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# Files in inputfiles Folder

|  |  |  |
| --- | --- | --- |
| No. | File name | File Contents |
| 1. | inputparameters.in | Input parameters specified by the user for setting up the GCMC simulations |
| 2. | hard\_sphere\_cutoffs.in | Hard sphere potential cutoff distances (Angstrom unit) for each pair of identical and non-identical particle types in the simulation |
| 3. | lennard\_jones\_cutoffs.in | Lennard-Jones potential cutoff distances (Angstrom unit) for each pair of identical and non-identical particle types in the simulation  Note: The Lennard-Jones potential cutoff distances can be specified for each particle pair type using this file. However, the current version uses the keyword LENNARD\_JONES\_CUTOFF (not the file) to specify the same cutoff distance for all particle pairs (typical value is 12.0 Angstrom) |
| 4. | lennard\_jones\_parameters.in | Lennard-Jones parameters for all particle types |
| 5. | square\_well\_parameters.in | Attractive square well potential parameters each pair of ion type and water |
| 6. | particle\_pair\_interactions.in | Matrix table of ones and zeroes to indicate which interactions exist for each pair of identical and non-identical particle types |
| 7. | pid\_init.in | PID parameters for each particle type in the simulation (used only for excess potential calculations) |
| 8. | molar\_mass.in | Molar mass of each particle type (used in PID method) |
| 9. | state\_0 | Initial state configuration of all the particles (ions, solvent) in the simulation box |

Examples of input files can be found in the simulation example folder:./gibs/Simulation\_Examples

# Keywords used in inputparameters.in file

### SIMULATION\_TYPE

|  |  |
| --- | --- |
| Keyword | SIMULATION\_TYPE |
| Purpose | To specify the type of GCMC simulation to run |
| Always used? | YES |
| Allowed values | GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION (For computing the excess chemical potential and mean activity coefficients of individual ions and salt) |
| GCMC\_WITH\_SOLUTE\_ALLATOM\_MODEL (For computing ion/solvent distributions around a fixed solute represented in atomic detail) |
| GCMC\_WITH\_SPHERICAL\_MACROION(For computing ion/solvent distributions around a fixed spherical macroion - this option is not implemented yet.) |
| GCMC\_WITH\_CYLINDRICAL\_POLYION (For computing ion distributions around a fixed cylindrical polyion of finite length - this option is not implemented yet) |
| Example Usage | SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION |

### CAVITY\_GRID\_SPACING

|  |  |
| --- | --- |
| Keyword | CAVITY\_GRID\_SPACING |
| Purpose | To specify the cavity grid spacing (in Angstrom units) to use in the grid insertion algorithm |
| Always Used? | YES |
| Allowed values | Non-zero integer |
| Example Usage | CAVITY\_GRID\_SPACING 0.5 |

### CAVITY\_GRID\_SEGMENTS

|  |  |
| --- | --- |
| Keyword | CAVITY\_GRID\_SEGMENTS |
| Purpose | To specify the number of segments into which the cavity grid cells are divided |
| Always used? | YES |
| Allowed values | Non-zero integer |
| Example Usage | CAVITY\_GRID\_SEGMENTS 1000 |

### SOLUTE\_MODEL\_TYPE

|  |  |
| --- | --- |
| Keyword | SOLUTE\_MODEL\_TYPE |
| Purpose | To specify the type of solute model |
| Always used? | YES |
| Allowed values | none (No solute model in the system)  [Usage requires specifying the following keywords/values]   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION |
| all\_atom  [Description]: Solute represented in atomic detail=  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_SOLUTE\_ALLATOM\_MODEL * SOLUTE\_ALLATOM\_COORDINATE\_FILETYPE * SOLUTE\_ALLATOM\_COORDINATE\_FILENAME |
| cylindrical\_polyion  [Description]: Solute is a cylindrical polyion; e.g., cylindrical model of B-DNA with discrete or continuous charge distribution  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_CYLINDRICAL\_POLYION * POLYION\_CYLINDER\_MONOMER\_LENGTH * POLYION\_CYLINDER\_NUM\_MONOMER * POLYION\_CYLINDER\_CHARGE\_PER\_MONOMER * POLYION\_CYLINDER\_RADIUS * POLYION\_CYLINDER\_LENGTH * SELECT\_POLYION\_CYLINDER\_POTENTIAL |
| spherical\_macroion  [Description]: Solute is a sphere with its center located at the center of  the simulation box, and carrying a charge, MACROION\_SPHERE\_CHARGE, in e units  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_SPHERICAL\_MACROION * MACROION\_SPHERE\_CHARGE * MACROION\_SPHERE\_RADIUS |
| Example Usage | SOLUTE\_MODEL\_TYPE all\_atom |

