

GEMC - ANALYSIS

This notebook analyses the results of a simulation.

Setup

Setup Configuration

```
ShowMonteCarloOverviewSimuSystem
If[ValueQ@custParam,
  ShowMonteCarloOverviewCstParam
]
ShowExtendedAnalysisTable;
markShowCell[EvaluationCell[]];
```

SIMULATION SYSTEM	
Directory	C:\gemc\GEMC - Intramolecular Energy\exampleSimulations\Example_4_LjArgon_FS_14000@Tast1.00@ constV_n500_CFC

(particleInsertionMode	CfcVlugt	trialMoveScaleMoves	False)
	trialMoveAdoption	acceptedPerCycle	trialMoveAdoptionLimit	10	
trialMoveAdoptionSetpoint	1	widomrOvl	0		
trialMoveAdoptionBoundary	0.025	eqAdjAvrCycles	1000		
trialMoveAdoptionAvg	10	-	-		
(trialMoveAdoptionMaximumSwaps	3000)
trialMoveAdoptionAdaptVolumeChanges	False				
trialMoveLimitsAdoptionMode	numberMoves				

Initial Conditions

Overview

Show Overview

```
ReleaseHold@ (ShowMonteCarloOverviewEnvironment /. Normal@simDef)
ExportGraphic [ "ShowMonteCarloOverviewEnvironment.pdf", ReleaseHold@ (ShowMonteCarloOverviewEnvironment /. Normal@simDef) ]
ReleaseHold@ (ShowMonteCarloOverviewDetails /. Normal@simDef)
ExportGraphic [ "ShowMonteCarloOverviewDetails.pdf", ReleaseHold@ (ShowMonteCarloOverviewDetails /. Normal@simDef) ]
ReleaseHold@ (ShowMonteCarloOverviewOPLS /. Normal@simDef)
ExportGraphic [ "ShowMonteCarloOverviewOPLS.pdf", ReleaseHold@ (ShowMonteCarloOverviewOPLS /. Normal@simDef) ]
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		
warm-up cycles	2000	
equilibration cycles	4000	
production cycles	10000	
translations per cycle	247	
rotations per cycle	0	
volume changes per cycle	5	
insertions per cycle	248	
ghost insertions per cycle	125	
total number of moves per cycles	625	
	BOX 1	BOX 2
cutoff distance [\AA]	14.	14.
overlap distance [\AA]	2.4	2.4
max translation distance [\AA] Argon	2.	2.
max rotation angle [rad] Argon	0.436332	0.436332
max volume change [\AA^3]	1201.21	1201.21

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

Simulation Results

General Information

```
ShowMonteCarloOverviewSimuSystemResults
markShowCell[EvaluationCell[]];
```

GENERAL INFORMATION	
Version (GIT SHA1)	64c727d486b4e446b2d9a3dfd68f504389d0ec6a
Timing Method	RepeatedTiming[RandomReal[1, {100, 100, 100}];, 1][[1]]*1000
Timing @ Start [ms]	4.55554
Timing @ End [ms]	4.69993
Total physical memory @ End [GB]	8.49299 GiB
Total physical memory @ End [GB]	8.90396 GiB
ENSEMBLE AVERAGES	
Average from cycle	4001
Average to cycle	14000

Evaluation Times

Define Grid

Show Information

```
ShowEvalTimesCode
ShowEvalTimesPhases
NormalizedTiming[]
markShowCell[EvaluationCell[]];
```

CODE PARTS					
Part	Time / total	t_{avr} / ms	t_{acc} / ms	t_{rejDu} / ms	t_{rej0v} / ms
Translation	0h 26min 48s	0.406911	0.520205	0.258251	0.184677
Rotation	0h 0min 0s	–	–	–	–
Volume Change	0h 16min 47s	14.3962	14.9077	13.8296	–
Insertion (CFC)	0h 8min 31s	0.536374	0.850392	0.361538	0.443101
Widom	0h 10min 0s	0.342918	0.342918	–	–

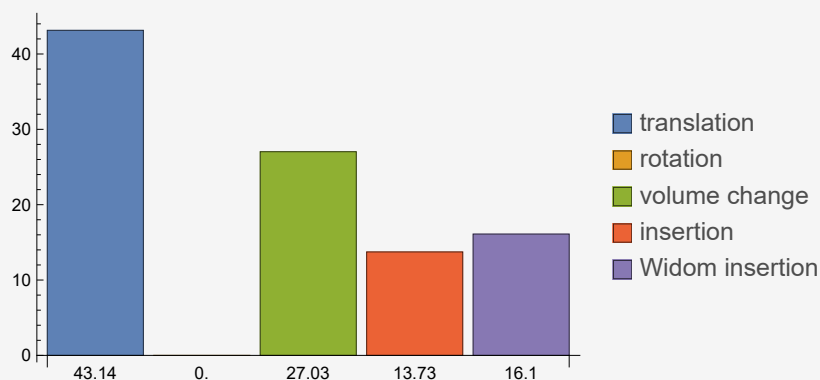
SIMULATION PHASES		
Part	Time / total	Time Fraction
Warm-Up Cycles	0h 2min 57s	3.274%
Equilibration Cycles	0h 24min 45s	27.44%
Production Cycles	1h 2min 30s	69.28%
Trial Move Execution	1h 2min 7s	68.86%
Tail Correction	0h 20min 38s	22.87%
Documentation	0h 6min 22s	7.06%
Other	0h 1min 5s	1.21%
Total	1h 30min 13s	

Normalized Timing	t'_{avr}	t'_{acc}	t'_{rejeDu}	t'_{rejeOv}	t' per succ. move
Translation	0.782	1.00	0.496	0.355	1.36
Rotation	–	–	–	–	–
Volume Change	27.7	28.7	26.6	–	52.7
Insertion (CFC)	1.03	1.63	0.695	0.852	117.
Widom	0.659	0.659	–	–	0.659

ShowEvalTimesBarChart

ExportGraphic["evaluationTimes.pdf", ShowEvalTimesBarChart];

markShowCell[EvaluationCell[]];



Calculations

Visual Check

Show Boxes

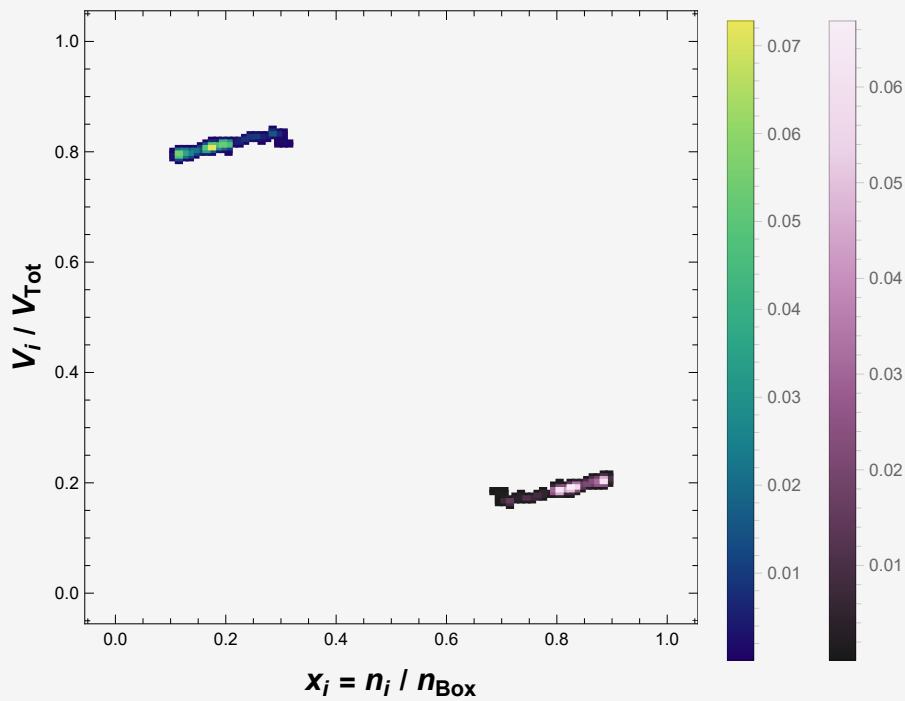
Probability Plot

acc. to (Frenkel 2002, p238)

