

GEMC - ANALYSIS

This notebook analyses the results of a simulation.

Setup

Setup Configuration

```
283 ShowMonteCarloOverviewSimuSystem
284 ShowMonteCarloOverviewCstParam
285 ShowExtendedAnalysisTable;
286 markShowCell[EvaluationCell[]];
```

SIMULATION SYSTEM	
Directory	C:\gemc\GEMC - Intramolecular Energy\exampleSimulations\Example_5_Methanol_FS_17000@T450K@ n500_nV100_Ewald-10-12-Inf\

trialMoveAdoption	acceptedPerCycle	eLRMethod	Ewald
trialMoveAdoptionSetpoint	1	eLRCKappa	{10, 10}
trialMoveAdoptionBoundary	0.025	eLRCKRange	{12, 12}
trialMoveAdoptionAvg	10	eLRCes	∞
trialMoveAdoptionLimit	10	rdfDocuMolec	True
trialMoveSpeciesSepcific	True	rdfDocuAtom	True
widomrOvl	0	rdfDocudr	0.01
eqAdjAvrCycles	1000	intraConfigDocu	True
trialMoveAdoptionMaximumSwaps	3000		
trialMoveAdoptionAddMoveChangeType	none		
trialMoveLimitsAdoptionMode	numberMoves		

Initial Conditions

Overview

Show Overview

```
305 ShowMonteCarloOverviewEnvironment@@(simDef[#] &/@ {"system","ensembleType","T","Psys"  
306 ShowMonteCarloOverviewDetails@@(simDef[#] &/@ {"system","nWarmUpCycles","nEquiCycles"  
307 ShowMonteCarloOverviewOPLS@@(simDef[#] &/@ {"system","ffLabelsNonBonded","ffLabelsBon  
308 markShowCell[EvaluationCell[]];
```

ENVIRONMENT			
Ensemble Type	Gibbs Ensemble with constant total Volume		
Components	Methanol		
T [K]	450.		
P [bar]	1.		
	BOX 1	BOX 2	TOTAL
L [Å]	50.0792	34.1347	
V [Å ³]	125595.	39772.9	165368.
ρ [Molecules/Å ³]	7.96212×10^{-4}	1.00571×10^{-2}	3.02357×10^{-3}
v [dm ³ /mol]	0.756349	0.0598795	0.199173
Number of Molecules	100	400	500
Methanol	100	400	500
Mole Fractions			
Methanol	1.	1.	1.

SIMULATION DETAILS		
warm-up cycles	2000	
equilibration cycles	5000	
production cycles	10000	
TRIAL MOVES PER CYCLE		
translations	500	
rotations	500	
volume changes	5	
insertions	250	
ghost insertions	125	
bond stretches	3000	
angle bends	3000	
torsion rotations	500	
total number of moves per cycles	7880	
	BOX 1	BOX 2
cutoff distance [\AA]	25.	17.
overlap distance [\AA]	0.	0.
max translation distance [\AA] Methanol	2.	2.
max rotation angle [rad] Methanol	0.436332	0.436332
max volume change [\AA^3]	397.729	397.729

OPLS-AA DEFINITIONS	
Component	Methanol
non-bonded	O,ROH C,CH ₃ OH and RCH ₂ OH H(C),CH ₃ OH H(C),CH ₃ OH H(C),CH ₃ OH H(O),ROH
bond stretching	{1, 2} → {CT-OH, 0.1} {1, 6} → {HO-OH, 0.1} {2, 3} → {HC-CT, 0.1} {2, 4} → {HC-CT, 0.1} {2, 5} → {HC-CT, 0.1}
angle bending	{2, 1, 6} → {CT-OH-HO, 15.} {1, 2, 3} → {HC-CT-OH, 15.} {1, 2, 4} → {HC-CT-OH, 15.} {1, 2, 5} → {HC-CT-OH, 15.} {3, 2, 4} → {HC-CT-HC, 15.} {3, 2, 5} → {HC-CT-HC, 15.} {4, 2, 5} → {HC-CT-HC, 15.}
torsion	{3, 1, 2, 6} → {alcohol H-C-O-H, 180.} {4, 1, 2, 6} → {alcohol H-C-O-H, 180.} {5, 1, 2, 6} → {alcohol H-C-O-H, 180.}

Simulation Results

General Information

```
323 ShowMonteCarloOverviewSimuSystemResults
324 markShowCell[EvaluationCell[]];
```

GENERAL INFORMATION	
Version (GIT SHA1)	a1ecf23e529dbc1e37e303a1b2ac9188f9e5686a
Timing Method	RepeatedTiming[RandomReal[1, {100, 100, 100}];, 1][[1]]*1000
Timing @ Start [ms]	5.2295
Timing @ End [ms]	4.85244
Total physcal memory @ End [GB]	11.3608 GiB
Total physcal memory @ End [GB]	11.4441 GiB
ESEMBLE AVERAGES	
Average from cycle	5001
Average to cycle	15 000

Evaluation Times

Define Grid

Show Information

```
657 ShowEvalTimesCode
658 ShowEvalTimesPhases
659 NormalizedTiming[]
660 markShowCell[EvaluationCell[]];
```

CODE PARTS					
Part	Time / total	t_{avr} / ms	t_{acc} / ms	t_{rejDu} / ms	t_{rejOv} / ms
Translation	2h 0min 55s	0.853617	0.859169	0.84793	–
Rotation	2h 0min 18s	0.8492	0.855415	0.842664	–
Volume Change	4h 36min 15s	221.008	221.462	220.516	–
Insertion	0h 19min 26s	0.991014	2.41725	0.969219	–
Widom	0h 23min 56s	0.765867	0.765867	–	–
Bond Stretch	11h 16min 6s	0.901485	0.916381	0.88615	–
Angle Bend	11h 35min 39s	0.927536	0.948516	0.905543	–
Torsion	2h 0min 31s	0.964157	1.0022	0.947468	–

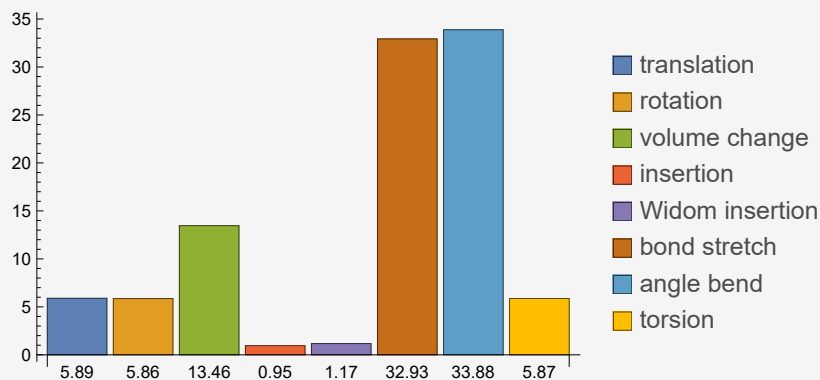
SIMULATION PHASES		
Part	Time / total	Time Fraction
Warm-Up Cycles	0h 29min 36s	1.217%
Equilibration Cycles	13h 36min 59s	33.58%
Production Cycles	26h 26min 6s	65.2%
Trial Move Execution	34h 13min 9s	84.4%
Virial & Tail Correction	5h 32min 30s	13.67%
Documentation	0h 28min 4s	1.15%
Other	0h 18min 57s	0.78%
Total	40h 32min 42s	

Normalized Timing	t'_{avr}	t'_{acc}	t'_{rejDu}	t'_{rejOv}	t' per succ. move
Translation	0.994	1.0	0.987	–	1.96
Rotation	0.988	0.996	0.981	–	1.93
Volume Change	257.	258.	257.	–	495.
Insertion	1.15	2.81	1.13	–	76.6
Widom	0.891	0.891	–	–	0.891
Bond Stretch	1.05	1.07	1.03	–	2.07
Angle Bend	1.08	1.10	1.05	–	2.11
Torsion	1.12	1.17	1.10	–	3.68

```

663 ShowEvalTimesBarChart
664 ExportGraphic["evaluationTimes.pdf",ShowEvalTimesBarChart];
665 markShowCell[EvaluationCell[]];

```



Calculations

Visual Check

Show Boxes

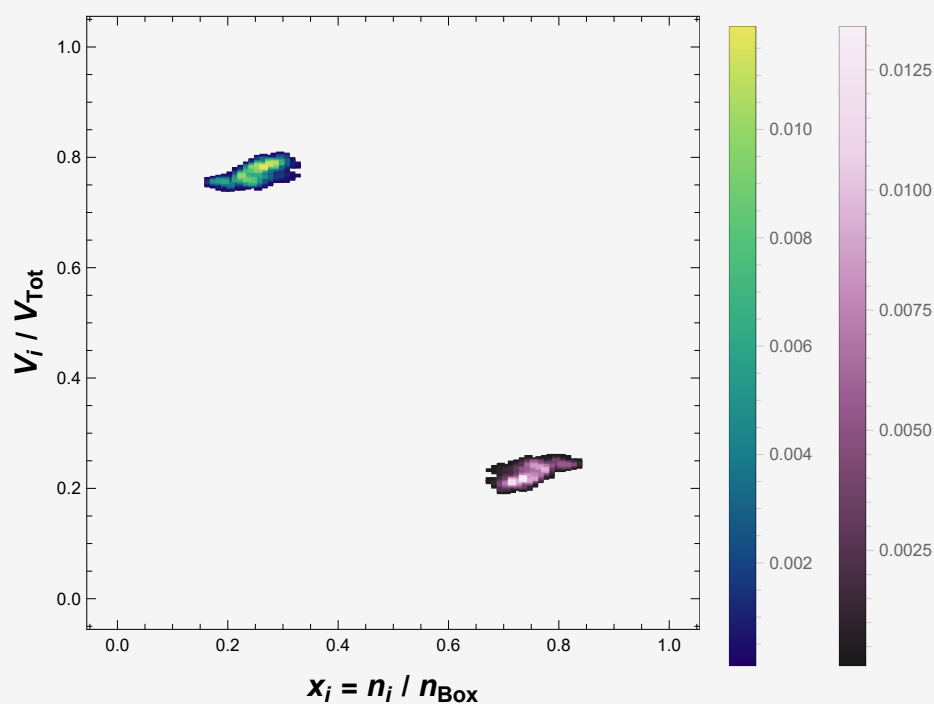
Probability Plot

acc. to (Frenkel 2002, p238)

```

699 Block[{lImageSize = Medium},plotProbabilityCheckV2[]]
700 ExportGraphic["plotProbabilityCheck.pdf",plotProbabilityCheckV2[]];
701 markShowCell[EvaluationCell[]];