### SOLUTE\_ALLATOM\_COORDINATE\_FILETYPE

|  |  |
| --- | --- |
| Keyword | SOLUTE\_ALLATOM\_COORDINATE\_FILETYPE |
| Purpose | To specify the format of the file containing the solute's atom coordinates, radius, and charge information |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SOLUTE\_MODEL\_TYPE all\_atom |
| Allowed values | PQR  [Description]: PQR file format |
| XYZR  [Description]: Tab-delimited columns of atom x,y,z, charge and radius values  [Use]: This option is not fully implemented |
| Example Usage | SOLUTE\_ALLATOM\_COORDINATE\_FILETYPE PQR |

### SOLUTE\_ALLATOM\_COORDINATE\_FILENAME

|  |  |
| --- | --- |
| Keyword | SOLUTE\_ALLATOM\_COORDINATE\_FILENAME |
| Purpose | To specify the path and the name of the solute's charge/atom-coordinate file |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SOLUTE\_MODEL\_TYPE all\_atom |
| Allowed values | <path-to-file>/<name-of-the-file>.pqr |
| Example Usage | SOLUTE\_ALLATOM\_COORDINATE\_FILENAME ../../polyA\_polyT\_DNA\_model/polyAT25.pqr |

### USE\_SPM

|  |  |
| --- | --- |
| Keyword | USE\_SPM |
| Purpose | To select whether to use the solvent primitive model, in which the solvent molecules are represented as hard spheres. |
| Always used? | YES |
| Allowed values | YES  [Usage requires specifying the following keywords/values]:   * SOLVENT\_LABEL * SOLVENT\_RADIUS * SOLVENT\_PACKING\_FRACTION <floating point number >= 0.3> * SOLVENT\_EXCESS\_CHEMICAL\_POTENTIAL * SOLVENT\_ION\_ATTRACTION |
| NO |
| Example Usage | USE\_SPM YES |

### USE\_MWATER

|  |  |
| --- | --- |
| Keyword | USE\_MWATER |
| Purpose | To select whether to use the monoatomic water model (Molinero and Moore 2008) |
| Always used? | YES  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES * SOLVENT\_LABEL Water |
| Allowed values | YES |
| NO |
| Example Usage | USE\_MWATER NO |

### USE\_PID

|  |  |
| --- | --- |
| Keyword | USE\_PID |
| Purpose | To use the PID controller method for updating the chemical potential |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION |
| Allowed values | YES |
| NO |
| Example Usage | USE\_PID YES |

### SOLVENT\_LABEL

|  |  |
| --- | --- |
| Keyword | SOLVENT\_LABEL |
| Purpose | To specify the label for identifying the solvent particle type |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES |
| Allowed values | Any string label (use 'Water' if the solvent is water) |
| Example Usage | SOLVENT\_LABEL Water |

### SOLVENT\_RADIUS

|  |  |
| --- | --- |
| Keyword | SOLVENT\_RADIUS |
| Purpose | To specify the radius of solvent hard sphere (in Angstrom) |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES |
| Allowed values | floating point number (double), typical value for water is 1.4 Angstrom |
| Example Usage | SOLVENT\_RADIUS 1.4 |

### SOLVENT\_PACKING\_FRACTION

|  |  |
| --- | --- |
| Keyword | SOLVENT\_PACKING\_FRACTION |
| Purpose | To specify the solvent packing fraction |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES |
| Allowed values | Floating point number (double) between 0 and 1 |
| Example Usage | SOLVENT\_PACKING\_FRACTION 0.3 |

