

GEMC - ANALYSIS

This notebook analyses the results of a simulation.

Setup

Setup Configuration

```
267 ShowMonteCarloOverviewSimuSystem
268 If[ValueQ@custParam,
269     ShowMonteCarloOverviewCstParam
270 ]
271 ShowExtendedAnalysisTable;
272 markShowCell[EvaluationCell[]];
```

SIMULATION SYSTEM	
Directory	C:\gemc\GEMC - Intramolecular Energy\exampleSimulations\Example_1_LjArgon_FS_14000@Tast1.00@ constV_n500\

```
( trialMoveAdoption      acceptedPerCycle  trialMoveScaleMoves  False )
trialMoveAdoptionSetpoint      1      trialMoveAdoptionLimit  10
trialMoveAdoptionBoundary      0.025      widomrOvl      0
( trialMoveAdoptionAvg      10      eqAdjAvrCycles      1000 )

( trialMoveAdoptionMaximumSwaps      3000
trialMoveAdoptionAdaptVolumeChanges      False
trialMoveLimitsAdoptionMode      numberMoves )
```

Initial Conditions

Overview

Show Overview

```

291 ShowMonteCarloOverviewEnvironment@@(simDef[#] &/@ {"system","ensembleType","T","Psys"
292 ShowMonteCarloOverviewDetails@@(simDef[#] &/@ {"system","nWarmUpCycles","nEquiCycles"
293 ShowMonteCarloOverviewOPLS@@(simDef[#] &/@ {"system","ffLabelsNonBonded","ffLabelsBon
294 markShowCell[EvaluationCell[]];

```

ENVIRONMENT			
Ensemble Type	Gibbs Ensemble with constant total Volume		
Components	Argon		
T [K]	116.79		
P [bar]	12.		
	BOX 1	BOX 2	TOTAL
L [Å]	46.0094	28.3251	
V [Å ³]	97395.5	22725.6	120121.
ρ [Molecules/Å ³]	1.54011×10^{-3}	1.54011×10^{-2}	4.16246×10^{-3}
v [dm ³ /mol]	0.39102	0.039102	0.144677
Number of Molecules	150	350	500
Argon	150	350	500
Mole Fractions			
Argon	1.	1.	1.

SIMULATION DETAILS		
warum-up cycles	2000	
equilibration cycles	2000	
production cycles	10000	
TRIAL MOVES PER CYCLE		
translations	500	
rotations	0	
volume changes	1	
insertions	150	
ghost insertions	125	
bond stretches	0	
angle bends	0	
torsion rotations	0	
total number of moves per cycles	776	
	BOX 1	BOX 2
cutoff distance [Å]	14.	14.
overlap distance [Å]	2.4	2.4
max translation distance [Å] Argon	2.	2.
max rotation angle [rad] Argon	0.436332	0.436332
max volume change [Å³]	1201.21	1201.21

OPLS-AA DEFINITIONS				
	non-bonded	bond stretching	angle bending	torsion
Argon	Ar,Tan			

Simulation Results

General Information

```
305 ShowMonteCarloOverviewSimuSystemResults
306 markShowCell[EvaluationCell[]];
```

GENERAL INFORMATION	
Version (GIT SHA1)	e1c0c937992f4dc7f0ab43aa8ab6e3412ce75441
Timing Method	RepeatedTiming[RandomReal[1, {100, 100, 100}];, 1][[1]]*1000
Timing @ Start [ms]	4.8343
Timing @ End [ms]	4.97914
Total physcal memory @ End [GB]	8.0465 GiB
Total physcal memory @ End [GB]	8.86367 GiB
ESEMBLE AVERAGES	
Average from cycle	2001
Average to cycle	12 000

Evaluation Times

Define Grid

Show Information

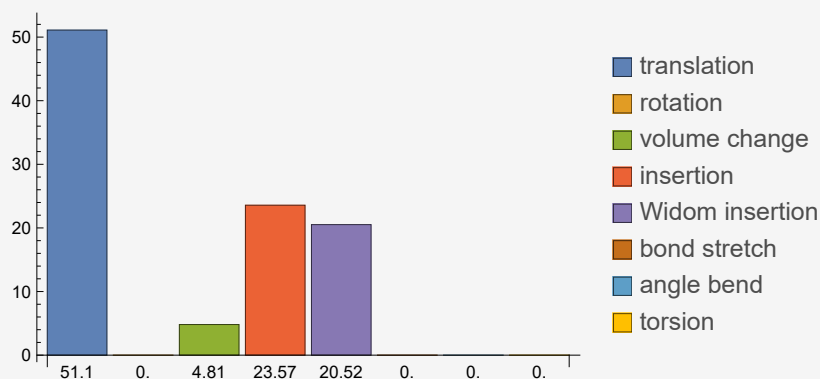
```
583 ShowEvalTimesCode
584 ShowEvalTimesPhases
585 NormalizedTiming[]
586 markShowCell[EvaluationCell[]];
```

CODE PARTS					
Part	Time / total	t _{avr} / ms	t _{acc} / ms	t _{rejDu} / ms	t _{rej0v} / ms
Translation	0h 10min 52s	0.0932741	0.0917334	0.0938742	0.121055
Rotation	0h 0min 0s	–	–	–	–
Volume Change	0h 1min 1s	5.12575	5.40872	4.82093	–
Insertion	0h 5min 1s	0.188045	1.3582	0.131172	0.239414
Widom	0h 4min 22s	0.174827	0.174827	–	–
Bond Stretch	0h 0min 0s	–	–	–	–
Angle Bend	0h 0min 0s	–	–	–	–
Torsion	0h 0min 0s	–	–	–	–

SIMULATION PHASES		
Part	Time / total	Time Fraction
Warm-Up Cycles	0h 1min 27s	4.374%
Equilibration Cycles	0h 5min 15s	15.81%
Production Cycles	0h 26min 35s	79.82%
Trial Move Execution	0h 21min 17s	63.93%
Virial & Tail Correction	0h 10min 36s	31.84%
Documentation	0h 0min 9s	0.49%
Other	0h 1min 14s	3.74%
Total	0h 33min 18s	

Normalized Timing	t' _{avr}	t' _{acc}	t' _{rejeDu}	t' _{reje0v}	t' per succ. move
Translation	1.02	1.00	1.02	1.32	1.73
Rotation	–	–	–	–	–
Volume Change	55.9	59.0	52.6	–	108.
Insertion	2.05	14.8	1.43	2.61	281.
Widom	1.91	1.91	–	–	1.91

```
589 ShowEvalTimesBarChart  
590 ExportGraphic["evaluationTimes.pdf", ShowEvalTimesBarChart];  
591 markShowCell[EvaluationCell[]];
```



