Very Draft Software Instructions

1. Run NanoEngineer-1 and create a single molecule per file - also referred to as a template. This file will have the **.mmp** file extension. If you create a polymer chain it counts as a single molecule. Use the "combine selected chunks" tool to insure the molecule or polymer chain created is a single entity.

2. Run PACKMOL to create a box of molecules using the template created above. Create an input file for the MD cell. This file is read by PACKMOL to create the box. This following file defines the box for a water urea system. This is a good simple system to practice with. Create a water and a dgeba template (e.g squarecff91.mmp - also contains crosslinked IPD). The box is 100.0 angstroms per side. The molecules are all placed 2 angstroms apart because the tolerance token is set to 2.0. The output file is .mmp because of the filetype token. The force field name in the template files are tested against the forcefieldname token value. If they do not match then PACKMOL will stop execution with an error message.

The following is a *.INP file for PACKMOL!!!

```
#
# A mixture of water and DGEBA/IPD oligomers
#

# All the atoms from different molecules will be separated at least 2.0
# Angstroms at the solution.

tolerance 2.0

# The file type of input and output files is MMP
# Added MMP as a new file type

filetype mmp

# The name of the output file to be created by PACKMOL

output dgebawater.mmp

# force field name This is a new token added by me to support force
# fields. Specify the force field in all uppercase letters. I need to
# handle case conversions in the software in the next release.

forcefieldname CFF91

# 20 water molecules and 400 urea molecules will be put in a box
# defined by the minimum coordinates x, y and z = 0. 0. 0. and maximum
# coordinates 100. 100. 100. That is, they will be put in a cube of side
```

```
# 100. (the keyword "inside cube 0. 0. 0. 100.") could be used as well.

structure squarecff91.mmp
  number 5
  inside box 0. 0. 0. 100. 100. 100.
end structure

structure water.mmp
  number 20
  inside box 0. 0. 0. 100. 100. 100.
end structure
```

$ packmol squarecff91.inp

The water template, water.mmp, and urea template, urea.mmp are defined above to fill the box. 25 total molecules are placed in the box. The file, dgeba.mmp, will contain 25 molecules. The file will be used by MSI2LMP to create the LAMMPS input file. Run packmol from the command line. Run the cmd program to access the command line under Windows.

3. Run MSI2LMP to create the LAMMPS input file. Run MSI2LMP from the command line. Run the cmd program to access the command line under Windows. **Prior to running the software define the environment variable BIOSYM_LIBRARY to point at any directory you have permission to access. Place the cff91_cff91v.frc file in the directory. This environment variable is necessary for Windows, Linux, etc...**

$ msi2lmp dgeba.mmp -class II -frc cff91_cff91v.frc

The dgebawater.mmp file contains the system created by PACKMOL - 25 molecules. Use a class 2 (II) force field - CFF91 is a class 2 force field. **The specific force field file used is cff91_cff91v.frc.**

The output file is **dgebawater.lammps05.**