```

lImageSize = Medium;
plotProbabilityCheckV2[]
lImageSize = Scaled[1];
ExportGraphic["plotProbabilityCheck.pdf",plotProbabilityCheck];
markShowCell[EvaluationCell[]];

```



Show Plots

```

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

```

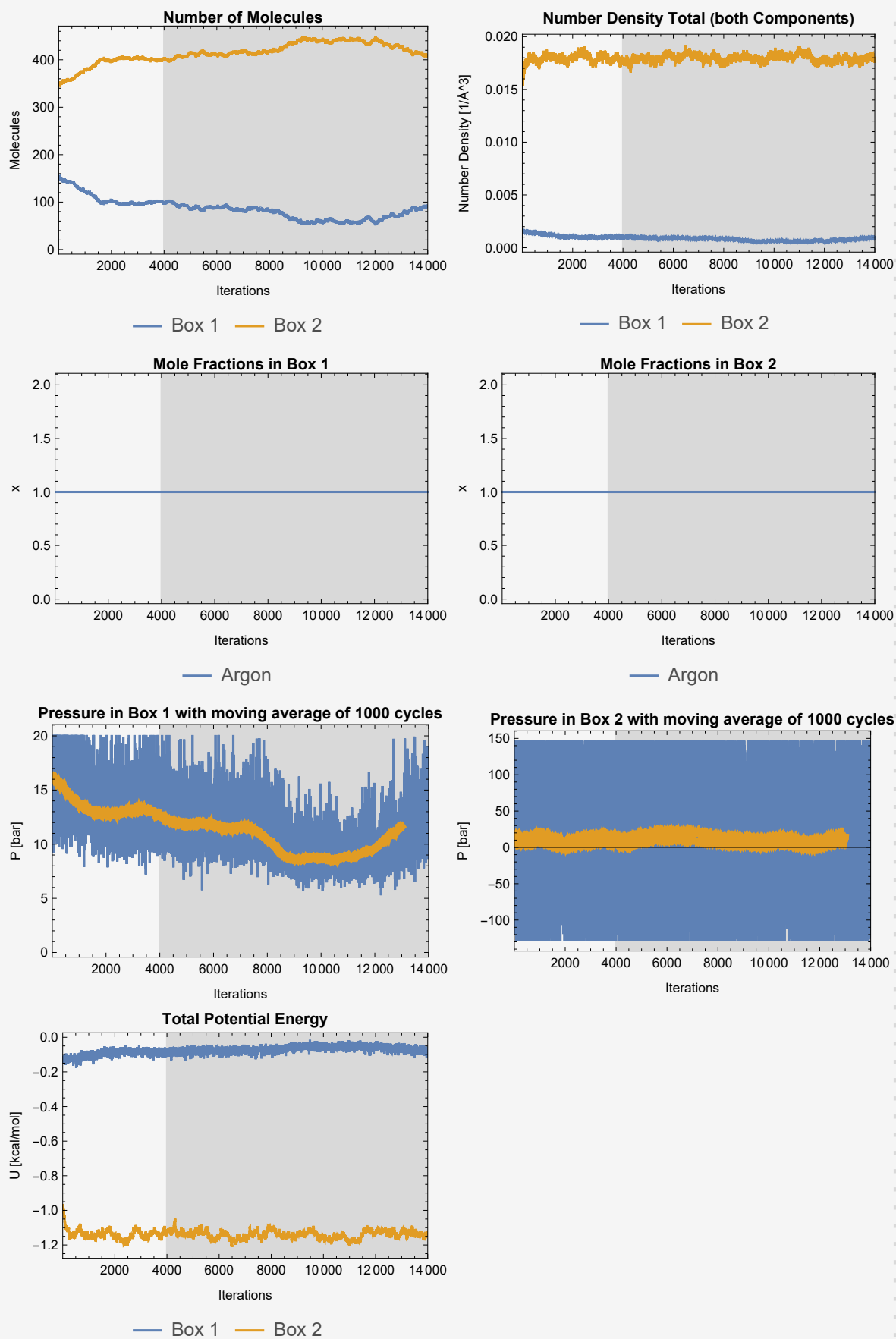
Values

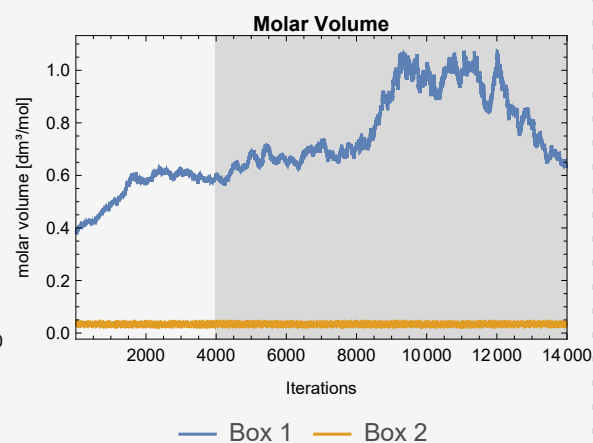
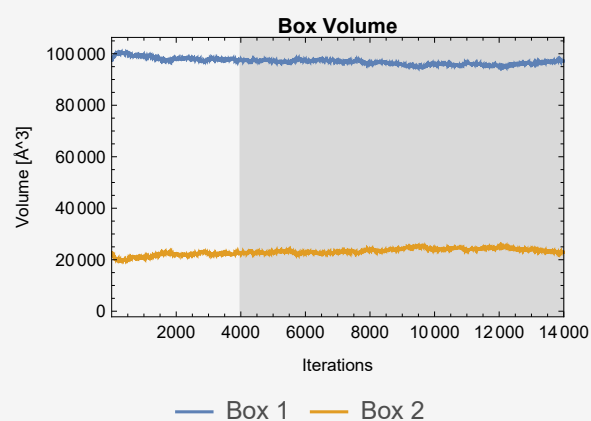
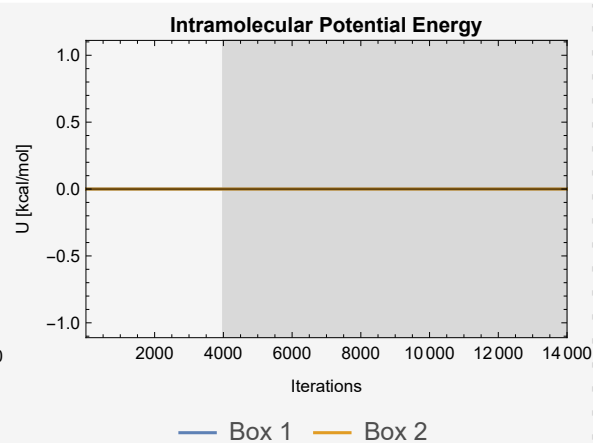
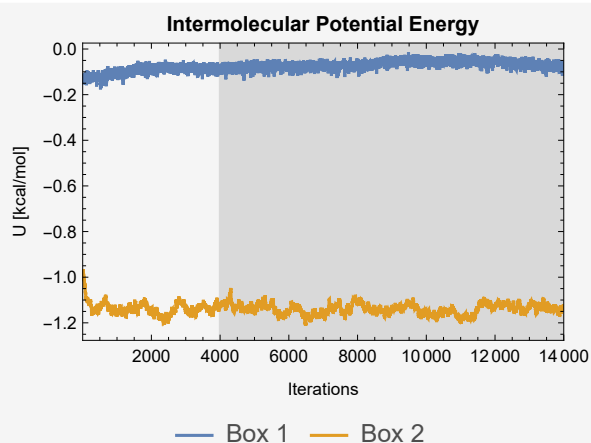
```