Calculations

Visual Check

Show Boxes

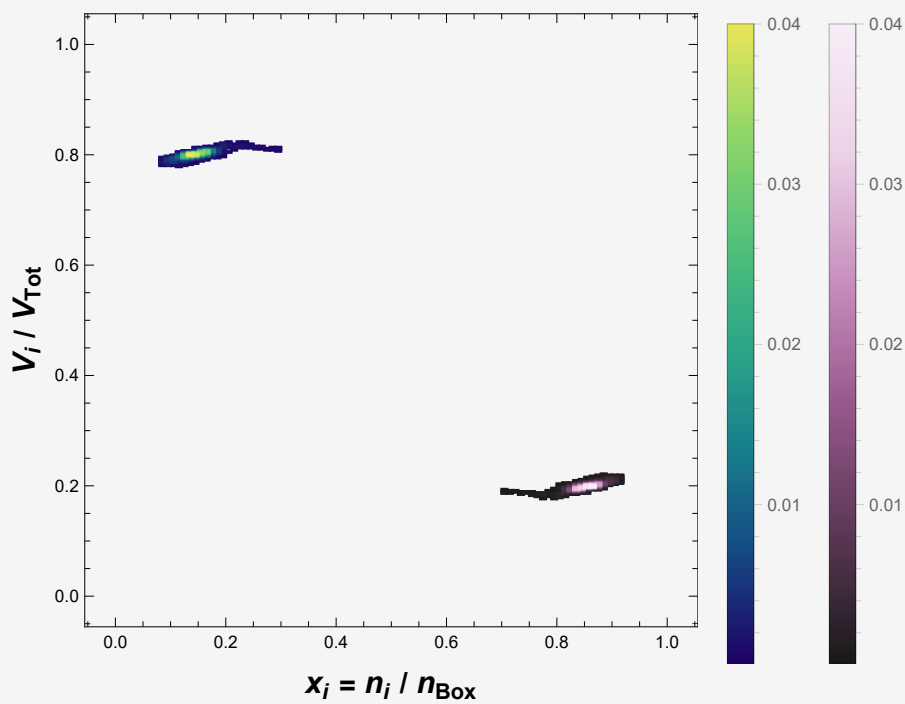
Probability Plot

acc. to (Frenkel 2002, p238)

```

625 lImageSize = Medium;
626 plotProbabilityCheckV2[]
627 lImageSize = Scaled[1];
628 ExportGraphic["plotProbabilityCheck.pdf",plotProbabilityCheck];
629 markShowCell[EvaluationCell[]];

```



Show Plots

```

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

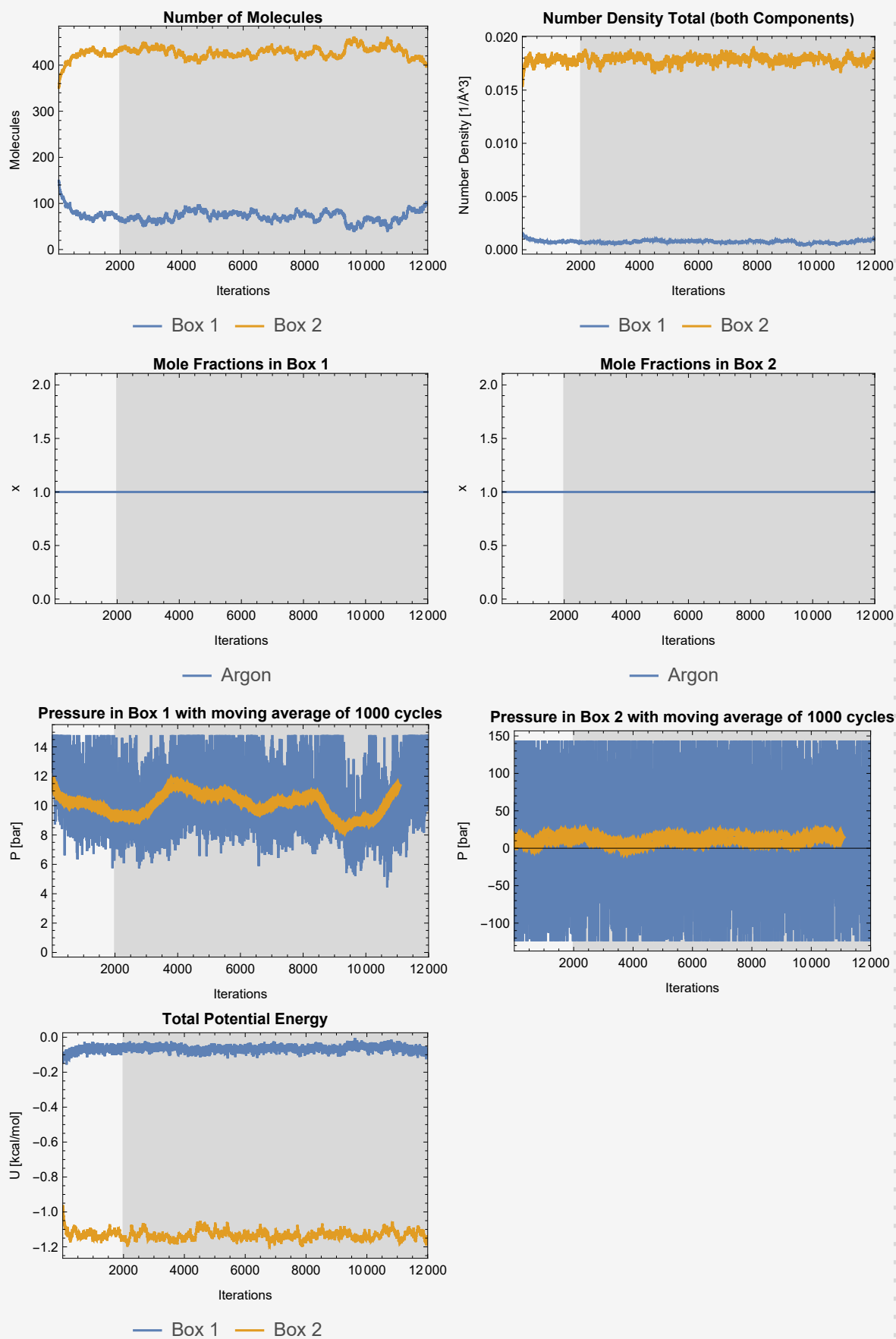
```