### SOLVENT\_CONCENTRATION

|  |  |
| --- | --- |
| Keyword | SOLVENT\_CONCENTRATION |
| Purpose | To specify the molar concentration of the solvent |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SOLVENT\_RADIUS * SOLVENT\_PACKING\_FRACTION * X\_LEN * Y\_LEN * Z\_LEN |
| Allowed values | Floating point number (double)  [Use] Currently, this keyword is not used to set the solvent concentration. The solvent concentration is internally calculated using the solvent packing fraction, solvent radius, and the simulation box volume. It is kept if in the future, one desires to directly specify the solvent concentration instead of indirectly calculating it through the solvent packing fraction. |
| Example Usage | SOLVENT\_CONCENTRATION 13.0 |

### SOLVENT\_EXCESS\_CHEMICAL\_POTENTIAL

|  |  |
| --- | --- |
| Keyword | SOLVENT\_EXCESS\_CHEMICAL\_POTENTIAL |
| Purpose | To specify the excess chemical potential of the solvent in kcal/mol units |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES |
| Allowed values | Floating point number (double) |
| Example Usage | SOLVENT\_EXCESS\_CHEMICAL\_POTENTIAL 1.076 |

### SOLVENT\_ION\_ATTRACTION

|  |  |
| --- | --- |
| Keyword | SOLVENT\_ION\_ATTRACTION |
| Purpose | To specify whether to include an attractive (short-range) interaction between solvent and ions |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * USE\_SPM YES |
| Allowed values | YES |
| NO |
| Example Usage | SOLVENT\_ION\_ATTRACTION NO |

### LENNARD\_JONES\_CUTOFF

|  |  |
| --- | --- |
| Keyword | LENNARD\_JONES\_CUTOFF |
| Purpose | To specify the same Lennard-Jones potential cutoff distance (in Angstrom units) for all particle pair types |
| Always used? | NO  Used only if Lennard-Jones interactions are turned on in the particle\_pair\_interactions.in file |
| Allowed values | Floating point number (double), typical value is 12.0 (Angstrom) |
| Example Usage | LENNARD\_JONES\_CUTOFF 12.0 |

### MAXIMUM\_NUMBER\_OF\_PARTICLES

|  |  |
| --- | --- |
| Keyword | MAXIMUM\_NUMBER\_OF\_PARTICLES |
| Purpose | To set the maximum allowed number of particles for pre-allocating the size of arrays and vectors that store particle data |
| Always used? | YES |
| Allowed values | Integer number |
| Example Usage | MAXIMUM\_NUMBER\_OF\_PARTICLES 3000 |

### NUM\_ITER

|  |  |
| --- | --- |
| Keyword | NUM\_ITER |
| Purpose | To specify the total number of iterations for updating excess chemical potential. |
| Always used? | YES |
| Allowed values | Integer number >=1  NUM\_ITER = 1 if the following keyword/value is used   * SIMULATION\_TYPE GCMC\_WITH\_SOLUTE\_ALLATOM\_MODEL     NUM\_ITER = 1 if all the following keywords/values are used   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION * USE\_PID YES     NUM\_ITER > 1 if all the following keywords/values are used   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION * USE\_PID NO |
| Example Usage | NUM\_ITER 1 |

### NUM\_STEPS

|  |  |
| --- | --- |
| Keyword | NUM\_STEPS |
| Purpose | To specify the total number of GCMC steps in the simulation. |
| Always used? | YES |
| Allowed values | Integer number |
| Example Usage | NUM\_STEPS 10000000 |

### NUM\_GCMCCYCL

|  |  |
| --- | --- |
| Keyword | NUM\_GCMCCYCL |
| Purpose | To specify the number of insertion/deletion cycles within a GCMC simulation step. |
| Always used? | YES |
| Allowed values | Integer number  Its value is set to a small number (e.g., 3), if the following keyword/value is used   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION   Otherwise, its value is typically set to the average expected number of total particles in the system |
| Example Usage | NUM\_GCMCCYCL 3 |

### NUM\_MOVCYCL

|  |  |
| --- | --- |
| Keyword | NUM\_MOVCYCL |
| Purpose | To specify the number of single-particle displacement cycles/steps within a GCMC simulation step |
| Always used? | YES |
| Allowed values | Integer number  Its value is set to a small number (typically greater than NUM\_GCMCCYCL), if the following keyword/value is used   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION   Otherwise, its value is set such that at least 50-70% of simulations steps are single-particle displacements. |
| Example Usage | NUM\_MOVCYCL 7 |

