

MAE 720: Molecular Level Modelling for Engineering Application

# Demonstration of MD Simulation using LAMMPS and OVITO

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## Software

In this class

- LAMMPS (MD Simulator)
- OVITO (Visualization, pre & post processing)
- WinScp (Transferring file from local computer to HPC and vice-versa)

Other Opensource Software

- VMD (preprocessing, visualization)
- Avogadro (preprocessing, GUI)
- AtomsK (preprocessing, cmd line)
- EMC (preprocessing, cmd line)

Commercial Software

- Material Studio (preprocessing, GUI)
- MedeA software (MD, DFT, GUI)



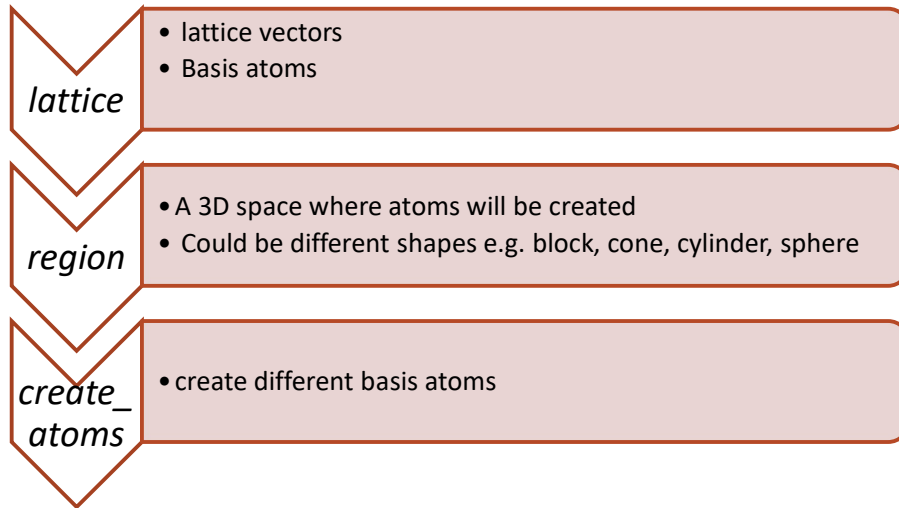
## Download Practice Files



<https://go.ncsu.edu/mae720>



## LAMMPS built-in commands for generating initial geometry



## Graphene

Bond length

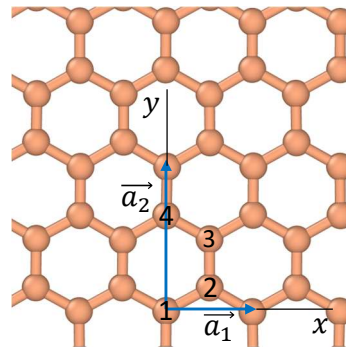
- $l = 1.42 \text{ \AA}$

Lattice Vectors

- $\vec{a}_1 = (\sqrt{3}, 0, 0)l$
- $\vec{a}_2 = (0, 3, 0)l$

Basis atoms

- $\text{basis1} = (0, 0, 0)l = 0\vec{a}_1 + 0\vec{a}_2$
- $\text{basis2} = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0\right)l = \frac{1}{2}\vec{a}_1 + \frac{1}{6}\vec{a}_2$
- $\text{basis3} = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}, 0\right)l = \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2$
- $\text{basis4} = (0, 2, 0)l = 0\vec{a}_1 + \frac{2}{3}\vec{a}_2$



## lattice command

### Syntax

```
lattice style scale keyword values ...
```

- `style` = `none` or `sc` or `bcc` or `fcc` or `hcp` or `diamond` or `sq` or `sq2` or `hex` or `custom`
- `scale` = scale factor between lattice and simulation box

`scale` = reduced density  $\rho^*$  (for LJ units)  
`scale` = lattice constant in distance units (for all other units)

- zero or more keyword/value pairs may be appended
- keyword = `origin` or `orient` or `spacing` or `a1` or `a2` or `a3` or `basis` or `triclinic/general`