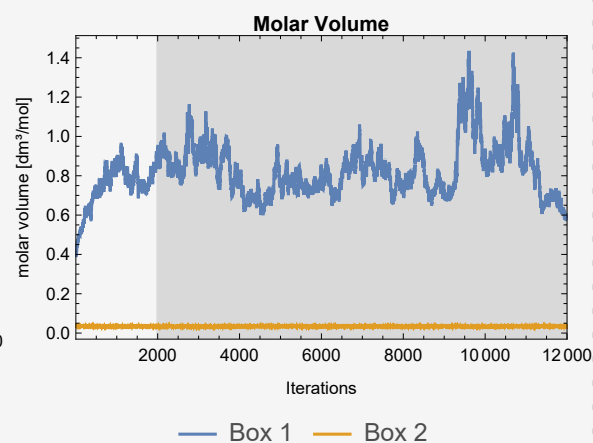
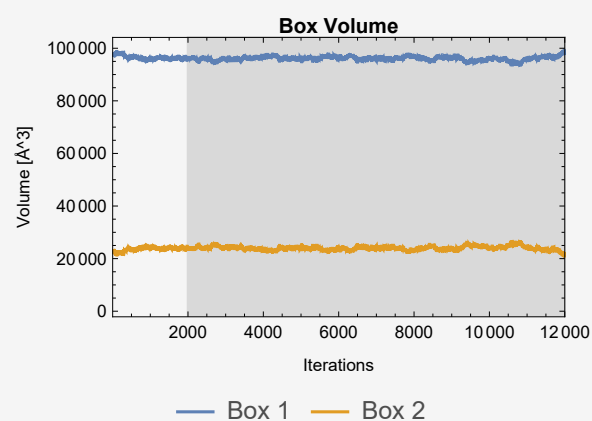
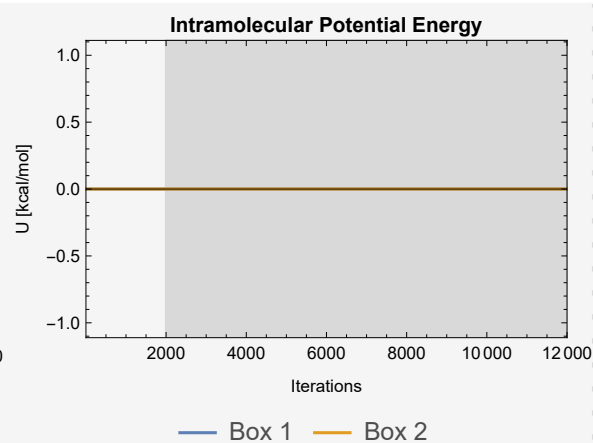
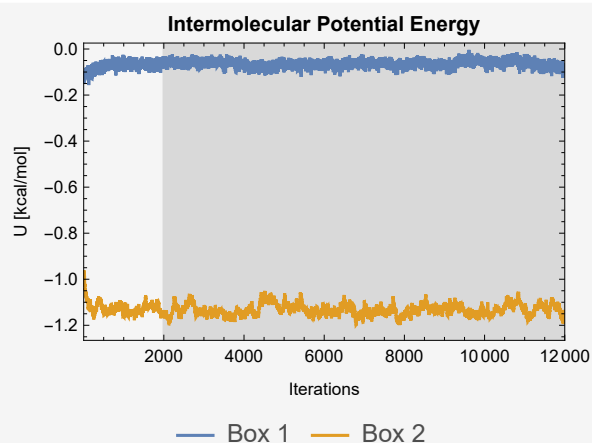
Values

```

646 plotValuesGrid = Grid[{
647     {plotNumOfMolecules,plotDensityTotal},
648     {plotMoleFractions1,plotMoleFractions2},
649     {plotPressure1,plotPressure2},
650     {plotTotalEnergy},
651     {plotInterEnergy,plotIntraEnergy},
652     {plotVolume,plotMolarVolume}
653 },Alignment→Center, ItemSize→Scaled[0.5]]
654
655 ExportGraphic["plotValues.pdf",plotValuesGrid];
656 markShowCell[EvaluationCell[]];