### NUM\_EQSTEPS

|  |  |
| --- | --- |
| Keyword | NUM\_EQSTEPS |
| Purpose | To specify the number of GCMC steps for equilibration |
| Always used? | YES |
| Allowed values | Integer number |
| Example Usage | NUM\_EQSTEPS 1000000 |

### MIN\_PTCL\_SPACING

|  |  |
| --- | --- |
| Keyword | MIN\_PTCL\_SPACING |
| Purpose | To specify the minimum spacing (Angstrom) between particles initially placed in the box without the grid-based insertion algorithm |
| Always used? | NO (not used or tested yet - may become deprecated) |
| Allowed values | Floating point number (double) |
| Example Usage | MIN\_PTCL\_SPACING 20.0 |

### INITIAL\_PTCL\_NUMBER

|  |  |
| --- | --- |
| Keyword | INITIAL\_PTCL\_NUMBER |
| Purpose | To set the initial number of particles in the system, when creating the initial state of the system instead of reading the state from a file. |
| Always used? | NO (not used – may become deprecated)  [Usage requires specifying the following keyword/value]:  START\_STATE 0 |
| Allowed values | Integer number |
| Example Usage | INITIAL\_PTCL\_NUMBER 100 |

### START\_STATE

|  |  |
| --- | --- |
| Keyword | START\_STATE |
| Purpose | To set the value (0 or 1) for specifying whether or not to create the initial state configuration of the system or read the state from a file (file name has to be state\_0). |
| Always used? | YES |
| Allowed values | Integer number, 0 or 1  0, if the initial configuration of the particles in the system should be randomly set by the program.  1, if the initial configuration of the particles should be read from a file. |
| Example Usage | START\_STATE 1 |

### RECORD\_PARTICLETYPE\_COUNT

|  |  |
| --- | --- |
| Keyword | RECORD\_PARTICLETYPE\_COUNT |
| Purpose | To set the option to record the count of each particle type in the simulation box after every RECORD\_EVERY\_N\_STEPS GCMC steps |
| Always used? | YES |
| Allowed values | YES  This will create output files in the format ./outputfiles/particlecount\_{particle type label}.out  [Usage requires specifying the following keywords/values]:   * RECORD\_EVERY\_N\_STEPS |
| NO |
| Example Usage | RECORD\_PARTICLETYPE\_COUNT YES |

### RECORD\_MOVE\_ACCEPTANCE\_RATE

|  |  |
| --- | --- |
| Keyword | RECORD\_MOVE\_ACCEPTANCE\_RATE |
| Purpose | To specify whether to record the acceptance rates for GCMC moves |
| Always used? | YES |
| Allowed values | YES  This will create output files,  ./outputfiles/insertion\_acceptance\_rate  ./outputfiles/deletion\_acceptance\_rate  ./outputfiles/displacement\_acceptance\_rate |
| NO |
| Example Usage | RECORD\_MOVE\_ACCEPTANCE\_RATE YES |

### RECORD\_SYSTEM\_ENERGY

|  |  |
| --- | --- |
| Keyword | RECORD\_SYSTEM\_ENERGY |
| Purpose | To specify whether to record the energy of the system (in kcal/mol) after every RECORD\_EVERY\_N\_STEPS GCMC steps |
| Always used? | YES |
| Allowed values | YES  This will create the output file, ./outputfiles/energy.out  [Usage requires other keywords/values to be specified]:  RECORD\_EVERY\_N\_STEPS |
| NO |
| Example Usage | RECORD\_SYSTEM\_ENERGY YES |

### RECORD\_EVERY\_N\_STEPS

|  |  |
| --- | --- |
| Keyword | RECORD\_EVERY\_N\_STEPS |
| Purpose | To set the step period for recording the particle counts and energy |
| Always used? | YES |
| Allowed values | integer number |
| Example Usage | RECORD\_EVERY\_N\_STEPS 100 |

### NUM\_RECORD\_STATES

|  |  |
| --- | --- |
| Keyword | NUM\_RECORD\_STATES |
| Purpose | The number of states to record after equilibration. |
| Always used? | YES |
| Allowed values | integer number |
| Example Usage | NUM\_RECORD\_STATES 20 |