plotValuesGrid = Grid[{
  {plotNumOfMolecules,plotDensityTotal},
  {plotMoleFractions1,plotMoleFractions2},
  {plotPressure1,plotPressure2},
  {plotTotalEnergy},
  {plotInterEnergy,plotIntraEnergy},
  {plotVolume,plotMolarVolume}
},Alignment→Center, ItemSize→Scaled[0.5]]

ExportGraphic["plotValues.pdf",plotValuesGrid];
markShowCell[EvaluationCell[]];

```



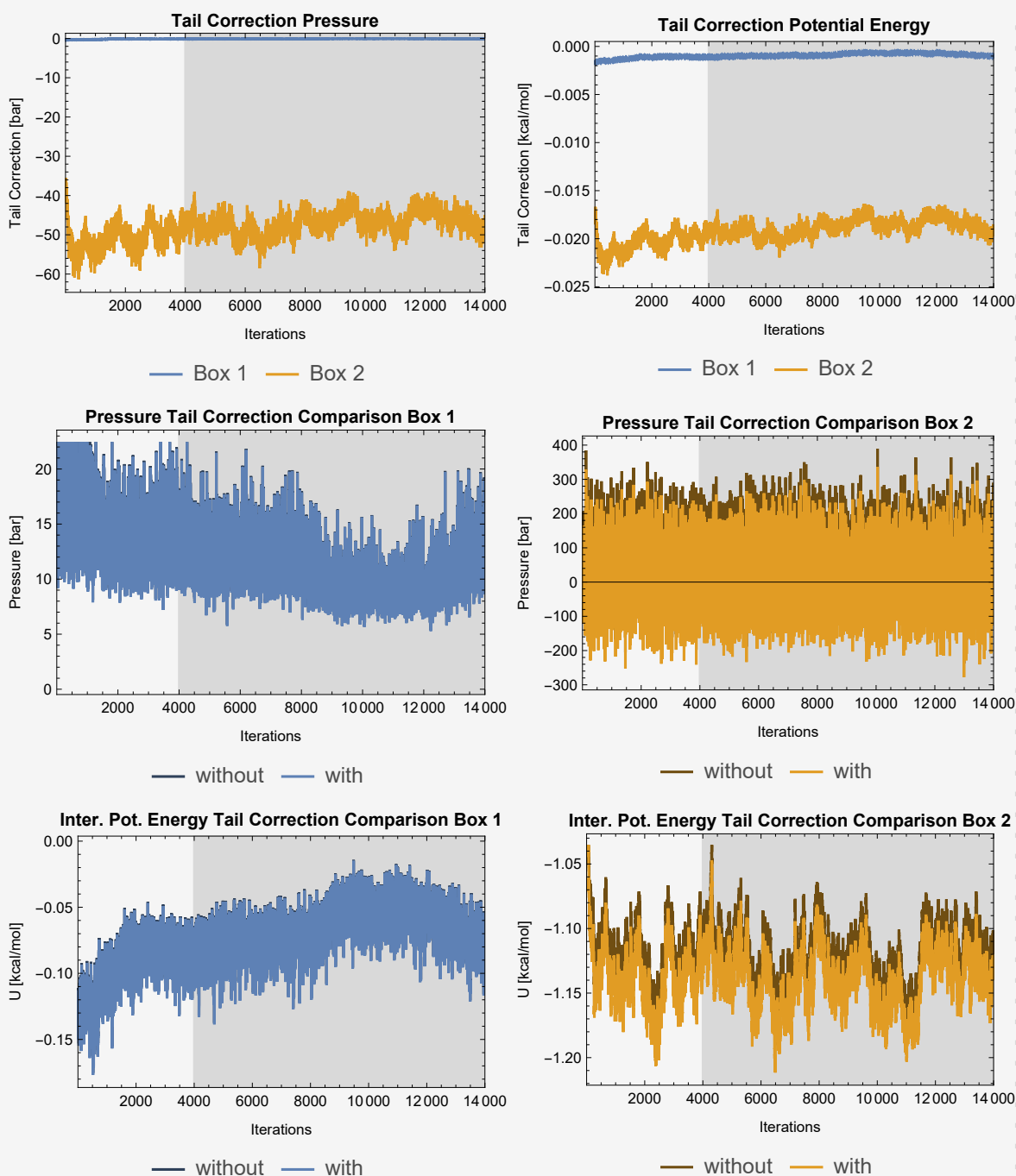


Tail Corrections

```
plotTailCorrGrid = Grid[{
  {plotTailCorrPressure,plotTailCorrEnergy},
  {plotTailComparisonPressure1,plotTailComparisonPressure2},
  {plotTailComparisonEnergy1,plotTailComparisonEnergy2}
}, ItemSize→Scaled[0.5],Alignment→Center]
```

