# Lab 3: Mass distribution in Simbody

3.1 Lab: Vector operations in Simbody

Dot-products and cross-products are fundamental vector operations and are useful for kinematics (motion), mass-distribution calculations, and kinetics (forces). Perform the following calculations first "by-hand" and then perform the calculations using the `Vec3` and `Mat33` classes in SimTK Simbody. Submit your "by-hand" calculations in-class. Submit your C^{++} program `HelloVector.cpp` to your SimTK project and include your nicely formatted output results `HelloVectorResults.txt`.
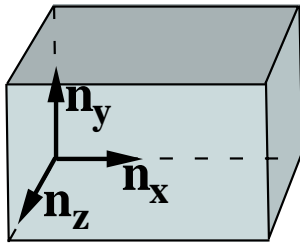
The figure to the left shows a right-handed set of orthogonal unit vectors $\mathbf{n}_x$, $\mathbf{n}_y$, $\mathbf{n}_z$. Given below are two vectors $\mathbf{v}$ and $\mathbf{w}$.

$$\mathbf{v} = 2\,\mathbf{n}_x \;+\; 3\,\mathbf{n}_y \;+\; 4\,\mathbf{n}_z$$
$$\mathbf{w} = 5\,\mathbf{n}_x \;-\; 6\,\mathbf{n}_y \;+\; 7\,\mathbf{n}_z$$

$$10\,\mathbf{v} \;=\; \boxed{}$$

$$\mathbf{v} * 10 \;=\; \boxed{}$$

$$\mathbf{v}/10 \;=\; \boxed{}$$

$$\mathbf{v} + \mathbf{w} \;=\; \boxed{}$$

$$\mathbf{v} - \mathbf{w} \;=\; \boxed{}$$

$$\mathbf{v} \cdot \mathbf{w} \;=\; \boxed{}$$

$$\mathbf{v} \times \mathbf{w} \;=\; \boxed{}$$

$$\mathbf{w} \times \mathbf{v} \;=\; \boxed{}$$

$$\mathbf{v}^2 \;=\; \boxed{}$$

$$\mathbf{v}^3 \;=\; \boxed{}$$

$$|\mathbf{v}| \;=\; \boxed{}$$

$$|\mathbf{w}| \;=\; \boxed{}$$

$$\texttt{UnitVector}(\mathbf{v}) \;=\; \frac{2\,\mathbf{n}_x + 3\,\mathbf{n}_y + 4\,\mathbf{n}_z}{\sqrt{29}}$$
$$= \; 0.3714\,\mathbf{n}_x + 0.5571\,\mathbf{n}_y + 0.7428\,\mathbf{n}_z$$

$$\angle(\mathbf{v}, \mathbf{w}) \;=\; \boxed{}\; \text{radians or} \; \boxed{}^{\circ}$$

$$\mathbf{v} * \mathbf{w} \;=\; 10\,\mathbf{n}_x\,\mathbf{n}_x \;-\; 12\,\mathbf{n}_x\,\mathbf{n}_y \;+\; 14\,\mathbf{n}_x\,\mathbf{n}_z$$
$$+ \; \boxed{}$$
$$+ \; \boxed{}$$

$$\mathbf{w} * \mathbf{v} \;=\; 10\,\mathbf{n}_x\,\mathbf{n}_x \;+\; 15\,\mathbf{n}_x\,\mathbf{n}_y \;+\; 20\,\mathbf{n}_x\,\mathbf{n}_z$$
$$- \; \boxed{}$$
$$+ \; \boxed{}$$

Prototypes for additional functions that you need to create and use are shown below.

```
bool  WriteVec3ToFile( const Vec3 &v, int precision, FILE *fptr );
bool  WriteMat33ToFile( const Mat33 &m, int precision, FILE *fptr );
```

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[0]Last updated May 2, 2007 by Paul Mitiguy.