```



Show Plots

```

708 (* show line plots with the following cycle range *)
709 plotRange = {1,nDocuCycles}; (* {from,to} or {1,nDocuCycles} to display everything *)
710 (* vertical (values) range *)
711 vertRange = Automatic; (* Automatic → adjust range for most relevant parts | All → in

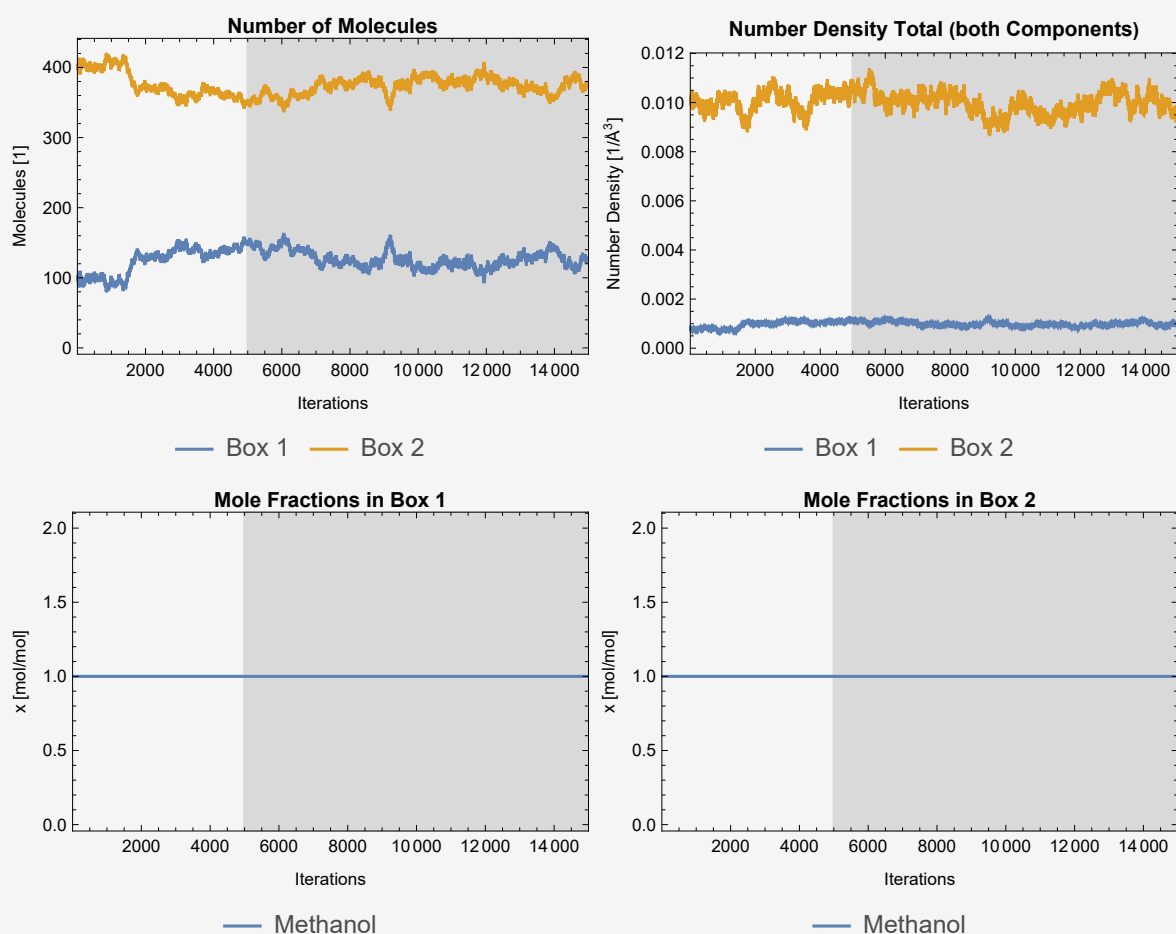
```

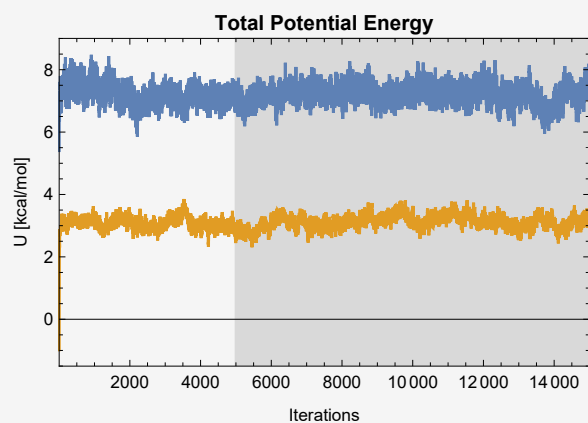
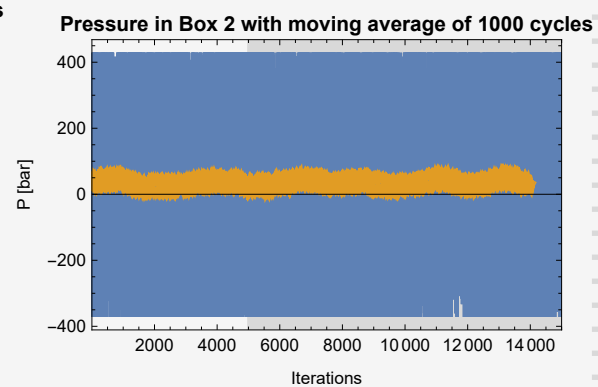
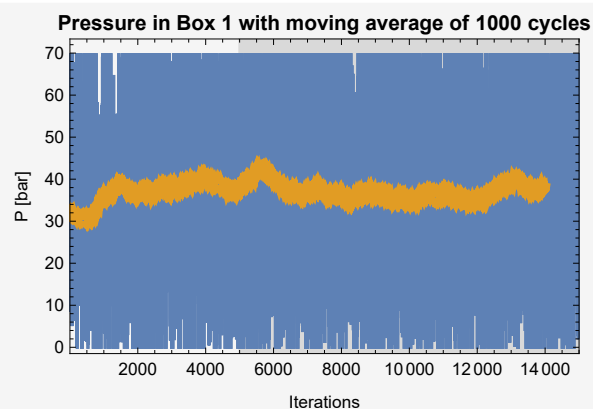
Values

```

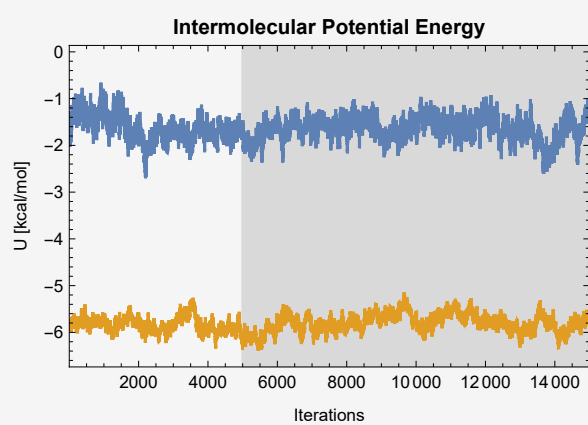
718 plotValuesGrid = Grid[{
719   {plotNumOfMolecules,plotDensityTotal},
720   {plotMoleFractions1,plotMoleFractions2},
721   {plotPressure1,plotPressure2},
722   {plotTotalEnergy},
723   {plotInterEnergy,plotIntraEnergy},
724   {plotVolume,plotMolarVolume}
725 },Alignment→Center, ItemSize→Scaled[0.5]]
726
727 ExportGraphic["plotValues.pdf",plotValuesGrid];
728 markShowCell[EvaluationCell[]];

```

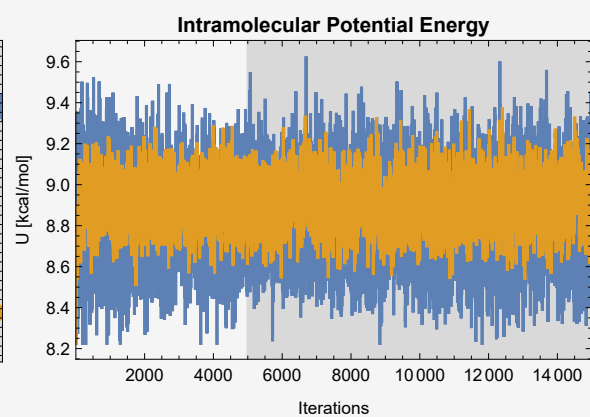




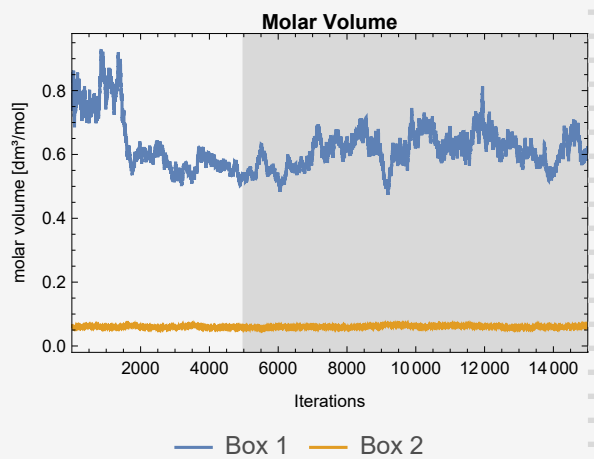
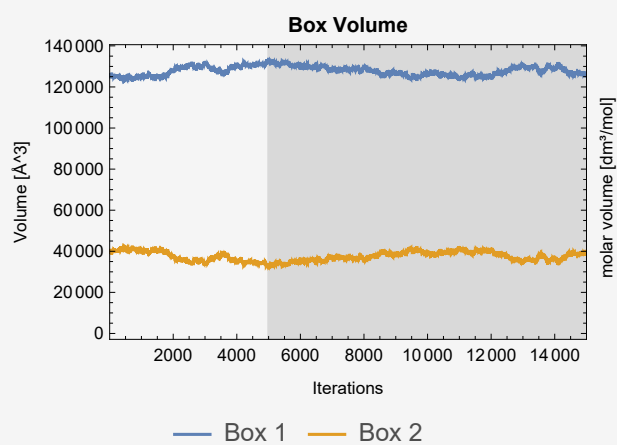
— Box 1 — Box 2