### LOOKUP\_PMF\_DELR

|  |  |
| --- | --- |
| Keyword | LOOKUP\_PMF\_DELR |
| Purpose | To specify the radial distance spacing (in Angstrom) with which the particle pair PMFs are listed in the look up table |
| Always used? | NO  Used only if ion pair PMFs are read from a look up table (Not fully implemented) |
| Allowed values | Floating point number (double) |
| Example Usage | LOOKUP\_PMF\_DELR 0.05 |

### LOOKUP\_PMF\_NUMR

|  |  |
| --- | --- |
| Keyword | LOOKUP\_PMF\_NUMR |
| Purpose | To specify the number of rows in the PMF lookup table |
| Always used? | NO  Used only if ion pair PMFs are read from a look up table (Not fully implemented) |
| Allowed values | Integer number |
| Example Usage | LOOKUP\_PMF\_NUMR 2000 |

### SLOTH\_SORENSEN\_CORRECTION

|  |  |
| --- | --- |
| Keyword | SLOTH\_SORENSEN\_CORRECTION |
| Purpose | To specify the value (0 or 1) for selecting the Sloth-Sorensen correction term in GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION simulation, with the adaptive GCMC algorithm (USE\_PID NO) |
| Always used? | NO  [Usage requires following keywords/values to be specified]:   * SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION * USE\_PID NO |
| Allowed values | Integer number (0 or 1)  0: Do not use Sloth-Sorensen correction term  1: Use the Sloth-Sorensen correction Term. |
| Example Usage | SLOTH\_SORENSEN\_CORRECTION 1 |

### CALCULATE\_SOLUTE\_PARTICLE\_RDF

|  |  |
| --- | --- |
| Keyword | CALCULATE\_SOLUTE\_PARTICLE\_RDF |
| Purpose | To specify whether or not to calculate the solute-particle RDF |
| Always used? | NO  [Usage requires specifying other keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_SOLUTE\_ALLATOM\_MODEL |
| Allowed values | YES  This option will create output files as ./outputfiles/rdf\_solute\_{particle type label}.out  [Usage requires specifying other keywords/values]:   * RDF\_MAX\_DISTANCE * RDF\_BIN\_SIZE * NUM\_RDF\_BINS * RDF\_REF * RDF\_REF\_AXIS\_LENGTH\_FRACTION * CYLINDRICAL\_RDF\_AXIS\_DIRECTION |
| NO |
| Example Usage | CALCULATE\_SOLUTE\_PARTICLE\_RDF YES |

### CALCULATE\_PARTICLE\_PAIR\_RDF

|  |  |
| --- | --- |
| Keyword | CALCULATE\_PARTICLE\_PAIR\_RDF |
| Purpose | To specify whether or not to calculate the particle pair RDFs. |
| Always used? | YES |
| Allowed values | YES  This option will create output files as ./outputfiles/rdfpair\_{particle pair type label}.out  [Usage requires specifying other keywords/values]:   * RDF\_MAX\_DISTANCE * RDF\_BIN\_SIZE * NUM\_RDF\_BINS |
| NO |
| Example Usage | CALCULATE\_PARTICLE\_PAIR\_RDF NO |

### RDF\_MAX\_DISTANCE

|  |  |
| --- | --- |
| Keyword | RDF\_MAX\_DISTANCE |
| Purpose | To specify the maximum radial distance (in Angstrom units) within which the RDFs are computed. |
| Always used? | NO  [Usage requires specifying one of the following keywords/values]:   * CALCULATE\_SOLUTE\_PARTICLE\_RDF YES * CALCULATE\_PARTICLE\_PAIR\_RDF YES |
| Allowed values | Floating point number (double)  The specified value is used only if the following keyword/value is set as  RDF\_BIN\_SIZE 0  Otherwise, it is internally computed. |
| Example Usage | RDF\_MAX\_DISTANCE 45 |

