Advanced System Building Features in LAMMPS

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Overview

- System setup and data model in LAMMPS
- Entering simulation system info into LAMMPS incrementally with:
  - create_atoms
  - read_data
- Commands to assist in building topologies
- Using the molecule command
- Using multiple force fields (hybrid styles)

How LAMMPS stores Topology Data

- LAMMPS uses a distributed data model
  → topology data is attached to atoms
  → as atoms move between sub-domains, so does the topology information
  → per sub-domain info (e.g. bondlist) and atom migration is part of neighbor list build
  → requires to know the sub-domain layout
  => can only be done after the box is defined
- Definition of the simulation cell locks is certain system properties (e.g. number of types)

Pre-Box Commands

- Certain commands in LAMMPS are only allowed before the simulation box is defined (via create_box or read_data or read_restart)
- Examples: atom_style, boundary, dimension, package, processors, newton, units
- When the box is created, most per-atom arrays are defined and then properties like number of types (atom/bond/angle/dihedral) and dimensioning of per-atom arrays (e.g. for storing topology data with atoms) are locked in

Simple Systems == No Problems

- Thus to set up a simple atomic system, you only set the number of atom types (create_box) and then once or more call create_atoms
- Or when using external tools, all topology info is provided in a single data file (cf. header section)

  LAMMPS can then infer the per-atom array dimensions from this data. it reads the file a first time for that purpose and then creates the box and then fills it with atoms and their associated info and topology data

Multiple Lattice Commands

- When using create_atoms multiple times and the lattice info is changed, some care is needed
- The lattice information is no system information, but simply provides a set of length measures that simplify setting up lattice based geometries
- Lattice information is applied when used and not retroactively altered with a new lattice
- Thus building systems with two components having different lattices settings, lengths have to be commensurate to avoid overlaps etc.

Building Complex Systems with External Build Tools

- Often the preferred option, as the options and tools in LAMMPS are limited by its nature of a parallel program with distributed data
- Examples:
  - charmm2lammps.pl (via psfgen / charmm)
  - msi2lmp (via Material Studio)
  - moltemplate (standalone, importing fragments)
  - TopoTools (via packmol, OpenBabel, scripting)

Advanced System Building Inside of LAMMPS

- Need to reserve space for additional type and topology data when creating the box:
  create_box 2 bond/types 1 angle/types 1 &
  extra/bond/per/atom 2 extra/angle/per/atom 1&
  extra/special/per/atom 4
- Similar options exist for read_data:

  read_data data.wrapped extra/atom/types 1 &
  extra/bond/types 1 extra/angle/types 1 &
  extra/dihedral/types 1 extra/bond/per/atom 9 &
  extra/angle/per/atom 10 ...

Simple Case: read_data plus create_atoms

- For example to create a metal slab system with a molecular system layered on top of it you can:
  - Read in the molecular system via read_data
  - Reserve space for the additional (metal) atom type
  - Create the metal slab atoms with create_atoms (usually restricted to a specific region)

Using read_data Multiple Times

- It is possible to use read_data multiple times
- **All** system info must be set with the **first** call
- Subsequent calls **must** use the “add” keyword
- There are different options to define how atom IDs and various types are determined
- **No** check is made for overlaps
- Added systems can be shifted around
- Final box is the combined maximum, care must be taken with respect to image flags

How to Handle Overlaps

- Avoid them by choosing box boundaries to be shifted from lattice grid positions
  → whether atoms are included or not is no longer ambiguous
- Avoid them by using box dimensions that are commensurate with multiple chosen lattices. N.b. this also applies to rotated lattices
- Use the delete_atoms overlap command
  it can delete topology data, but cannot use compress option with molecular data (reset_ids)

