Building LAMMPS data files with car/mdf files and the msi2lmp utility

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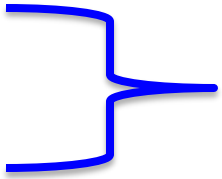
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- Description of files
  - LAMMPS data file
  - Structure files (car/mdf)
  - Force field files (frc)
  - msi2lmp.exe



Biosym/Discover software

- Mineral with limited bonding (kaolinite)
- Bonded organic molecule (toluene)

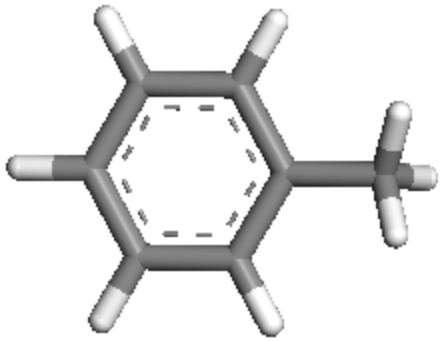
LAMMPS Data Files

- http://lammps.sandia.gov/doc/read_data.html

- Typical components (toluene.lammps05)
  - Summary of molecular connectivity
  - Cell dimensions
  - Force field parameters (pair, bond, angle, dihedral, improper)
  - Atom info (molecule #, atom type #, charge, xyz coordinates)
  - Bond info (bonds, angles, etc)

- Examples in LAMMPS distribution

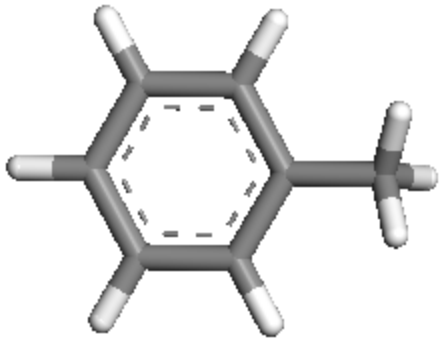
Structure Files



- car file (coordinates, atom type, charge)

```
C1    -0.692663292  -0.094096410  0.003399037 XXXX 1   cp   C  -0.100
C2     0.080988729  -1.425449986  0.004347065 XXXX 1   cp   C  -0.100
C3     1.620876319  -1.420834453  0.005671437 XXXX 1   cp   C  -0.100
C4     2.386905208  -0.085003697 -0.002079692 XXXX 1   cp   C  -0.100
C5     1.613536848   1.246298529 -0.026904058 XXXX 1   cp   C   0.000
C6     0.073572216   1.241704742 -0.004902500 XXXX 1   cp   C  -0.100
C7     2.379381006   2.581705596  0.007764760 XXXX 1   c3   C  -0.300
H1    -1.832488967  -0.097446130  0.009999447 XXXX 1   h    H   0.100
H2    -0.486334530  -2.414248925  0.007052748 XXXX 1   h    H   0.100
H3     2.193596249  -2.406396682  0.013631449 XXXX 1   h    H   0.100
H4     3.526773693  -0.081542221  0.008067005 XXXX 1   h    H   0.100
H5    -0.499289128   2.227113274  0.002830637 XXXX 1   h    H   0.100
H6     2.624394086   2.906106279 -1.057242639 XXXX 1   h    H   0.100
H7     3.346362304   2.450326318  0.597088580 XXXX 1   h    H   0.100
H8     1.733495243   3.376908124  0.507943882 XXXX 1   h    H   0.100
```