— Box 1 — Box 2



— Box 1 — Box 2

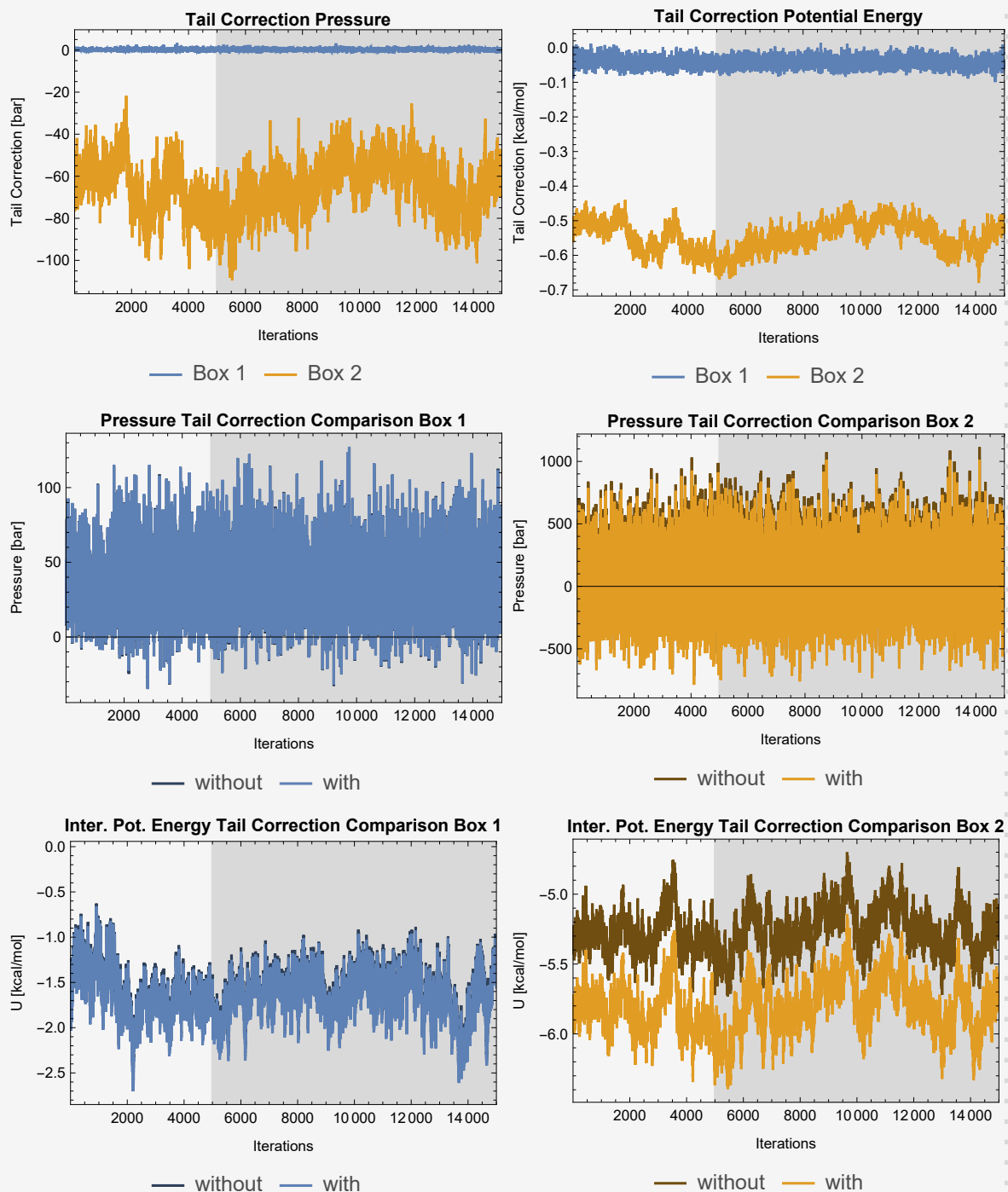


Tail Corrections

```

739 plotTailCorrGrid = Grid[{
740   {plotTailCorrPressure,plotTailCorrEnergy},
741   {plotTailComparisonPressure1,plotTailComparisonPressure2},
742   {plotTailComparisonEnergy1,plotTailComparisonEnergy2}
743 }, ItemSize→Scaled[0.5],Alignment→Center]
744
745 ExportGraphic["plotTailCorr.pdf",plotTailCorrGrid];
746 markShowCell[EvaluationCell[]];

```

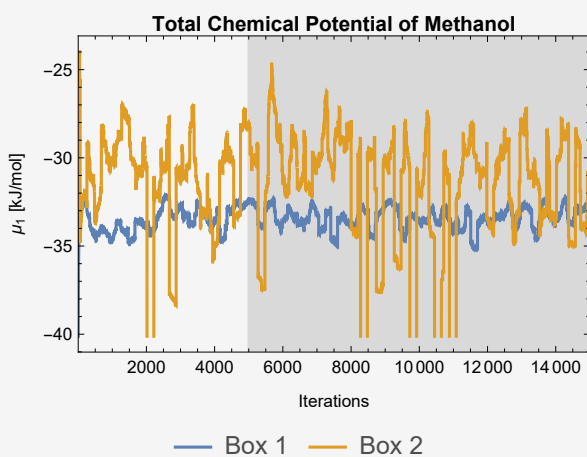
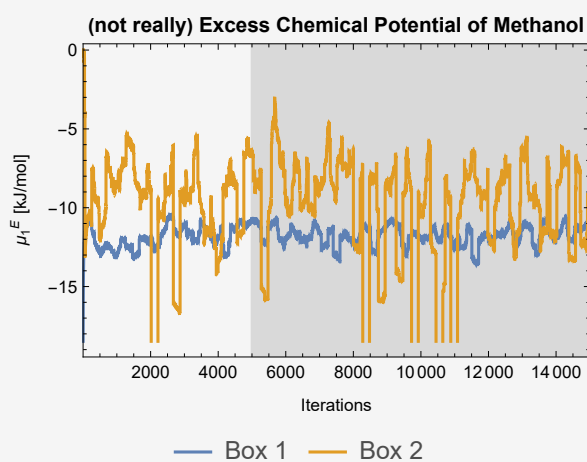
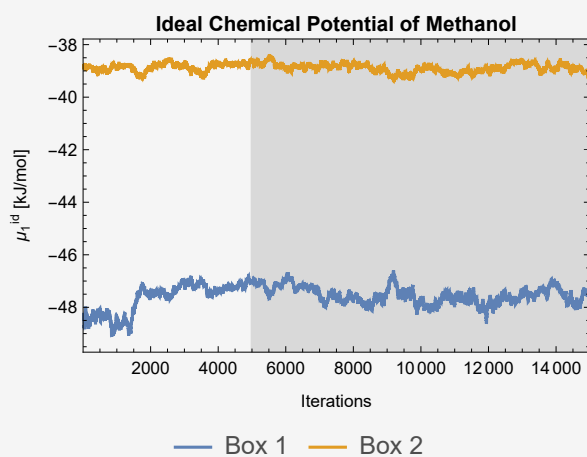


Chemical Potentials

```

753 plotChemPotGrid = Grid[{
754     plotIdealChemPotential,
755     plotExcessChemPotential,
756     plotTotalChemPotential
757 }, ItemSize→Scaled[0.5], Alignment→Center]
758
759 ExportGraphic["plotChemPot.pdf", plotChemPotGrid];
760 markShowCell[EvaluationCell[]];

