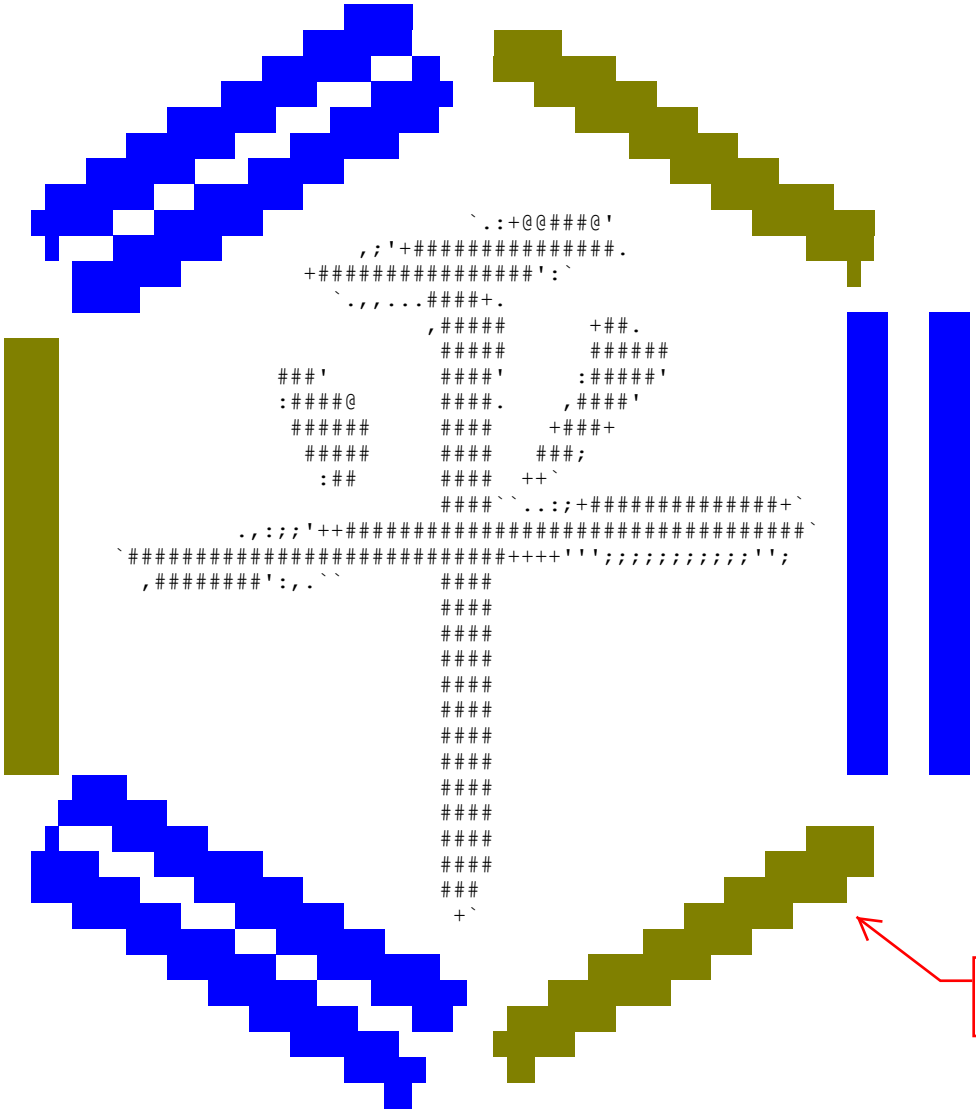
```
#########################################################################
###              Welcome to ForceBalance version 1.0! =D              ###
###                  Force Field Optimization System                  ###
###                       Author: Lee-Ping Wang                       ###
#########################################################################
```

This is an annotated ForceBalance output file. I'm experimenting with this format for creating documentation. - LPW



Sorry for the drab colors.

```
Reading options from file: optimize.in

#########################################################
###  Options at their default values are not printed   ###
###        Use 'verbose_options True' to Enable        ###
#########################################################
Reading force field from file: chlorine.prm

#############################################################
### Starting parameter indices, physical values and IDs ###
#############################################################
   0 [  4.1300e+00 ] : VDWS3
   1 [  3.4000e-01 ] : VDWT3
-------------------------------------------------------------

#########################################################
###    Rescaling Factors (Lower Takes Precedence):    ###
#########################################################
   VDWS                                 : 5.00000e+00
   VDWT                                 : 5.00000e-01
   VDWS                                 : 5.00000e+00
   VDWT                                 : 5.00000e-01
   VDWD                                 : 1.00000e+00
```

The force field file is parsed, and parameters are given names. Throughout the program, force field parameters are referred to by their name.