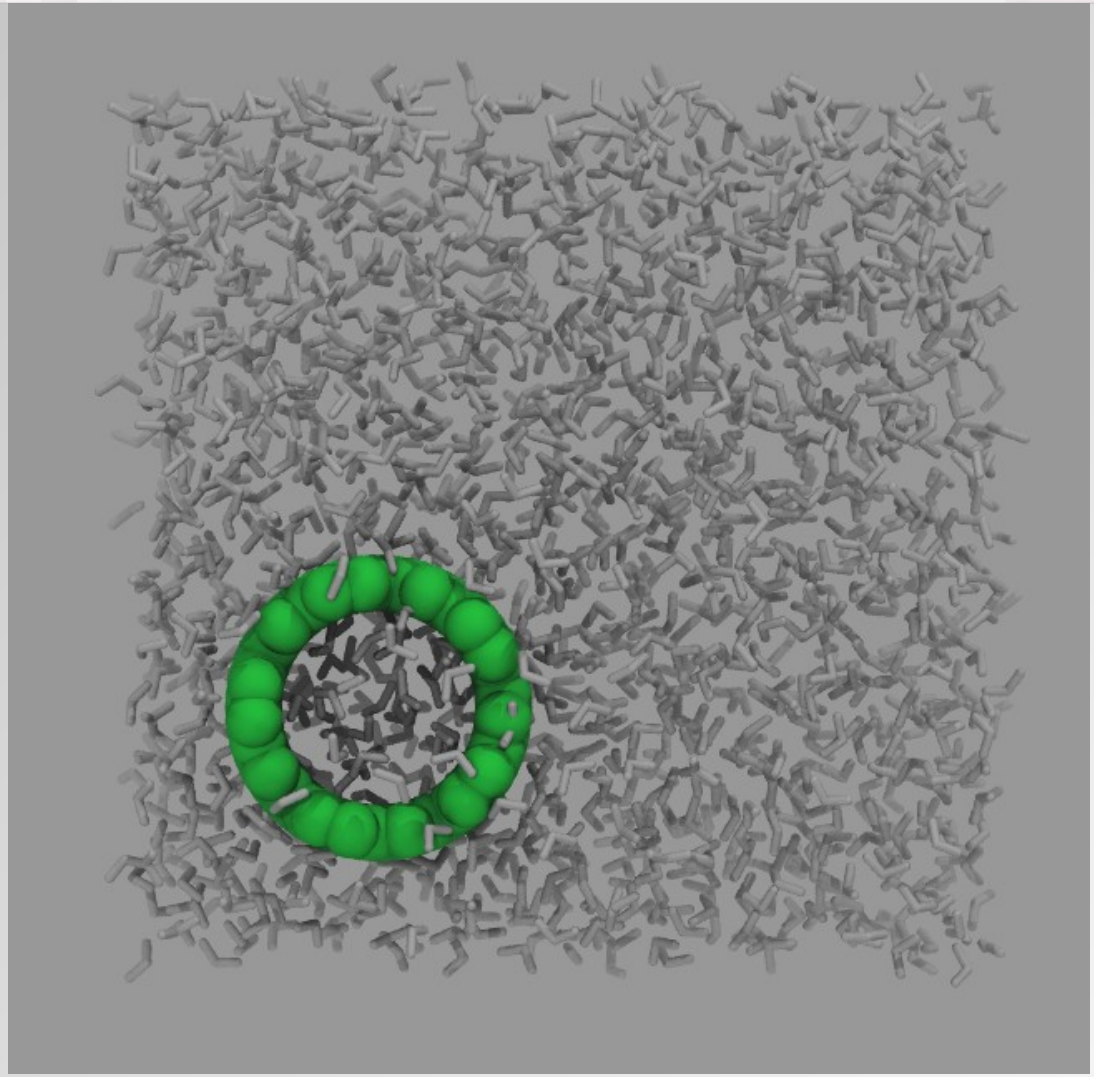
Molecule Command and Files

- Molecule command allows to store information for a group of atoms, e.g. a molecule
- Information is read from a file similar (but not the same) as a data file
- Molecule information is not part of system Identified with a Molecule ID string
- Several commands that can insert atoms into the system, can also insert molecules similar to read_data type offsets can be used
- Space must be available for topology data

Using Multiple Force Fields

- LAMMPS has provisions to do simulations with having **different parts** of the system represented by **different** force fields
- Convenient, but has implications that can easily render the resulting total forces **bogus**
- Best when different **parts** are **separate** entities
- Contact interactions between different force fields **must** be pair-wise additive
- Must not be used to “mix” manybody potentials

Partial Computation of Forces



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