```



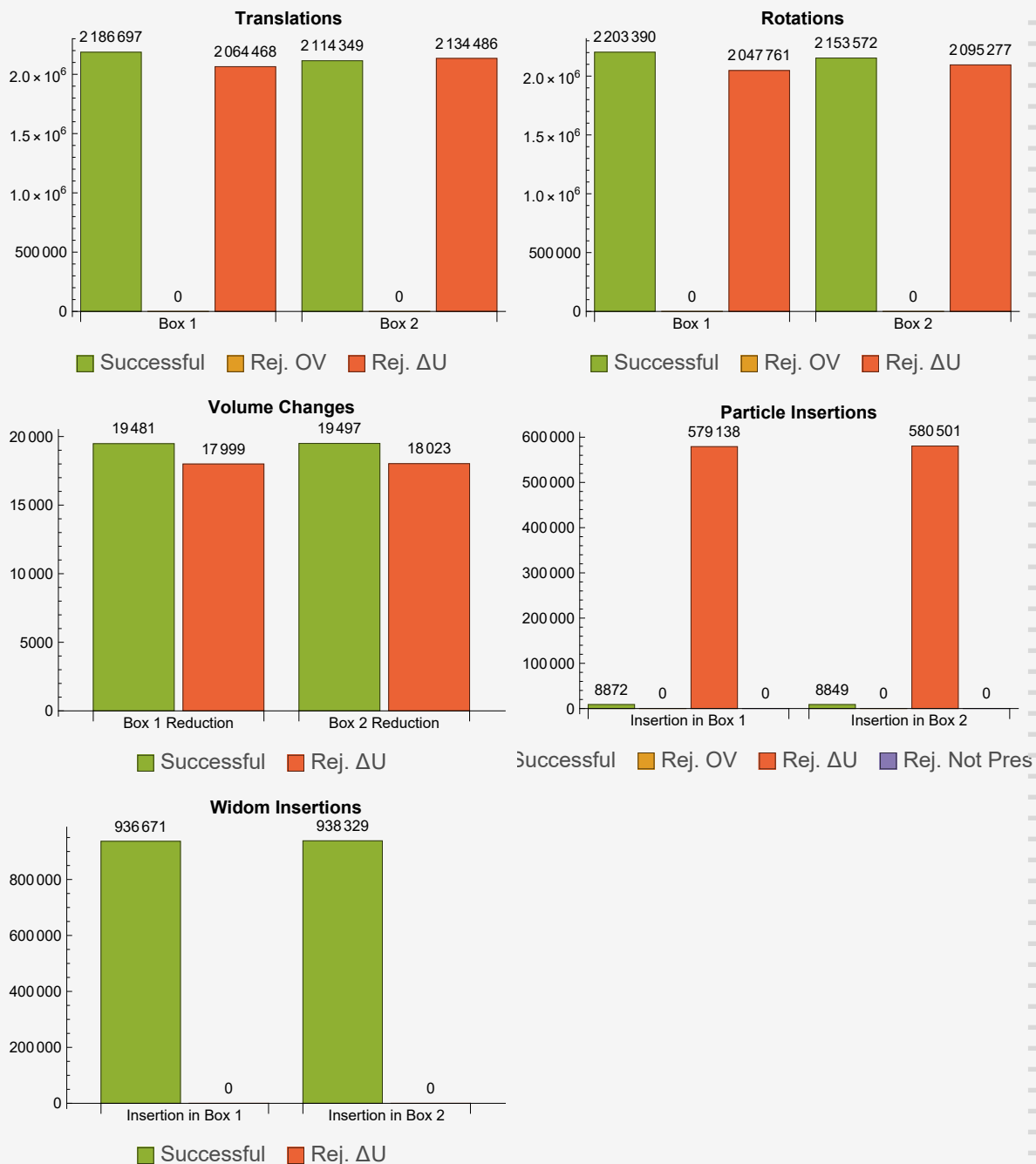
Plot of the Standard Deviation of the molar volume

Counters

```

778 plotCountersGrid
779 ExportGraphic["plotCounters.pdf",plotCountersGrid];
780 markShowCell[EvaluationCell[]];

```



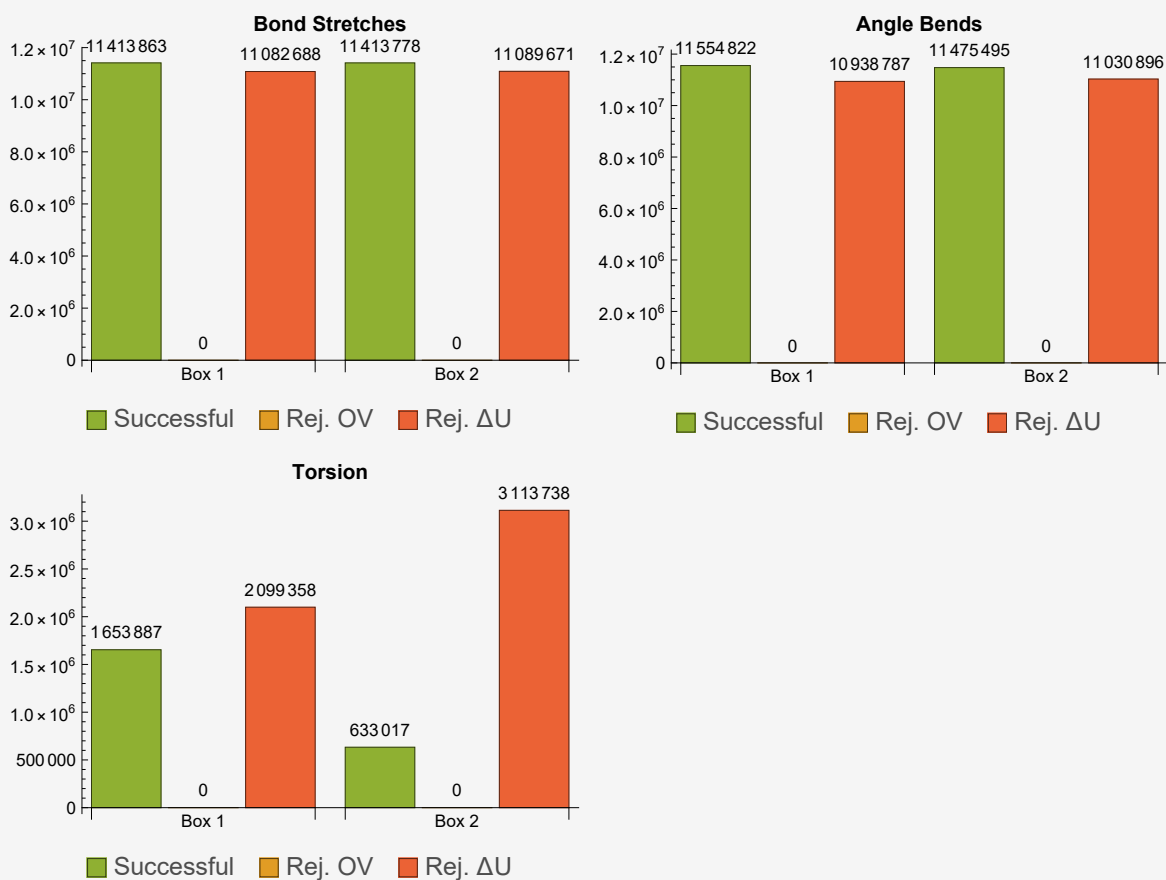
Species specific Counters

```
787 plotSpeciesCountersGrid
788 markShowCell[EvaluationCell[]];
```

No species specific plots if only one species is simulated

Intramolecular Trial Moves

```
795 plotIntraCountersGrid
796 markShowCell[EvaluationCell[]];
```

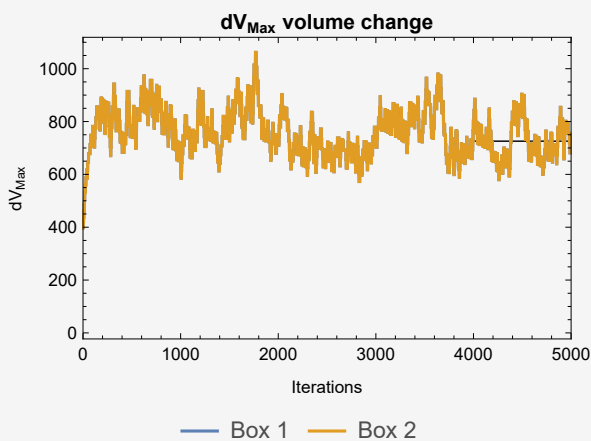
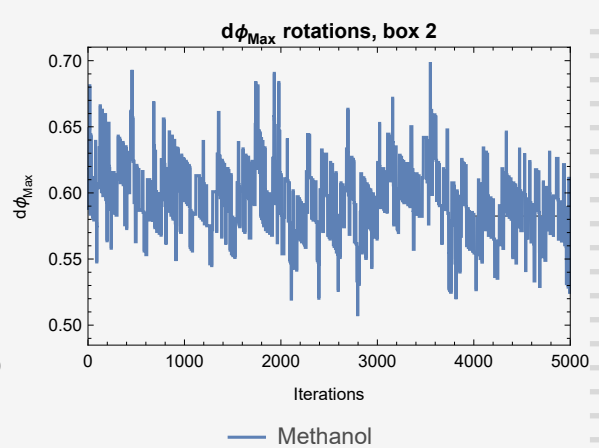
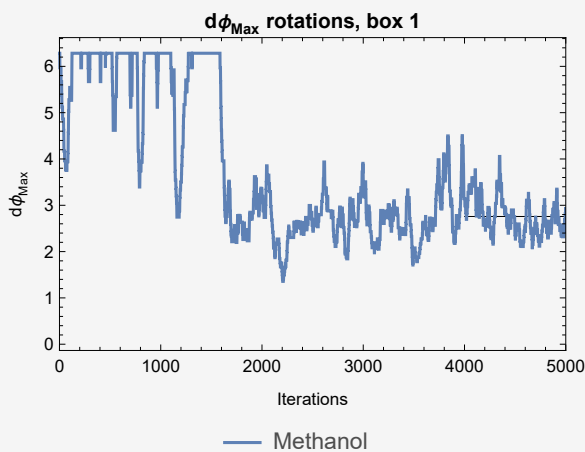
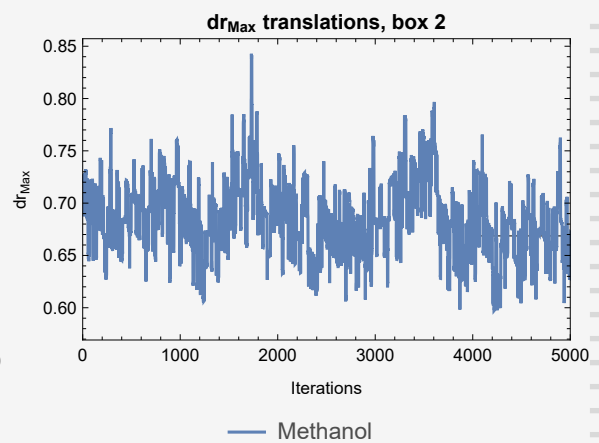
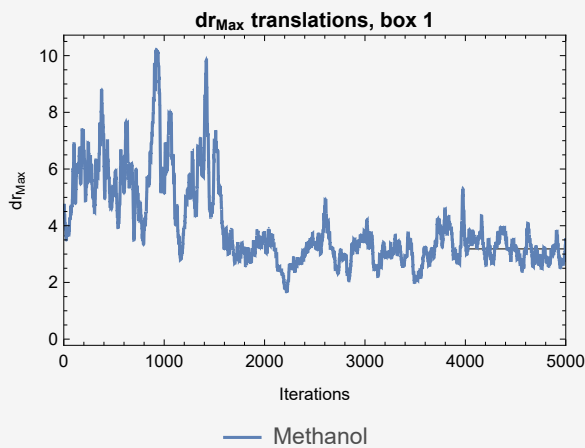


