**Ice Generation Coding Plan**

Algorithm

1. Using LAMMPS:
   1. Generate Oxygen Lattice in a tetrahedral arrangement.
      1. O – O distance = 2.75 Å
      2. O – O – O Angle = Perfect Tetrahedral = 109.5°
   2. Generate data output file
2. Using Python:
   1. Generate axis (a line) between each O with 2 possible sites – each site 1 Å away from either Oxygen and on this axis.
   2. Assign 1 Hydrogen atom randomly on each axis in 1 of the 2 possible sites such that it would be considered chemically bonded to the nearest Oxygen.
   3. Perform a Monte Carlo Simulation until all Oxygen’s have a Coordination Number = 2
   4. Output a new data output file

PLAN:

LAMMPS:

* Custom lattice command to get the Oxygens in the needed orientation.
* Very simple LAMMPS Code

PYTHON:

* Will use the principles of Object Oriented coding
* Classes:
  + Atom Class= Parent Class for the Elemental Classes
  + Oxygen and Hydrogen = Children Classes
    - Properties:
      * ID?
      * Position
        + x y z positions (Å)
      * Chemical Bonds = List of Hydrogen Atoms’ addresses that the Oxygen is bonded to.
      * Axes = List of Axes’ addresses that are associated with the Oxygen and a single Axes instance address for the Hydrogen.
  + Axis Class = the class representation of the axis between 2 Oxygens
  + Properties:
    - ID?
    - Oxygen1, Oxygen2 = the 2 Oxygen atoms on each end of the axis
    - Site1, Site2 = the 2 possible sites for a Hydrogen to be associated with, Site1 is 1Å from Oxygen1. Same for Site2/Oxygen2
    - Length?
  + Site Class = the class representation of a possible location for a Hydrogen Atom insertion
  + Properties:
    - ID?
    - Connected Axis
    - Position
      * x y z coordinates (Å)
    - Occupied = true or false
    - Nearest Oxygen = address of the closest associated Oxygen Object
* Algorithm
  + Read in the information from the data file
    - Generate a list of Oxygen Objects that represent every oxygen from the data file and their position.
    - Store the simulation box dimensions.
  + Loop through the list of Oxygen Atoms and find each of their neighbors
    - Use the Distance Formula [O(n2)?] to find all Oxygens that are 2.75 Å away.
    - Generate Axes b/w an Oxygen and its neighbors if not already generated. Add each generated Axis to the Axis List.
      * With each Axis Generation, generate the 2 Site objects associated with the 1 Å distance from each Oxygen.
  + Iterate through the Axis list.
    - Generate a Hydrogen on each axis, randomly choosing between the 2 sites. This will cause some Oxygens to have more or less than the needed number of bonds, which is addressed in the next step.
    - Assign the new Hydrogen as a chemical bond with the Oxygen it is nearest to.
  + Perform a Monte Carlo Simulation to ensure that the coordination number of each Oxygen is exactly 2.
  + Write the Data File according to the following format:

#Header Information

# atoms

# atom types

# bonds

# bond types

# angle

# angle types

# # xlo xhi

# # ylo yhi

# # zlo zhi

Masses

1 15.994

2 1.008

Atoms

<atomID> <MoleculeID> <atomType> <q> <x> <y> <z>

Velocities

<atomID> <vx> <vy> <vz>

Bonds

<bondID> <bondType> <IDatom1> <IDatom2>

Angles

<angleID> <angleType> <IDatom1> <IDatom2> <IDatom3>