3.2 Lab: Calculating a simple inertia dyadic and inertia matrix

The figure to the right shows a point O and a molecule (particle) Q of mass m. The position vector of Q from O is expressed in terms of x, y, and the right-handed orthogonal unit vectors $\mathbf{n_x}$, $\mathbf{n_y}$, $\mathbf{n_z}$ as

$$\mathbf{r}^{Q/O} = x\,\mathbf{n_x} + y\,\mathbf{n_y}$$
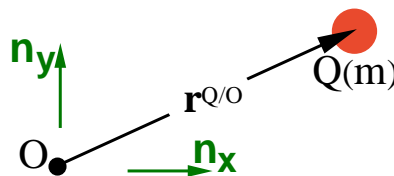
The purpose of this example is to find $\underline{\mathbf{I}}^{Q/O}$, the inertia dyadic of Q about O using its definition, i.e.,

$$\underline{\mathbf{I}}^{Q/O} \triangleq m\left[\underline{\mathbf{1}} * (\mathbf{r}^{Q/O} \cdot \mathbf{r}^{Q/O}) - \mathbf{r}^{Q/O} * \mathbf{r}^{Q/O}\right]$$

Calculate the symbolic inertia dyadic $\underline{\mathbf{I}}^{Q/O}$ (the unit dyadic can be expressed as $\underline{\mathbf{1}} = \mathbf{n_x}*\mathbf{n_x} + \mathbf{n_y}*\mathbf{n_y} + \mathbf{n_z}*\mathbf{n_z}$.).

$$
\begin{aligned}
\underline{\mathbf{I}}^{Q/O} \;=\; & m\,y^2\,\mathbf{n_x}*\mathbf{n_x} &+& \quad\boxed{}\;\mathbf{n_x}*\mathbf{n_y} &+& \quad\boxed{}\;\mathbf{n_x}*\mathbf{n_z} \\
+\; & \boxed{}\;\mathbf{n_y}*\mathbf{n_x} &+& \quad\boxed{}\;\mathbf{n_y}*\mathbf{n_y} &+& \quad\boxed{}\;\mathbf{n_y}*\mathbf{n_z} \\
+\; & \boxed{}\;\mathbf{n_z}*\mathbf{n_x} &+& \quad\boxed{}\;\mathbf{n_z}*\mathbf{n_y} &+& \quad\boxed{}\;\mathbf{n_z}*\mathbf{n_z}
\end{aligned}
$$

Calculate (without Simbody) Q's **inertia matrix** about O for $\mathbf{n_x}$, $\mathbf{n_y}$, $\mathbf{n_z}$ when Q is a single carbon-12 atom of mass[1] $m = \frac{12}{6.0221415 \times 10^{23}}$ g that is located at $x = 1 \times 10^{-10}$ m and $y = 2 \times 10^{-10}$ m.

$$
I^{Q/O} = 10^{-43} * \begin{bmatrix} 7.97059 & -3.98529 & 0 \\ -3.98529 & 1.99265 & 0 \\ 0 & 0 & 9.96323 \end{bmatrix}_{\mathbf{n_{xyz}}}
$$

## 3.3 Lab: Determining the mass properties of an oxygen molecule

The following figure shows two oxygen **atoms**[2] (particles), each of mass m. The atoms are double-**bonded**[3] to form an oxygen **molecule**.[4] This double-bonded oxygen molecule is modeled as a massless rigid rod B of length L, where L is the **bond length**.[5] Right-handed orthogonal unit vectors $\mathbf{b_x}$, $\mathbf{b_y}$, $\mathbf{b_z}$ are fixed in B with $\mathbf{b_x}$ directed from one atom to the other.

The point of this problem is to calculate the oxygen molecule's mass, mass center, and central inertia matrix.

Given: $m = 15.9994$ amu (atomic mass units)

Given: $L = 121$ picometers

(Note: L is sometimes given in units of **angstroms** (Å), an internationally-recognized non-SI unit of length equal to 1×10^{-10} meters or 100 picometers.)
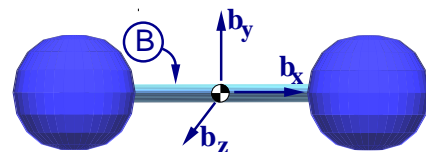
- Calculate the molecule's mass: $\boxed{}$ amu

- Calculate the distance from the left-most oxygen atom to the molecules mass center: $\boxed{}$ Å

- Show that the molecule's central inertia dyadic is: $\underline{\mathbf{I}}^{B/B_{cm}} = I\,\mathbf{b_y}\,\mathbf{b_y} + I\,\mathbf{b_z}\,\mathbf{b_z}$
  where $I = \frac{1}{2}\,m\,L^2 = 1.17084077 \times 10^{-19}$ amu $*\,\text{m}^2$

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[1] A **mole** of carbon-12 atoms is defined to be the number of carbon-12 atoms that is exactly equal to 12 grams. The current best estimate of the number of carbon-12 atoms in a mole is called **Avogadro's number** (or **Avogadro's constant**), equal to 6.0221415×10^{23} atoms/mole.