```



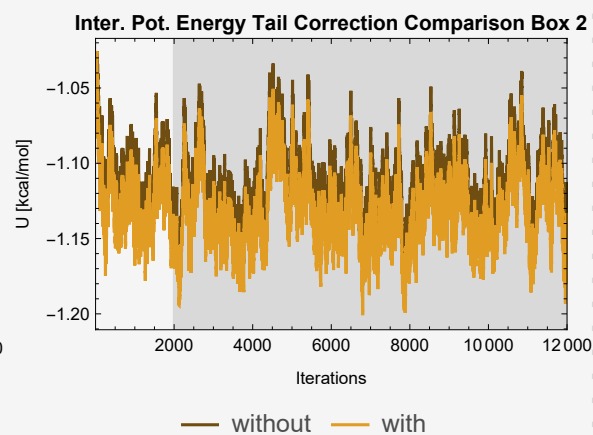
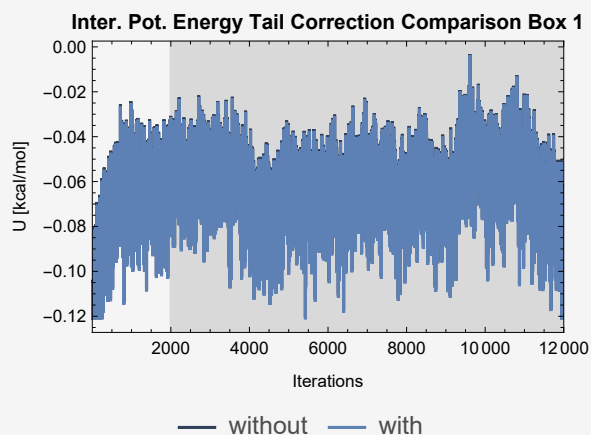
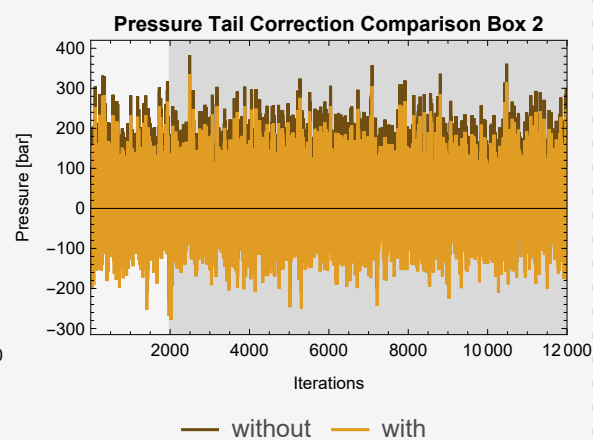
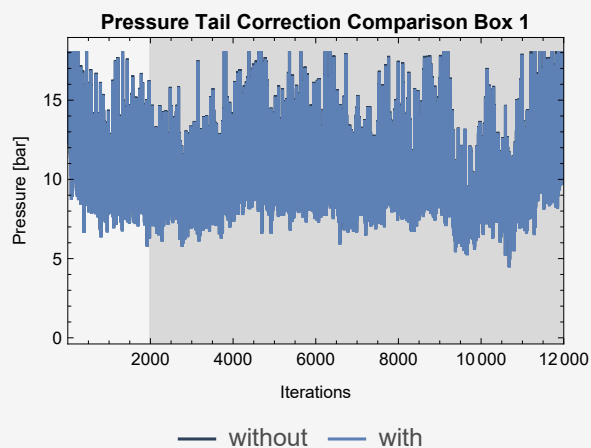
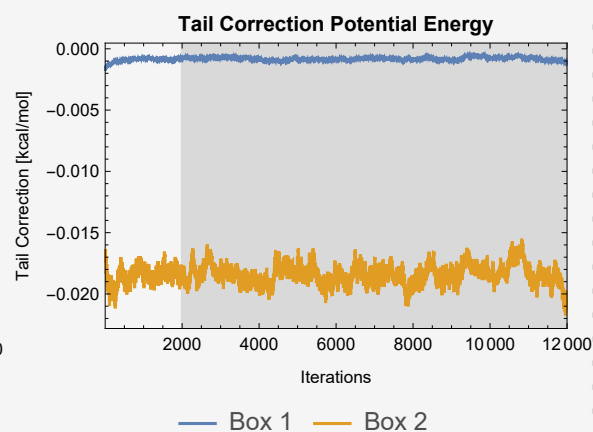
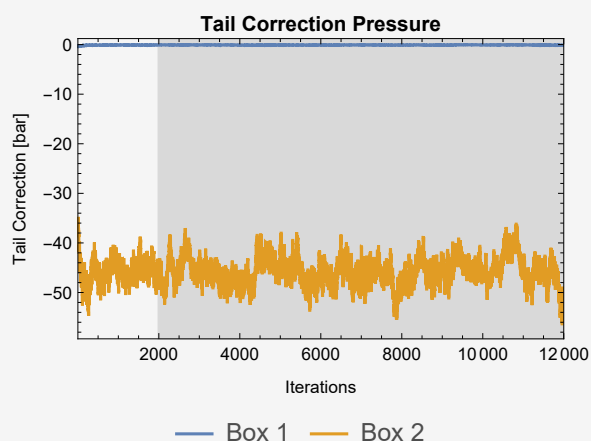


Tail Corrections

```

667 plotTailCorrGrid = Grid[{
668   {plotTailCorrPressure,plotTailCorrEnergy},
669   {plotTailComparisonPressure1,plotTailComparisonPressure2},
670   {plotTailComparisonEnergy1,plotTailComparisonEnergy2}
671 }, ItemSize→Scaled[0.5],Alignment→Center]
672
673 ExportGraphic["plotTailCorr.pdf",plotTailCorrGrid];
674 markShowCell[EvaluationCell[]];

```

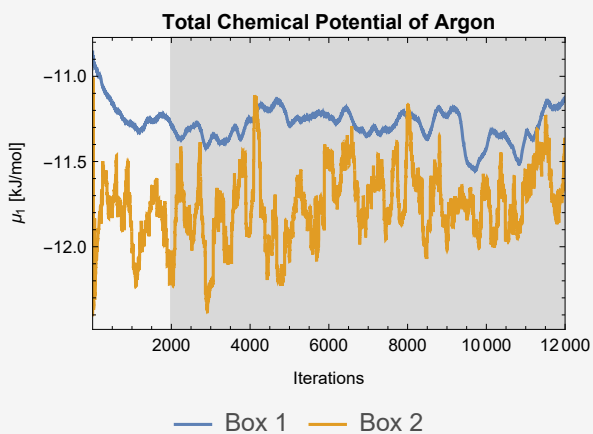
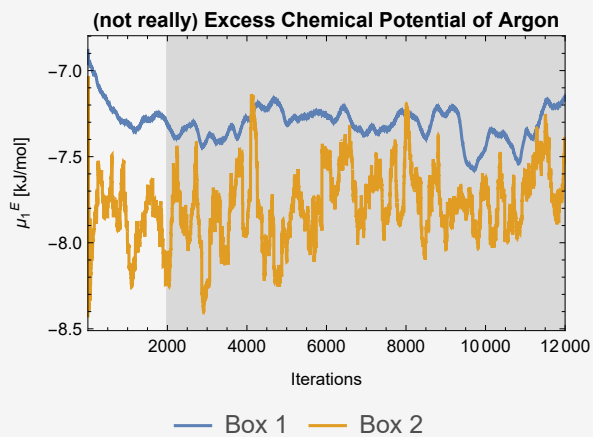
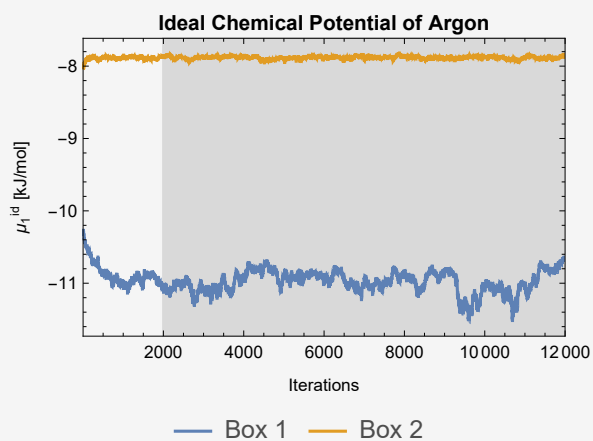


