Tips for conversion between KISSMD-2NN MEAM and LAMMPS-2NN MEAM

1. library.meam (extracted from LAMMPS User Manual)

The MEAM library file provided with LAMMPS has the name potentials/ library.meam. It is the "meamf" file used by other MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, it is formatted as a series of entries, each of which has 19 parameters and can span multiple lines:

elt, lat, z, ielement, atwt, alpha, b0, b1, b2, b3, alat, esub, asub, t0, t1, t2, t3, rozero, ibar

# CAUTION: KISSMD-2NN MEAM uses t0=1.0.

The ibar parameter selects the form of the function G(Gamma) used to compute the electron density; options are

```
       0: G = sqrt(q+Gamma)
       1: G = exp(Gamma/2)
       2: not implemented
       3: G = 2/(1+exp(-Gamma))
       4: G = sqrt(1+Gamma)
      -5: G = +-sqrt(abs(1+Gamma)).
```

# CAUTION: KISSMD-2NN MEAM uses option 3 for ibar.

2. MEAM parameter file (extracted from LAMMPS User Manual)

If used, the MEAM parameter file contains settings that override or complement the library file settings. Examples of such parameter files are in the potentials directory with a ".meam" suffix. Their format is the same as is read by other Fortran MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, each line has one of the following forms. Each line can also have a trailing comment (starting with #) which is ignored.

```
keyword = value
keyword(I) = value
keyword(I,J) = value
keyword(I,J,K) = value
```

The recognized keywords are as follows:

```
rc          = cutoff radius for cutoff function; default = 4.0

delr        = length of smoothing distance for cutoff function; default = 0.1

rho0(I)     = relative density for element I (overwrites value read from meamf
              file)

Ec(I,J)     = cohesive energy of reference structure for I-J mixture

delta(I,J)  = heat of formation for I-J alloy; if Ec_IJ is input as zero, then
              LAMMPS sets Ec_IJ = (Ec_II + Ec_JJ)/2 - delta_IJ

alpha(I,J)  = alpha parameter for pair potential between I and J can be computed
              from bulk modulus of reference structure

re(I,J)     = equilibrium distance between I and J in the reference structure

Cmax(I,J,K) = Cmax screening parameter when I-J pair is screened by K (I<=J);
              default = 2.8

Cmin(I,J,K) = Cmin screening parameter when I-J pair is screened by K (I<=J);
              default = 2.0
```

```
# CAUTION: The sequence of i, j, k is different in KISSMD and LAMMPS. In the
          current KISSMD, Cmin(i,j,k) means when i-k pair is screeened by j
          while in LAMMPS, when i-j pair is screened by k.
```

```
lattce(I,J) = lattice structure of I-J reference structure:
    dia = diamond (interlaced fcc for alloy)
    fcc = face centered cubic
    bcc = body centered cubic
    dim = dimer
    b1  = rock salt (NaCl structure)
    hcp = hexagonal close-packed
    c11 = MoSi2 structure
    l12 = Cu3Au structure (lower case L, followed by 12)
    b2  = CsCl structure (interpenetrating simple cubic)

# CAUTION: KISSMD-2NN MEAM does not support 'c11' lattice structure.
# CAUTION: l12 AB3 structure is not supported as an reference structure in
          LAMMPS. If you have a KISSMD parameter set based on the l12 AB3
          structure, you can use l12 A3B structure as a reference by reversing
          the order of elements, Cmin, and Cmax instead.

nn2(I,J)   = turn on second-nearest neighbor MEAM formulation for I-J pair.
    0 = second-nearest neighbor formulation off
    1 = second-nearest neighbor formulation on
    default = 0

# CAUTION: KISSMD-2NN MEAM uses option 1 for nn2(I,J).

erose_form  = integer value to select the form of the Rose energy function
    astar = alpha * (r/re - 1.d0)
    if erose_form = 0: erose = -Ec*(1+astar+a3*(astar**3)/(r/re))
                               *exp(-astar)
    if erose_form = 1: erose = -Ec*(1+astar+(-attrac+repuls/r)*(astar**3))
                               *exp(-astar)
    if erose_form = 2: erose = -Ec*(1 +astar + a3*(astar**3))*exp(-astar)
    a3 = repuls, astar <0
    a3 = attrac, astar >= 0
    default = 0

# CAUTION: KISSMD-2NN MEAM uses option 2 for erose_form.

attrac(I,J) = additional cubic attraction term in Rose energy I-J pair
              potential; default = 0
repuls(I,J) = additional cubic repulsive term in Rose energy I-J pair potential;
              default = 0

# CAUTION: KISSMD-2NN MEAM uses the same value for attrac and repuls
```

```
zbl(I,J)    = blend the MEAM I-J pair potential with the ZBL potential for small
              atom separations (ZBL); default = 1
# CAUTION: KISSMD-2NN MEAM uses zbl(I,J) = 0.

gsmooth_factor = factor determining the length of the G-function smoothing
                 region; only significant for ibar=0 or ibar=4.
# CAUTION: KISSMD-2NN MEAM uses option 3 for ibar, therefore gsmooth_factor is
         negligible.

augt1       = integer flag for whether to augment t1 parameter by 3/5*t3 to
              account for old vs. new meam formulations;
    0 = don't augment t1
    1 = augment t1
    default = 1
# CAUTION: KISSMD-2NN MEAM uses option 0 for augt1.

ialloy      = integer flag to use alternative averaging rule for t parameters,
              for comparison with the DYNAMO MEAM code
    0 = standard averaging (matches ialloy=0 in DYNAMO)
    1 = alternative averaging (matches ialloy=1 in DYNAMO)
    2 = no averaging of t (use single-element values)
    default = 0
# CAUTION: KISSMD-2NN MEAM uses option 2 for ialloy.

mixture_ref_t = integer flag to use mixture average of t to compute the
                background reference density for alloys, instead of the single-
                element values
    0 = do not use mixture averaging for t in the reference density
    1 = use mixture averaging for t in the reference density
    default = 0
# CAUTION: KISSMD-2NN MEAM uses option 0 for mixture_ref_t.

emb_lin_neg = integer value to select embedding function for negative densities
    0 = F(rho)=0
    1 = F(rho) = -asub*esub*rho (linear in rho, matches DYNAMO)
    default = 0
# CAUTION: KISSMD-2NN MEAM uses option 0 for emb_lin_neg.

bkgd_dyn    = integer value to select background density formula
    0 = rho_bkgd = rho_ref_meam(a) (as in the reference structure)
    1 = rho_bkgd = rho0_meam(a)*Z_meam(a) (matches DYNAMO)
    default = 0
# CAUTION: KISSMD-2NN MEAM uses option 0 for bkgd_dyn.
```