[2] An **atom** is the smallest collection of protons, electrons, and neutrons that retains its chemical properties.

[3] A **bond** is the word for the attractive interaction between atoms and molecules. These attractive interactions are described by **quantum electrodynamics** and are associated with the sharing or transfer of electrons between atoms.

[4] A **molecule** is a combination of two or more **atoms** that are held together in a definite configuration by **chemical bonds**.

[5] **Bond length** (also called **bond distance**) is the distance between two bonded atoms.

- Find the molecule's central inertia matrix for $\mathbf{b}_x$, $\mathbf{b}_y$, $\mathbf{b}_z$: $\quad I^{B/B_{cm}} =$
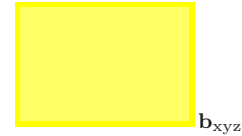
$$\boxed{}_{\mathbf{b_{xyz}}}$$

3.4 Lab: Centroid, mass center, and inertia matrix of a set of molecules

There are three "ingredients" in Newton's law for a particle, namely $\mathbf{F}$, m, and $\mathbf{a}$. Each ingredient affects the motion of biological structures. In the investigation of the motion of a system of molecules (particles), it can be helpful to track the location of the system's **mass center** (also called its **center of mass**).

Perform the following calculations "by-hand" and then perform the calculations using the `Vec3` and `Inertia` classes in SimTK Simbody. Submit your "by-hand" calculations in-class. Submit your C++ program `HelloCenterOfMass.cpp` to your SimTK project.

The system S shown below consists of molecules (particles) Q_1, Q_2, Q_3, Q_4, each which is 1 meter from point O. The purpose of this example is to first use physical intuition to locate the **centroid** and **mass center** of the four molecules and then to use mathematical definitions to find $\mathbf{r}^{S_{centroid}/O}$ (the position vector of the centroid of S from O) and $\mathbf{r}^{S_{cm}/O}$ (the position vector of the mass center of S from O).[6]
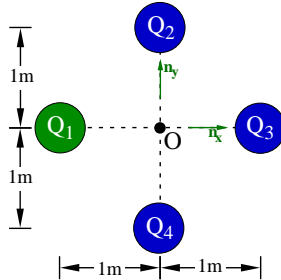
Particle	m^{Q_i} (kg)	$\mathbf{r}^{Q_i/O}$	$m^{Q_i} * \mathbf{r}^{Q_i/O}$
Q_1	1	$\text{-}\mathbf{n}_x$	$\text{-}\mathbf{n}_x$
Q_2	2		
Q_3	2		
Q_4	2		
Sums	$m^S = \boxed{}$	$\sum_{i=1}^{n} \mathbf{r}^{Q_i/O} = \boxed{}$	$\sum_{i=1}^{n} m^{Q_i} * \mathbf{r}^{Q_i/O} = \boxed{}$

$$\mathbf{r}^{S_{centroid}/O} \triangleq \frac{1}{n} * \sum_{i=1}^{n} \mathbf{r}^{Q_i/O} = \boxed{} \qquad \mathbf{r}^{S_{cm}/O} \triangleq \frac{1}{m^S} * \sum_{i=1}^{n} m^{Q_i} * \mathbf{r}^{Q_i/O} = \boxed{}$$

Using the `Vec3` and `Mat33` classes in Simbody, calculate the system's inertia matrix about point O. Next, calculate the system's inertia matrix about S_{cm} for $\mathbf{n}_x$, $\mathbf{n}_y$, $\mathbf{n}_z$.

Results

$$I^{S/O}_{\mathbf{n}_{xyz}} = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 7 \end{bmatrix} \qquad\qquad I^{S/S_{cm}}_{\mathbf{n}_{xyz}} = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 2.85714 & 0 \\ 0 & 0 & \boxed{} \end{bmatrix}$$

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[6]The **centroid** is the center of a set of **points** whereas the **center of mass** is the center of a set of **particles**. The center of mass is located with a "weighted average" of position vectors whereas the centroid is located with an "unweighted average". **Conceptually**, if one were located at the center of mass of a system, there would be the same amount of **mass** to the left and right, front and back, and above and below. If one were located at the centroid, the **volume** (or number of particles) would be equally distributed (the centroid does not depend on whether the matter is lead or styrofoam).