`basis` values = `x y z`  
`x,y,z` = fractional coords of a basis atom ( $0 \leq x,y,z < 1$ )

### Lattice command parameters of graphene

- `style` = `custom`
- `scale` = 1.42
- `a1`  $\sqrt{3}$  0 0
- `a2` 0 3 0
- `basis` 0 0 0
- `basis`  $\frac{1}{2}$   $\frac{1}{6}$  0
- `basis`  $\frac{1}{2}$   $\frac{1}{2}$  0
- `basis` 0  $\frac{3}{2}$  0



## region command

### Syntax

```
region ID style args keyword arg ...
```

- ID = user-assigned name for the region
- `style` = `delete` or `block` or `cone` or `cylinder` or `ellipsoid` or `plane` or `prism` or `sphere` or `union` or `intersect`

`block` args = `xlo xhi ylo yhi zlo zhi`  
`xlo,xhi,ylo,yhi,zlo,zhi` = bounds of block in all dimensions (distance units)  
`xlo,xhi,ylo,yhi,zlo,zhi` can be a variable (see below)

zero or more keyword/arg pairs may be appended

`units` value = `lattice` or `box`  
`lattice` = the geometry is defined in lattice units  
`box` = the geometry is defined in simulation box units

### Parameters of region command for graphene

- ID = mybox (could be anything)
- `style` = `block`
- `xlo xhi` = 0 \$L
- `ylo yhi` = 0 \$W
- `zlo zhi` = -10 10  
(doesn't matter as simulation will be 2D)



## create\_atoms command

### Syntax

```
create_atoms type style args keyword values ...
```

- **type** = atom type (1-Ntypes or type label) of atoms to create (offset for molecule creation)
- **style** = *box* or **region** or *single* or *mesh* or *random*

**region** args = **region-ID**  
 region-ID = particles will only be created if contained in the region

create\_atoms parameters for graphene

- type = 1 (only carbon atoms)
- style = region
- region = mybox (previously defined ID of the region command)

Imp –in graphene.lmp



## Visualization

Two LAMMPS command to extract data for visualization

- **write\_data**
  - A single snapshot of the simulation state. Also used as a lammps input file.
  - atomic position, topology (bond, angle, dihedral etc.), force coefficient etc.
- **dump**
  - Multiple snapshots of simulation state with time. Can't be used as an input file.
  - extract atomic position, velocity etc.

### write\_data command

#### Syntax

```
write_data file keyword value ...
```

- file = name of data file to write out
- zero or more keyword/value pairs may be appended
- keyword = *nocoeff* or *nofix* or *nolabelmap* or *triclinic/general* or *types* or *pair*