Structure Files



- mdf file (atom type, charge, bonding information)

```
XXXX_1:C1      C  cp    ?    0  0   -0.1000 0 0 8 1.0000  0.0000 C2/1.5 C6/1.5 H1
XXXX_1:C2      C  cp    ?    0  0   -0.1000 0 0 8 1.0000  0.0000 C3/1.5 C1/1.5 H2
XXXX_1:C3      C  cp    ?    0  0   -0.1000 0 0 8 1.0000  0.0000 C2/1.5 C4/1.5 H3
XXXX_1:C4      C  cp    ?    0  0   -0.1000 0 0 8 1.0000  0.0000 C3/1.5 C5/1.5 H4
XXXX_1:C5      C  cp    ?    0  0    0.0000 0 0 8 1.0000  0.0000 C4/1.5 C6/1.5 C7
XXXX_1:C6      C  cp    ?    0  0   -0.1000 0 0 8 1.0000  0.0000 C5/1.5 C1/1.5 H5
XXXX_1:C7      C  c3    ?    0  0   -0.3000 0 0 8 1.0000  0.0000 C5 H6 H7 H8
XXXX_1:H1      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C1
XXXX_1:H2      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C2
XXXX_1:H3      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C3
XXXX_1:H4      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C4
XXXX_1:H5      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C6
XXXX_1:H6      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C7
XXXX_1:H7      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C7
XXXX_1:H8      H  h     ?    0  0    0.1000 0 0 8 1.0000  0.0000 C7
```

Force Field Files

- These files are in the Biosym/Discover format and available in the LAMMPS distribution (…/tools/msi2lmp)
  - cff91.frc
  - cvff.frc
  - cvff_aug.frc
  - pcff.frc (pcff.rlb and pcff_templates.dat also needed)
- Information contained in frc files
  - Atom types
  - Energy expressions and parameters
  - Atomic charge assignments (not used by msi2lmp)
- Build you own frc file (clayff.frc)

msi2lmp.exe

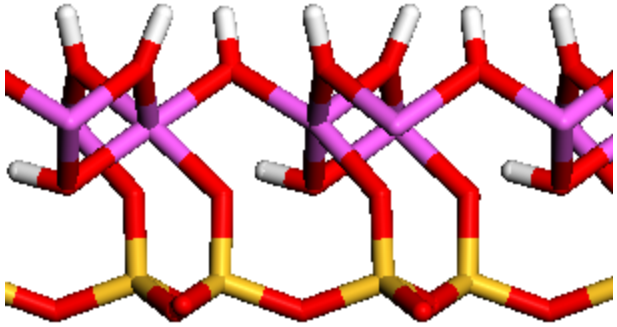
- Available in LAMMPS distribution (…/tools/msi2lmp)
- Written in C
- Updated as of LAMMPS 2005
- Reads molecular information from structure files and produces a LAMMPS data file
- Syntax:

  msi2lmp.exe *root* –frc *frc_file*

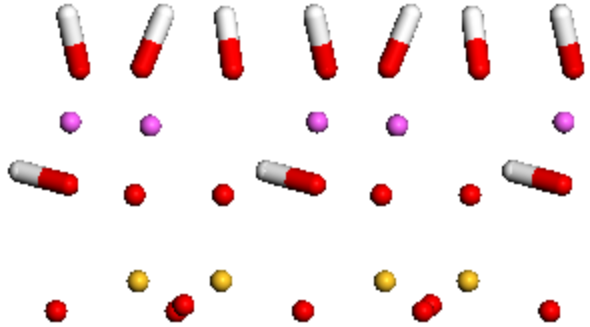
  root = root name of car/mdf files (toluene.car, toluene.mdf)

  frc_file = Biosym/Discover force field file

Example – kaolinite $Al_2Si_2O_5(OH)_4$



- Fully bonded model
  - Created with Materials Studio software
  - Atom types assigned manually



- Nonbonded model for LAMMPS simulations (except for hydroxyl groups)
- Build kaolinite data file from kaolinite.car and kaolinite.mdf

Example – toluene vapor

- Atom types and charges assigned automatically with Materials Studio software
- All other parameters assigned automatically from cvff.frc
  - pair coeffs
  - bond coeffs
  - angle coeffs
  - dihedral coeffs
  - improper coeffs
- Build toluene data file from toluene.car and toluene.mdf