4. Input & Output Files

4.1. POSCAR files

GCVC code requires following multiple POSCAR files that contains different information.

> **❶ Note**
>
> 1. File format is based on VASP code without line of "Selective dynamics".
> 2. Lines of internal positions should NOT contain comment out or other character.
>   e.g., "0.000 0.000 0.000" is ok. "0.000 0.000 0.000 # Cu" is incorrect.
> 3. File name of POSCAR files below should not be changed. Captical and lower-case letters should be distinguished.

4.1.1. POSCAR.cluster

POSCAR specifying ideal positions of lattice points

1. Axis and internal positions are the ideal value (should NOT use relaxed values after DFT calc.)
2. The line of number of atoms always contain SINGLE element, just specifying number of total lattice points:
   e.g., "256" is ok. "128 128" is incorrect.

> **❶ Note**
>
> 1. The cell size should be larger than twice of maximum distance of used clusters due to the periodic boundary condition.

4.1.2. POSCAR.lattice

POSCAR specifying information about user-defined sublattice.

1. The line of number of atoms specifies sublattice information.
   e.g., "8 16 12" means the first 8 sites are sublattice-1, following 16 are sub-2, and the last 12 are sub-3.
2. Axis and set of internal positions are the same as POSCAR.cluster. (Sequence of internal position can differ from POSCAR.cluster)

4.1.3. POSCAR.spin

POSCAR specifying occupation of elements at each lattice point.

1. Line of number of atoms specifies number of constituent elements (i.e., the definition is the same as VASP)
2. Axis and set of internal positions are the same as POSCAR.cluster. (Sequence of internal position can differ from POSCAR.cluster)

4.1.4. POSCAR.canarea

POSCAR specifying sets of lattice points where their compositions are kept fixed

1. The line of number of atoms specifies sublattice-like index (similar to POSCAR.lattice)
   e.g., "8 16 12" means the first 8 sites are index-1, following 16 are index-2, and the last 12 are index-3.
2. Axis and set of internal positions are the same as POSCAR.cluster. (Sequence of internal position can differ from POSCAR.cluster or POSCAR.lattice)

4.1.5. POSCAR.disp

POSCAR specifying atomic displacement. (VLCE / CS-VLCE)

1. Sequence of internal position is the same as POSCAR.spin.
2. Lines of axis as well as internal positions can be different from ideal value. (e.g., after relaxation by DFT calc.)
3. Line of number of atoms is the same as POSCAR.spin.

> **❶ Note**
>
> 1. To get POSCAR.disp, typically, POSCAR.spin in small cell is applied to program to get atomic displacement, and then perform mksupercell.rb. In this case, mksupercell.rb for POSCAR.spin and POSCAR.disp does not give the same sequence of internal position, resulting in error in GCVC program. So, if you

perform mksupercell.rb to get POSCAR.spin and POSCAR.disp, please check the sequence of internal posisions.
2. If sequence of internal position in POSCAR.disp differs from that in POSCAR.spin, you can generate new POSCAR.disp with corrected sequence by using sortPoscarDisp program.

4.2. gcvc-.in files

gcvc-*.in files determines main calculation conditions for GCVC.

File format of gcvc-*.in is:

```
# Comment out line
Tag : value(s)
Tag : value(s)
...
```

The 1st line is always for comment. You can describe any comment. The following lines consists of "Tag", space, ":", space, "value(s)". (Double quotation is not required in gcvc-*.in file)

> ❶ Note
>
> 1. "Tag" should be ALL capital letters.
> 2. Explanation of tag below is e.g.: TRUNCATION[0-3]. This means that Tag of "TRUNCATION" has 4 values (i.e., [0-3]) separated by space character, so you should write for instance:
>   TRUNCATION : 0.0 0.3 1.0 0.8

4.2.1. gcvc-cluster.in

Input for getCluster

- MAXBODY
    Maximum dimension of cluster to be searched (MAXBODY <=4)
- TRUNCATION[0-3]
    [0] : Lower limit of truncation of cluster search (angstrom)
    [1-3] : Upper limit of truncation for pair, triplet, quartet (angstrom)
- FACTOR (Default: 100000)
    Determine accuracy to calculate pair distance. Number of zeros (default: 5

zeros) determine number of digits after the decimal point considered. Example:

```
MAXBODY : 4
TRUNCATION : 0.0 7.0 5.5 5.5
FACTOR : 10000000
```