```
ExportGraphic["plotTailCorr.pdf",plotTailCorrGrid];
```

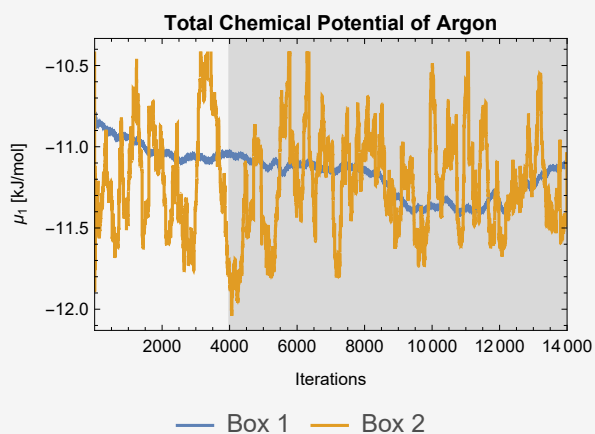
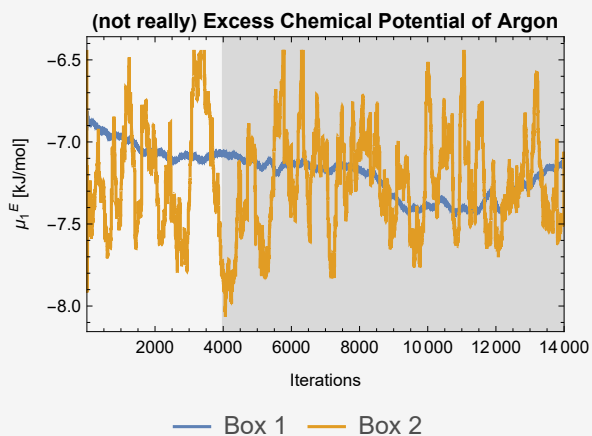
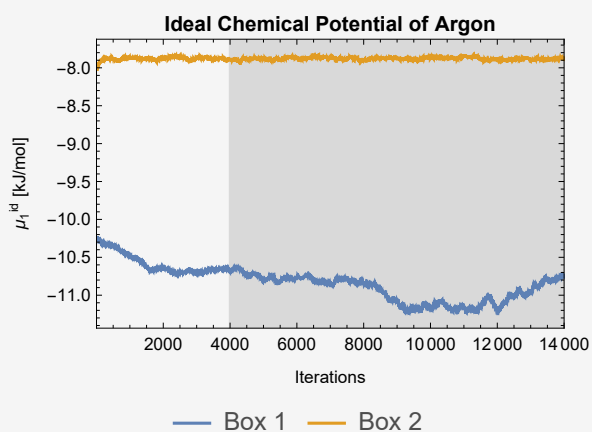
```
markShowCell[EvaluationCell[]];
```



Chemical Potentials

```
plotChemPotGrid = Grid[{
  plotIdealChemPotential,
  plotExcessChemPotential,
  plotTotalChemPotential
}, ItemSize→Scaled[0.5], Alignment→Center]

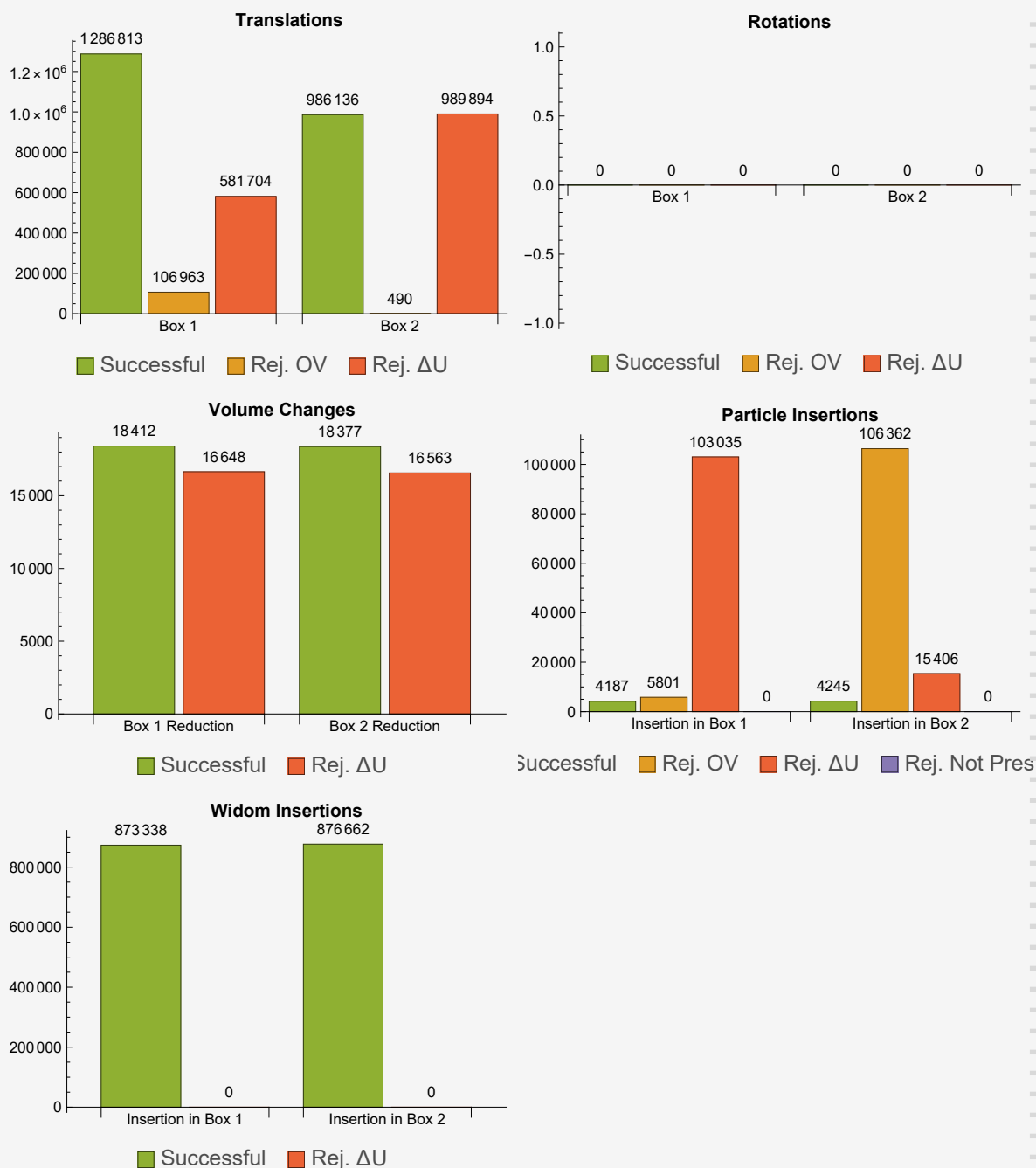
ExportGraphic["plotChemPot.pdf", plotChemPotGrid];
markShowCell[EvaluationCell[]];
```



Plot of the Standard Deviation of the molar volume

Counters