Trial Move Limits Course

```

807 If[ValueQ@transMaxVecDoc,
808   ExportGridGraphic[{"transLimits_box" <> ToString@#, courseTransMax[#]} &/@ boxVec,
809   ExportGridGraphic[{"rotaLimits_box" <> ToString@#, courseRotaMax[#]} &/@ boxVec,
810   ExportGridGraphic[{"volumLimits", courseVolMax[]}], False];
811 markShowCell[EvaluationCell[]];
812 ];

```



```

815 If[nEquiCycles>0, Do[
816     ExportGridGraphic[{"transMax - Box " <> ToString@# <> " " <> system[[iCp]], histo
817     , {iCp, Length@system}]];

820 If[nEquiCycles>0, Do[
821     ExportGridGraphic[{"rotaMax - Box " <> ToString@# <> " " <> system[[iCp]], histoR
822     , {iCp, Length@system}]];

825 If[nEquiCycles>0, ExportGridGraphic[{"volMax - Box " <> ToString@#, histoVolMax[#]} &

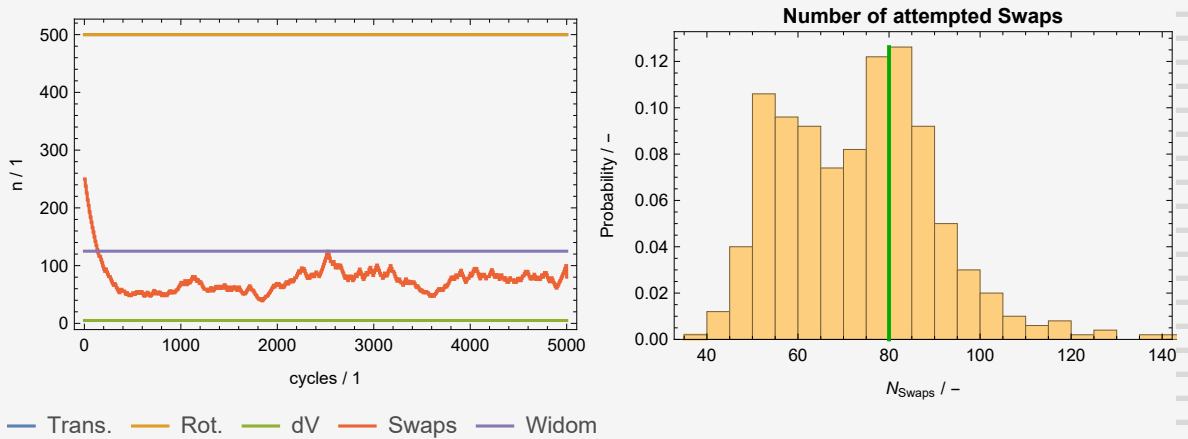
```

Number of Trial Moves

```

832 If[ValueQ@nMovesDocu,
833     ExportGridGraphic[{"TrialMovesCourse", pltCourseTrialMoves[]}, {"TrialMovesHisto
834     markShowCell[EvaluationCell[]];
835 ];

```

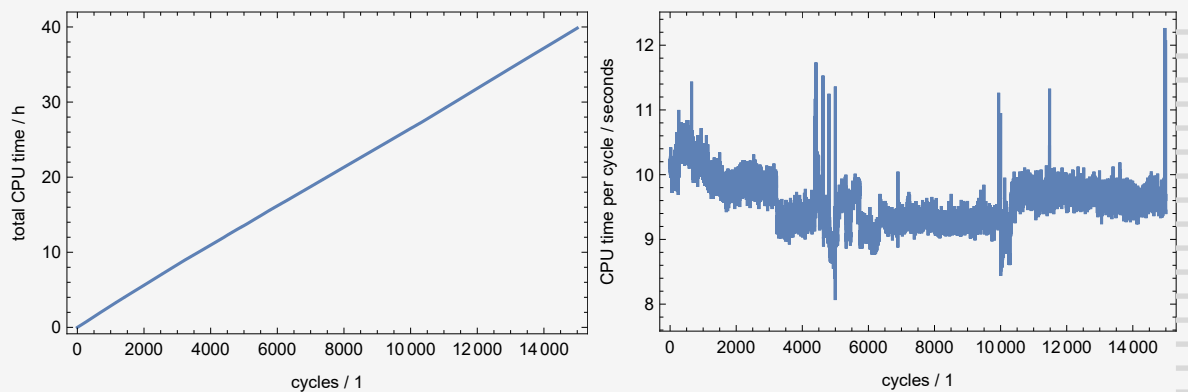


CPU Time Usage

```

842 If[ValueQ@timingCPUList,
843     ExportGridGraphic[{"TimingCPUTotal", pltTimingCPUTotal[]}, {"TimingCPUPerCycle",
844     markShowCell[EvaluationCell[]];
845 ];

```



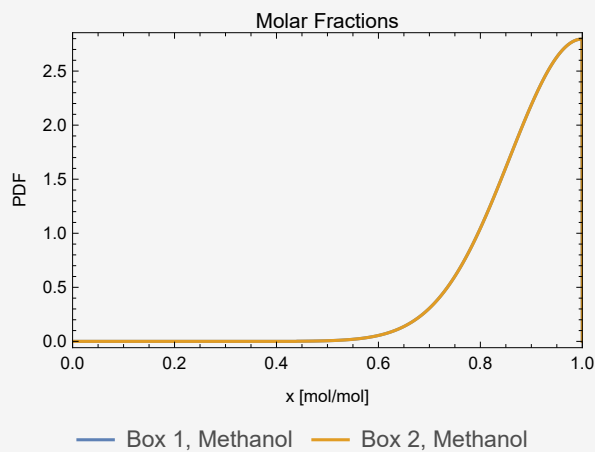
Ensemble Averages

Average Cycles as defined in section "Setup" / "Ensemble Averages"

Density Plots

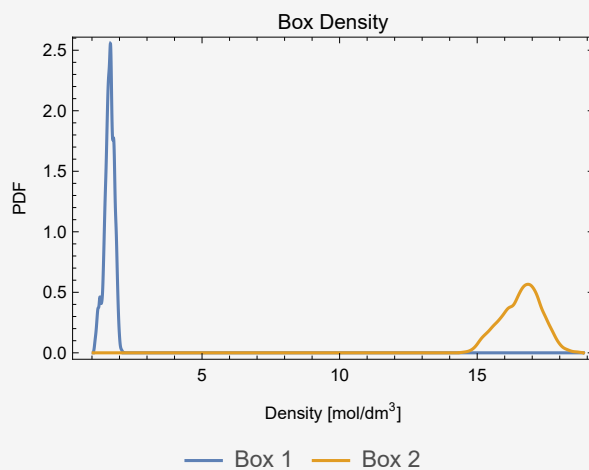
Mole Fractions

```
868 ExportGridGraphic[{"moleFractionsHistogram", plotMolarFractions[]}, False];
869 markShowCell[EvaluationCell[]];
```



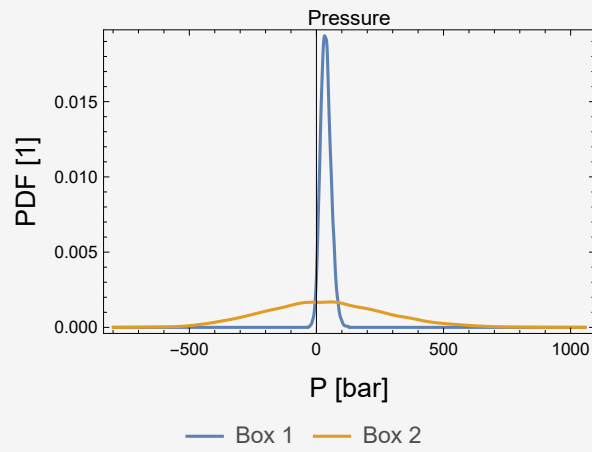
Box Densities

```
876 ExportGridGraphic[{"densityHistogram", plotDensityHistogram[]}, False];
877 markShowCell[EvaluationCell[]];
```



Pressure

```
884 ExportGridGraphic[{"pressureHistogram", plotPressureHistogram[]}, False];  
885 markShowCell[EvaluationCell[]];
```



Averaged Values

```

896 assocResults = <| |>;
897 showAveragedValues
898 ExportGraphic["simResultsAveragedValues.pdf",showAveragedValues];
899 markShowCell[EvaluationCell[]];

```

AVERAGED VALUES				
averaged from 5001 to 15000				
Box V corresponds to Box 1, Box L corresponds to Box 2				
System	Box V		Box L	
	mean	std	mean	std
T [K]	450.	–	450.	–
v [dm ³ / mol]	0.612623	0.0508783	0.0605282	0.00274054
rho [mol / dm ³]	1.64382	0.139118	16.5548	0.743146
n [1]	126.634	11.8813	373.366	11.8813
Pressure				
P ideal [bar]	61.5035	5.20509	619.4	27.8049
P viral [bar]	–24.561	20.7629	–520.122	236.326
P tail [bar]	0.144406	0.596215	–65.2603	12.3399
P [bar]	37.0869	20.5848	34.0175	238.707
Internal Energy				
U Inter [kcal/mol]	–1.63666	0.256684	–5.79603	0.194046
U Intra [kcal/mol]	8.8446	0.193743	8.91538	0.116568
U Total [kcal/mol]	7.20795	0.309855	3.11935	0.218933
Mole Fractions				
Methanol	1.0000	0	1.0000	0
Ideal μ [kJ/mol]				
Methanol	–47.541	0.31340	–38.890	0.16863
Excess μ [kJ/mol]				
Methanol	11.749	0.59651	10.361	3.9575
Total μ [kJ/mol]				
Methanol	–33.394	0.59651	–32.005	3.9575