4.2.2. gcvc-cluster-couple.in

Input for getCluster-couple

- MAXCOUPLE
    Maximum coupling order. Example:
       maxCouple=2 is: [conf-x, conf-y, conf-z, x-y, x-z, y-z].
       maxCouple=3 is: [conf-x, conf-y, ..., conf-x-y, conf-y-z, ..., x-y-z]
- MAXORDER
    Maximum summed dimenstion of coupled clusters for pair (couple=2), triplet (couple=3), and quartet (couple=4) coupling. Example:
       maxOrder : 5 7 9 is:
          for conf-x (couple=2): point-point, point-pair,...,point-quartet, pair-pair,...,pair-triplet. (Sum of dimension is below 5).
          for conf-x-y (couple=3): point-point-point, ... , point-tri-tri, pair-pair-pair, pair-pair-tri. (Sum of dimension is below 7).
- TRUNCATION[0-3]
    [0]: Lower limit of truncation of distance between coupling clusters
    [1-3]: Upper limit of truncation for pair, triplet, and quartet coupling
- IDDISTANCE[0-2]
    When coupled-cluster distance for pair, triplet, and quartet, (d[0], d[1], d[2]), satisfy
       d[i] > iddistance[i], (i = 0, 1, 2)
    these coupled-clusters are classified only by the geometrical figure (Most rough approximation)
- EMDISTANCE[0-2]
    When coupled-cluster distance for pair, triplet, and quartet, (d[0], d[1], d[2]), satisfy
       iddistance[i] >= d[i] > emdistance,
    these coupled-clusters consisting of the same set of lattice points are treated as the same
    (i.e., direction-dependence of coupled clusters are neglected -> This is effective medium approx.)

- CELLSIZE[0-2]

  If POSCAR.cluster is 2x4x4 extension of the unit cell, then write "2 4 4".

  This tag tells the program the size of unit cell, then the program determine special vectors for coupled-cluster search.

4.2.3. gcvc-basis-conf.in

Input for getBasis-conf

- SPINCE[0-(J-1)]

  For J-component system, specify spin variables to construct basis functions.

  Sequence of spin variables can be arbitrary.

- SPINPOSCAR[0-(K-1)]

  Specify spin variables in POSCAR.spin including K (K <= J) elements.

  Sequence of spin variables should be consistent with POSCAR.spin.

- DEFBASIS (Default : -1)

  If DEFBASIS = 1, user-defined basis function (specified by PSI) is used to calculate correlation functions.

- PSI[0-(J^2-1)] (Default : not required)

  The first J-components are coefficients of sigma^0, sigma^1, sigma^2, ..., sigma^(J-1) for basis_0.

  The second J-components are coefficients of sigma^0, sigma^1, sigma^2, ..., sigma^(J-1) for basis_1.

  The third ... ... for basis_2.

  ...

4.2.4. gcvc-basis-disp.in

Input for getBasis-disp based on CS-VLCE

- MAXORDER

  Maximum order of basis function used in CS-VLCE.

- NORMDISP

  (angstrom) Normalization displacement for spin variable, tau.

- CALCDIR[0-2]

  Specify whether basis function for x, y, z (i.e., [0-2]) is calculated (=1) or not calculated (=0). Example:

  calcdir="1 1 0" means basis function along x, y are calculated, while along z is not calculated.

4.2.5. gcvc-basis-couple.in

Input for getBasis-couple

Tags of SPINCE, SPINPOSCAR, MAXORDER, NORMDISP, CALCDIR is required (Meaning is the same as gcvc-basis-*.in)

4.2.6. gcvc-graph.in

Input for getGraphLap

- SPINCE[0-(J-1)]

  For J-component system, specify spin variables to construct basis functions.

  Sequence of spin variables can be arbitrary.

- SPINPOSCAR[0-(K-1)]

  Specify spin variables in POSCAR.spin including K (K <= J) elements.

  Sequence of spin variables should be consistent with POSCAR.spin.

- PAIRINDEX[0-(M-1)]

  For graph calc.: Pair cluster indices (differ from that in info-cluster. Typically, PAIRINDEX = 0 denotes 1NN pair, 1 denotes 2NN pair, ... Each Pair constructs each A matrix.

- MODULE (Default : -1)

  If MODULE > 0, then linear combination of A matrix for each pair is constructed.

- COEFF[N*(0-(M-1))]

  (MODULE > 0 only) First M values corresponds to the first set of coefficients for module of A. Following second M values to the second set of ...

- BASIS0, BASIS1

  For graph calc.: Basis index (differ from basis index itself in CE) for two lattice points that make pair of PAIRINDEX. Basis index for CE = BASIS0 (or BASIS1) + 1.

- DEFBASIS (Default : -1)

  If DEFBASIS = 1, user-defined basis function (specified by PSI) is used to calculate correlation functions.

- PSI[0-(J^2-1)] (Default : not required)

  The first J-components are coefficients of sigma^0, sigma^1, sigma^2, ..., sigma^(J-1) for basis_0.

  The second J-components are coefficients of sigma^0, sigma^1, sigma^2, ...,

sigma^(J-1) for basis_1.

The third ... ... for basis_2.

...

