### Geometric classes

Geometric classes represent objects in three-dimensional space. There are three board geometric classes: Point, Vector, and Shape. The first is pretty self-explanatory; it represents a point. Vector and Shape are more detailed classes and are explained below.

#### Vector

The Vector class represents any 2-D or 3-D vector quantity. It also supports vector arithmetics, including dot and cross products. The dot() function is also used to define the L2-norm. All Vectors are explicitly convertible to bools - if a Vector does not have any NaN value, then it can be converted to true. This can be used to check whether a Vector has any NaN value, similar to how a pointer can be checked if it's a nullptr. A derived class called MutableVector can be used to modify any of the coordinates, though it's not sure whether it will be useful. The more important derived class is the Direction class, which dictates that the L2-norm be 1. Any non-zero Vector can be converted into a non-NaN Direction.

#### Shape

The abstract Shape class provides a template for volumetric objects. All classes derived from Shape must implement the following functions in order to be instantiated:

- xMin(), xMax(), and so on: locate the extremum points in each of the three coordinates.
- 2. surfaceArea()
- 3. volume()
- surfaceContains(const Point&): checks whether the Point is strictly on the surface.
- 5. encloses(const Point&): checks whether the Point is strictly inside \*this (i.e. not on the surface or outside).
- 6. encloses(const Shape&): checks whether the other Shape is completely contained within \*this. This function evaluates to true even if the two Shapes intersect on the surface of \*this.
- 7. overlaps(const Shape&): checks whether the two Shapes overlap (i.e. the region of intersection is non-zero in volume).
- 8. contentsOverlap(const Shape&): checks whether the other Shape overlap with any Shape contained within \*this. This function may only differ from overlaps() if \*this is of type BoundingBox (see below).

- 9. distanceToSurface(const Point&, const Direction&): calculates the smallest, positive distance that a point has to travel to reach the surface.
  - If the point is inside the shape, the distance equation will have positive and negative roots, and only the smallest positive root is returned
  - If the point is on the surface, returns 0 if it leaves the surface, and the distance to the other end if it enters the surface.
  - If the point is outside the shape, returns NAN if it never enters the shape, else the smallest distance to the surface.
- 10. normal(const Point&): checks if the point is on the surface, and returns the outward normal vector if it is.
- 11. print(std::ostream& os): outputs the shape into std::cout.

Additionally, Shape also has two member variables that represent the index of refraction and the total macroscopic cross section, respectively. They are both doubles and therefore assumed to be constant. In the future, it might make sense to have them as a separate class (let's say, Property), in order to captures their respective dependencies on various parametes.

Right now, there are two implemented derived classes of Shape: Sphere and Box. Sphere requires a Point representing the origin and a radius. Box requires two Point representing the two opposing vertices. The Sphere class is our current representation of droplet particles, which has the advantage of easy implementations of the aforementioned functions. A more accurate geometric class may be implemented in the future to account for the affects of surface tension and gravity. The Box class probably will never be used to represent physical objects, but rather to construct a derived BoundingBox class. In this context, a Box is not a terminal shape, but a Sphere is.

## Tree classes

The motive for using a Tree data structure is to quickly locate which —Shape—object (potentially out of thousands or millions) that a ray of photon will enter next, which is our version of the nearest neighbor search algorithm. A brute-force approach will have a time-complexity of order  $\mathcal{O}(N)$ , which in itself is not ideal. Furthermore, distance calculations are expensive because of the use of the square-root function (in case of the Sphere class) or some other functions that are potentially more expensive. A tree is a hierarchical data structure that groups objects based on certain common features. In this case, an Octree is used to group 3D shapes into each of the 8 octants of equal volume. Using a tree structure, the average time-complexity is down to  $\mathcal{O}(\log N)$ , which scales extremely well for large datasets. The majority of distance calculations involving those octants are to a surface of a box, and therefore are linear in nature, leaving a very few expensive calculations at the end.

## BoundingBox

The BoundingBox class is derived from Box and represents an axis-aligned bounding box (AABB). It is the building block of an Octree and therefore is constrained to have at most 8 children. A Node is defined as a pointer to a Shape - more specifically, a std::unique\_ptr<Shape> - that is contained within a BoundingBox. The pointed-to Shape itself can be either another BoundingBox (which means there are further subdivisions within that particular octant) or a terminal shape (which means they are leaf nodes).

#### Octree

# Snell's Law and Orientation of the Transmitted Ray

Let  $\hat{\imath}$  be the incident vector,  $\hat{n}$  be the (outward) normal vector, and  $\hat{t}$  be the transmitted vector. Also the index of refraction of a medium is labeled n.