### RDF\_BIN\_SIZE

|  |  |
| --- | --- |
| Keyword | RDF\_BIN\_SIZE |
| Purpose | To specify the bin size for calculating the radial distribution functions (RDFs). |
| Always used? | NO  [Usage requires specifying one of the following keywords/values]:   * CALCULATE\_SOLUTE\_PARTICLE\_RDF YES * CALCULATE\_PARTICLE\_PAIR\_RDF YES |
| Allowed values | Any floating point number (double) greater than or equal to zero  If the value is zero, it is computed internally based on the number of bins (NUM\_RDF\_BINS) |
| Example Usage | RDF\_BIN\_SIZE 0.5 |

### NUM\_RDF\_BINS

|  |  |
| --- | --- |
| Keyword | NUM\_RDF\_BINS |
| Purpose | To specify the number of bins over which to compute the RDFs |
| Always used? | NO  [Usage requires specifying one of the following keywords/values]:   * CALCULATE\_SOLUTE\_PARTICLE\_RDF YES * CALCULATE\_PARTICLE\_PAIR\_RDF YES |
| Allowed values | Integer number  The specified value is used only if the following keyword/value is set as  RDF\_BIN\_SIZE 0  Otherwise, it is internally computed. |
| Example Usage | NUM\_RDF\_BINS 90 |

### RDF\_REF

|  |  |
| --- | --- |
| Keyword | RDF\_REF |
| Purpose | To compute the RDF from a reference line or from a reference point. |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_SOLUTE\_ATOM\_MODEL |
| Allowed values | AXIS\_OF\_CYLINDER  This value is used to calculate the cylindrical RDF where the reference line is the cylindrical axis of a solute (e.g., DNA molecule or a cylindrical polyion). |
| CENTER\_OF\_SPHERE  This value is used to calculate the spherical RDF where the reference point is the center of a sphere (atom or spherical macroion) |
| Example Usage | RDF\_REF AXIS\_OF\_CYLINDER |

### RDF\_REF\_AXIS\_LENGTH\_FRACTION

|  |  |
| --- | --- |
| Keyword | RDF\_REF\_AXIS\_LENGTH\_FRACTION |
| Purpose | To specify the fraction of the solute's principal axis length from which the cylindrical RDF is computed. For example, if the solute is B-DNA, one can use a value 1.0 to include the whole length of the B-DNA or a fraction of that length (e.g, 0.8) to minimize Coulombic end-effects. |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * RDF\_REF AXIS\_OF\_CYLINDER |
| Allowed values | Floating point number between 0 and 1 |
| Example Usage | RDF\_REF\_AXIS\_LENGTH\_FRACTION 0.8 |

### CYLINDRICAL\_RDF\_AXIS\_DIRECTION

|  |  |
| --- | --- |
| Keyword | CYLINDRICAL\_RDF\_AXIS\_DIRECTION |
| Purpose | To specify the cylindrical axis direction, perpendicular to which the cylindrical radial distribution functions have to be computed |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * RDF\_REF AXIS\_OF\_CYLINDER * RDF\_REF\_AXIS\_LENGTH\_FRACTION |
| Allowed values | X\_AXIS Used if the longest principal axis of the solute molecule aligns with the x-axis |
| Y\_AXIS  Used if the longest principal axis of the solute molecule aligns with the y-axis |
| Z\_AXIS  Used if the longest principal axis of the solute molecule aligns with the z-axis |
| Example Usage | CYLINDRICAL\_RDF\_AXIS\_DIRECTION Z\_AXIS |

### ION

|  |  |
| --- | --- |
| Keyword | ION |
| Purpose | To specify the ion label, charge (in e units) , radius (in Angstroms), molar concentration (M), and excess chemical potential (in kcal/mol) |
| Always used? | YES |
| Allowed values | ION {ion label} {charge} {radius} {conc} {excess chemical potential} |
| Example Usage | ION Sr 2.0 1.25 0.1 -0.273594  ION Cl -1.0 1.81 0.2 0.8938194 |

### X\_LEN

|  |  |
| --- | --- |
| Keyword | X\_LEN |
| Purpose | To specify the length of the simulation box along x-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number  For excess chemical potential calculations (SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION) use a cubic box (X\_LEN = Y\_LEN = Z\_LEN) |
| Example Usage | X\_LEN 100 |

### Y\_LEN

|  |  |
| --- | --- |
| Keyword | Y\_LEN |
| Purpose | To specify the length of the simulation box along y-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number  For excess chemical potential calculations (SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION) use a cubic box (X\_LEN = Y\_LEN = Z\_LEN) |
| Example Usage | Y\_LEN 100 |

