pair_style ufm command

pair_style ufm/gpu command

pair_style ufm/omp command

pair_style ufm/opt command

pair_style ufm/rw command

Syntax:

```
pair_style style args
```

- style = *ufm* or *ufm/rw*
- args = list of arguments for a particular style

```
ufm args = cutoff
    cutoff = global cutoff for Lennard Jones interactions (distance units)
ufm/rw args = otype htype epsilon sigma cutoff
    otype,htype = atom types for O and H
    epsilon = energy scale resulting from p*kB*T product (energy units)
    sigma = characteristic UF distance (distance units)
    cutoff = global cutoff for UF/Rw (distance units)
```

Examples:

```
pair_style ufm 5.0
pair_coeff 1 1 100.0 1.0 2.5
pair_coeff * * 100.0 1.0

pair_style ufm/rw 1 2 44.01 2.0 10.0
pair_coeff * *
variable lambda equal ramp(1.0,0.0)
fix f1 all adapt 1 pair ufm/rw fscale * * v_lambda
```

Description:

Style *ufm* computes pairwise interactions using the Uhlenbeck-Ford (UF) potential (Paula Leite2016) which is given by

$$E = -\varepsilon \ln\left[1 - \exp\left(-r^2/\sigma^2\right)\right] \qquad r < r_c$$

$$\varepsilon = p\, k_B\, T$$

where rc is the cutoff radius, sigma is a distance-scale and epsilon is an energy-scale, i.e., a product of Boltzmann constant kB, temperature T and the UF p-parameter which is responsible to control the softness of the interactions (Paula Leite2017).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global *ufm* cutoff is used.

Style *ufm/rw* computes the UF interaction between two rigid water molecules with the interparticle distance between them defined as the distance between their centers of masses (Paula Leite2018). The atomic types of the oxygen and hydrogen atoms, epsilon, sigma and cutoff parameters are specified as pair_style arguments.

NOTE: The *ufm/rw* style is based on LAMMPS implementation of TIP4P water model. Therefore, for each rigid water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a rigid water molecule is 100, then its 2 H atoms must have IDs 101 and 102.

The fix adapt command can be used to vary epsilon, sigma or fscale variables of these pair styles over the course of a simulation, in which case *pair_style*/*pair_coeff* settings for epsilon and sigma must still be specified, but will be overridden. For example these commands will vary the prefactor epsilon for all pairwise interactions from 10.0 at the beginning to 100.0 at the end of a run:

```
variable prefactor equal ramp(10,100)
fix f1 all adapt 1 pair ufm epsilon * * v_prefactor
```

NOTE: These models are useful as a reference system for fluid-phase free-energy calculations. It can be done performing thermodynamic integration procedure using fix adapt, which will rescale the forces on each atom by varying a scale variable, which always starts with value 1.0. The syntax is the same described above, however, changing epsilon to fscale. A detailed explanation of how to use this command and perform nonequilibrium thermodynamic integration procedure to compute absolute free energies of fluids in LAMMPS is given in PaulaLeite2018.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the Speed packages doc page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Build package doc page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See the Speed packages doc page for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is always mixed via a *geometric* rule. The cutoff is mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table and tail are not relevant for this pair style.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: sigma parameter must be greater than zero.

Related commands:

pair_coeff, fix adapt

Default: none

(Paula Leite2016) Paula Leite , Freitas, Azevedo, and de Koning, J Chem Phys 126, 044509 (2016).

(Paula Leite2017) Paula Leite, Santos-Florez, and de Koning, Phys Rev E 96, 32115 (2017).

(Paula Leite2018) Paula Leite and de Koning, Comp. Mat. Sc. XXX, XXX (2018).