Scaling factors (i.e. priors) are specified here. This is how much we expect the parameters to vary. Values that are printed lower will take priority. These can be specified in the input file.

```
------------------------------------------------------------

############################################################
###                Setup for force field                 ###
############################################################
priors                    OrderedDict([('VDWS', 5.0), ('VDWT', 0.5), ('VDWD', 1.0)])
constrain_charge          False
------------------------------------------------------------
Backing up: temp/chloroform to: backups/chloroform.0.tar.bz2
There are 940 snapshots in this simulation
QM forces are not present, only fitting energies.

############################################################
###     Setup for fitting simulation chloroform :        ###
############################################################
name                      chloroform
simtype                   ABINITIO_TINKER
simdir                    simulations/chloroform
w_energy                  1.0
------------------------------------------------------------
Backing up: temp/dichloromethane to: backups/dichloromethane.0.tar.bz2
There are 1057 snapshots in this simulation
QM forces are not present, only fitting energies.

############################################################
###   Setup for fitting simulation dichloromethane :     ###
############################################################
name                      dichloromethane
simtype                   ABINITIO_TINKER
simdir                    simulations/dichloromethane
w_energy                  1.0
------------------------------------------------------------
Using parabolic regularization (Gaussian prior) with strength 1.0e-02 (+), 0.0e+00 (x)

############################################################
###            Setup for objective function :            ###
############################################################
penalty_additive          0.01
normalize_weights         False
------------------------------------------------------------

############################################################
###                 Setup for optimizer                  ###
############################################################
jobtype                   NEWTON
trust0                    -0.1
adapt_fac                 0.2
adapt_damp                1.0
err_tol                   0.5
------------------------------------------------------------

############################################################
###                    Main Optimizer                    ###
###       Newton-Raphson Mode (Adaptive Radius)          ###
############################################################

Sim: chloroform      Errors: Energy =   3.2035 kJ/mol (83.7509%) Objective = 7.01422e-01
Sim: dichloromethane Errors: Energy =   2.4220 kJ/mol (64.6000%) Objective = 4.17316e-01

######################################################################
###                  Objective Function Breakdown                  ###
###  Simulation Name          Residual  x  Weight  =  Contribution ###
######################################################################
chloroform                    0.70142      1.000      7.01422e-01
dichloromethane               0.41732      1.000      4.17316e-01
Regularization                0.00000      1.000      0.00000e+00
Total                                               1.11874e+00
----------------------------------------------------------------------
  Step       |k|         |dk|        |grad|       -=X2=-      Stdev(X2)     StepQual
     0   0.000e+00   0.000e+00   3.959e+01   1.11874e+00   0.000e+00        1.000


############################################################
###                   Total Gradient                     ###
```

Settings related to the force field are printed out here.

Settings for each of the fitting simulations (i.e. the reference data set plus the protocol for computing the corresponding MM data) are printed out here.

Settings for the objective function and the optimizer are printed out here. There are lots of options that we read from the input file. You can create an input file using MakeInputFile.py

ForceBalance loops through the data sets, calls TINKER to compute the MM data, and computes parameteric derivatives using finite difference. "Indicators" are printed out to show qualitatively how well the force field is doing.

The objective function components are broken down and displayed.