Reduced Units

```
906 NormalizedUnits[];
907 markShowCell[EvaluationCell[]];
```

name	dimensional	unit	critical norm	
T	450.	K	$T_{\text{red}}=T/T_c$	0.878
p_v	37.1	bar	$p_{\text{red}}=p/p_c$	0.458
p_L	34.0	bar		0.420
ρ_v	1.64	mol / dm ³	$\rho_{\text{red}}=\rho/\rho_c$	0.194
ρ_L	16.6	mol / dm ³		1.95
μ_v	-33.4	kJ / mol	$\mu_{\text{red}}=\mu/\mu_c$	-
μ_L	-32.0	kJ / mol		-

Comparison & Checks

Comparison Functions

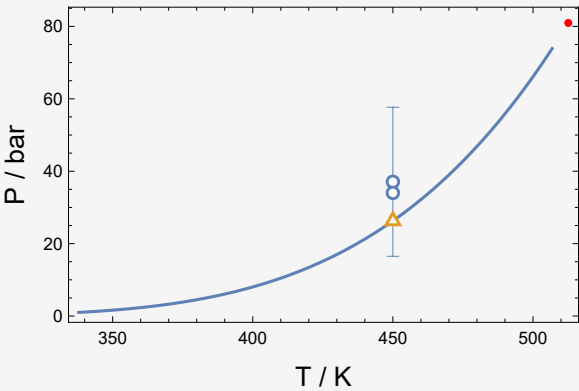
Equation of State Comparison

Comparison to a pure LJ EOS (Thol, 2016), a t-PR-LJ EoS (Harismiadis, 1994) or the SRK EoS

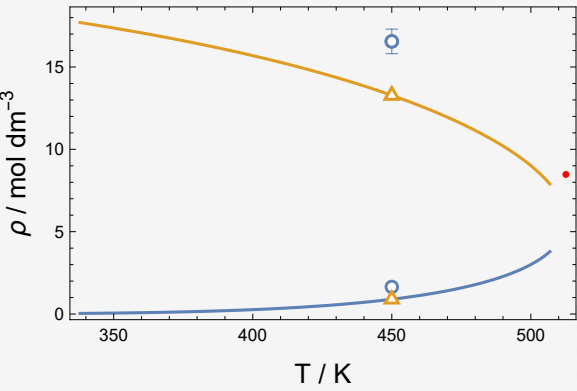
```
1723 CalculateEosComparison[]; Pause[1];
1724 markShowCell[EvaluationCell[]];
```

SRK Comparison, Methanol at T = 450 K
Defintion relative error: $\text{Abs}[\zeta_{\text{Sim}} - \zeta_{\text{EOS}}] / \zeta_{\text{EOS}}$

Unit	Box V			Box L		
	Sim	SRK-EoS	$\Delta_{\text{rel}} / \%$	Sim	SRK-EoS	$\Delta_{\text{rel}} / \%$
$\rho / \text{mol dm}^{-3}$	1.64	0.896	83.5	16.6	13.3	24.7
P / bar	37.1	26.3	41.1	34.0	26.3	29.4



○ Simulation △ SRK EOS ● Critical point



○ Simulation △ SRK EOS ● Critical point

Equilibrate State

```
1731 Showcheckfinalvalues
1732 markShowCell[EvaluationCell[]];
```

Checking minimum particle and length of the simulation	
min 10 particles in gas phase	😊
min 200 particles in liquid phase	😊
gas partilces make up more than 20% of the total particles	😊
Accepted insertions 10 times or more over equilibration period	😊
Accepted insertions 10 times or more over production period	😊

Test specific evaluations

Setup

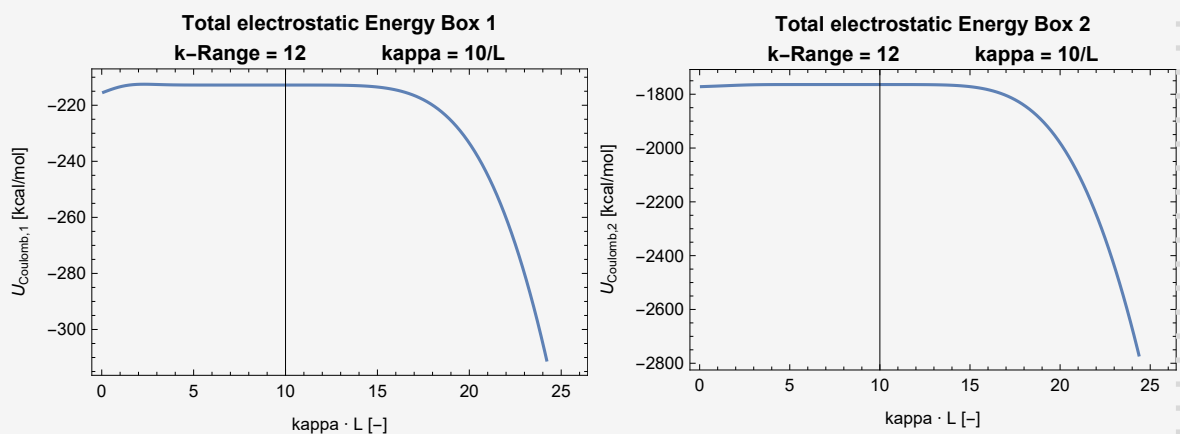
CFC Vlugt

SwapMove Species Choice probabilities

PAN Binary Swaps

Ewald Electrostatic Long-Range Correction

```
1797 If[SameQ[checkGetAssocParameter[custParam, "eLRCEMethod"], "Ewald"],
1798   VisualizeELRCEwald[exportFlag];
1799   markShowCell[EvaluationCell[]];];
```



Wolf Electrostatic Long-Range Correction

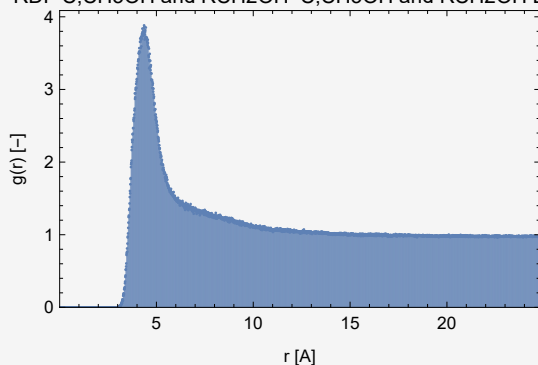
Radial Distribution Function per Atom

```

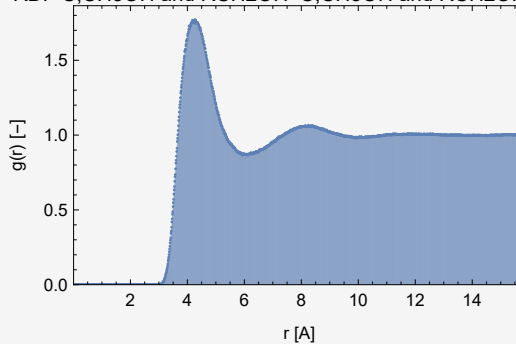
1815 If[checkGetAssocParameter[custParam, "rdfDocuAtom"],
1816     VisualizeRDFAtom[];
1817     markShowCell[EvaluationCell[]];];

```

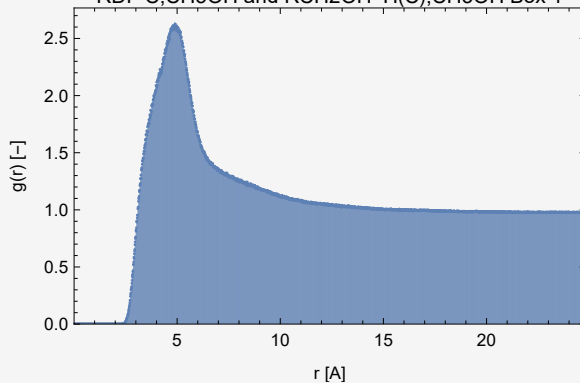
RDF C,CH3OH and RCH2OH-C,CH3OH and RCH2OH Box 1



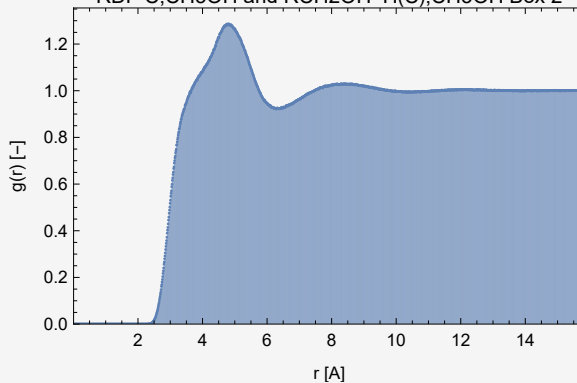
RDF C,CH3OH and RCH2OH-C,CH3OH and RCH2OH Box 2