Chemical Potentials

```

681 plotChemPotGrid = Grid[{
682     plotIdealChemPotential,
683     plotExcessChemPotential,
684     plotTotalChemPotential
685 }, ItemSize→Scaled[0.5], Alignment→Center]
686
687 ExportGraphic["plotChemPot.pdf", plotChemPotGrid];
688 markShowCell[EvaluationCell[]];

```



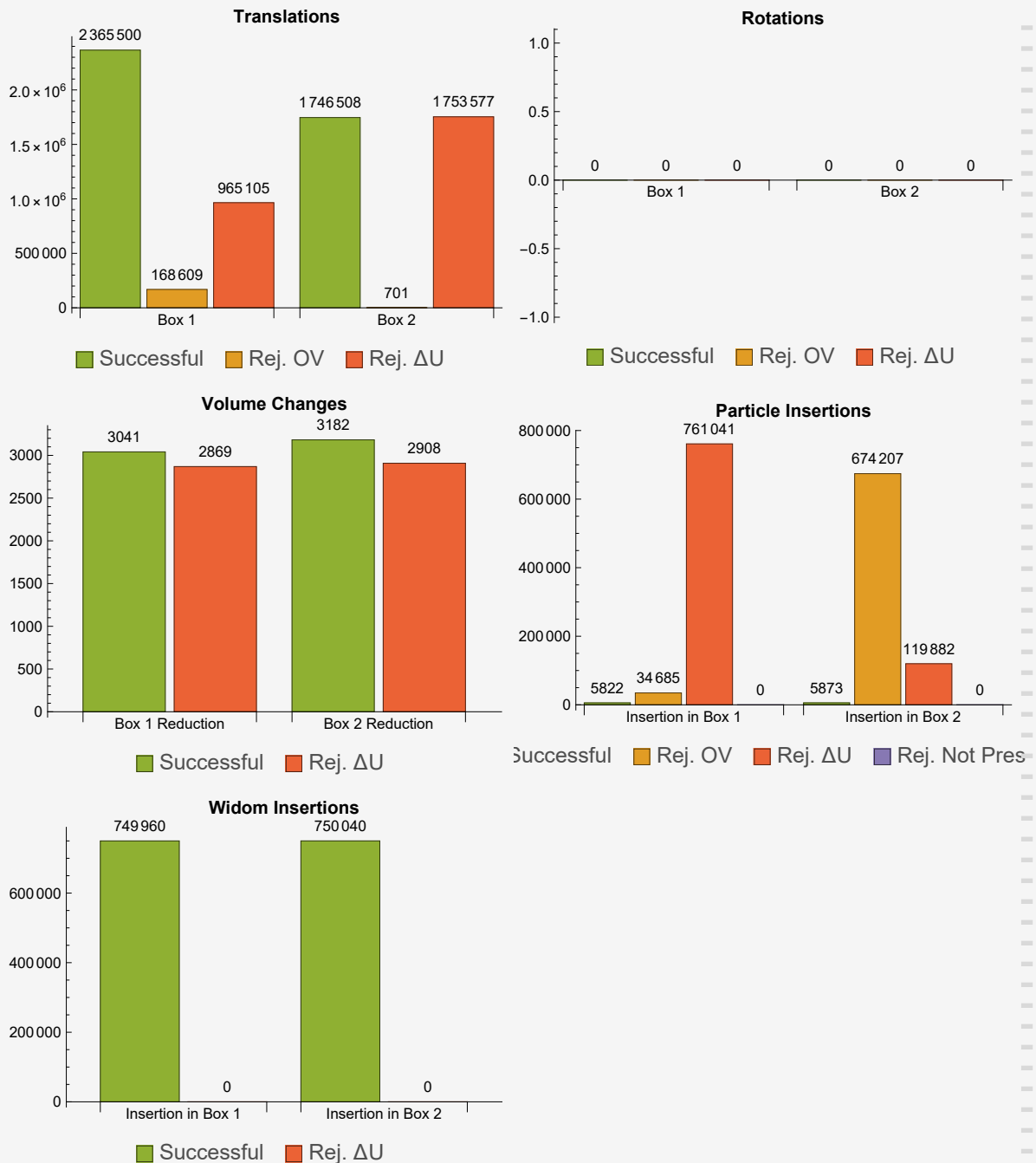
Plot of the Standard Deviation of the molar volume

Counters

```

706 plotCountersGrid
707 ExportGraphic["plotCounters.pdf",plotCountersGrid];
708 markShowCell[EvaluationCell[]];

```



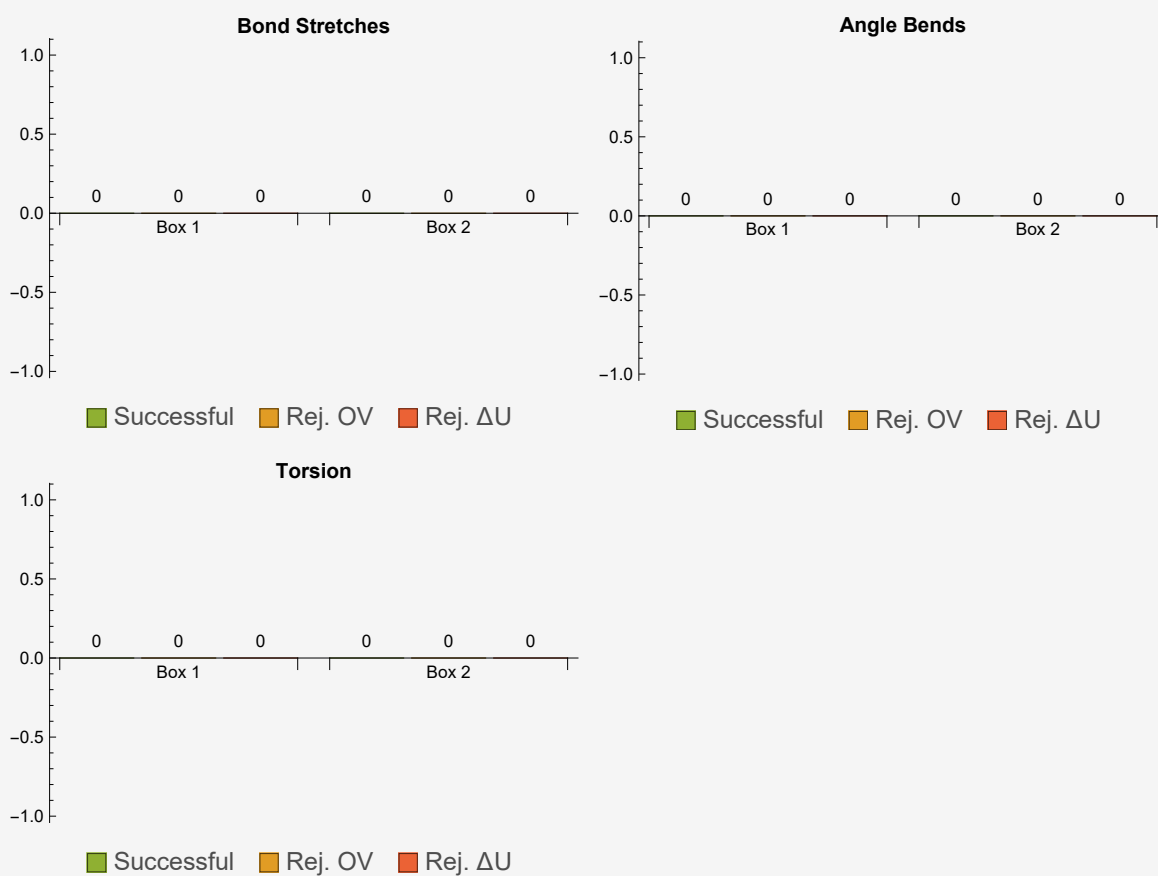
Species specific Counters

```
715 plotSpeciesCountersGrid
716 markShowCell[EvaluationCell[]];
```

