Even though the local density potential isn’t actually a pair potential, it seems most natural to implement it as a pair style based on examples in the MANYBODY package. Our starting point has been the code for the pair style eam/alloy. Our current implementation strategy is presented below:

Name of the pair style in LAMMPS input script: localdensity

How input parameters are taken: pair\_style localdensity <input file>

(no pair\_coeff command)

Input file format:

Line 1: comment or blank (this line is ignored)

Line 2: comment or blank (ignored)

Line 3: (number of LD potentials)

Line 4: blank (ignored)

Line 5: (lower and upper cutoffs)

Line 6: centraltypes (central atom types separated by spaces)

Line 7: neighbortypes (neighbor atom types separated by spaces)

Line 8: (number of values of and tabulated)

Line 9:

Line 10:

Line 11:

Line 11:

…

Line 9+:

Line 10+: blank (ignored)

Block 2

Block 3

…

Block

Thus the input file is separated into blocks each representing a separate local density potential and each specifying its own upper and lower cutoffs, central and neighbor atoms, and potential. In general, blank lines anywhere are ignored.