```
plotCountersGrid
ExportGraphic["plotCounters.pdf",plotCountersGrid];
markShowCell[EvaluationCell[]];
```



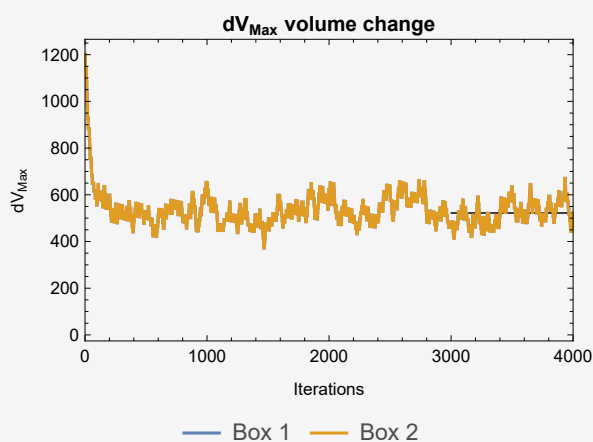
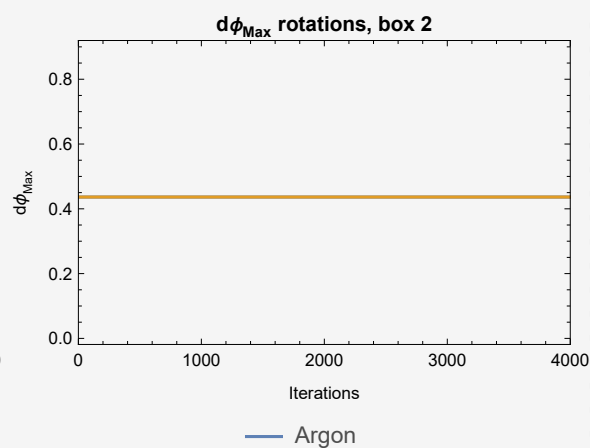
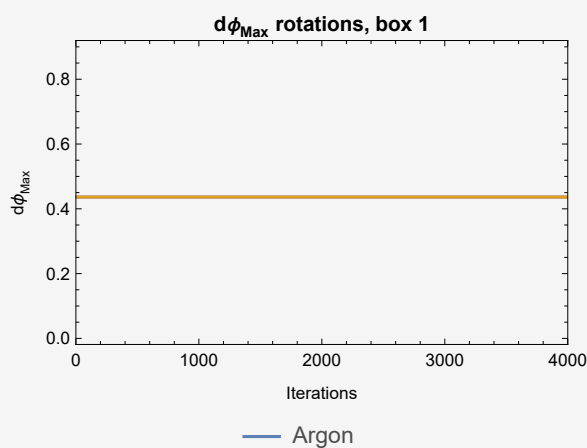
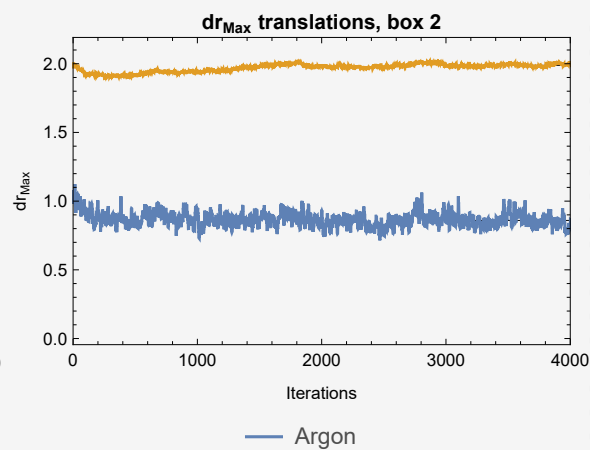
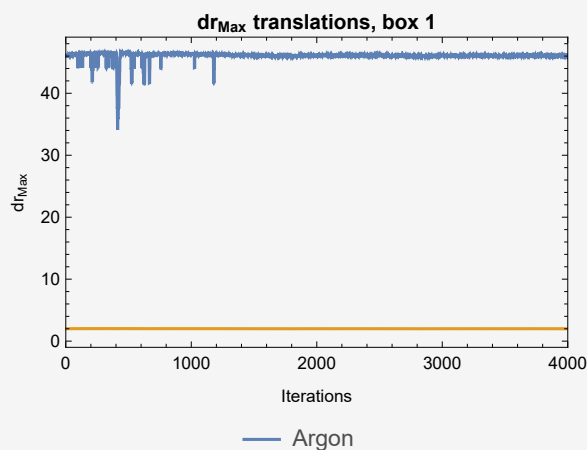
Species specific Counters

```
plotSpeciesCountersGrid  
markShowCell[EvaluationCell[]];
```

No species specific plots if only one species is simulated

Trial Move Limits Course

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