Lab 3: Mass distribution in Simbody

3.5   Lab: Determining the mass properties of the molecule 1G2S

The following figure shows the "***ribbon view***" and "***atoms and bonds view***" of the molecule 1G2S.pdb.[7]
The point of this problem is to calculate this molecule's mass, mass center, and central inertia matrix.
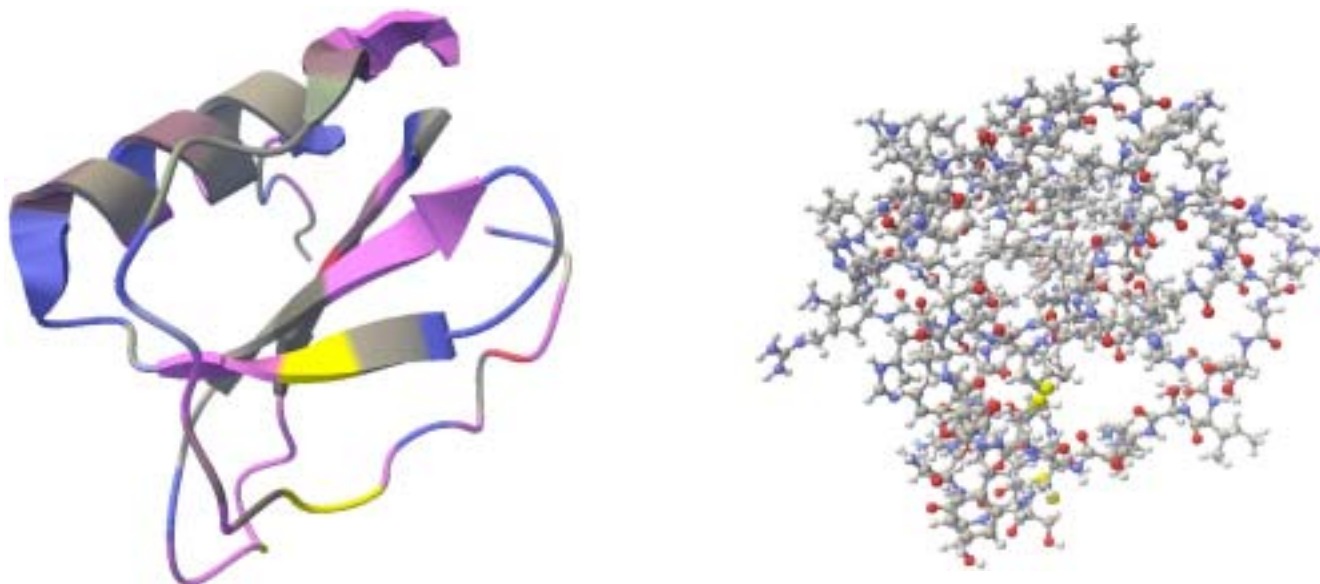
Modify the C^{++} program `InertiaPropertiesOfPDBMolecules.cpp`. This program queries the user for a `.pdb`
file and does the following (see the detailed description of the .pdb file in Section 3.6):

- Calculates and prints out the molecule's mass
- Calculates and prints out the molecule's mass center location
- Calculates and prints out the molecule's ***central inertia matrix***
- Visualizes the atom locations using VTK (from within your Simbody program)
- Determine the size of the bounding box determined by the ground's "x, y, z" axes.
- Visualize the bounding box along with the molecules (use opacity and different colors to see both)
- Optional**: Determine the molecule's central ***principal moments of inertia***
- Optional**: Determine the molecule's central ***principal directions***
- Optional**: Determine the size of the bounding box determined by the principal "x, y, z" axes.
- Optional**: Visualize both bounding boxes (ground and principal) along with the molecules

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[7]This molecule is freely available for download from www.pdb.org. These pictures were produced by ***SimTK ToRNAdo***
(free to download from www.simtk.org/home/rna-viz-proto). Alternately, this molecule can be viewed with the free molecule
viewers ***Pymol*** or ***VMD***.