### dump command

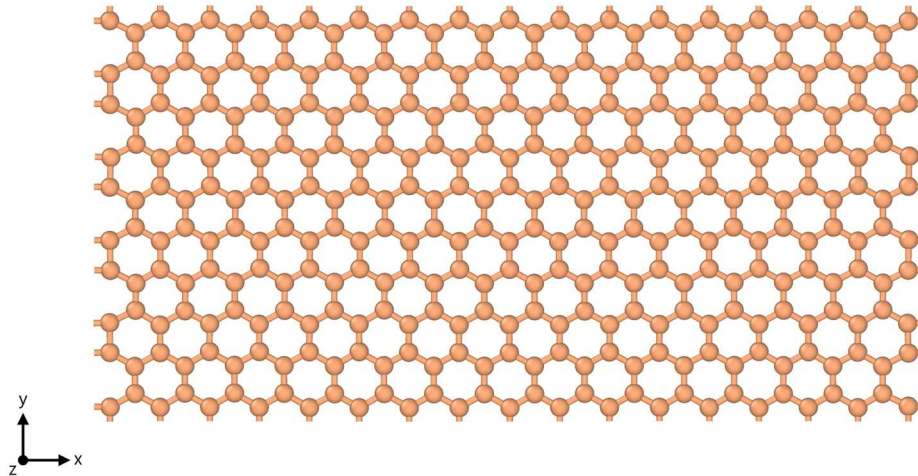
#### Syntax

```
dump ID group-ID style N file attribute1 attribute2 ...
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- style = *atom* or *atom/adios* or *atom/gz* or *atom/zstd* or *cfg* or *cfg/gz* or *cfg/zstd* or *cfg/uef* or *custom/zstd* or *custom/adios* or *dcd* or *extxyz* or *grid* or *grid/vtk* or *h5md* or *image* or *local* or *molfile* or *movie* or *netcdf* or *netcdf/mpiio* or *vtk* or *xtc* or *xyz* or *xyz/gz* or *xyz/zstd* or *yaml*
- N = dump on timesteps which are multiples of N
- file = name of file to write dump info to



## OVITO for Visualization



## read\_data command

- Load initial geometry generated from other software.
- File format: lammps data file.
- Can read multiple data files. add, offset, shift operation can be performed.

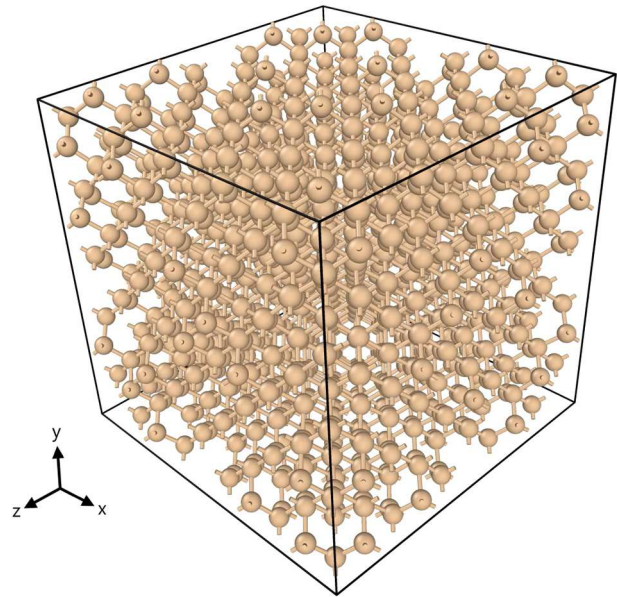
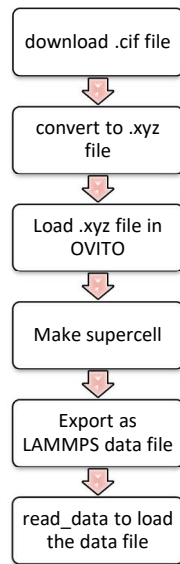
### Syntax