No species specific plots if only one species is simulated

Intramolecular Trial Moves

```
723 plotIntraCountersGrid
724 markShowCell[EvaluationCell[]];
```

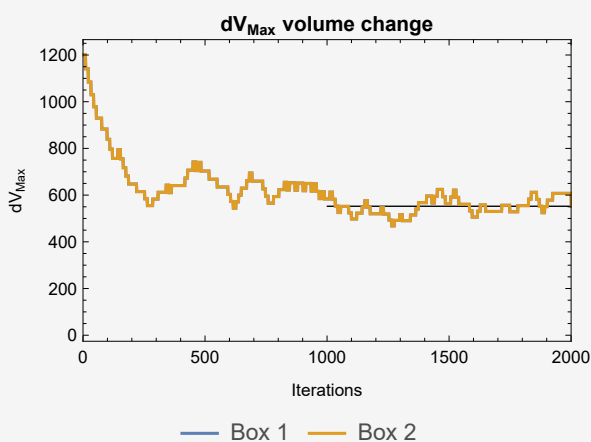
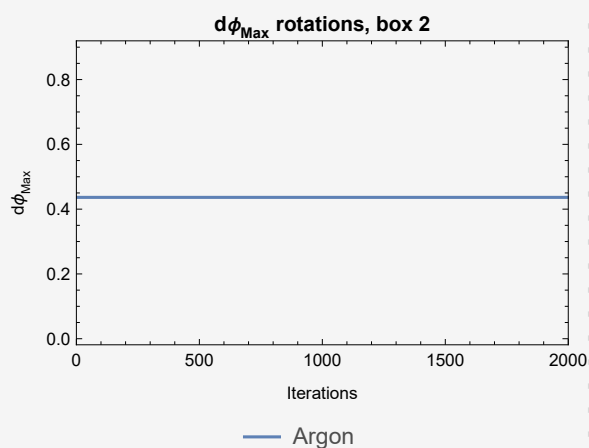
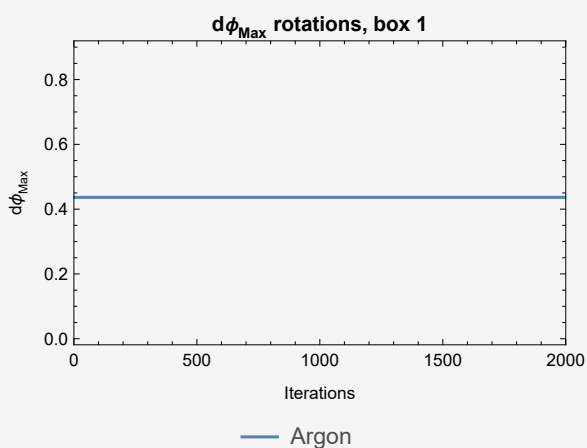
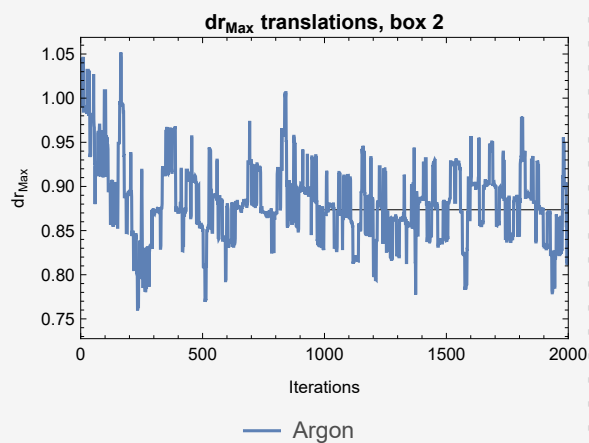
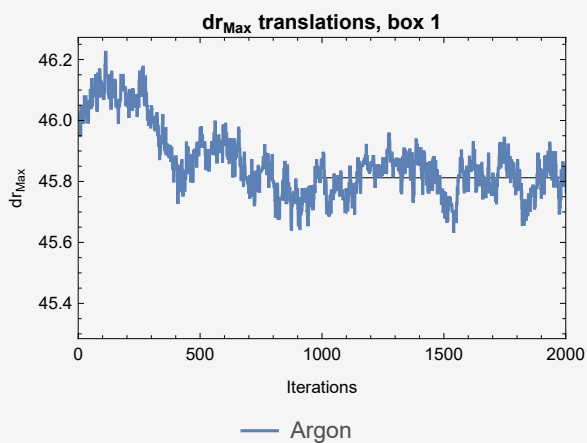


Trial Move Limits Course

```

735 If[ValueQ@transMaxVecDoc,
736   ExportGridGraphic[{"transLimits_box" <> ToString@#, courseTransMax[#]} &/@ boxVec,
737   ExportGridGraphic[{"rotaLimits_box" <> ToString@#, courseRotaMax[#]} &/@ boxVec,
738   ExportGridGraphic[{"volumLimits", courseVolMax[]}], False];
739 markShowCell[EvaluationCell[]];
740 ];