The "0th" optimization step is complete.

```
#########################################################
   0 [  3.9586e+01 ] : VDWS3
   1 [  7.7870e-01 ] : VDWT3
---------------------------------------------------------

Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 2.5142e-01, result -9.0465e-01
Searching! Hessian diagonal scaling = 1.0000e+01, L =  4.0000e+00, length 2.9139e-02, result -1.7941e-01
Searching! Hessian diagonal scaling = 2.4562e+01, L = -3.8541e+00, length 1.3038e-02, result -7.9462e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 2.5142e-01, result -9.0465e-01
Searching! Hessian diagonal scaling = 4.4377e+00, L = -8.5410e-01, length 5.2243e-02, result -3.4582e-01
Searching! Hessian diagonal scaling = 2.3131e+00, L =  2.1459e+00, length 5.8236e-02, result -5.4259e-01
Searching! Hessian diagonal scaling = 1.0379e+00, L =  8.0526e-01, length 2.0965e-01, result -8.9006e-01
Searching! Hessian diagonal scaling = 1.0010e+00, L =  1.0311e+00, length 2.5025e-01, result -9.0431e-01
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0010e+00, length 2.5142e-01, result -9.0465e-01
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0001e+00, length 2.5142e-01, result -9.0465e-01
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9990e-01, length 2.5142e-01, result -9.0465e-01

#########################################################
###  Mathematical Parameters (Current + Step = Next)   ###
#########################################################
   0 [  0.0000e+00 - 5.3045e-02 = -5.3045e-02 ] : VDWS3
   1 [  0.0000e+00 + 2.4576e-01 =  2.4576e-01 ] : VDWT3
---------------------------------------------------------

#########################################################
###    Physical Parameters (Current + Step = Next)    ###
#########################################################
   0 [  4.1300e+00 - 2.6522e-01 =  3.8648e+00 ] : VDWS3
   1 [  3.4000e-01 + 1.2288e-01 =  4.6288e-01 ] : VDWT3
---------------------------------------------------------
Sim: chloroform      Errors: Energy =   1.4200 kJ/mol (37.1241%) Objective = 1.37820e-01
Sim: dichloromethane Errors: Energy =   1.0311 kJ/mol (27.5013%) Objective = 7.56322e-02

#############################################################################################
###                          Objective Function Breakdown                                 ###
###  Simulation Name          Residual  x  Weight  =  Contribution (Current-Prev)  ###
#############################################################################################
chloroform                     0.13782      1.000      1.37820e-01 ( -5.636e-01 )
dichloromethane                0.07563      1.000      7.56322e-02 ( -3.417e-01 )
Regularization                 0.00063      1.000      6.32127e-04 ( +6.321e-04 )
Total                                                  2.14084e-01 ( -9.047e-01 )
---------------------------------------------------------------------------------------------
  Step       |k|         |dk|        |grad|        -=X2=-      Stdev(X2)     StepQual
     1   2.514e-01   2.514e-01   3.431e+00   2.14084e-01   4.523e-01      1.000


#########################################################
###                  Total Gradient                   ###
#########################################################
   0 [  3.4310e+00 ] : VDWS3
   1 [ -4.1164e-02 ] : VDWT3
---------------------------------------------------------

Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+01, L =  4.0000e+00, length 5.3252e-03, result -4.6582e-03
Searching! Hessian diagonal scaling = 2.4562e+01, L = -3.8541e+00, length 2.1431e-03, result -1.9630e-03
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 4.4377e+00, L = -8.5410e-01, length 1.2293e-02, result -9.7377e-03
Searching! Hessian diagonal scaling = 2.3131e+00, L =  2.1459e+00, length 2.4519e-02, result -1.6378e-02
Searching! Hessian diagonal scaling = 1.0183e+00, L =  8.6475e-01, length 6.1406e-02, result -2.4531e-02
Searching! Hessian diagonal scaling = 1.0011e+00, L =  9.6653e-01, length 6.2640e-02, result -2.4583e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9800e-01, length 6.2721e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9990e-01, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9980e-01, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9911e-01, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9954e-01, length 6.2722e-02, result -2.4586e-02
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9970e-01, length 6.2722e-02, result -2.4586e-02

#########################################################
###  Mathematical Parameters (Current + Step = Next)   ###
#########################################################
   0 [ -5.3045e-02 - 1.3935e-02 = -6.6980e-02 ] : VDWS3
   1 [  2.4576e-01 + 6.1154e-02 =  3.0692e-01 ] : VDWT3
---------------------------------------------------------
```

Print out objective function gradient (also possible to print Hessian)

Line search over Levenberg-Marquardt parameter. Cheap; no derivatives.