```
read_data file keyword args ...
```

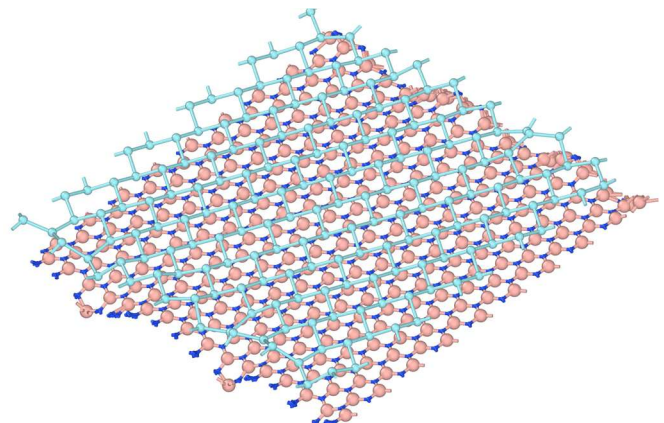
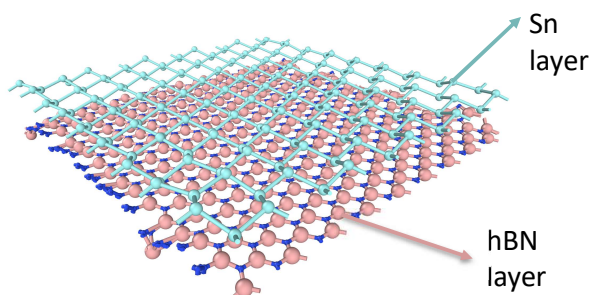
- file = name of data file to read in
- zero or more keyword/arg pairs may be appended



## Silicon (Diamond lattice)

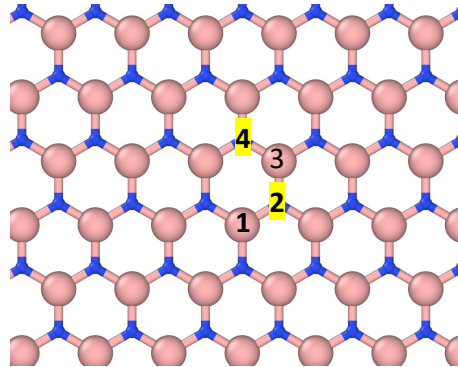


## hexagonal Boron-Nitride and Stanene (hBN-Sn) bilayer

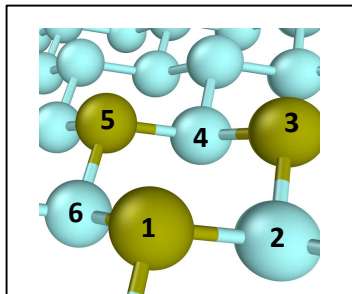


## hBN layer

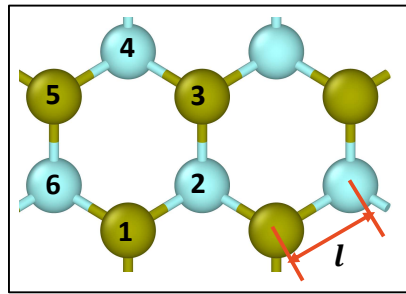
- Similar to graphene
- Two types of basis atoms
  - 1,3 – Boron (type 1 atom)
  - 2,4 – Nitrogen (type 2 atom)
- create\_atoms command to change the basis atoms types
- Syntax:
  - create\_atoms type region region-ID basis M itype
  - M – id of basis atom to change
  - itype – changed atom type



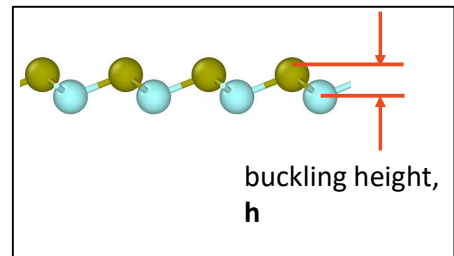
## Sn layer



3D view



Top View



Front View

- 1,3,5 atoms are coplanar
- 2,4,6 atoms are coplanar

