

## 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:

1. `xMin()`, `xMax()`, and so on: locate the extremum points in each of the three coordinates.
2. `surfaceArea()`
3. `volume()`
4. `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 capture their respective dependencies on various parameters.

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 effects 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

## Propogation of light in matter

Light is a manifestation of travelling electric and magnetic field. The two fields oscillate perpendicular to each other and to the direction at which light travels. They both have wavenumber  $k$  and frequency  $\omega$ . Let  $x$  be the direction of propogation of the electric field, the field can be expressed as

$$\mathbf{E}(x, t) = \mathbf{E}_0 \Re \left[ e^{i(kx - \omega t)} \right] \quad (1)$$

To be precise, the term "wavenumber" refers to the angular wavenumber and is defined as the number of radians per unit length. In a vacuum with no attenuation, it is related to the phase velocity  $v_p$  as

$$k = \frac{\omega}{v_p}. \quad (2)$$

Since the phase velocity is a fraction  $n$  lower than the speed of light in vacuum  $c$ , the relation between wavenumber and refractive index is

$$k = \frac{\omega n}{c} \quad (3)$$

In an unattenuated medium,  $k$  is a real number, and the variable  $n$  is known as the refractive index. This only holds in vacuum; in any other material,  $k$  is a complex number, with its imaginary part accounting for the extent of attenuation.  $n$  therefore must also be a complex number. From now on, the variable  $n$  refers the real part of  $n + i\kappa$ , and the imaginary part  $\kappa$  is called the extinction coefficient. In other words,

$$k = \frac{\omega}{c}(n + i\kappa) \quad (4)$$

To show that attenuation is accounted for by the imaginary component, Equation 1 can be expanded as

$$\begin{aligned} \mathbf{E}(x, t) &= \mathbf{E}_0 \Re \left[ \exp \left[ -\frac{\omega}{c}\kappa x + i \left( \frac{\omega}{c}nx - \omega t \right) \right] \right] \\ &= \mathbf{E}_0 \exp \left( -\frac{\omega}{c}\kappa x \right) \cos \left( \frac{\omega}{c}nx - \omega t \right) \end{aligned} \quad (5)$$

Here, the electric field strength falls off exponentially with distance travelled, and the decay extent is characterized by the extinction coefficient. This resembles the linear attenuation of light intensity

$$I(x) = I_0 e^{-\sigma x}, \quad (6)$$

and the two equations are in fact related. Since the medium of interest is non-magnetic,  $\mathbf{B} \approx \mu \mathbf{H}$ , and the magnetic permeability  $\mu$  can be readily approximated as its vacuum value  $\mu_0 = 4\pi \times 10^{-7}$  H/m. The Poynting vector, defined as

$$\mathbf{S} \equiv \mathbf{E} \times \mathbf{H}, \quad (7)$$

can be written in terms of the  $\mathbf{B}$  field:

$$\mathbf{S} = \frac{1}{\mu} \mathbf{E} \times \mathbf{B}. \quad (8)$$

Thanks to Maxwell's Equations, the  $\mathbf{E}$  and  $\mathbf{B}$  are in phase in both spatial and temporal domains. In terms of magnitude, the two fields are proportional by a factor of  $c/n$ , or the wave speed. As a result,

$$\mathbf{S}(x, t) = \frac{n}{\mu c} \|\mathbf{E}_0\|^2 \exp\left(-\frac{2\omega}{c}\kappa x\right) \cos^2\left(\frac{\omega}{c}nx - \omega t\right) \hat{\mathbf{x}}. \quad (9)$$

The light intensity is defined as the time-averaged magnitude of the Poynting vector:

$$I(x) = \langle \|\mathbf{S}(x, t)\| \rangle \quad (10)$$

$$= \frac{n}{\mu c} \|\mathbf{E}_0\|^2 \exp\left[-\frac{2\omega}{c}\kappa x\right] \cdot \frac{1}{T} \int_0^T \cos^2\left(\frac{\omega}{c}nx - \omega t\right) dt. \quad (11)$$

Assume the integrating time  $T$  is much larger than the wave period - i.e.  $T \gg \frac{2\pi}{\omega}$ , then the averaging integral in Equation 11 will approach the average value over one single period, which is  $\frac{1}{2}$ . Therefore,

$$I(x) = \frac{n}{2\mu c} \|\mathbf{E}_0\|^2 \exp\left[-\frac{2\omega}{c}\kappa x\right]. \quad (12)$$