```



```

743 Do[
744     ExportGridGraphic[{"transMax - Box " <> ToString@# <> " " <> system[[iCp]], histo
745     , {iCp, Length@system}];

748 Do[
749     ExportGridGraphic[{"rotaMax - Box " <> ToString@# <> " " <> system[[iCp]], histoR
750     , {iCp, Length@system}];

753 ExportGridGraphic[{"volMax - Box " <> ToString@#, histoVolMax[#]} &/@ boxVec, False]

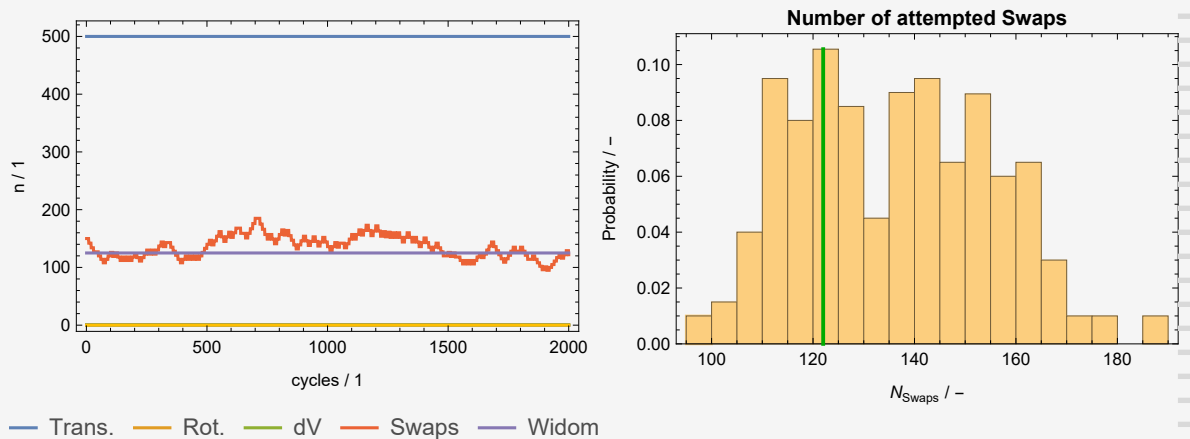
```

Number of Trial Moves

```

760 If[ValueQ@nMovesDocu,
761     ExportGridGraphic[{"TrialMovesCourse", pltCourseTrialMoves[]}, {"TrialMovesHisto
762     markShowCell[EvaluationCell[]];
763 ];

```

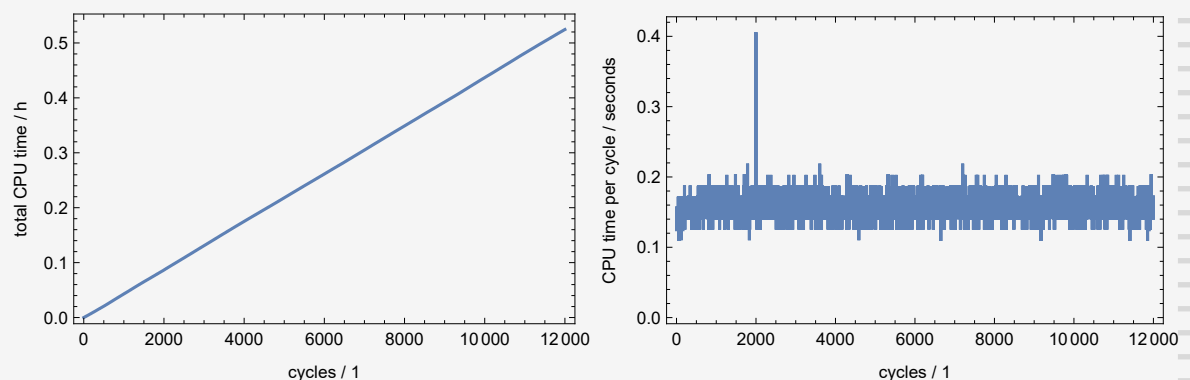


CPU Time Usage

```

770 If[ValueQ@timingCPUList,
771     ExportGridGraphic[{"TimingCPUTotal", pltTimingCPUTotal[]}, {"TimingCPUPerCycle",
772     markShowCell[EvaluationCell[]];
773 ];

```



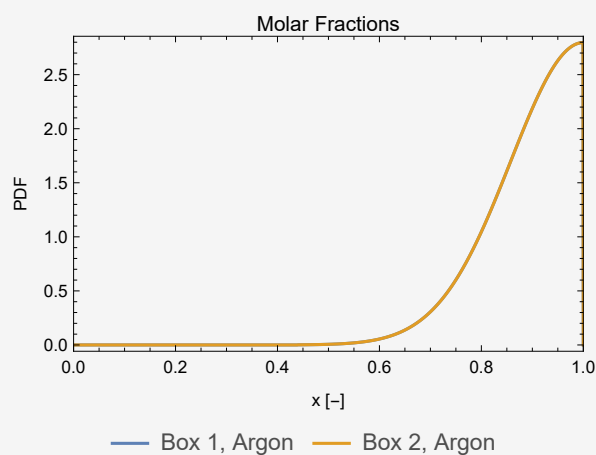
Ensemble Averages

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

Density Plots

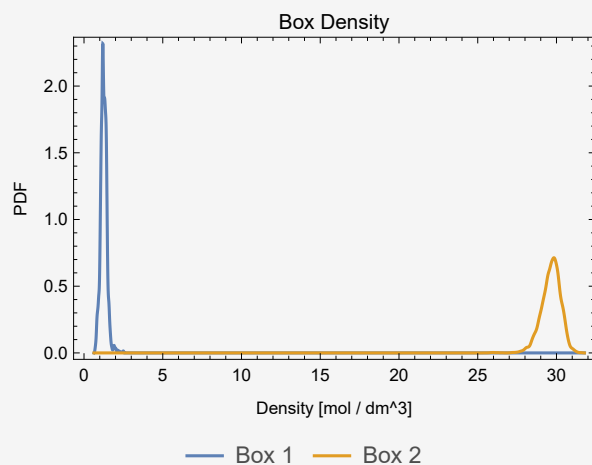
Mole Fractions

```
792 ExportGridGraphic[{"moleFractionsHistogram", plotMolarFractions[]}, False];
793 markShowCell[EvaluationCell[]];
```



