Example 2: Calculating Excess Chemical Potential Using the Proportional Integral-Derivative (PID) Controller Approach

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# Example file folders

Uncompress the files listed in the table below, using the command

$ tar –zxvf {filename}.tar.gz

|  |  |
| --- | --- |
| Simulation Examples | Compressed files |
| Example 2 A: Excess chemical potential calculation for 100 mM NaCl, using the Solvent Primitive Model (SPM) | ./gibs/Simulation\_Examples/excess\_chempot\_nacl\_100mM\_PID\_SPM.tar.gz |

# Example 2 A: Excess chemical potential calculation for 100 mM NaCl, using the Solvent Primitive Model (SPM)

In this example, we calculate the excess chemical potential of Na+ and Cl- in 100 mM NaCl water with solvent packing fraction of 0.3 in a 100 Angstrom cube box, using the PID method and the solvent primitive model (SPM).

**Simulation run Directory**: ./gibs/Simulation\_Examples/excess\_chempot\_nacl\_100mM\_PID\_SPM

* Create inputfiles and outputfiles sub-directories
* Output files will be written out in the outputfiles folder
* Copy the input files from Example 1B to the inputfiles directory.

## Setting the parameters in the ./inputfiles/inputparameters.in file

Copy the input files from the first simulation of Example 1B to the inputfiles directory.

**Step 1:** Set the following parameters

USE\_PID YES

NUM\_ITER 1

NUM\_STEPS 16000000

## 

In a 100 Angstrom cube box, a solvent packing fraction of 0.3 corresponds to 22.693 M concentration of water.

## Setting the parameters in ./inputfiles/pid\_init.in file

PARTICLE\_TYPE MU\_EX BI EPSI

Na 0.0 1.0 0.01

Cl 0.0 1.0 0.01

Water 0.0 1.0 0.01

In the PID method, the initial guess values for the excess chemical potential are read from the 2nd column of the pid\_init.in file, and not from the inputparameters.in file. The BI and EPSI are parameters used in the PID algorithm.

## Set the molar masses of each particle type in the ./inputfiles/molar\_mass.in file

PARTICLE\_TYPE MOLAR\_MASS

Na 23.0

Rb 85.47

Sr 87.62

CoHex 160.93

Cl 35.45

Water 18.02

The molar mass is used for computing the target mass density, against which the PID method is used to calibrate the excess chemical potential.

## Setting the hard sphere cut-off distances in ./inputfiles/hard\_sphere\_cutoffs.in file

The hard sphere cut-off distances are set equal to the sum of the hard sphere radii of the particle types.

PARTICLE\_TYPE PARTICLE\_TYPE HARD\_SPHERE\_CUTOFF

Na Na 2.04

Cl Cl 3.62

Water Water 2.80

Na Cl 2.83

Na Water 2.42

Cl Water 3.21

## Setting the types of Interactions in the ./inputfiles/particle\_pair\_interactions.in file

In this example, ions interact via hard sphere repulsions and Coulomb potentials. Ions and water interact via hard sphere repulsions.

ParticleType ParticleType HARD\_SPHERE\_REPULSION COULOMB\_POTENTIAL LENNARD\_JONES\_POTENTIAL SQUARE\_WELL\_POTENTIAL LOOKUP\_TABLE

Na Na 1 1 0 0 0

Cl Cl 1 1 0 0 0

Water Water 1 0 0 0 0

Na Cl 1 1 0 0 0

Na Water 1 0 0 0 0

Cl Water 1 0 0 0 0

## Starting the simulation

To start the simulation in the simulation run folder (if executable file is located in the same folder), do

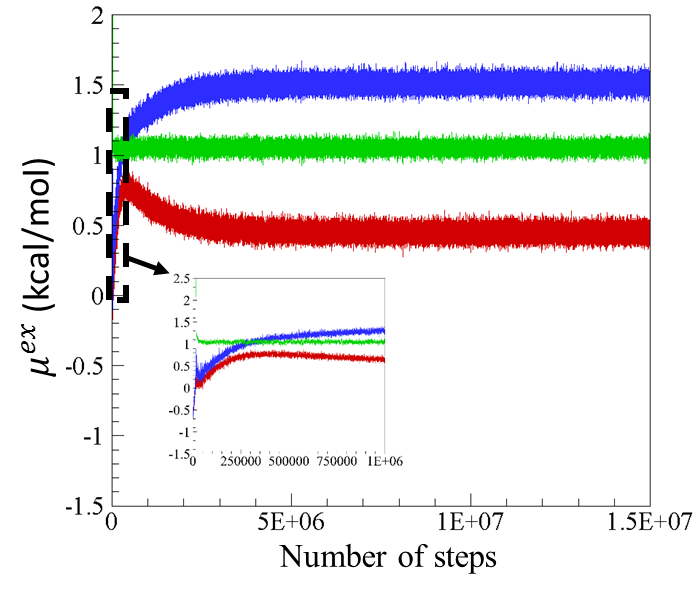
$ ./gibs.exe > run\_2\_13\_2017\_r1.out

The screen output is written out to run\_2\_13\_2017\_r1.out file.

## Checking convergence

In the PID method, the excess chemical potential values are written out in the 4th column of the particlecount\_Na.out, particlecount\_Cl.out, and particlecount\_Water.out files.

The figure below shows the plot of the excess chemical potential () versus number of simulation steps for Na+ (red), Cl- (green), and water (blue) in 100 mM NaCl and water (solvent packing fraction is 0.3, equivalent to 22.693 M in 100 Angstrom cube box). On average, the values start to converge within the first steps. The plot shows the convergence in the excess chemical potential calculation based on the PID method.



## Computing the average excess chemical potential and the number of ions and water molecules

Average excess chemical potential based on the last steps:

kcal/mol

kcal/mol, and

kcal/mol.

Number of Na+ and Cl- ions =

Number of water molecules =