4.2.7. gcvc-gs-graph-can.in

Input for gs-graph-can

- SPINCE

  Meaning is the same as gcvc-basis-conf.in.
- MININDEX (Integer)

  0 <= MININDEX < MAXINDEX.

  MININDEX specify minimum index of structure in gs-search.
- MAXINDEX (Integer)

  MININDEX < MAXINDEX <= [component^(NumAtom in gs-cell) - 1] .

  MAXINDEX specify maximum index of structure in gs-search.
- GSCELLSIZE[0-2]

  If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to
  perform gs-search within 2x1x1 supercell, then write:

  "2 4 4" (i.e., 4/2, 4/1, 4/1).
- COMPOSITION[0-(J-1)] (gs-conf-can only)

  Write compositions (0.0 - 1.0) for each element. Sequence should be
  consistent with SPINCE.
- NUMSTR (gs-conf-can only) (Default: -1)

  Number of structures having m-th lowest (m <= NUMSTR) energy whose
  POSCAR is written into poscar.gs file.
- WRITESPIN (gs-conf-can only) (Default: 1)

  If WRITESPIN = 1, write spins on each site to gscar file. Otherwise, spins
  are NOT written in gscar file.
- WRITECORR (Default: 0)

  If WRITECORR = 1, write correlaions of cluster in ecicar (excluding empty)
  for all configurations.
- WRITEGRAPH (Default: 1)

  If WRITEGRAPH < 0, graph information is not written in output files
- NUMPAIR

  Number of pairs used in the gs-graph-can calculation. This should be
  consistent with the information in ecicar file.

  e.g., If ecicar contains three pairs, then NUMPAIR = 3
- MODULE (Default : -1)

  If MODULE > 0, then linear combination of A matrix for each pair is

constructed.
- COEFF[N*(0-(M-1))]

  (MODULE > 0 only) First M values corresponds to the first set of
  coefficients for module of A. Following second M values to the second set
  of ...

  M should be equal to NUMPAIR. This leads to totaly considering N
  modules.

> **🛈 Note**
>
> 1. If MININDEX or MAXINDEX is not written in *.in file, automatically set:
>   MININDEX = 0
>   MAXINDEX = [component^(NumAtom in gs-cell) - 1]

4.2.8. gcvc-lsfit.in

Input for lsfit

- NUMCLUSTER

  Number of clusters (including empty) for one structure written in
  CORRELATION file (i.e., clusters by getCluster + empty cluster).
- CLUSTER

  Set of cluster index (empty is always zero) that you want to include for LS-
  fitting. Set of cluster index should be written in a single line.
- FIXCLUSTER

  (Default: -1) If FIXCLUSTER >= 0, energy contribution from ECIs of [cluster
  index = FIXCLUSTER] is subtracted from energies of each structures, and
  then lsfit is performed. This should be used only for debug or special case.
- FIXECI

  (Default: Not required. Only for FIXCLUSTER >=0) ECIs for fixcluster.

4.2.9. gcvc-opt-basis.in

Input for opt-basis

- Tags of TEMPERATURE, MCSTEP are required

  (meaning is the same as gcvc-cmc-conf.in)
- NUMALLCLUSTER

  Number of all clusters (NOT basis!) for ONE structure in CORRELATION
  file

- BASECLUSTER[0-J]

    Cluster indices that are always included in optimized clusters
- NUMADDCLUSTER

    Number of clusters to be added to BASECLUSTER to obtain optimal clusters

    (i.e., total cluster = [BASECLUSTER] + added clusters
- MININDEX

    Minimum cluster index for added clusters.
- MAXINDEX

    Maximum cluster index for added clusters.
- NUMEXCHANGE

    Maximum number of clusters to be exchanged during MC simulation

    (Therefore, NUMEXCHANGE < NUMADDCLUSTER)
- DEFDET (Default: -1.0)

    If DEFDET > 0.0, lower-threshold for allowed determinant in CV-calculation is set to DEFDET. Otherwise, opt-basis automatically determines the threshold.
- LSR (Default: 1.0)

    New set of clusters are accepted only when [squared ls-fitted error: $1/(Nstr)(dEave)^2$] <= [CV-score] * lsr.
- FIXCLUSTER

    (Default: -1) If FIXCLUSTER >= 0, energy contribution from ECIs of [cluster index = FIXCLUSTER] is subtracted from energies of each structures, and then lsfit is performed. This should be used only for debug or special case.
- FIXECI

    (Default: Not required. Only for FIXCLUSTER >=0) ECIs for fixcluster.

> ❶ Note
>
> 1. When your DFT inputs contains single composition, DO NOT include point cluster in BASECLUSTER, since it always results in linear dependence of empty and point correlations.
> 2. When your DFT inputs contains multiple compositions, you should ALWAYS include point cluster in BASECLUSTER except for special reasons.