The parameter step is printed. Mathematical vs. physical parameters = internal optimization variables vs. physical values. Can be pasted into input file to restart; enclose this with read_mvals and / read_mvals in $options section.

The indicators show better agreement with updated parameters.

The 1st optimization step is complete.

The objective function decreases by less compared to the previous step.

```
#########################################################
###    Physical Parameters (Current + Step = Next)     ###
#########################################################
   0 [  3.8648e+00 - 6.9677e-02 =  3.7951e+00 ] : VDWS3
   1 [  4.6288e-01 + 3.0577e-02 =  4.9346e-01 ] : VDWT3
---------------------------------------------------------
Sim: chloroform      Errors: Energy =   1.3557 kJ/mol (35.4432%) Objective = 1.25622e-01
Sim: dichloromethane Errors: Energy =   0.9402 kJ/mol (25.0778%) Objective = 6.28896e-02

#################################################################################
###                          Objective Function Breakdown                     ###
###  Simulation Name          Residual  x  Weight  =  Contribution (Current-Prev) ###
#################################################################################
chloroform                     0.12562      1.000      1.25622e-01 ( -1.220e-02 )
dichloromethane                0.06289      1.000      6.28896e-02 ( -1.274e-02 )
Regularization                 0.00099      1.000      9.86839e-04 ( +3.547e-04 )
Total                                                  1.89498e-01 ( -2.459e-02 )
---------------------------------------------------------------------------------
  Step       |k|         |dk|       |grad|       -=X2=-     Stdev(X2)    StepQual
     2   3.141e-01   6.272e-02   2.824e-01   1.89498e-01   4.324e-01      1.000


#########################################################
###                   Total Gradient                  ###
#########################################################
   0 [  2.8185e-01 ] : VDWS3
   1 [  1.7923e-02 ] : VDWT3
---------------------------------------------------------

Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 2.4017e-02, result -5.5108e-04
Searching! Hessian diagonal scaling = 1.0000e+01, L =  4.0000e+00, length 2.3749e-03, result -8.7020e-05
Searching! Hessian diagonal scaling = 2.4562e+01, L = -3.8541e+00, length 9.6618e-04, result -3.6289e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 2.4017e-02, result -5.5108e-04
Searching! Hessian diagonal scaling = 4.4377e+00, L = -8.5410e-01, length 5.3600e-03, result -1.8603e-04
Searching! Hessian diagonal scaling = 2.3131e+00, L =  2.1459e+00, length 1.0310e-02, result -3.2508e-04
Searching! Hessian diagonal scaling = 1.0316e+00, L =  8.2231e-01, length 2.3273e-02, result -5.4468e-04
Searching! Hessian diagonal scaling = 1.0002e+00, L =  1.0134e+00, length 2.4012e-02, result -5.5105e-04
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0001e+00, length 2.4017e-02, result -5.5108e-04
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0009e+00, length 2.4017e-02, result -5.5108e-04
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0004e+00, length 2.4017e-02, result -5.5108e-04
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0002e+00, length 2.4017e-02, result -5.5108e-04

#########################################################
###  Mathematical Parameters (Current + Step = Next)  ###
#########################################################
   0 [ -6.6980e-02 - 1.7283e-03 = -6.8708e-02 ] : VDWS3
   1 [  3.0692e-01 - 2.3954e-02 =  2.8296e-01 ] : VDWT3
---------------------------------------------------------

#########################################################
###    Physical Parameters (Current + Step = Next)     ###
#########################################################
   0 [  3.7951e+00 - 8.6415e-03 =  3.7865e+00 ] : VDWS3
   1 [  4.9346e-01 - 1.1977e-02 =  4.8148e-01 ] : VDWT3
---------------------------------------------------------
Sim: chloroform      Errors: Energy =   1.3537 kJ/mol (35.3921%) Objective = 1.25260e-01
Sim: dichloromethane Errors: Energy =   0.9399 kJ/mol (25.0678%) Objective = 6.28395e-02

#################################################################################
###                          Objective Function Breakdown                     ###
###  Simulation Name          Residual  x  Weight  =  Contribution (Current-Prev) ###
#################################################################################