Our job is to find  $\hat{t}$ , given  $\hat{i}$ ,  $\hat{n}$ ,  $n_1$  and  $n_2$ . The vectors are related through Snell's Law, and in vector notation it reads

$$n_1 \left( \hat{\boldsymbol{i}} \times \hat{\boldsymbol{n}} \right) = n_2 \left( \hat{\boldsymbol{t}} \times \hat{\boldsymbol{n}} \right), \tag{1}$$

or

$$\hat{\boldsymbol{t}} \times \hat{\boldsymbol{n}} = \boldsymbol{c},\tag{2}$$

for the new vector  $\boldsymbol{c}$  defined as  $\boldsymbol{c} = \frac{n_1}{n_2} (\hat{\boldsymbol{i}} \times \hat{\boldsymbol{n}})$ . Note that  $\boldsymbol{c}$  and  $\hat{\boldsymbol{n}}$  are orthogonal

We start solving for  $\hat{t}$  by decomposing it into two components: one parallel and one orthogonal to  $\hat{n}$ :

$$\hat{\boldsymbol{t}} = t_{\parallel} \hat{\boldsymbol{n}} + t_{\perp} \hat{\boldsymbol{p}} \tag{3}$$

Since the cross product of the parallel component and  $\hat{n}$  is the zero vector, we require the cross product of the orthogonal component and  $\hat{n}$  be equal to c.

$$t_{\perp}\hat{\boldsymbol{p}} \times \hat{\boldsymbol{n}} = \boldsymbol{c} \tag{4}$$

Since c and  $\hat{n}$  are already orthogonal, one of the possible values for the unit vector  $\hat{p}$  is  $\hat{p} = \hat{n} \times \hat{c}$  (the other possibility is its additive inverse). Note that the unit vector  $\hat{c}$  is c normalized to unit length. Using the vector triple product identity  $a \times (b \times c) = (a \cdot c)b - (a \cdot b)c$ , it can be showed that

$$\hat{\boldsymbol{p}} \times \hat{\boldsymbol{n}} = (\hat{\boldsymbol{n}} \times \hat{\boldsymbol{c}}) \times \hat{\boldsymbol{n}} 
= \hat{\boldsymbol{n}} \times (\hat{\boldsymbol{c}} \times \hat{\boldsymbol{n}}) 
= (\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{n}})\hat{\boldsymbol{c}} - (\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{c}})\hat{\boldsymbol{n}} 
= 1\hat{\boldsymbol{c}} - 0\hat{\boldsymbol{n}} 
\hat{\boldsymbol{p}} \times \hat{\boldsymbol{n}} = \hat{\boldsymbol{c}}$$
(5)

Substituting the above expression into Equation 4, we arrive at the expression for  $t_{\perp}$ :

$$t_{\perp}\hat{\boldsymbol{p}} \times \hat{\boldsymbol{n}} = \boldsymbol{c}$$

$$t_{\perp}\hat{\boldsymbol{c}} = \boldsymbol{c}$$

$$t_{\perp} = \|\boldsymbol{c}\|$$
(6)

The parallel component of  $\hat{\boldsymbol{t}}$  does not contribute to the cross product, so theoretically  $t_{\parallel}$  can assume any value and Equation 2 will hold true. However, since  $\hat{\boldsymbol{t}}$  is a unit vector, we require that

$$t_{\parallel}^2 + t_{\perp}^2 = 1$$
 
$$t_{\parallel} = \pm \sqrt{1 - t_{\perp}^2}$$

The choice of sign on  $t_{\parallel}$  now depends on the orientation of the incident vector  $\hat{\imath}$ . When the incident ray **enters** a surface, the transmitted vector  $\hat{t}$  will point inwards, away from the normal vector. Conversely, when the incident ray **exits** the surface,  $\hat{t}$  will point outwards. Therefore,

$$t_{\parallel} = egin{cases} -\sqrt{1-t_{\perp}^2} &, \hat{m{\imath}} \cdot \hat{m{n}} < 0 \ \sqrt{1-t_{\perp}^2} &, \hat{m{\imath}} \cdot \hat{m{n}} > 0 \end{cases}$$

Therefore, the final form of the transmitted vector  $\hat{t}$  is

$$\hat{\boldsymbol{t}} = \|\boldsymbol{c}\| \left( \hat{\boldsymbol{n}} \times \hat{\boldsymbol{c}} \right) + \operatorname{sgn} \left( \hat{\boldsymbol{i}} \cdot \hat{\boldsymbol{n}} \right) \sqrt{1 - \|\boldsymbol{c}\|^2} \hat{\boldsymbol{n}}$$

$$\boldsymbol{c} = \frac{n_1}{n_2} \left( \hat{\boldsymbol{i}} \times \hat{\boldsymbol{n}} \right)$$
(7)

There are two special considerations. First, if  $\|\mathbf{c}\| > 1$ , the radical in Equation 7 is complex-valued, and no refraction occurs. This phenomenon is known as total internal reflection. Second, if the incident ray to tangent to the surface it intersects with  $(\hat{\imath} \cdot \hat{n} = 0)$ , it neither enters or exits the surface. As a result, there is no refraction either.