```

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

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

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

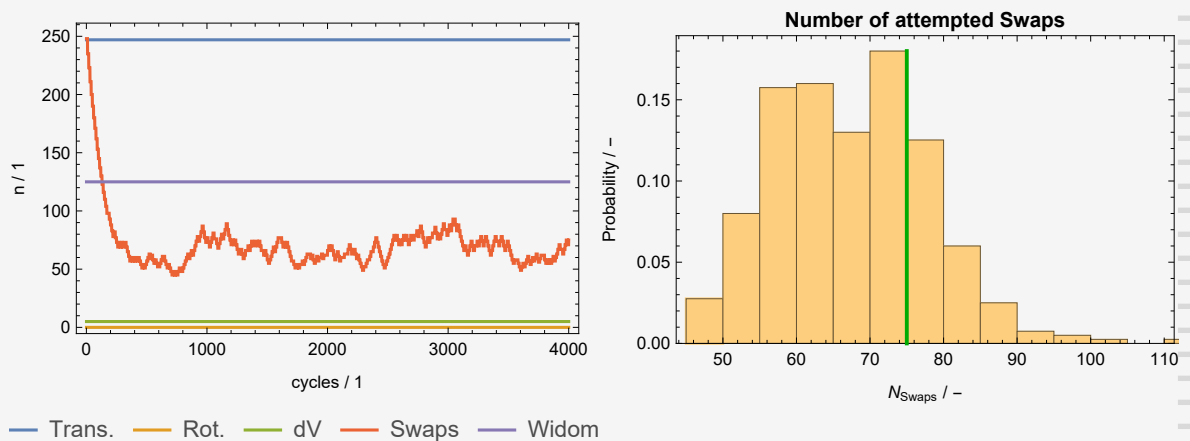
```

Number of Trial Moves

```

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

```

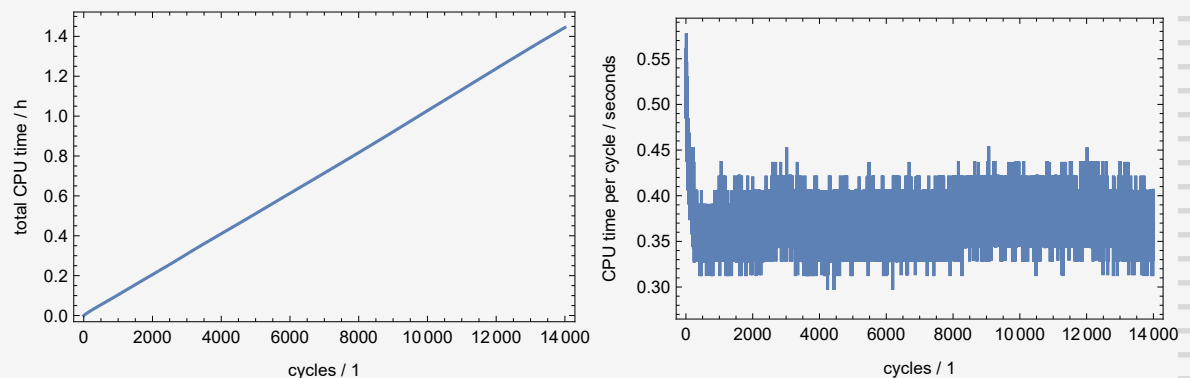


CPU Time Usage

```

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

```



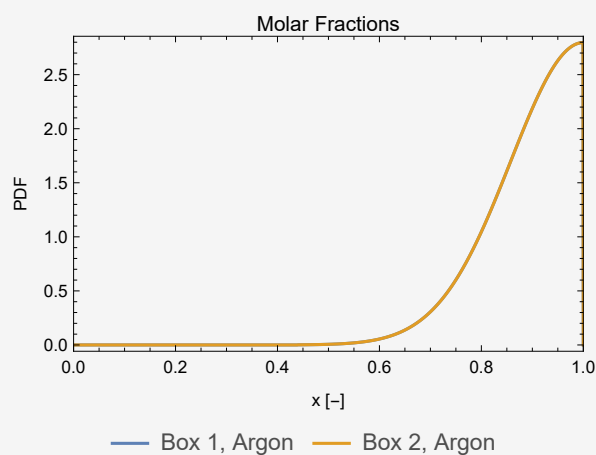
Ensemble Averages

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

Density Plots

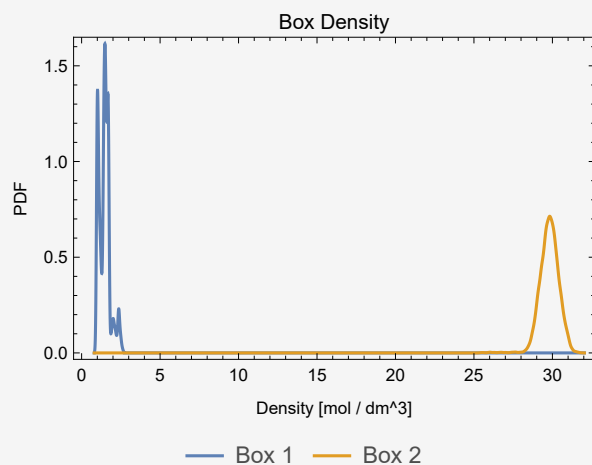
Mole Fractions

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



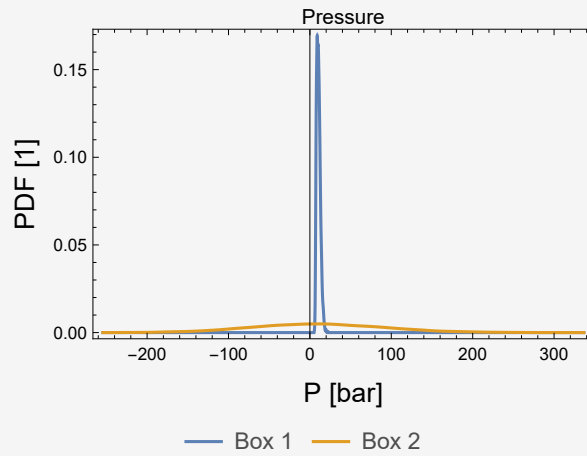
Box Densities

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



Pressure

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



Averaged Values

```
assocResults = <| |>;
showAveragedValues
ExportGraphic["simResultsAveragedValues.pdf", showAveragedValues];
markShowCell[EvaluationCell[]];
```

AVERAGED VALUES averaged from 4001 to 14000 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]	0.793006	0.144048	0.0335338	0.000624428
rho [mol / dm ³]	1.30178	0.226285	29.831	0.555121
n [1]	75.7452	13.6888	424.255	13.6888
Pressure				
P ideal [bar]	12.6409	2.19733	289.672	5.39048
P virial [bar]	–1.98076	1.89309	–231.912	79.764
P tail [bar]	–0.0961372	0.031633	–46.9179	2.85234
P [bar]	10.564	2.33244	10.8425	80.9242
Internal Energy				
U Inter [kcal/mol]	–0.0661878	0.0170742	–1.13984	0.0227061
U Intra [kcal/mol]	0.	0.	0.	0.
U Total [kcal/mol]	–0.0661878	0.0170742	–1.13984	0.0227061
Mole Fractions				
Argon	1.0000	0	1.0000	0
Ideal μ [kJ/mol]				
Argon	–10.934	0.17352	–7.8777	0.018074
Excess μ [kJ/mol]				
Argon	7.2447	0.11545	7.2574	0.30624
Total μ [kJ/mol]				
Argon	–11.219	0.11545	–11.232	0.30624

Reduced Units

```
NormalizedUnits[];
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	10.6	bar	$p_{\text{red}}=p/p_C$	$p^*=p \cdot \sigma^3/\epsilon$
p_L	10.8	bar		
ρ_V	1.30	mol / dm ³	$\rho_{\text{red}}=\rho/\rho_C$	$\rho^*=\rho \cdot \sigma^3$
ρ_L	29.8	mol / dm ³		
μ_V	-11.2	kJ / mol	$\mu_{\text{red}}=\mu / \mu_C$	$\mu^*=\mu / \epsilon$
μ_L	-11.2	kJ / mol		