chloroform                     0.12526      1.000      1.25260e-01 ( -3.620e-04 )
dichloromethane                0.06284      1.000      6.28395e-02 ( -5.012e-05 )
Regularization                 0.00085      1.000      8.47883e-04 ( -1.390e-04 )
Total                                                  1.88947e-01 ( -5.511e-04 )
---------------------------------------------------------------------------------
  Step       |k|         |dk|       |grad|       -=X2=-     Stdev(X2)    StepQual
     3   2.912e-01   2.402e-02   7.318e-02   1.88947e-01   1.172e-02      1.000


#########################################################
###                   Total Gradient                  ###
```

```
############################################################
   0 [  7.3117e-02 ] : VDWS3
   1 [  2.9105e-03 ] : VDWT3
------------------------------------------------------------

Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 3.9977e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+01, L =  4.0000e+00, length 3.8939e-04, result -4.5117e-06
Searching! Hessian diagonal scaling = 2.4562e+01, L = -3.8541e+00, length 1.5825e-04, result -1.8799e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 3.9977e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 4.4377e+00, L = -8.5410e-01, length 8.8068e-04, result -9.6608e-06
Searching! Hessian diagonal scaling = 2.3131e+00, L =  2.1459e+00, length 1.6999e-03, result -1.6922e-05
Searching! Hessian diagonal scaling = 1.0318e+00, L =  8.2167e-01, length 3.8710e-03, result -2.8442e-05
Searching! Hessian diagonal scaling = 1.0002e+00, L =  1.0129e+00, length 3.9970e-03, result -2.8776e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0006e+00, length 3.9977e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0046e+00, L =  9.3188e-01, length 3.9787e-03, result -2.8730e-05
Searching! Hessian diagonal scaling = 1.0007e+00, L =  9.7398e-01, length 3.9949e-03, result -2.8771e-05
Searching! Hessian diagonal scaling = 1.0001e+00, L =  9.9006e-01, length 3.9973e-03, result -2.8777e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9728e-01, length 3.9976e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9774e-01, length 3.9977e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9452e-01, length 3.9976e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9623e-01, length 3.9976e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9688e-01, length 3.9976e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9746e-01, length 3.9977e-03, result -2.8778e-05
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9713e-01, length 3.9976e-03, result -2.8778e-05

############################################################
###  Mathematical Parameters (Current + Step = Next)   ###
############################################################
   0 [ -6.8708e-02 - 4.9258e-04 = -6.9201e-02 ] : VDWS3
   1 [  2.8296e-01 - 3.9672e-03 =  2.7899e-01 ] : VDWT3
------------------------------------------------------------

############################################################
###    Physical Parameters (Current + Step = Next)     ###
############################################################
   0 [  3.7865e+00 - 2.4629e-03 =  3.7840e+00 ] : VDWS3
   1 [  4.8148e-01 - 1.9836e-03 =  4.7950e-01 ] : VDWT3
------------------------------------------------------------
Sim: chloroform      Errors: Energy =   1.3538 kJ/mol (35.3945%) Objective = 1.25277e-01
Sim: dichloromethane Errors: Energy =   0.9397 kJ/mol (25.0629%) Objective = 6.28149e-02

################################################################################
###                          Objective Function Breakdown                    ###
###  Simulation Name          Residual  x  Weight  =  Contribution (Current-Prev) ###
################################################################################
chloroform                    0.12528      1.000      1.25277e-01 ( +1.744e-05 )
dichloromethane               0.06281      1.000      6.28149e-02 ( -2.460e-05 )
Regularization                0.00083      1.000      8.26268e-04 ( -2.161e-05 )
Total                                               1.88918e-01 ( -2.878e-05 )
--------------------------------------------------------------------------------
  Step       |k|         |dk|       |grad|       -=X2=-     Stdev(X2)    StepQual
     4   2.874e-01   3.998e-03   1.370e-02   1.88918e-01   2.668e-04      1.000