Box Densities

```
800 ExportGridGraphic[{"densityHistogram", plotDensityHistogram[]}, False];
801 markShowCell[EvaluationCell[]];
```

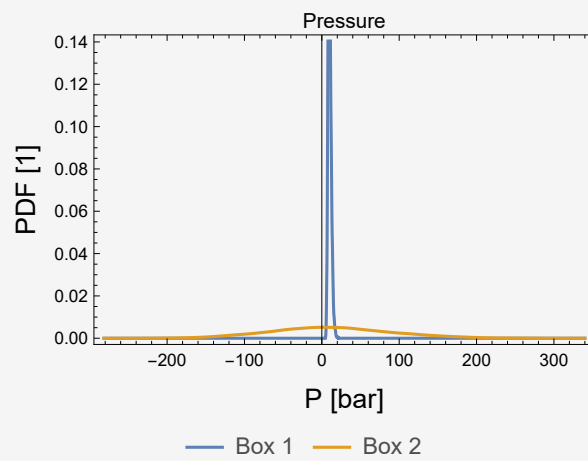


Pressure

```

808 ExportGridGraphic[{"pressureHistogram", plotPressureHistogram[]}, False];
809 markShowCell[EvaluationCell[]];

```



Averaged Values

```

820 assocResults = <| |>;
821 showAveragedValues
822 ExportGraphic["simResultsAveragedValues.pdf",showAveragedValues];
823 markShowCell[EvaluationCell[]];

```

AVERAGED VALUES				
averaged from 2001 to 12000				
Box V corresponds to Box 1, Box L corresponds to Box 2				
System	Box V		Box L	
	mean	std	mean	std
T [K]	116.79	–	116.79	–
v [dm ³ / mol]	0.832986	0.135727	0.0336985	0.000685633
rho [mol / dm ³]	1.22972	0.183571	29.6871	0.598584
n [1]	71.248	11.0058	428.752	11.0058
Pressure				
P ideal [bar]	11.9411	1.78256	288.276	5.81252
P viral [bar]	–1.71756	1.76498	–230.764	77.3576
P tail [bar]	–0.0855249	0.0244252	–45.7471	2.80881
P [bar]	10.1381	2.11942	11.7647	78.6085
Internal Energy				
U Inter [kcal/mol]	–0.0620866	0.0152787	–1.13322	0.0241377
U Intra [kcal/mol]	0.	0.	0.	0.
U Total [kcal/mol]	–0.0620866	0.0152787	–1.13322	0.0241377
Mole Fractions				
Argon	1.0000	0	1.0000	0
Ideal μ [kJ/mol]				
Argon	–10.985	0.15055	–7.8824	0.019666
Excess μ [kJ/mol]				
Argon	7.3188	0.089463	7.7715	0.20750
Total μ [kJ/mol]				
Argon	–11.293	0.089463	–11.746	0.20750

Reduced Units

```
830 NormalizedUnits[];
831 markShowCell[EvaluationCell[]];
```

name	dimensional	unit	critical norm	LJ norm
T	117.	K	$T_{\text{red}}=T/T_C$	$T^* = k_B T / \epsilon$
p_V	10.1	bar	$p_{\text{red}}=p/p_C$	$p^*=p \cdot \sigma^3/\epsilon$
p_L	11.8	bar		
ρ_V	1.23	mol / dm ³	$\rho_{\text{red}}=\rho/\rho_C$	$\rho^*=\rho \cdot \sigma^3$
ρ_L	29.7	mol / dm ³		
μ_V	-11.3	kJ / mol	$\mu_{\text{red}}=\mu / \mu_C$	$\mu^*=\mu / \epsilon$
μ_L	-11.7	kJ / mol		

Comparison & Checks

Comparison Functions

Equation of State Comparison

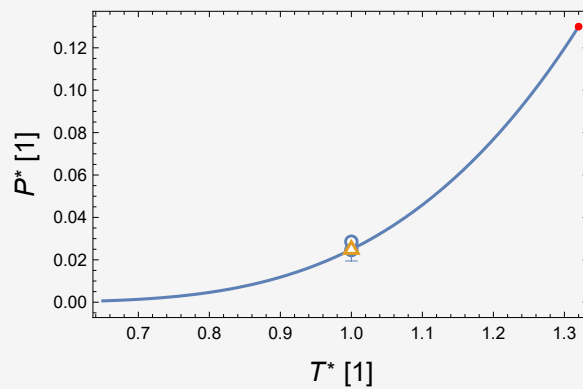
Comparison to a pure LJ EOS (Thol, 2016), a t-PR-LJ EoS (Harismiadis, 1994) or the SRK EoS

```
1959 EosResultsAssoc = <| |>;
1960 CalculateEosComparison[]; Pause[1];
1961 markShowCell[EvaluationCell[]];
```

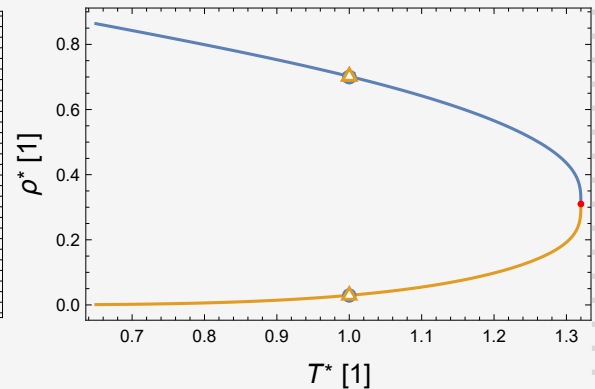
LJ Comparison, Argon at $T^* = 1$.

Defintion relative error: $\text{Abs}[\zeta_{\text{Sim}} - \zeta_{\text{EOS}}] / \zeta_{\text{EOS}}$

Unit	Box V			Box L		
	Sim	LJ-EoS	$\Delta_{\text{rel}} / \%$	Sim	LJ-EoS	$\Delta_{\text{rel}} / \%$
$\rho^* / 1$	0.0290	0.0295	1.60	0.700	0.702	0.306
$P^* / 1$	0.0246	0.0249	1.13	0.0286	0.0249	14.7



○ Simulation △ LJ-Fluid EOS ● Critical point



○ Simulation △ LJ-Fluid EOS ● Critical point

Equilibrate State

```
1968 Showcheckfinalvalues
1969 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

Export Analysis Results

Credits