t$ ▷ Case 3
      else
        $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, Determining other side(z_{Mi}), σ_i) ▷ Case 2 with other end of pore
      end if
    end if
  end if
end if

The next scenario differs from the first only in that the z-velocity is negative, following the identical logic as before.

Algorithm 6 Computing t_M, second scenario

if $v_{iz} < 0$ **and** $((z_i \geq \frac{\sigma_i}{2}$ **and** $z_i \leq Z_1 - \frac{\sigma_i}{2})$ **or** $(z_i \geq Z_2 + \frac{\sigma_i}{2}$ **and** $z_i \leq L_z - \frac{\sigma_i}{2}))$ **then**
  if $d_i == 0$ **then**
    $t_M \leftarrow \frac{z_{Mi}+\sigma_i/2-z_i}{v_{iz}}$
  else if $\sigma_i > d_i$ **then**
    $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, z_{Mi}, σ_i)
  else
    $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, z_{Mi}, σ_i)
    if $t_M == \infty$ **or** $z_i + v_{zi}t_M < z_{Mi}$ **then**
      $\cos\theta_1 \leftarrow \frac{(x_{Mi}-x_i)v_{xi}+(y_{Mi}-y_i)v_{yi}}{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\sqrt{v_{xi}^2+v_{yi}^2}}$
      $\sin\theta_2 \leftarrow \sqrt{1-\cos^2\theta_1}\cdot\frac{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}}{(d_i-\sigma_i)/2}$
      $t^2 \leftarrow (x_{Mi}-x_i)^2 + (y_{Mi}-y_i)^2 + \left(\frac{d_i-\sigma_i}{2}\right)^2 + (d_i-\sigma_i)\cdot\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\left(\cos\theta_1\sqrt{1-\sin^2\theta_2}-\sqrt{1-\cos^2\theta_1}\sin\theta_2\right)$
      if $z_i + v_{zi}t \leq$ Determining other side(z_{Mi}) **then**
        $t_M \leftarrow t$
      else
        $t_M \leftarrow$ Quartic equation solutions(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, Determining other side(z_{Mi}), σ_i)
      end if
    end if
  end if
end if

The third is when the particle is completely inside a pore.

Algorithm 7 Computing t_M, third scenario

if $(z_i == 0$ **and** $v_{iz} < 0)$ **or** $(z_i \geq Z_1$ **and** $z_i \leq Z_2)$ **or** $(z_i \geq Z_3$ **and** $z_i \leq L_z)$ **then**
    if $z_i \geq Z_1$ **and** $z_i \leq Z_2$ **then**
        if $v_{zi} > 0$ **then**
            $z_{Mi} \leftarrow Z_2$
        else
            $z_{Mi} \leftarrow Z_1$
        end if
    else if $z_i \geq Z_3$ **and** $z_i \leq L_z$ **then**
        if $v_{zi} > 0$ **then**
            $z_{Mi} = L_z$
        else
            $z_{Mi} \leftarrow Z_3$
        end if
    else
        $z_{Mi} \leftarrow Z_3 - L_z$
    end if
end if ▷ Reassign z_{Mi}

$\cos\theta_1 \leftarrow \frac{(x_{Mi}-x_i)v_{xi}+(y_{Mi}-y_i)v_{yi}}{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\sqrt{v_{xi}^2+v_{yi}^2}}$

$\sin\theta_2 \leftarrow \sqrt{1-\cos^2\theta_1}\cdot\frac{\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}}{(d_i-\sigma_i)/2}$

$t^2 \leftarrow (x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2+\left(\frac{d_i-\sigma_i}{2}\right)^2+(d_i-\sigma_i)\cdot\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2}\cdot\left(\cos\theta_1\sqrt{1-\sin^2\theta_2}-\sqrt{1-\cos^2\theta_1}\sin\theta_2\right)$

if $|v_{zi}|t \leq |z_{Mi}-z_i|$ **then** ▷ Determine if particle will hit pore interior or rim
    $t_M \leftarrow t$ ▷ Case 3
else
    $t_M \leftarrow$ Quartic equation solutions$(d_i, x_i, v_{xi}, x_{Mi}, y_i, v_{yi}, y_{Mi}, z_i, v_{zi}, z_{Mi}, \sigma_i)$ ▷ Case 2
end if

Finally, the particle could be partially embedded.
When implementing, Algorithms 5 to 8 should be assembled together.