4.2.10. gcvc-conf-space.in

Input for conf-space

- INDEX : Set of index (start from 0) to choose which row-data are used for conf-space calc.

    Note: When 1st index is negative, then ALL row-data are automatically used.
- MAXMOMENT : (Default: 4) Maximum order of moment to be calculated.

4.2.11. gcvc-cmc-graph.in

Input for cmc-graph

- SPINCE, SPINPOSCAR, TEMPERATURE, MCSTEP, AVESTEP, WRITECORR, WRITEENG, INITRAND, MCCELLSIZE, DEFBASIS, PSI

    Meaning are the same as gcvc-cmc-conf.in.
- WRITEGRAPH (Default : +1) : If it has negative value, then graph information is not calculated.

4.2.12. gcvc-wl.in

Input for wang-landau

- SPINCE, SPINPOSCAR, WRITEENG, INITRAND, DEFBASIS, PSI

    Meaning are the same as gcvc-cmc-conf.in.
- WRITESTEP (Default: 10000)

    WL simulation progress is written for every WRITESTEP.
- EMIN

    Minimum energy for WL simulation considered.
- EMAX

    Maximum energy for WL simulation considered.
- NUMBIN

    Number of bins.
- FLATSTEP (Default: 100)

    Flatness of histgram, H(E), is checked for every FLATSTEP.
- FLATNESS (Default: 0.9)

    When H(E) for all possible E satisfies [H(E) >= FLATNESS * (average of H(E))], then WL proceeds next iteration (i.e., renewal f factor).
- LOGFINIT (Default: e=2.718...)

    Initial value of f factor.
- LOGFFIN (Default: $e^{(10^{(-8)})}$=1.00000001)

    Final value of f factor. If f becomes equal or less than LOGFFIN, WL simulation finishes.
- SINGLEFLIP (Default: -1)

If this is > 0, then single-flip WL simulation (i.e., composition variable) is performed. Otherwise, standard two-spin flip (composition is fixed) is performed.

- MACROSTATE (Default: 1)

    If MACROSTATE > 0, then POSCAR of macro-state for each bin is written in macro-state.wl file. Value of MACROSTATE determines number of output structures (as POSCAR) to macro-state.wl file. (Structures having MACROSTATE-lowest energy are written). Therefore, MACROSTATE =1 means writing gs-state POSCAR only.

- FTHRESHOLD (Default: -1.0)

    If FTHRESHOLD > 0: When WL finds new bin (between emin and emax) with current f <= FTHRESHOLD, then log(g(E)) += [value of log(g(E)) for before-flipping state] to acceralate WL simulation. This is not usually recommended except for special reason.

- NUMGS (Default: 2)

    Since final DOS of g(E) takes relative value, g(E_gs) is subtracted from simulated g(E). i.e., Log of practical DOS = log[g(E)] - log[g(E_gs)] + log(numgs). Therefore, numgs means number of degenerated ground-state. If this value is unknown, please first use the default.

4.2.13. gcvc-f-wl.in

Input for f-wang-landau

- TEMPERATURE

    Meaning and format is the same as gcvc-cmc-conf.in.

4.2.14. gcvc-wl-2d.in

Input for wang-landau-2d

- SPINCE, SPINPOSCAR, WRITEENG, INITRAND, DEFBASIS, PSI, WRITESTEP, FLATSTEP, FLATNESS, LOGFINIT, LOGFFIN, SINGLEFLIP, FTHRESHOLD, NUMGS

    Meaning are the same as gcvc-wl.in.

- MAXSTEP (Default = -1)

    If maxstep > 0 and WL-step > maxstep, then WL simluation go to next iteratio regardless that H(E) does not get flat.

- NUMBIN

    Number of bins along one coordination (i.e., Total number of bins in 2d space is NUMBIN * NUMBIN)

- XMIN

    Minimum value of 1st correlation

- XMAX

    Maximum value of 1st correlation

- YMIN

    Minimum value of 2nd correlation

- YMAX

    Maximum value of 2nd correlation

- XBASIS (Default = 0)

    Specifying which basis-indes set is used for 1st correlation.
    e.g., If the cluster has basis indes set of (1,1,1), (1,1,2), (1,2,2) and (2,2,2), XBASIS = 0 is (1,1,1), XBASIS = 2 is (1,2,2).
    Therefore, for binary system, default value should be used.

- YBASIS (Default = 0)

    Specifying which basis-indes set is used for 2nd correlation.

> **❶ Note**
>
> 1. Cluster indices used for wang-landau-2d are specified by ecicar file.

4.2.15. gcvc-cmc-conf.in, gcvc-cmc-conf-div.in

Input for cmc-conf: configurational MC simulation (canonical). gcvc-cmc-conf.in for cmc-conf, and gcvc-cmc-conf-div.in for cmc-conf-div

- SPINCE, SPINPOSCAR

    Meaning is the same as gcvc-basis-*.in.