Comparison & Checks

Comparison Functions

Equation of State Comparison

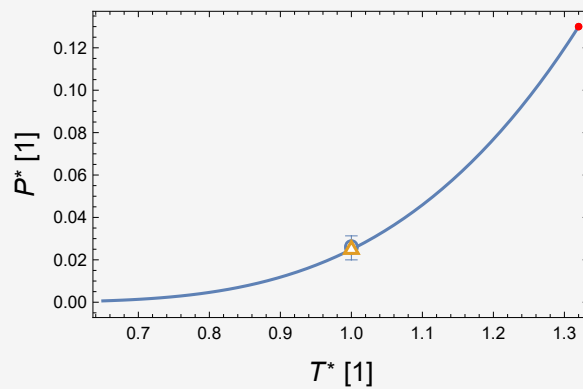
Comparison to a pure LJ EOS (Thol, 2016), a t-PR-LJ EoS (Harismiadis, 1994) or the SRK EoS

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

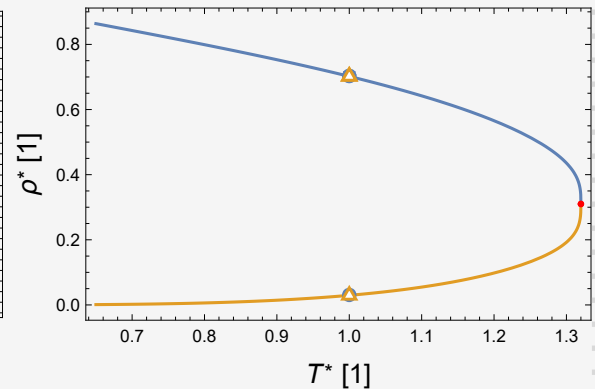
LJ Comparison, Argon at $T^* = 1$.

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	$\Delta_{\text{rel}} / \%$
$\rho^* / 1$	0.0307	0.0295	4.17	0.703	0.702	0.178
$P^* / 1$	0.0256	0.0249	3.02	0.0263	0.0249	5.74



○ Simulation △ LJ-Fluid EOS ● Critical point



○ Simulation △ LJ-Fluid EOS ● Critical point

Equilibrate State

```
Showcheckfinalvalues
markShowCell[EvaluationCell[]];
```

Checking minimum particle and length of the simulation	
min 10 particles in gas phase	😊
min 200 particles in liquid phase	😊
gas particles 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

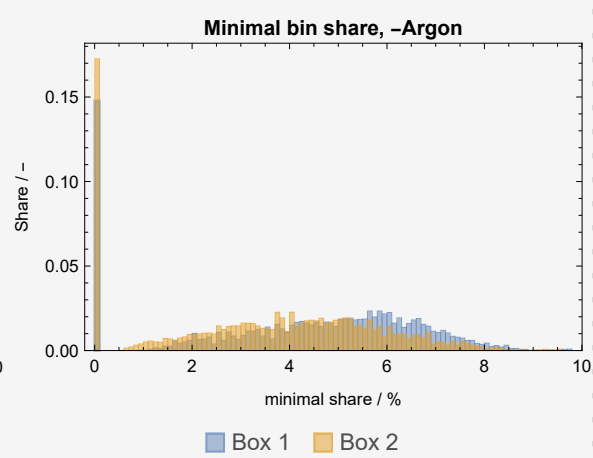
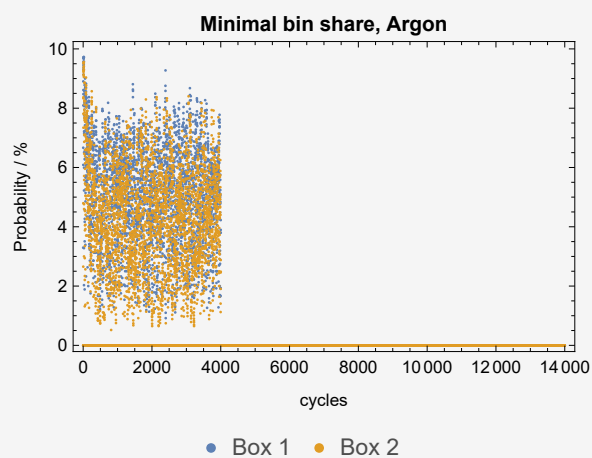
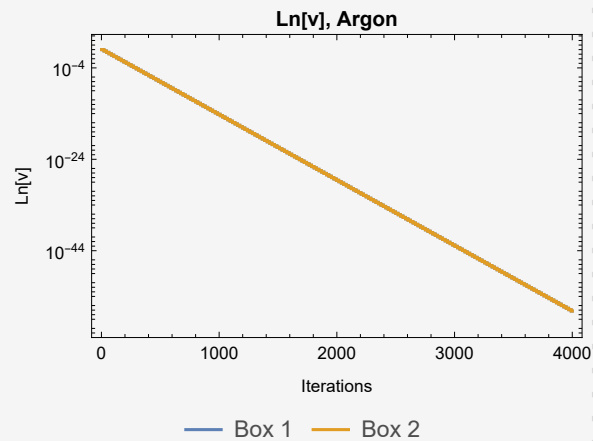
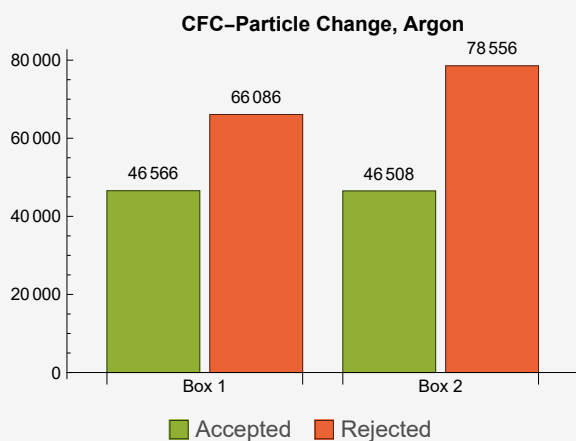
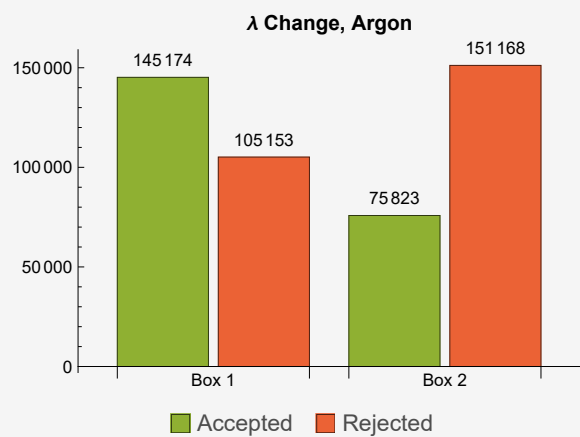
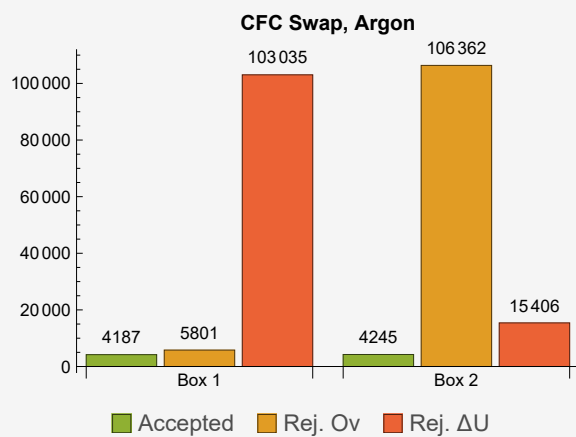
Setup