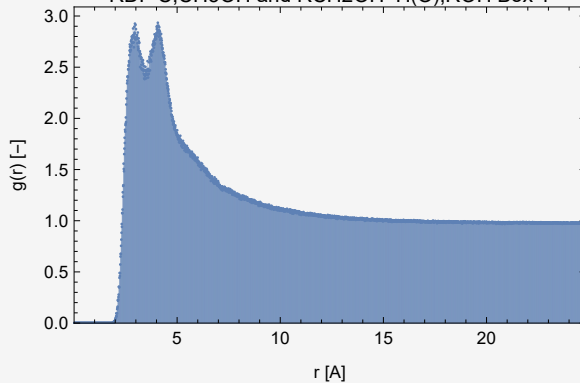
RDF C,CH3OH and RCH2OH-H(C),CH3OH Box 1



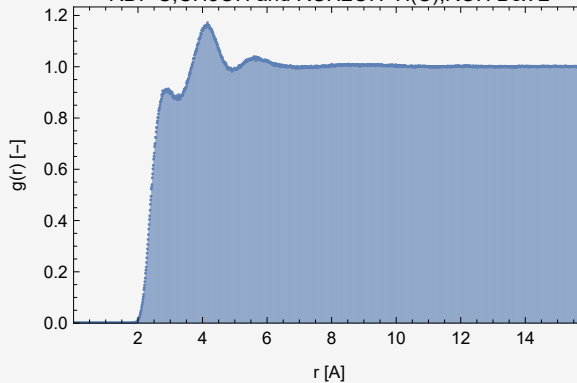
RDF C,CH3OH and RCH2OH-H(C),CH3OH Box 2

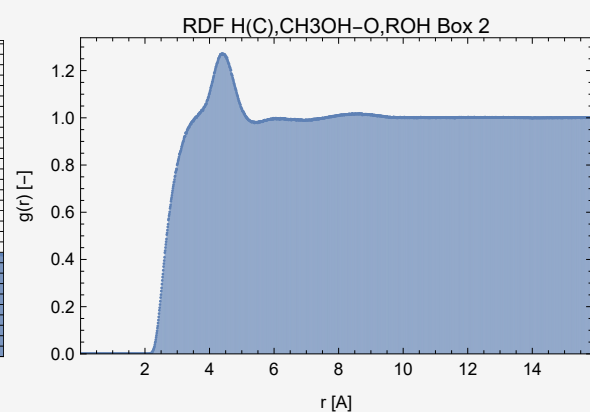
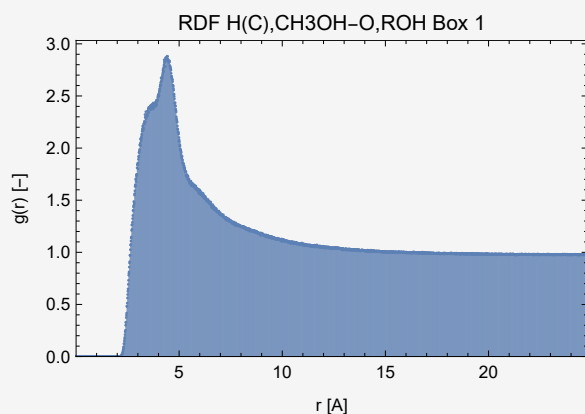
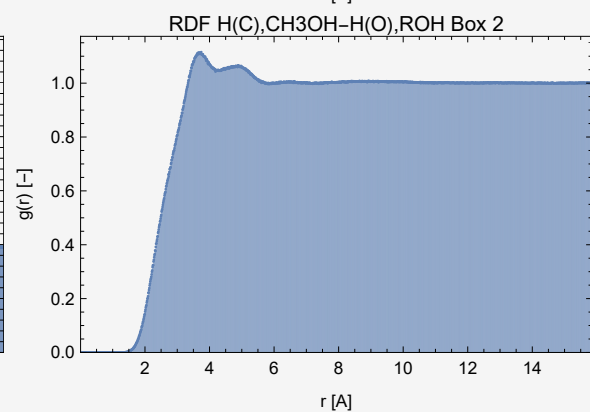
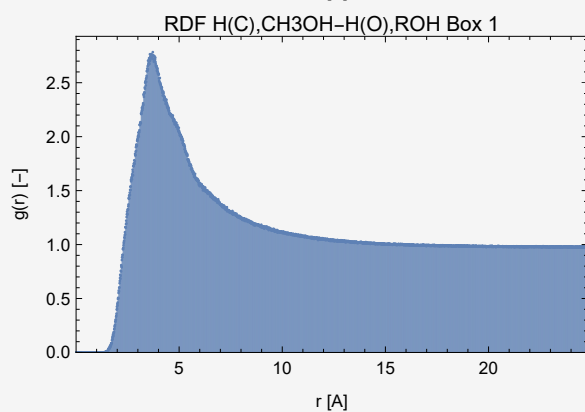
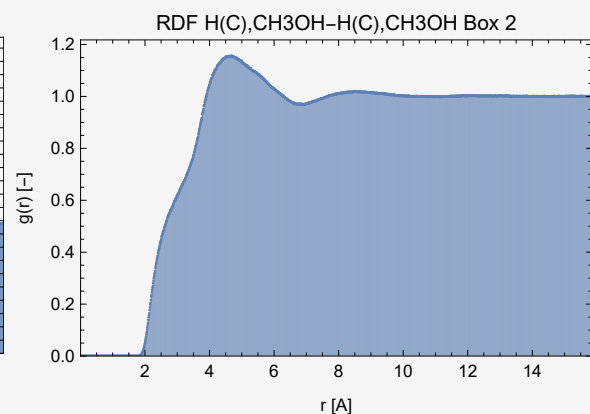
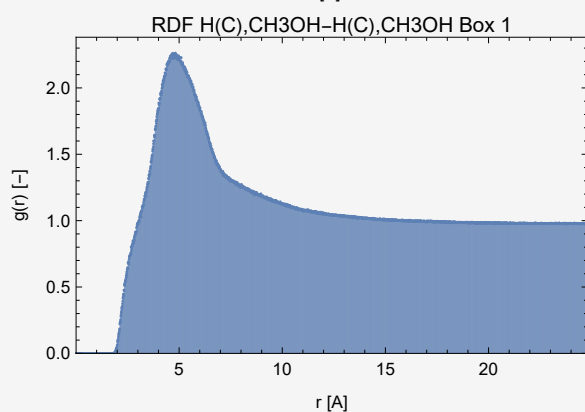
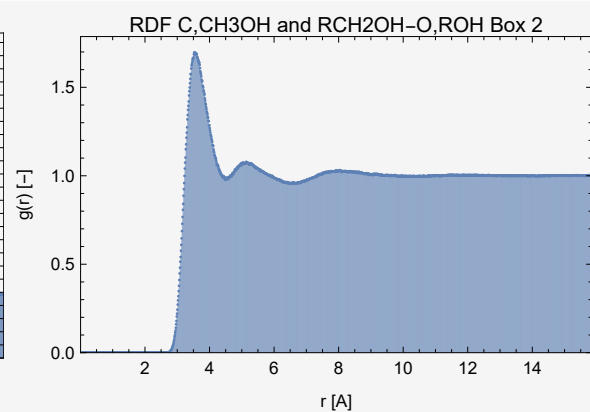
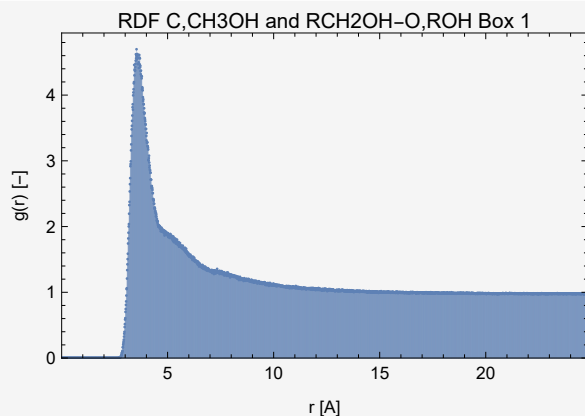