- TEMPERATURE[0-J]

    Temperature for MC.
    If more than three element, it means: [Tinit, stepT, Tfin, Tinit, stepT, Tfin, ...] (When stepT < 0 and Tinit < Tfin, cmc-simulation with incrase of temperature is performed, and when stepT >0 and Tinit > Tfin, vice versa.)
    If one element, it just means: Temperature.

- MCSTEP

    Number of MC-steps per site for annealing temperature

- AVESTEP

    Number of MC-steps per site for final (i.e., taking average) temperature

- WRITECORR (Default = 0)

    If WRITECORR > 0, write correlations for each MC-step at annealing

temperature to corr.cmc file. WRITECORR should be integer value.

- WRITEENG (Default = 0)
  If WRITEENG > 0, write energy for each MC-step at annealing temperature to energy.cmc file. WRITEENG should be integer value.
- INITRAND (Default = +1)
  If INITRAND < 0, initialization of random-number seed is NOT performed. In this case, MC always has the same result.
- MCCELLSIZE (cmc-conf-div only)
  If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform MC simulation within 2x1x1 supercell, then write:
    "2 4 4" (i.e., 4/2, 4/1, 4/1).
- DEFBASIS (Default : -1)
  If DEFBASIS = 1, user-defined basis function (specified by PSI) is used to calculate correlation functions.
- PSI[0-(J^2-1)] (Default : not required)
  The first J-components are coefficients of sigma^0, sigma^1, sigma^2, ..., sigma^(J-1) for basis_0.
  The second J-components are coefficients of sigma^0, sigma^1, sigma^2, ..., sigma^(J-1) for basis_1.
  The third ... ... for basis_2.
  ...
- MAXDECUT (Default : -1.0)
  If MAXDECUT > 0.0, MC step with dE >= MAXDECUT is skipped, then goto next loop. (stepSum does NOT increase).

4.2.16. gcvc-cmc-conf-fix.in

Input for cmc-conf-fix

Tags of SPINCE, SPINPOSCAR, TEMPERATURE, MCSTEP, AVESTEP, WRITECORR are required
  (meaning is the same as gcvc-cmc-conf.in)
One additional tag is:

- FIXPOINTS[0-J]
  Specifying set of lattice points whose occupation is kept fixed to initial configuration during MC simulation.
  Index of lattice points is based on POSCAR.cluster, and index starts from "0".

4.2.17. gcvc-cmc-conf-pmb.in

Input for cmc-conf-pmb

Tags of SPINCE, SPINPOSCAR, TEMPERATURE, MCSTEP, AVESTEP are required.
  (meaning is the same as gcvc-cmc-conf.in)
There are three additional tags:

- CLUSTERINDEX
  Cluster index (based on getCluster. 0 is empty.) for pmb calculation
- BASISINDEX
  Integer value to specify basis index with cluster=CLUSTERINDEX for pmb calculation.
  In the case of ternary system and pair cluster, we have basis index of (1,1), (1,2) and (2,2).
  When you want to perform pmb calculation for (1,2), BASISINDEX = 1. ((1,1)=0, (1,2)=1, (2,2)=2).
- PMBASIS
  Value of basis function for cluster=CLUSTERINDEX and basis=BASISINDEX for pmb calculation.

4.2.18. gcvc-gcmc-conf.in

Input for gcmc-conf

- SPINCE, SPINPOSCAR[0-(K-1)], TEMPERATURE, MCSTEP, AVESTEP, WRITECORR, WRITEENG, INITRAND, DEFBASIS, PSI, MAXDECUT
  Meaning is the same as gcvc-cmc-conf.in.
- MU[0-(K-1)]
  Chemical potential for constituent elements for K-component system.
  Order is the same as SPINPOSCAR.

4.2.19. gcvc-stat-cluster.in

Input for stat-cluster

- STATFLAG (Default: 1)
  If STATFLAG = 0, statistical information calculation (average, variance, covariance etc.) is NOT performed.

- CORRINDEX[0-J]

  Set of correlation index where statistical information are calculated.

  Index is based on corr.cmc (i.e., 1st-row of corr.cmc is 0, 2nd-row is 1, ...)
- PFLAG (Default: -1)

  If PFLAG > 0, then calculate partial average (i.e., q > qmean) of correlations for data-indices = CORRINDEX. Value of qmean for each index are specified by PMB.
- PMB[0-J]

  (PFLAG > 0 only) Value of qmean for each data index.
- SIGMA

  When you want to calculate probability distribution of basis function for clusters of CORRINDEX, set SIGMA >= 0.0: Calculate the prob-distribution with gaussian width (=SIGMA) of each data.
- CMIN

  (SIGMA >= 0.0 only) Minimum value of basis function where prob-distribution is calculated.
- CMAX

  (SIGMA >= 0.0 only) Maximum value of basis function where prob-distribution is calculated.
- DC

  (SIGMA >= 0.0 only) One step of basis function for prob-distribution calculation.
- CORRINDEX2[0-1]

  (SIGMA2 >= 0.0 only) Two correlation index where bivariate probability distribution (BPD) is calculated.