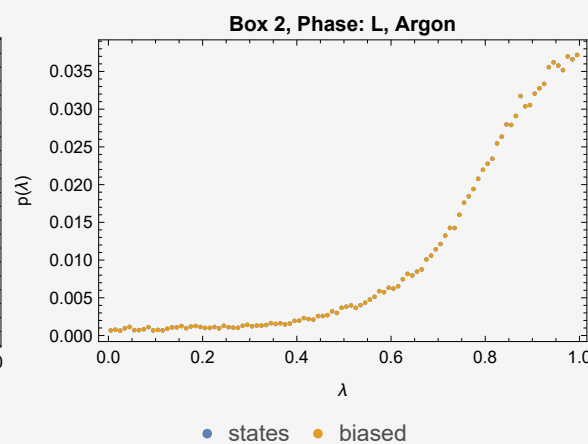
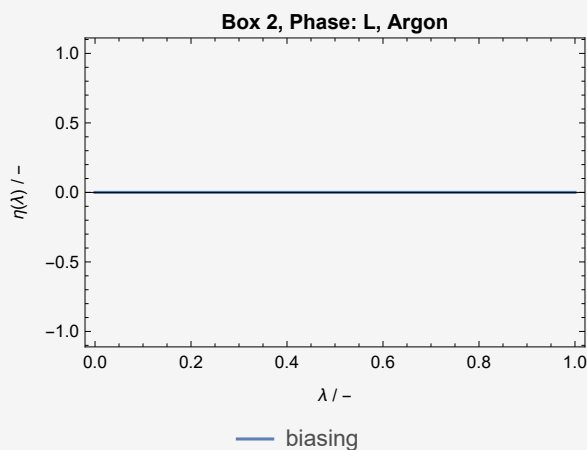
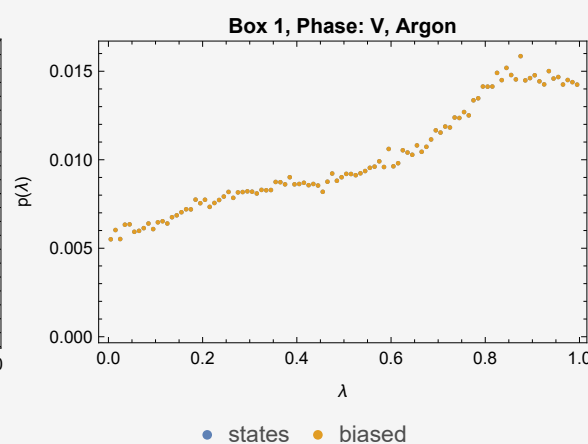
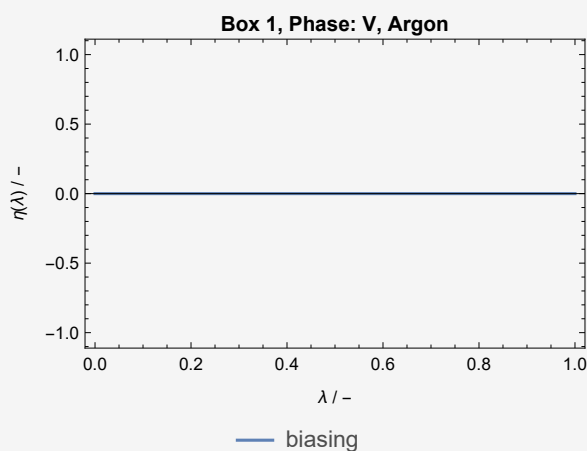
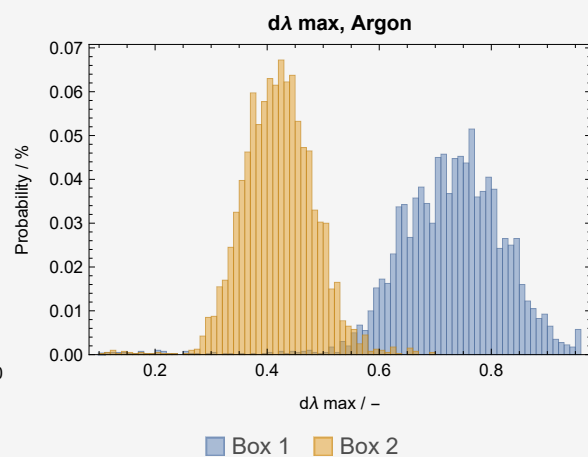
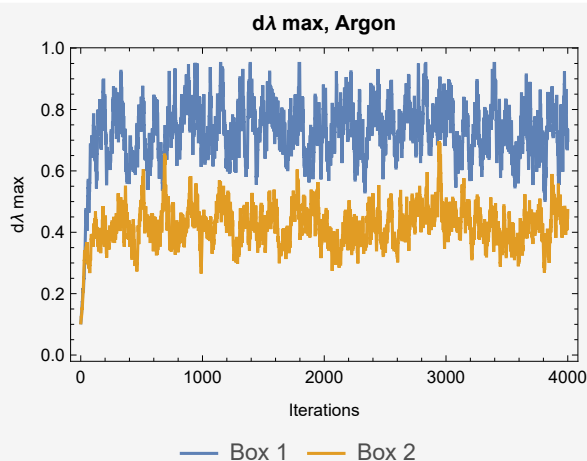
CFC Vlugt

Basic

```
visualizeCfcVlugtBasic[];
```

CFC Vlugt Trial Move Timing						
Part	Time / total	t_{total} / %	t_{avr} / ms	t_{acc} / ms	t_{rejDu} / ms	t_{rejOv} / ms
Lambda Change	0h 2min 43s	31.95	0.342538	0.568841	0.147422	–
Exchange	0h 3min 54s	45.77	0.985357	1.42931	0.699681	–
Swap	0h 1min 54s	22.28	0.476929	1.8394	0.411967	0.443101





type calculation	$\mu_{V,Ex}$	$\mu_{L,Ex}$
widom	-0.326	-3.34
last recorded bin	-0.923	-3.89
linear fit, 5 bins	-0.932	-4.08
linear fit, 10 bins	-0.888	-3.80
linear fit, 15 bins	-0.897	-3.83
linear fit, 20 bins	-0.935	-3.92
linear fit, 25 bins	-0.963	-3.88

Extensive

SwapMove Species Choice probabilities

PAN Binary Swaps

Ewald Electrostatic Long Range Correction

Wolf Electrostatic Long Range Correction

Custom Evaluations

Export Analysis Results

Credits