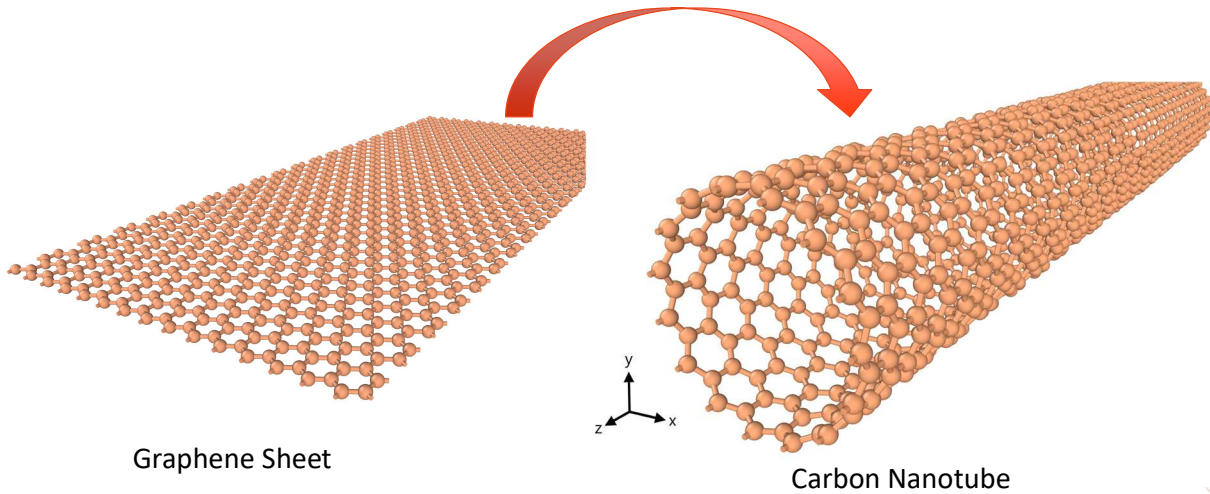
- Bond length
- $l = 2.69 \text{ \AA}$
  - $h = 0.88 \text{ \AA}$

- Lattice Vectors
- $\vec{a}_1 = (\sqrt{3}l, 0, 0)$
  - $\vec{a}_2 = (0, 3l, 0)$
  - $\vec{a}_3 = (0, 0, -2h)$

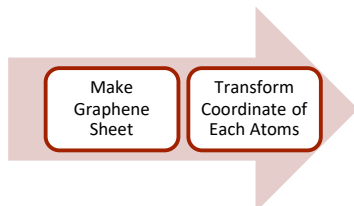
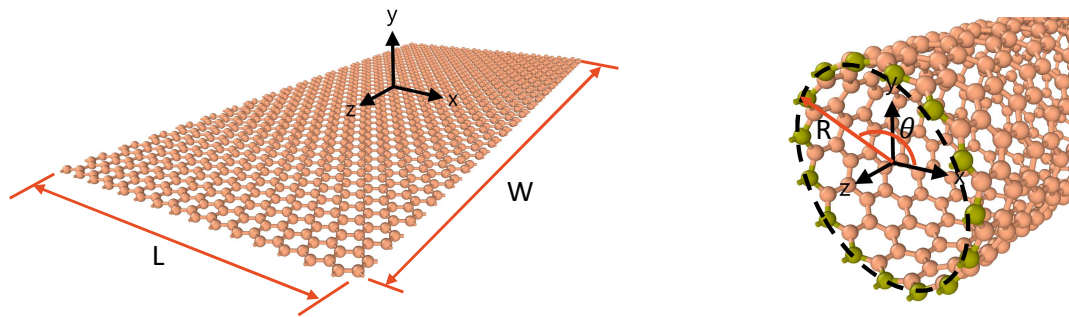
### Basic Vectors

- basis1 =  $0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3$
- basis2 =  $\frac{1}{2}\vec{a}_1 + \frac{1}{6}\vec{a}_2 + \frac{1}{2}\vec{a}_3$
- basis3 =  $\frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2 + 0\vec{a}_3$
- basis4 =  $0\vec{a}_1 + \frac{2}{3}\vec{a}_2 + \frac{1}{2}\vec{a}_3$

## Carbon Nano-Tube (CNT)



## Coordinate Transformation



Equations for co-ordinate Transformation

- $R = \frac{L}{2\pi}$
- $\theta_i = \frac{2\pi x_i}{L}$
- center = (a, b)
- $x'_i = R \cos \theta_i + a$
- $y'_i = R \sin \theta_i + b$
- $z'_i = z_i$



## displace\_atoms command

### Syntax