  Index is based on corr.cmc (i.e., 1st-row of corr.cmc is 0, 2nd-row is 1, ...)
- SIGMA2

  When you want to calculate BPD for clusters of CORRINDEX2, set SIGMA2 >= 0.0: Calculate the BPD with gaussian width (=SIGMA2) of each data.
- CMIN2

  (SIGMA2 >= 0.0 only) Minimum value of basis function where BPD is calculated.
- CMAX2

  (SIGMA2 >= 0.0 only) Maximum value of basis function where BPD is calculated.
- DC2

  (SIGMA2 >= 0.0 only) One step of basis function for BPD calculation.
- RCORR (Default = 0.0)

  (SIGMA2 >= 0.0 only) Correlation coefficient of bivariate gaussian for

smearing.

> **❶ Note**
>
> 1. 1st-row of corr.cmc obtained by MC simulation is always correlation for empty cluster. So avoid including CORRINDEX of 0 without special reason.
> 2. If stat-cluster code results in core dumped or segmentation fault, check the last line of corr.cmc file.
>   When the last line of corr.cmc contains only linefeed code or EOF, then remove the last line.

4.2.20. gcvc-find-r.in

Input for find-r

- SDE

  Standard deviation (s.d.) of energy for certain cell size (Cell size should be consistent with pmb simulation)
- SDC

  S.D. of (pair) correlation for the cell (Cell size should be consistent with pmb simulation)
- AVEE

  Energy of ideally random state (When PME below is measured from energy of random state, AVEE should be 0)
- AVEC

  (Pair) correlation of ideally random state
- PME

  Energy of special structure whose correlations corresponds to those obtained by cmc-pmb simulation. Unit is [eV / atoms in the above cell size]
- PMC

  (Pair) correlation of special structure whose correlations corresponds to those obtained by cmc-pmb simulation. Value is for the above cell size.
- FRANGE (positive value)

  Factor for integration range of probability density. Integral is performed for [-frange*sigma(E) : frange*sigma(E)]
- MINC

  Minimum value of integration range for correlation.
- MAXC

  Maximum value of integration range for correlation.
- SIGN

When PME and PMC are the "above" pmb value, SIGN >= 0. When they are the "below" value, SIGN < 0.

- MESH
  Number of meshes in one direction to numerically construct E-C distribution. Therefore, total number of mesh is (MESH * MESH).
- DR
  find-r program search optimal R value with grid of r = -1.0 + n * DR. (-1.0 + dr <= r <= 1.0 - dr)
- TEMPERATURE
  Set of temperature where ensemble-averaged (pair) correlation is calculated with optimal R. Interpretation of temperature is the same as cmc-conf.
- RAE (optional)
  Correlation coefficient for property A and energy.
- SDA (optional)
  Standard deviation for property A (Cell size should be consistent with data for SDE and SDC)
- AVEA (optional)
  Property of ideally random state

4.2.21. gcvc-gs-conf.in, gcvc-gs-conf-can.in

Input for gs-conf (gcvc-gs-conf.in) and gs-conf-can (gcvc-gc-conf-can.in)

- SPINCE
  Meaning is the same as gcvc-basis-conf.in.
- MININDEX (Integer)
  0 <= MININDEX < MAXINDEX.
  MININDEX specify minimum index of structure in gs-search.
- MAXINDEX (Integer)
  MININDEX < MAXINDEX <= [component^(NumAtom in gs-cell) - 1] .
  MAXINDEX specify maximum index of structure in gs-search.
- GSCELLSIZE[0-2]
  If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform gs-search within 2x1x1 supercell, then write:
    "2 4 4" (i.e., 4/2, 4/1, 4/1).
- COMPOSITION[0-(J-1)] (gs-conf-can only)
  Write compositions (0.0 - 1.0) for each element. Sequence should be consistent with SPINCE.
- NUMSTR (gs-conf-can only) (Default: -1)

Number of structures having m-th lowest (m <= NUMSTR) energy whose POSCAR is written into poscar.gs file.

- WRITESPIN (gs-conf-can only) (Default: 1)
  If WRITESPIN = 1, write spins on each site to gscar file. Otherwise, spins are NOT written in gscar file.
- WRITECORR (Default: 0)
  If WRITECORR = 1, write correlaions of cluster in ecicar (excluding empty) for all configurations.