3.6   Lab: Determining the mass properties of the molecule 2CDT

The following figure shows the "***ribbon view***" and "***atoms and bonds view***" of the molecule 2CDT.pdb.[8] The point of this problem is to calculate this molecule's mass distribution properties.
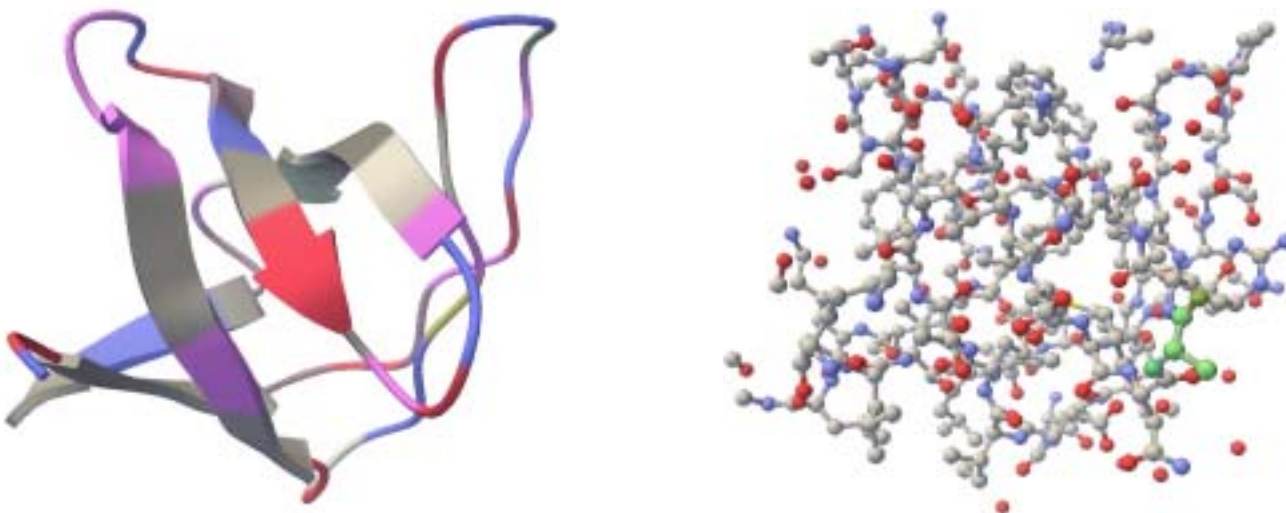
Enhance and submit your C++ program `InertiaPropertiesOfPDBMolecules.cpp` to your SimTK project. This program should calculate and print out the molecules mass distribution properties (mass, mass center location, and central inertia matrix) for the following:

- The molecule's mass distribution properties when `HETAM` are ignored.

- The molecule's mass distribution properties when `HETAM` are included.

- The molecule's mass distribution properties when hydrogen atoms are added from:
  http://biophysics.cs.vt.edu/H++/
  (See the Lab3 file `2CDTWithHydrogensAddedFromH++Website.pdb`)

```
//-------------------------------------------------------------------------
// PDB ATOM record format from
// http://www.wwpdb.org/documentation/format23/sect9.html
// COLUMNS       DATA TYPE        FIELD       DEFINITION
// -------------------------------------------------------------------------
//  1 -  6       Record name      "ATOM    "
//  7 - 11       Integer          serial      Atom serial number.
// 13 - 16       Atom             name        Atom name.
// 17            Character        altLoc      Alternate location indicator.
// 18 - 20       Residue name     resName     Residue name.
// 22            Character        chainID     Chain identifier.
// 23 - 26       Integer          resSeq      Residue sequence number.
// 27            AChar            iCode       Code for insertion of residues.
// 31 - 38       Real(8.3)        x           Orthogonal coordinates for X in Angstroms
// 39 - 46       Real(8.3)        y           Orthogonal coordinates for Y in Angstroms
// 47 - 54       Real(8.3)        z           Orthogonal coordinates for Z in Angstroms
// 55 - 60       Real(6.2)        occupancy   Occupancy.
// 61 - 66       Real(6.2)        tempFactor  Temperature factor.
// 77 - 78       LString(2)       element     Element symbol, right-justified.
// 79 - 80       LString(2)       charge      Charge on the atom.
//-------------------------------------------------------------------------
```

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[8]This molecule's is freely available for download from www.pdb.org. These pictures were produced by ***SimTK ToRNAdo***.