```
displace_atoms group-ID style args keyword value ...
```

- `group-ID` = ID of group of atoms to displace
- `style` = `move` or `ramp` or `random` or `rotate`

```
move args = delx dely delz
```

`delx,dely,delz` = distance to displace in each dimension (distance units)  
any of `delx,dely,delz` can be a variable (see below)

### Parameters

- `group-ID` = group of each atom
- `style` = `move`
- $\text{delx} = x'_i - x_i$
- $\text{dely} = y'_i - y_i$
- `delz` = 0



## Loop in LAMMPS

### variable command

#### Syntax

```
variable name style args ...
```

### next command

#### Syntax

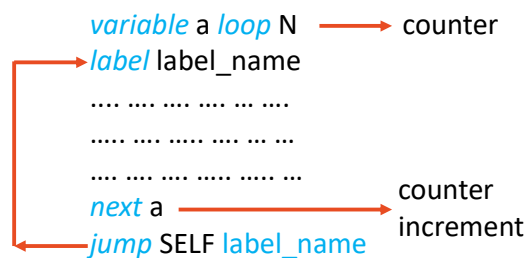
```
next variables
```

### jump command

#### Syntax

```
jump file label
```

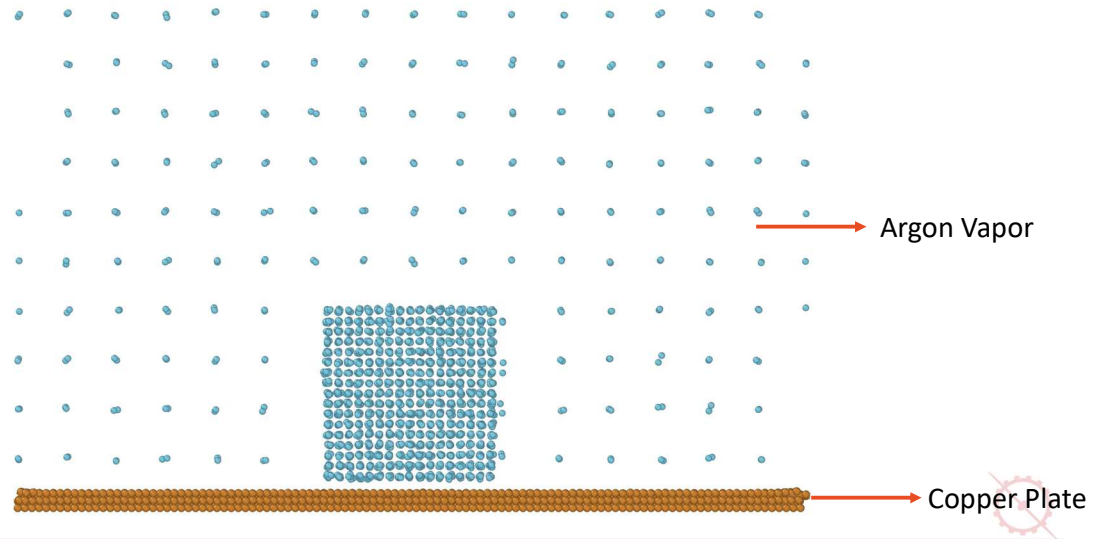
- `file` = filename of new input script to switch to
- `label` = optional label within file to jump to



- For CNT, variable will be atoms id which loop over all the atoms
- Need to perform calculation for co-ordinate transformation
- finally, `displace_atom` command to move the atom.



## Cylindrical Droplet on a Surface



## delete\_atoms command

### Syntax

```
delete_atoms style args keyword value ...
```

- style = group or region or overlap or random or variable

```
group args = group-ID  
region args = region-ID
```

Lattice constant for Ar and Cu

$$\rho = \frac{nM}{N_a a^3}$$

- For copper (FCC), density is 8.96 gm/cc
- For liquid argon (FCC), density 1.33 gm/cc @ 90K
- For vapor argon (FCC), density 0.0168 gm/cc @ 90K

create copper atoms

create vapor argon  
atoms on top

delete droplet region

create liquid argon in  
the deleted region

## Running simulation in NCSU HPC

### Login to HPC node

- Open terminal/cmd/bash
- type: `ssh unityid@login.hpc.ncsu.edu`
- provide password and due security code

### Running LAMMPS

- [change directory] type: `cd /share/$GROUP/$USER`
- [make directory ] type: `mkdir Imp_test`
- [change directory] type: `cd ./Imp_test`
- [submitting job] type: `bsub<run_Imp.sh`

### Check Status of your simulation

- [ongoing jobs] type: `bjobs`
- [stop a job] type: `bkill jobid`
- [check log file] type : `less stdout.***`

### run\_Imp.sh

```
#!/bin/bash
#BSUB -n 32
#BSUB -R "span[hosts=1]"
#BSUB -W 60
#BSUB -J Imp_job
#BSUB -o stdout.%J
#BSUB -e stderr.%J

module load lammps/2022Jun23/intel/cpu
mpirun Imp_hazel -in droplet.Imp
```



## Nano-confined liquid: Try yourself