> **❶ Note**
>
> 1. If MININDEX or MAXINDEX is not written in *.in file, automatically set:
>   MININDEX = 0
>   MAXINDEX = [component^(NumAtom in gs-cell) - 1]

4.2.22. gcvc-es.in

Input for equiv-str

- SPINCE
  Meaning is the same as gcvc-basis-conf.in.
- SPINPOSCAR[0-(K-1)]
  Spin variables for POSCAR.spin
- ESCELLSIZE[0-2]
  If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform es-search within 2x1x1 supercell, then write:
    "2 4 4" (i.e., 4/2, 4/1, 4/1).

4.2.23. gcvc-ss.in, gcvc-ss-can.in

Input for str-select (gcvc-ss.in) and str-select-can (gcvc-ss-can.in)

- SPINCE[0-(J-1)]
  Meaning is the same as gcvc-basis-conf.in.
- SSCELLSIZE[0-2]
  If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform str-selectwithin 2x1x1 supercell, then write:
    "2 4 4" (i.e., 4/2, 4/1, 4/1).
- NUMSTRADD
  Number of input strutures you want to search.

- TEMPERATURE[0-J]
  - Meaning is the same as gcvc-cmc-conf.in
- SSSTEP
  - Number of steps per site for one temperature. (Total step in one T = ssstep * num-atom in supercell * numstradd)
- ALPHA
  - MWV factor (If alpha < 0, MWV-weight is zero: i.e., statistical ensemble is NOT considered.)
  - Typically, alpha ranges from around 0.8 to 1.2. Larger alpha decrease constraint of melting temperature.
- EQATGSE
  - Ground-state energy at (near or exactly) equiatomic composition. Unit should be per atom.
- EZERO[0-(J-1)]
  - Energy for pure elements. Sequence should be consistent with SPINCE. Unit should be per atom.
- TM[0-(J-1)]
  - Measured melting temperature (K) for pure elements. Sequence should be consistent with SPINCE.
- COMPOSITION[0-(J-1)] (str-select-can only)
  - Write compositions (0.0 - 1.0) for each element.
  - Sequence should be consistent with SPINCE. Note: Number of total (input + add) structures should be larger than number of correlations (with non-zero eci, and excluding empty) in ecicar.

4.2.24. gcvc-qr.in

Input for qr-search

- SPINCE[0-(J-1)]
  - Meaning is the same as gcvc-basis-conf.in.
- QRCELLSIZE[0-2]
  - If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform str-select within 2x1x1 supercell, then write:
    - "2 4 4" (i.e., 4/2, 4/1, 4/1).
- COMPOSITION[0-(J-1)]
  - Write compositions (0.0 - 1.0) for each element. Sequence should be consistent with SPINCE.
- TEMPERATURE[0-J]
  - Meaning is the same as gcvc-cmc-conf.in

- QRSTEP
  - Number of steps per site for one temperature. (Total step in one T = qrstep * num-atom in qr-cell * numstr)
- NUMEXCHANGE
  - Maximum number of atoms in qr-unit cell to be flipped (numexchangex2 atoms are totally flipped) during simulation.
- CUTOFF (CUTOFF > 0.0. Default: Not required)
  - If CUTOFF is specified, qr-search automatically stops when minimum distance becomes less than cutoff.
- LPNORM (Default: 2)
  - LPNORM = 2 means minimize correlation distance for Euclidean metric. Other positive value of LPNORM minimize distance in terms of LPNORM.

4.2.25. gcvc-qrm.in

Input for qrm-search

- SPINCE[0-(J-1)]
  - Meaning is the same as gcvc-basis-conf.in.
- QRCELLSIZE[0-2]
  - If POSCAR.cluster is 4x4x4 extension of unit-cell, and if you want to perform str-select within 2x1x1 supercell, then write:
    - "2 4 4" (i.e., 4/2, 4/1, 4/1).
- COMPOSITION[0-(J-1)]
  - Write compositions (0.0 - 1.0) for each element. Sequence should be consistent with SPINCE.
- TEMPERATURE[0-J]
  - Meaning is the same as gcvc-cmc-conf.in
- QRSTEP
  - Number of steps per site for one temperature. (Total step in one T = qrstep * num-atom in qr-cell * numstr)
- NUMSTR
  - Number of input strutures you want to search.
- READPOS (Default = 0)
  - If READPOS = 1, initial configuration is generated from POSCAR.spin.
  - If READPOS = 0, initial configuration is automatically generated.
- SPINPOSCAR[0-(K-1)] (READPOS = 1 only)
  - Specify spin variables for POSCAR.spin.

