fix deposit command¶

Syntax¶

```
fix ID group-ID deposit N type M seed keyword values ...
```

- ID, group-ID are documented in fix command
- deposit = style name of this fix command
- N = # of atoms or molecules to insert
- type = atom type to assign to inserted atoms (offset for molecule insertion; -1 for random selection from type list)
- M = insert a single atom or molecule every M steps
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword
  = *region* or *id* or *global* or *local* or *near* or *gaussian* or *attempt* or *rate* or *vx* or *vy* or *vz* or *mol* or *rigid* or *shake* or *types* or *units*

- *region* value = region-ID
- region-ID = ID of region to use as insertion volume
- *id* value = *max* or *next*
- max = atom ID for new atom(s) is max ID of all current atoms plus one
- next = atom ID for new atom(s) increments by one for every deposition
- *global* values = lo hi
- lo,hi = put new atom/molecule a distance lo-hi above all other atoms (distance units)
- *local* values = lo hi delta
- lo,hi = put new atom/molecule a distance lo-hi above any nearby atom beneath it (distance units)
- delta = lateral distance within which a neighbor is considered "nearby" (distance units)

- *near* value = R
- R = only insert atom/molecule if further than R from existing particles (distance units)
- *gaussian* values = xmid ymid zmid sigma
- xmid,ymid,zmid = center of the gaussian distribution (distance units)
- sigma = width of gaussian distribution (distance units)
- *attempt* value = Q
- Q = attempt a single insertion up to Q times
- *rate* value = V
- V = z velocity (y in 2d) at which insertion volume moves (velocity units)
- *vx* values = vxlo vxhi
- vxlo,vxhi = range of x velocities for inserted atom/molecule (velocity units)
- *vy* values = vylo vyhi
- vylo,vyhi = range of y velocities for inserted atom/molecule (velocity units)
- *vz* values = vzlo vzhi
- vzlo,vzhi = range of z velocities for inserted atom/molecule (velocity units)
- *target* values = tx ty tz
- tx,ty,tz = location of target point (distance units)
- *mol* value = template-ID
- template-ID = ID of molecule template specified in a separate molecule command
- *molfrac* values = f1 f2 ... fN

- f1 to fN = relative probability of creating each of N molecules in template-ID
- *rigid* value = fix-ID
- fix-ID = ID of fix rigid/small command
- *shake* value = fix-ID
- fix-ID = ID of fix shake command
- *orient* values = rx ry rz
- rx,ry,rz = vector to randomly rotate an inserted molecule around
- *units* value = *lattice* or *box*
- lattice = the geometry is defined in lattice units
- box = the geometry is defined in simulation box units
- *types* value = list of types to be randomly selected for deposit
- (allowed only if the given type value = -1

Examples¶

```
fix 3 all deposit 1000 2 100 29494 region myblock local 1.0 1.0 1.0 units box
fix 2 newatoms deposit 10000 1 500 12345 region disk near 2.0 vz -1.0 -0.8
fix 4 sputter deposit 1000 2 500 12235 region sphere vz -1.0 -1.0 target 5.0 5.0 0.0
units lattice
fix 5 insert deposit 200 2 100 777 region disk gaussian 5.0 5.0 9.0 1.0 units box
fix 2 flmatoms deposit 200 -1 100 5268 region addfilm local 1.5 1.5 1.5 vz -0.1 -0.1
units box types 3 4 5 6 7 8 9 10 11 12 13 14
```

Description¶

Insert a single atom or molecule into the simulation domain every M timesteps until N atoms or molecules have been inserted. This is useful for simulating deposition onto a surface. For the remainder of this doc page, a single inserted atom or molecule is referred to as a “particle”.

If inserted particles are individual atoms, they are assigned the specified atom type or, if the specified type is -1, they are randomly assigned a type from the types list. If they are molecules, the type of each atom in the inserted molecule is specified in the file read by the molecule command, and those values are added to the specified atom type. E.g. if the file specifies atom types 1,2,3, and those are the atom types you want for inserted molecules, then specify *type* = 0. If you specify *type* = 2, the in the inserted molecule will have atom types 3,4,5.

All atoms in the inserted particle are assigned to two groups: the default group "all" and the group specified in the fix deposit command (which can also be "all").

If you are computing temperature values which include inserted particles, you will want to use the compute_modify dynamic option, which insures the current number of atoms is used as a normalizing factor each time the temperature is computed.

Care must be taken that inserted particles are not too near existing atoms, using the options described below. When inserting particles above a surface in a non-periodic box (see the boundary command), the possibility of a particle escaping the surface and flying upward should be considered, since the particle may be lost or the box size may grow infinitely large. A fix wall/reflect command can be used to prevent this behavior. Note that if a shrink-wrap boundary is used, it is OK to insert the new particle outside the box, however the box will immediately be expanded to include the new particle. When simulating a sputtering experiment it is probably more realistic to ignore those atoms using the thermo_modify command with the *lost ignore* option and a fixed boundary.

The fix deposit command must use the *region* keyword to define an insertion volume. The specified region must have been previously defined with a region command. It must be defined with side = *in*.

Note

LAMMPS checks that the specified region is wholly inside the simulation box. It can do this correctly for orthonormal simulation boxes. However for triclinic boxes, it only tests against the larger orthonormal box that bounds the tilted simulation box. If the specified region includes volume outside the tilted box, then an insertion will likely fail, leading to a "lost atoms" error. Thus for triclinic boxes you should insure the specified region is wholly inside the simulation box.

The locations of inserted particles are taken from uniform distributed random numbers, unless the *gaussian* keyword is used. Then the individual coordinates are taken from a gaussian distribution of width *sigma* centered on *xmid*,*ymid*,*zmid*.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the molecule command, which reads files that define one or more molecules. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the molecule command for details. The only settings required to be in each file are the coordinates and types of atoms in the molecule.