### Z\_LEN

|  |  |
| --- | --- |
| Keyword | Z\_LEN |
| Purpose | To specify the length of the simulation box along z-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number  For excess chemical potential calculations (SIMULATION\_TYPE GCMC\_FOR\_CHEMICAL\_POTENTIAL\_CALCULATION) use a cubic box (X\_LEN = Y\_LEN = Z\_LEN) |
| Example Usage | Z\_LEN 100 |

### HX

|  |  |
| --- | --- |
| Keyword | HX |
| Purpose | To specify the simulation box grid spacing along x-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number (typical value for chemical potential calculations is 1.0) |
| Example Usage | HX 1.0 |

### HY

|  |  |
| --- | --- |
| Keyword | HY |
| Purpose | To specify the simulation box grid spacing along y-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number (typical value for chemical potential calculations is 1.0) |
| Example Usage | HY 1.0 |

### HZ

|  |  |
| --- | --- |
| Keyword | HZ |
| Purpose | To specify the simulation box grid spacing along z-axis in Angstrom units. |
| Always used? | YES |
| Allowed values | Floating point number (typical value for chemical potential calculations is 1.0) |
| Example Usage | HZ 1.0 |

### X\_MIN

|  |  |
| --- | --- |
| Keyword | X\_MIN |
| Purpose | To specify the lowest x-axis value of a right-handed coordinate system, where the leftmost bottom corner of the simulation box is located. |
| Always used? | YES |
| Allowed values | Floating point number (double) |
| Example Usage | X\_MIN -50.0 |

### Y\_MIN

|  |  |
| --- | --- |
| Keyword | Y\_MIN |
| Purpose | To specify the lowest y-axis value of a right-handed coordinate system, where the leftmost bottom corner of the simulation box is located. |
| Always used? | YES |
| Allowed values | Floating point number (double) |
| Example Usage | Y\_MIN -50.0 |

### Z\_MIN

|  |  |
| --- | --- |
| Keyword | Z\_MIN |
| Purpose | To specify the lowest z-axis value of a right-handed coordinate system, where the leftmost bottom corner of the simulation box is located. |
| Always used? | YES |
| Allowed values | Floating point number (double) |
| Example Usage | Z\_MIN -50.0 |

### TEMPERATURE

|  |  |
| --- | --- |
| Keyword | TEMPERATURE |
| Purpose | To specify the temperature in Kelvin units |
| Always used? | YES |
| Allowed values | Floating point number (double) |
| Example Usage | TEMPERATURE 298.0 |

### SOLVENT\_DIELECTRIC

|  |  |
| --- | --- |
| Keyword | SOLVENT\_DIELECTRIC |
| Purpose | To specify the solvent dielectric constant |
| Always used? | YES |
| Allowed values | Floating point number (double) |
| Example Usage | SOLVENT\_DIELECTRIC 78.5 |

### SOLUTE\_DIELECTRIC

|  |  |
| --- | --- |
| Keyword | SOLUTE\_DIELECTRIC |
| Purpose | To specify the solute dielectric constant |
| Always used? | NO  Currently, this keyword is not used. |
| Allowed values | Floating point number (double) |
| Example Usage | SOLUTE\_DIELECTRIC 2.0 |

### MACROION\_SPHERE\_CHARGE

|  |  |
| --- | --- |
| Keyword | MACROION\_SPHERE\_CHARGE |
| Purpose | To specify the charge of the spherical macro-ion (e units), located at its center (0,0,0) |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE spherical\_macroion |
| Allowed values | Floating point number (double) |
| Example Usage | MACROION\_SPHERE\_CHARGE 8.0 |

### MACROION\_SPHERE\_RADIUS

|  |  |
| --- | --- |
| Keyword | MACROION\_SPHERE\_RADIUS |
| Purpose | To specify the radius of the spherical macro-ion (in Angstrom) |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE spherical\_macroion |
| Allowed values | Floating point number (double) |
| Example Usage | MACROION\_SPHERE\_RADIUS 5.0 |