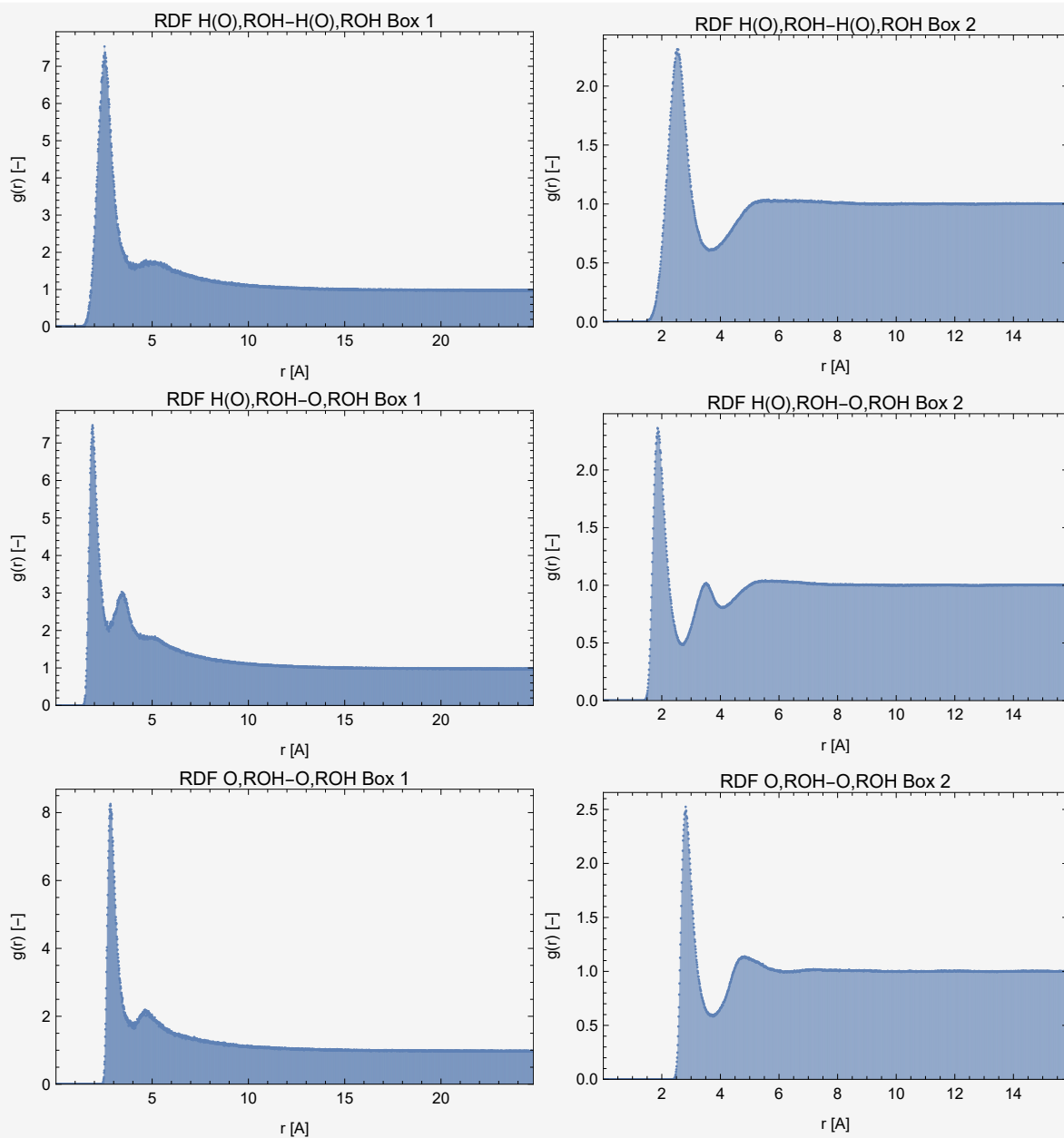
RDF C,CH3OH and RCH2OH-H(O),ROH Box 1



RDF C,CH3OH and RCH2OH-H(O),ROH Box 2





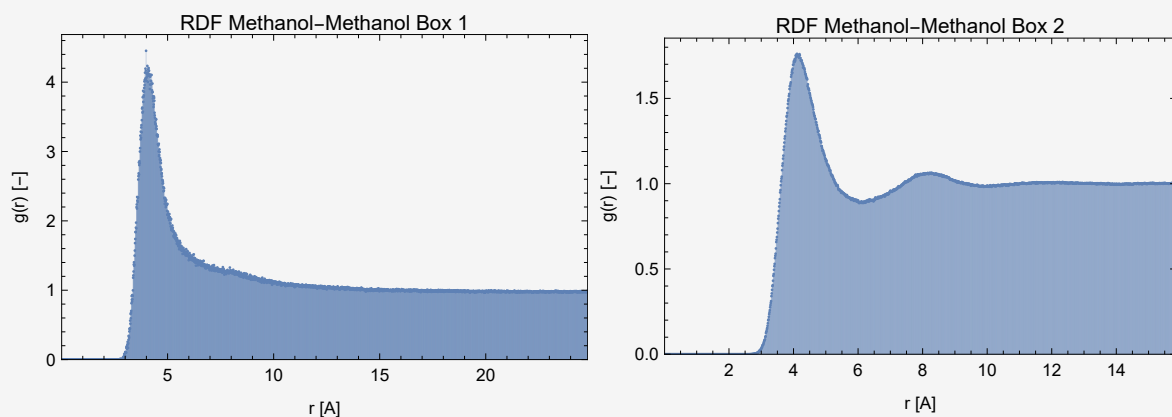


Radial Distribution Function per Molecule

```

1824 If[checkGetAssocParameter[custParam, "rdfDocuMolec"],
1825     VisualizeRDFMolec[];
1826     markShowCell[EvaluationCell[]];];

```

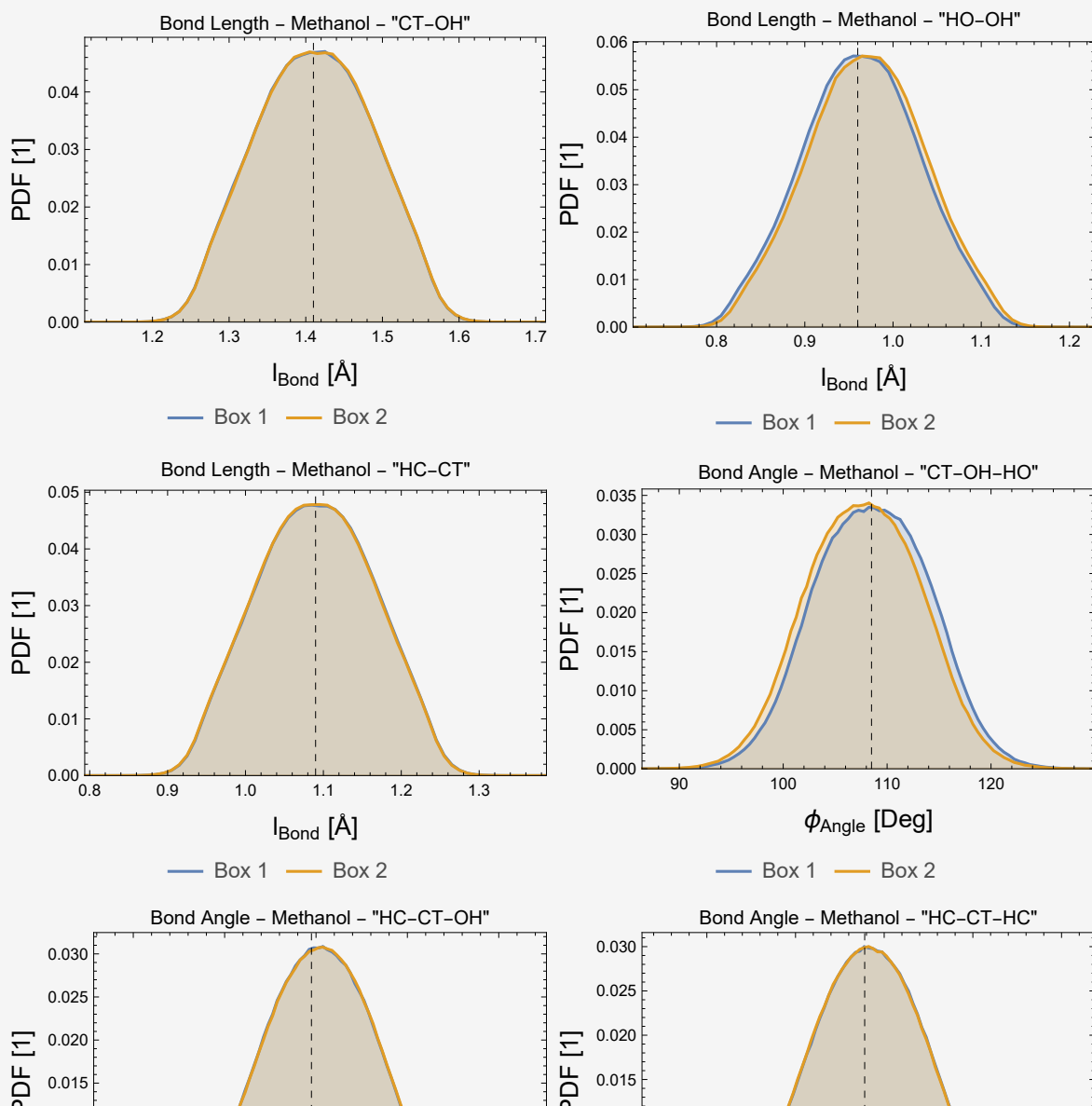


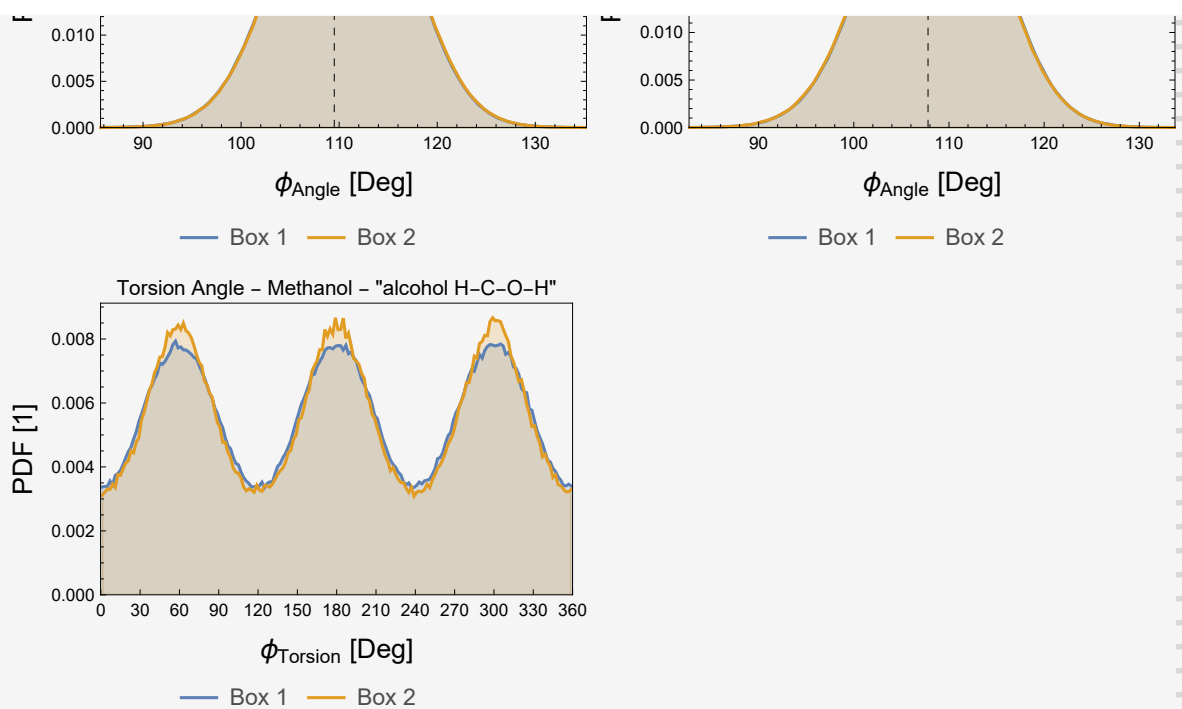
Intramolecular Configuration Distributions

```

1833 If[checkGetAssocParameter[custParam, "intraConfigDocu"],
1834     VisualizeIntraConfigDocu[];
1835     markShowCell[EvaluationCell[]];];

```





Custom Evaluations

Export Analysis Results

Credits