The relation between the attenuation coefficient  $\sigma$  and the extinction coefficient  $\kappa$  is then

$$\boxed{\sigma = \frac{2\omega\kappa}{c}}. \quad (13)$$

## Snell's Law and Orientation of the Transmitted Ray

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

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

$$n_1 (\hat{\mathbf{i}} \times \hat{\mathbf{n}}) = n_2 (\hat{\mathbf{t}} \times \hat{\mathbf{n}}), \quad (14)$$

or

$$\hat{\mathbf{t}} \times \hat{\mathbf{n}} = \mathbf{c}, \quad (15)$$

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

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

$$\hat{\mathbf{t}} = t_{\parallel} \hat{\mathbf{n}} + t_{\perp} \hat{\mathbf{p}} \quad (16)$$

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

$$t_{\perp} \hat{\mathbf{p}} \times \hat{\mathbf{n}} = \mathbf{c} \quad (17)$$

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

$$\begin{aligned} \hat{\mathbf{p}} \times \hat{\mathbf{n}} &= (\hat{\mathbf{n}} \times \hat{\mathbf{c}}) \times \hat{\mathbf{n}} \\ &= \hat{\mathbf{n}} \times (\hat{\mathbf{c}} \times \hat{\mathbf{n}}) \\ &= (\hat{\mathbf{n}} \cdot \hat{\mathbf{n}})\hat{\mathbf{c}} - (\hat{\mathbf{n}} \cdot \hat{\mathbf{c}})\hat{\mathbf{n}} \\ &= 1\hat{\mathbf{c}} - 0\hat{\mathbf{n}} \\ \hat{\mathbf{p}} \times \hat{\mathbf{n}} &= \hat{\mathbf{c}} \end{aligned} \quad (18)$$

Substituting the above expression into Equation 17, we arrive at the expression for  $t_{\perp}$ :

$$\begin{aligned} t_{\perp} \hat{\mathbf{p}} \times \hat{\mathbf{n}} &= \mathbf{c} \\ t_{\perp} \hat{\mathbf{c}} &= \mathbf{c} \\ t_{\perp} &= \|\mathbf{c}\| \end{aligned} \quad (19)$$

The parallel component of  $\hat{\mathbf{t}}$  does not contribute to the cross product, so theoretically  $t_{\parallel}$  can assume any value and Equation 15 will hold true. However, since  $\hat{\mathbf{t}}$  is a unit vector, we require that

$$\begin{aligned} t_{\parallel}^2 + t_{\perp}^2 &= 1 \\ t_{\parallel} &= \pm \sqrt{1 - t_{\perp}^2} \end{aligned}$$

The choice of sign on  $t_{\parallel}$  now depends on the orientation of the incident vector  $\hat{\mathbf{i}}$ . When the incident ray **enters** a surface, the transmitted vector  $\hat{\mathbf{t}}$  will

point inwards, away from the normal vector. Conversely, when the incident ray **exits** the surface,  $\hat{\mathbf{t}}$  will point outwards. Therefore,

$$t_{\parallel} = \begin{cases} -\sqrt{1-t_{\perp}^2} & , \hat{\mathbf{i}} \cdot \hat{\mathbf{n}} < 0 \\ \sqrt{1-t_{\perp}^2} & , \hat{\mathbf{i}} \cdot \hat{\mathbf{n}} > 0 \end{cases}$$

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

$$\begin{aligned} \hat{\mathbf{t}} &= \|\mathbf{c}\| (\hat{\mathbf{n}} \times \hat{\mathbf{c}}) + \text{sgn}(\hat{\mathbf{i}} \cdot \hat{\mathbf{n}}) \sqrt{1 - \|\mathbf{c}\|^2} \hat{\mathbf{n}} \\ \mathbf{c} &= \frac{n_1}{n_2} (\hat{\mathbf{i}} \times \hat{\mathbf{n}}) \end{aligned} \tag{20}$$

There are two special considerations. First, if  $\|\mathbf{c}\| > 1$ , the radical in Equation 20 is complex-valued, and no refraction occurs. This phenomenon is known as total internal reflection. Second, if the incident ray is tangent to the surface it intersects with  $(\hat{\mathbf{i}} \cdot \hat{\mathbf{n}} = 0)$ , it neither enters or exits the surface. As a result, there is no refraction or reflection.