### POLYION\_CYLINDER\_MONOMER\_LENGTH

|  |  |
| --- | --- |
| Keyword | POLYION\_CYLINDER\_MONOMER\_LENGTH |
| Purpose | To specify the length (in Angstrom units) of each monomer unit of the cylindrical polyion |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion |
| Allowed values | Floating point number (double) |
| Example Usage | POLYION\_CYLINDER\_MONOMER\_LENGTH 1.7 |

### POLYION\_CYLINDER\_NUM\_MONOMERS

|  |  |
| --- | --- |
| Keyword | POLYION\_CYLINDER\_NUM\_MONOMERS |
| Purpose | To specify the number of monomers in the cylindrical polyion |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion |
| Allowed values | Non-zero integer  Used to calculate the length of the cylindrical polyion (POLYION\_CYLINDER\_NUM\_MONOMERS x POLYION\_CYLINDER\_MONOMER\_LENGTH) |
| Example Usage | POLYION\_CYLINDER\_NUM\_MONOMERS 10 |

### POLYION\_CYLINDER\_CHARGE\_PER\_MONOMER

|  |  |
| --- | --- |
| Keyword | POLYION\_CYLINDER\_CHARGE\_PER\_MONOMER |
| Purpose | To specify the charge (in e units) per monomer |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion |
| Allowed values | Floating point value (double)  Used to calculate the total charge of the cylindrical polyion (POLYION\_CYLINDER\_NUM\_MONOMERS x POLYION\_CYLINDER\_CHARGE\_PER\_MONOMER) |
| Example Usage | POLYION\_CYLINDER\_CHARGE\_PER\_MONOMER 1.0 |

### POLYION\_CYLINDER\_RADIUS

|  |  |
| --- | --- |
| Keyword | POLYION\_CYLINDER\_RADIUS |
| Purpose | To specify the radius of the cylindrical polyion (in Angstrom) |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keyword/value]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion |
| Allowed values | Floating point value (double) |
| Example Usage | POLYION\_CYLINDER\_RADIUS 8.0 |

### POLYION\_CYLINDER\_LENGTH

|  |  |
| --- | --- |
| Keyword | POLYION\_CYLINDER\_LENGTH |
| Purpose | To specify the length of the cylindrical polyion (in Angstrom). |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keywords/values]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion * SELECT\_POLYION\_CYLINDER\_POTENTIAL 1 |
| Allowed values | Floating point value (double) |
| Example Usage | POLYION\_CYLINDER\_LENGTH 17 |

### SELECT\_POLYION\_CYLINDER\_POTENTIAL

|  |  |
| --- | --- |
| Keyword | SELECT\_POLYION\_CYLINDER\_POTENTIAL |
| Purpose | To specify whether to determine the charges of the cylindrical polyion are discretely or continuously distributed along the cylindrical axis |
| Always used? | NO (not implemented yet)  [Usage requires specifying the following keywords/values]:   * SOLUTE\_MODEL\_TYPE cylindrical\_polyion |
| Allowed values | Integer number, 0 or 1  Value is 0 if a discrete charge of 1 e unit is placed at the center of each monomer. Value is 1 for continuous charge distribution, in which case the interaction energy is computed using the formula for the potential between a cylindrical polyion (continuous charge distribution) and an ion. |
| Example Usage | SELECT\_POLYION\_CYLINDER\_POTENTIAL 1 |

### ELECTROSTATIC\_POTENTIAL\_DX\_MAP

|  |  |
| --- | --- |
| Keyword | ELECTROSTATIC\_POTENTIAL\_DX\_MAP |
| Purpose | To specify the name of the open DX formatted file comprising the solute electrostatic potential values at every grid point. The potential is read in units of kT/e but internally converted to kcal/(mol e). The potential is computed in the absence of ions using an external Poisson solver (APBS). |
| Always used? | NO  [Usage requires specifying the following keywords/values]:   * SIMULATION\_TYPE GCMC\_WITH\_SOLUTE\_ALLATOM\_MODEL * SOLUTE\_MODEL\_TYPE all\_atom |
| Allowed values | <path-to-file-directory>/<file-name>.dx |
| Example Usage | ELECTROSTATIC\_POTENTIAL\_DX\_MAP  ../../polyA\_polyT\_DNA\_model/pot\_polyAT25\_npbe\_pdie2.dx |