############################################################
###                   Total Gradient                     ###
############################################################
   0 [  1.3671e-02 ] : VDWS3
   1 [  8.6149e-04 ] : VDWT3
------------------------------------------------------------

Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 1.1685e-03, result -1.4035e-06
Searching! Hessian diagonal scaling = 1.0000e+01, L =  4.0000e+00, length 1.1474e-04, result -2.1789e-07
Searching! Hessian diagonal scaling = 2.4562e+01, L = -3.8541e+00, length 4.6659e-05, result -9.0733e-08
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0000e+00, length 1.1685e-03, result -1.4035e-06
Searching! Hessian diagonal scaling = 4.4377e+00, L = -8.5410e-01, length 2.5921e-04, result -4.6737e-07
Searching! Hessian diagonal scaling = 2.3131e+00, L =  2.1459e+00, length 4.9939e-04, result -8.2081e-07
Searching! Hessian diagonal scaling = 1.0323e+00, L =  8.2028e-01, length 1.1312e-03, result -1.3866e-06
Searching! Hessian diagonal scaling = 1.0002e+00, L =  1.0138e+00, length 1.1683e-03, result -1.4034e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  9.9874e-01, length 1.1685e-03, result -1.4035e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0026e+00, length 1.1685e-03, result -1.4034e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0010e+00, length 1.1685e-03, result -1.4036e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0016e+00, length 1.1685e-03, result -1.4036e-06
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0011e+00, length 1.1685e-03, result -1.4035e-06
```

```
Searching! Hessian diagonal scaling = 1.0000e+00, L =  1.0009e+00, length 1.1685e-03, result -1.4035e-06

##########################################################
###  Mathematical Parameters (Current + Step = Next)   ###
##########################################################
   0 [ -6.9201e-02 - 9.4859e-05 = -6.9296e-02 ] : VDWS3
   1 [  2.7899e-01 - 1.1646e-03 =  2.7783e-01 ] : VDWT3
----------------------------------------------------------

##########################################################
###    Physical Parameters (Current + Step = Next)     ###
##########################################################
   0 [  3.7840e+00 - 4.7429e-04 =  3.7835e+00 ] : VDWS3
   1 [  4.7950e-01 - 5.8231e-04 =  4.7892e-01 ] : VDWT3
----------------------------------------------------------
Sim: chloroform      Errors: Energy =   1.3538 kJ/mol (35.3945%) Objective = 1.25277e-01
Sim: dichloromethane Errors: Energy =   0.9397 kJ/mol (25.0639%) Objective = 6.28199e-02

#####################################################################################
###                         Objective Function Breakdown                          ###
###  Simulation Name          Residual  x  Weight  =  Contribution (Current-Prev) ###
#####################################################################################
chloroform                     0.12528      1.000      1.25277e-01 ( -5.313e-08 )
dichloromethane                0.06282      1.000      6.28199e-02 ( +5.003e-06 )
Regularization                 0.00082      1.000      8.19915e-04 ( -6.354e-06 )
Total                                                  1.88917e-01 ( -1.404e-06 )
-------------------------------------------------------------------------------------
  Step       |k|        |dk|       |grad|       -=X2=-     Stdev(X2)    StepQual
     5   2.863e-01   1.168e-03   3.287e-03   1.88917e-01   1.391e-05      1.000

Convergence criterion reached for objective function (1.00e-04)

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@@@             Final objective function value         @@@
@@@  Full:  1.889170e-01  Un-penalized:  1.880971e-01  @@@
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

##########################################################
###                 Final parameter values             ###
###             Paste to input file to restart         ###
###                  Choose pvals or mvals             ###
##########################################################
read_pvals
   0 [  3.7835e+00 ] : VDWS3
   1 [  4.7892e-01 ] : VDWT3
/read_pvals
read_mvals
   0 [ -6.9296e-02 ] : VDWS3
   1 [  2.7783e-01 ] : VDWT3
/read_mvals
----------------------------------------------------------
```

When convergence criteria are reached, the final parameter values are printed and the force field is saved to the "result" directory.