Algorithm 8 Computing t_M, fourth scenario

```
if (z_i ≤ Z_1 and z_i ≥ Z_1 − σ_i/2) or (z_i ≤ Z_3 and z_i ≥ Z_3 − σ_i/2) or (z_i ≥ 0 and z_i ≤ σ_i/2) or (z_i ≥ Z_2 and z_i ≤ Z_2 + σ_i/2) then
    if z_i ≤ Z_1 and z_i ≥ Z_1 − σ_i/2 then
        z_Mi ← Z_1
    else if z_i ≤ Z_3 and z_i ≥ Z_3 − σ_i/2 then
        z_Mi ← Z_3
    else if z_i ≥ 0 and z_i ≤ σ_i/2 then
        z_Mi ← 0
    else
        z_Mi ← Z_2
    end if                                                            ▷ Reassign z_Mi

    if σ_i > d_i then                         ▷ Particle larger than pore, only case 2 possible
        t_M ← Quartic equation solutions(d_i, x_i, v_xi, x_Mi, y_i, v_yi, y_Mi, z_i, v_zi, z_Mi, σ_i)
    else
        t_M ← Quartic equation solutions(d_i, x_i, v_xi, x_Mi, y_i, v_yi, y_Mi, z_i, v_zi, z_Mi, σ_i)   ▷ Case 2

        if t_M == ∞ or (v_zi > 0 and z_i + v_zi t_M > z_Mi) or (v_zi < 0 and z_i + v_zi t_M < z_Mi) then ▷ If no solution in previous step or solution non-physical
            if (z_Mi − z_i)v_zi > 0 then                              ▷ Particle flies towards/into pore
                cos θ_1 ← ((x_Mi − x_i)v_xi + (y_Mi − y_i)v_yi) / (sqrt((x_Mi − x_i)^2 + (y_Mi − y_i)^2) · sqrt(v_xi^2 + v_yi^2))
                sin θ_2 ← sqrt(1 − cos^2 θ_1) · sqrt((x_Mi − x_i)^2 + (y_Mi − y_i)^2) / ((d_i − σ_i)/2)
                t^2 ← (x_Mi − x_i)^2 + (y_Mi − y_i)^2 + ((d_i − σ_i)/2)^2 + (d_i − σ_i) · sqrt((x_Mi − x_i)^2 + (y_Mi − y_i)^2) · (cos θ_1 sqrt(1 − sin^2 θ_2) − sqrt(1 − cos^2 θ_1) sin θ_2)
                if z_i + v_zi t ≥ min(z_Mi, Determining other side(z_Mi)) and z_i + v_zi t ≤ max(z_Mi, Determining other side(z_Mi)) then
                    t_M ← t                                                           ▷ Case 3
                else
                    t_M ← Quartic equation solutions(d_i, x_i, v_xi, x_Mi, y_i, v_yi, y_Mi, z_i, v_zi, Determining other side(z_Mi), σ_i)   ▷ Case 2 with other end of pore
                end if
            else                                                   ▷ Particle flies away from/out of pore
                t_M ← Quartic equation solutions(d_i, x_i, v_xi, x_Mi, y_i, v_yi, y_Mi, z_i, v_zi, z_Mi, σ_i)   ▷ Case 2
            end if
        end if
    end if
end if
```

2.2. Collision dynamics

After t_M units of time passed, one particle-membrane collision would happen. Using the relevant mathematics described, we could write the following algorithm. It accounts for the rare case where a particle whose diameter is larger than that of the pore happens to touch the pore rim at every point. In this case, the dynamics is identical to colliding with a non-pore region.

Algorithm 9 Collision dynamics algorithm

if $(z_i \geq Z_1$ **and** $z_i \leq Z_2)$ **or** $(z_i \geq Z_3$ **and** $z_i \leq L_z)$ **then** ▷ Case 3
  $n_x \leftarrow \frac{x_{Mi}-x_i}{d_i-\sigma_i}\sigma_i$
  $n_y \leftarrow \frac{y_{Mi}-y_i}{d_i-\sigma_i}\sigma_i$ ▷ Normal vector, only x and y

  $v_{\|x} \leftarrow \frac{n_x v_{xi}+n_y v_{yi}}{n_x^2+n_y^2} n_x$
  $v_{\|y} \leftarrow \frac{n_x v_{xi}+n_y v_{yi}}{n_x^2+n_y^2} n_y$ ▷ Velocity along normal vector

  $v_{xi} \leftarrow v_{xi} - 2v_{\|x}$
  $v_{yi} \leftarrow v_{yi} - 2v_{\|y}$ ▷ Modifying velocity
else
  if $d_i == 0$ **or** $(\sigma_i > d_i$ **and** $\sqrt{(x_{Mi}-x_i)^2+(y_{Mi}-y_i)^2} < 10^{-6})$ **then** ▷ Case 1 or rare case
    $v_{zi} \leftarrow -v_{zi}$
  else ▷ Case 2
    $n_x \leftarrow \left(\frac{d_i/2}{\sqrt{(x_i-x_{Mi})^2+(y_i-y_{Mi})^2}} - 1\right)(x_{Mi}-x_i)$
    $n_y \leftarrow \left(\frac{d_i/2}{\sqrt{(x_i-x_{Mi})^2+(y_i-y_{Mi})^2}} - 1\right)(y_{Mi}-y_i)$ ▷ Normal vector, x and y

    if $\min(\min(|z_i|, |z_i - Z_1|), \min(|z_i - Z_2|, |z_i - Z_3|)) == |z_i|$ **then**
      $n_z \leftarrow z_i$
    else if $\min(\min(|z_i|, |z_i - Z_1|), \min(|z_i - Z_2|, |z_i - Z_3|)) == |z_i - Z_1|$ **then**
      $n_z \leftarrow z_i - Z_1$
    else if $\min(\min(|z_i|, |z_i - Z_1|), \min(|z_i - Z_2|, |z_i - Z_3|)) == |z_i - Z_2|$ **then**
      $n_z \leftarrow z_i - Z_2$
    else
      $n_z \leftarrow z_i - Z_3$
    end if ▷ Normal vector, z component

    $v_{\|x} \leftarrow \frac{n_x v_{xi}+n_y v_{yi}+n_z v_{zi}}{n_x^2+n_y^2+n_z^2} n_x$
    $v_{\|y} \leftarrow \frac{n_x v_{xi}+n_y v_{yi}+n_z v_{zi}}{n_x^2+n_y^2+n_z^2} n_y$
    $v_{\|z} \leftarrow \frac{n_x v_{xi}+n_y v_{yi}+n_z v_{zi}}{n_x^2+n_y^2+n_z^2} n_z$ ▷ Velocity along normal vector

    $v_{xi} \leftarrow v_{xi} - 2v_{\|x}$
    $v_{yi} \leftarrow v_{yi} - 2v_{\|y}$
    $v_{zi} \leftarrow v_{zi} - 2v_{\|z}$ ▷ Modifying velocity
  end if
end if