If the molecule template contains more than one molecule, the relative probability of depositing each molecule can be specified by the *molfrac* keyword. N relative probabilities, each from 0.0 to 1.0, are specified, where N is the number of molecules in the template. Each time a molecule is deposited, a random number is used to sample from the list of relative probabilities. The N values must sum to 1.0.

If you wish to insert molecules via the *mol* keyword, that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate fix rigid/small command which also appears in your input script.

Note

If you wish the new rigid molecules (and other rigid molecules) to be thermostatted correctly via fix rigid/small/nvt or fix rigid/small/npt, then you need to use the "fix_modify dynamic/dof yes" command for the rigid fix. This is to inform that fix that the molecule count will vary dynamically.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate fix shake command which also appears in your input script.

Each timestep a particle is inserted, the coordinates for its atoms are chosen as follows. For insertion of individual atoms, the "position" referred to in the following description is the coordinate of the atom. For insertion of molecule, the "position" is the geometric center of the molecule; see the molecule doc page for details. A random rotation of the molecule around its center point is performed, which determines the coordinates all the individual atoms.

A random position within the region insertion volume is generated. If neither the *global* or *local* keyword is used, the random position is the trial position. If the *global* keyword is used, the random x,y values are used, but the z position of the new particle is set above the highest current atom in the simulation by a distance randomly chosen between lo/hi. (For a 2d simulation, this is done for the y position.) If the *local* keyword is used, the z position is set a distance between lo/hi above the highest current atom in the simulation that is "nearby" the chosen x,y position. In this context, "nearby" means the lateral distance (in x,y) between the new and old particles is less than the *delta* setting.

Once a trial x,y,z position has been selected, the insertion is only performed if no current atom in the simulation is within a distance R of any atom in the new particle, including the effect of periodic boundary conditions if applicable. R is defined by the *near* keyword. Note that the default value for R is 0.0, which will allow atoms to strongly overlap if you are inserting where other atoms are present. This distance test is performed independently for each atom in an inserted molecule, based on the randomly rotated configuration of the molecule. If this test fails, a new random position within the insertion volume is chosen and another trial is made. Up to Q attempts are made. If the particle is not successfully inserted, LAMMPS prints a warning message.

Note

If you are inserting finite size particles or a molecule or rigid body consisting of finite-size particles, then you should typically set R larger than the distance at which any inserted particle may overlap with either a previously inserted particle or an existing particle. LAMMPS will issue a warning if R is smaller than this value, based on the radii of existing and inserted particles.

The *rate* option moves the insertion volume in the z direction (3d) or y direction (2d). This enables particles to be inserted from a successively higher height over time. Note that this parameter is ignored if the *global* or *local* keywords are used, since those options choose a z-coordinate for insertion independently.

The vx, vy, and vz components of velocity for the inserted particle are set using the values specified for the *vx*, *vy*, and *vz* keywords. Note that normally, new particles should be a assigned a negative vertical velocity so that they move towards the surface. For molecules, the same velocity is given to every particle (no rotation or bond vibration).

If the *target* option is used, the velocity vector of the inserted particle is changed so that it points from the insertion position towards the specified target point. The magnitude of the velocity is unchanged. This can be useful, for example, for simulating a sputtering process. E.g. the target point can be far away, so that all incident particles strike the surface as if they are in an incident beam of particles at a prescribed angle.

The *orient* keyword is only used when molecules are deposited. By default, each molecule is inserted at a random orientation. If this keyword is specified, then (rx,ry,rz) is used as an orientation vector, and each inserted molecule is rotated around that vector with a random value from zero to 2*PI. For a 2d simulation, rx = ry = 0.0 is required, since rotations can only be performed around the z axis.

The *id* keyword determines how atom IDs and molecule IDs are assigned to newly deposited particles. Molecule IDs are only assigned if molecules are being inserted. For the *max* setting, the atom and molecule IDs of all current atoms are checked. Atoms in the new particle are assigned IDs starting with the current maximum plus one. If a molecule is inserted it is assigned an ID = current maximum plus one. This means that if particles leave the system, the new IDs may replace the lost ones. For the *next* setting, the maximum ID of any atom and molecule is stored at the time the fix is defined. Each time a new particle is added, this value is incremented to assign IDs to the new atom(s) or molecule. Thus atom and molecule IDs for deposited particles will be consecutive even if particles leave the system over time.

The *units* keyword determines the meaning of the distance units used for the other deposition parameters. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. Note that the units choice affects all the keyword values that have units of distance or velocity.

The *types* keyword is used only if the insertion type is given as -1. In that case the inserted type is randomly chosen from the list of types following the *types* keyword.

Note

If you are monitoring the temperature of a system where the atom count is changing due to adding particles, you typically should use the compute_modify dynamic yes command for the temperature compute you are using.

Restart, fix_modify, output, run start/stop, minimize info¶

This fix writes the state of the deposition to binary restart files. This includes information about how many particles have been deposited, the random number generator seed, the next timestep for deposition, etc. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Note

For this to work correctly, the timestep must **not** be changed after reading the restart with reset_timestep. The fix will try to detect it and stop with an error.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions¶

The specified insertion region cannot be a “dynamic” region, as defined by the region command.

Related commands¶

fix pour, region

Default¶

Insertions are performed for individual atoms, i.e. no *mol* setting is defined. If the *mol* keyword is used, the default for *molfrac* is an equal probabilities for all molecules in the template. Additional option defaults are id = max, delta = 0.0, near = 0.0, attempt = 10, rate = 0.0, vx = 0.0 0.0, vy = 0.0 0.0, vz = 0.0 0.0, and units = lattice.