ⓘ Note

1. When READPOS = 1, NUMSTR is automatically set to 1 (i.e., single structure search.)

4.2.26. gcvc-qra.in

Input for qrma-search

Tags of SPINCE, QRCELLSIZE, COMPOSITION, TEMPERATURE, QRSTEP, NUMSTR are required. One additional tag is:

- R[0-M]

    Set of values, which are multiplied to correlations in qrccar (except for empty). Write format is the same as TEMPERATURE.

4.2.27. gcvc-qrl.in

Input for qrl-search

Tags of SPINCE, QRCELLSIZE, COMPOSITION, TEMPERATURE, QRSTEP are required. Additional tag is:

- SPINPOSCAR[0-(K-1)]

    Specify spin variables for POSCAR.spin.

4.2.28. gcvc-ca.in

Input for convert-axis

- AXIS0[0-2]

    User-defined 1st lattice vector (in angstrom)
- AXIS1[0-2]

    User-defined 2nd lattice vector (in angstrom)
- AXIS2[0-2]

    User-defined 3rd lattice vector (in angstrom)
- ORIGIN[0-2]

    Origin of user-defined lattice vectors in terms of FRACTIONAL coordinates of POSCAR file.
- EXPANDCELL (Integer value)

    If EXPANDCELL = r, searching new positions for user-defined axis within(2r+1)*(2r+1)*(2r+1) expansion of POSCAR (i.e., from (-r)*axis to (+r)*axis for each direction).

    Use large value of EXPANDCELL (typicall, 2-4) that user-defined cell should be contained in the expanding cell of POSCAR.

4.2.29. gcvc-tp.in

Input for trans-pos

- TRANSLATION[0-2]

    Translation (fractional coordinates), which is added to internal positions in POSCAR.
    The value shoule range from 0.0-1.0.
    If you do NOT want to translate position, write: 0.0 0.0 0.0
- MAGNIFY[0-2]

    Magnification factor, which is multiplied to internal posisions in POSCAR.
    If you do NOT want to magnify position, write: 1.0 1.0 1.0
    Magnification is especially useful to construct interface structure where length of lattice vector normal to the interface is different.

4.3. Other input files

4.3.1. CORRELATION

Input for opt-basis and lsfit

CORRELATION file contains values of basis functions for structures whose scalar property (e.g., energy) is estimated by DFT calculation.
You should write correlations for all clusters obtained by getCluster as well as that for empty.

- The file format for binary system is:

```
structure:001
1
-0.8
- - -
structure:002
1
0.5
- - -
structure:003
- - -
```

You should write "structure:[structure index]" before lines of correlations. Definition of structure index should be the same as enecar or ENERGY file. The 1st line after "structure:[structure index]" line should always be correlation for empty. The following lines are correlations whose sequence should be identical to definition by getCluster.

- The file format for multicomponent (here, ternary for instance) is:

```
structure:001
1
0.5 0.77
1.13 -2.5 0.01
...
structure:002
...
```

The 1st line after "structure:[structure index]" is also correlation for empty. The following lines are correlations with basis index for the clusters. Preferable (not enforced) sequence of correlations in one line is based on lexical order. For instance:

A certain triplet cluster in ternary system has (1,1,1), (2,2,2), (1,1,2), and (1,2,2) basis index.
In this case, sequence of correlations is: corr of (1,1,1), (1,1,2), (1,2,2), (2,2,2).

4.3.2. enecar

Information of DFT energies used for lsfit

Write structure index (definition should be the same as CORRELATION file) and scalar value (e.g., energy) for each line:

```
001 -35.112
002 -40.231
003 -29.872
...
```

If unit of energy is for instance (eV/4-atom), then unit of ECIs and CV score obtained by lsfit or opt-basis is also (eV/4-atom).

4.4. Output files

4.4.1. info-cluster

Detailed cluster information (getCluster)

File format is:

```
...
15  ::  [2.7, 2.7, 3.9 : 1, 2, 2] : (0, 8, 64)
...
```

Here, "15" means cluster index (0 is ALWAYS empty).
"2.7, 2.7, 3.9" means pair distance in the cluster (Therefore, cluster-index 15 is triplet cluster).
"1, 2, 2" means sublattice index (start from 1) in the cluster
"(0, 8, 64)" means representative set of lattice points which form the cluster (index of lattice point is based on POSCAR.cluster)

4.4.2. clucar

Lattice point information forming each cluster (getCluster)

Each line contains set of all lattice points that forms corresponding cluster: e.g., 15-th line in clucar corresponds to 15-th line in dimcar and info-cluster.

4.4.3. dimcar

Dimension and number of clusters (getCluster)

Each line consists of dimension of cluster and number of clusters in POSCAR.cluster.

4.4.4. cogcar

Position of center of gravity for individual clusters (getCluster)

It is used only for VLCE. Usual CE do not use this information.

4.4.5. mccar.conf

Cluster coordination information

mccar.conf is generated from setMC-conf code. This file is used for MC, qr-search and other codes.