

**Project:** Modifying LAMMPS tool msi2Imp  
**Data :** 10/05/2010  
**By:** SLTM

**Objective:** The LAMMPS tool msi2Imp converts a material studios file to a lamps input file. In its current formulation, msi2Imp only works for orthogonal simulations boxes. However, there is a need for msi2Imp to work for both orthogonal and non-orthogonal (triclinic) boxes.

Additionally, to comply with newer versions of lammps the dihedral coefficients and improper coefficients output should be changed from doubles to integers for all but the first coefficients.

For an **orthogonal box**, lammps input takes the following form where ValueLow indicates a number should be substituted for the keyword (based on lamps documentation for version Aug 2010:

```
ValueLow ValueHi xlo xhi  
ValueLow ValueHi ylo yhi  
ValueLow ValueHi zlo zhi
```

For a **triclinic box**, lammps input takes the following form:

```
ValueLow ValueHi xlo xhi  
ValueLow ValueHi ylo yhi  
ValueLow ValueHi zlo zhi  
Value_xy Value_xz Value_yz xy, xz, yz
```

The code msi2Imps needs to be modified to include both a triclinic box option along with the original orthogonal box conversion option. Bases on the lamps documentation

$$\begin{aligned} a &= lx \\ b^2 &= ly^2 + xy^2 \\ c^2 &= lz^2 + xz^2 + yz^2 \\ \cos \alpha &= \frac{xy * xz + ly * yz}{b * c} \\ \cos \beta &= \frac{xz}{c} \\ \cos \gamma &= \frac{xy}{b} \end{aligned}$$

## **Important variables:**

### Original definition

1. periodic – a flag set to 1 if system obeys periodic boundary conditions, set to 0 if it doesn't
2. pbc[0] – box length in the x direction
3. pbc[1] – box length in the y direction
4. pbc[2] – box length in the z direction
5. pbc[3] – alpha angle
6. pbc[4] – beta angle
7. pbc[5] – gamma angle

### Modified definition

#### Orthogonal

1. pbc[0] – xlow
2. pbc[1] – xhi
3. pbc[2] – ylow
4. pbc[3] – yhi
5. pbc[4] – zlow
6. pbc[5] – zhi

#### Triclinic

1. pbc[0] – box length in the x direction
2. pbc[1] – box length in the y direction
3. pbc[2] – box length in the z direction
4. pbc[3] – xy
5. pbc[4] – xz
6. pbc[5] – yz

## **Modifications:**

1. MSI2LMP.h
  - a. Line 65 – added integer variable TriclinicFlag, which is set to 0 for an orthogonal box and 1 for a triclinic box.
2. ReadCarFile.c
  - a. Variables added (Line 16-21)
    - i. cos\_alpha, cos\_gamma, sin\_gamma, cos\_beta, sin\_beta, A, B, C
  - b. Line 50 – added check for variable TriclinicFlag, based on the pbc variables read in from the .car file
  - c. Line 155, line 169 – added if/else statement because triclinic implementation only for periodic box

- d. Line 177 – 201 – Added if/else statement to treat triclinic vs. orthogonal boxes differently
    - i. Line 177 – if statement contains original code for orthogonal box (the pbc variables change meaning , see above)
    - ii. Line 182 – else statement contains conversions for lammps triclinic boxes (the pbc variables change meaning , see above)
3. WriteDataFile05.c
- a. Lines 56-68 – modified code to output needed data for either a triclinic box or an orthogonal box.
  - b. Line 129 and 144, the output for dihedral angles and improper coefficients are changed to be integers for all but the first coefficient.