

# 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_2_CO2_FS_4500@270K_n500 _Ewald-10-12-Inf

(	trialMoveAdoption	acceptedPerCycle	widomrOvl	0	)
trialMoveAdoptionSetpoint	1	eqAdjAvrCycles	100		
trialMoveAdoptionBoundary	0.025	eLRMethod	Ewald		
trialMoveAdoptionAvg	10	eLRCKappa	{10, 10}		
trialMoveScaleMoves	False	eLRCKRange	{12, 12}		
trialMoveAdoptionLimit	10	eLRces	∞		
(	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	CarbonDioxide		
T [K]	270.		
P [bar]	1.		
	BOX 1	BOX 2	TOTAL
L [Å]	59.3604	28.0649	
V [Å <sup>3</sup> ]	209165.	22105.1	231270.
$\rho$ [Molecules/Å <sup>3</sup> ]	$1.19523 \times 10^{-3}$	$1.13096 \times 10^{-2}$	$2.16197 \times 10^{-3}$
v [dm <sup>3</sup> /mol]	0.503849	0.053248	0.278549
Number of Molecules	250	250	500
CarbonDioxide	250	250	500
Mole Fractions			
CarbonDioxide	1.	1.	1.

SIMULATION DETAILS		
warm-up cycles	500	
equilibration cycles	2000	
production cycles	2000	
translations per cycle	1000	
rotations per cycle	1000	
volume changes per cycle	1	
insertions per cycle	75	
ghost insertions per cycle	125	
total number of moves per cycles	2201	
	BOX 1	BOX 2
cutoff distance [ $\text{\AA}$ ]	29.6	14.
overlap distance [ $\text{\AA}$ ]	1.91386	1.91386
max translation distance [ $\text{\AA}$ ] CarbonDioxide	2.	2.
max rotation angle [rad] CarbonDioxide	0.436332	0.436332
max volume change [ $\text{\AA}^3$ ]	574.569	574.569

OPLS-AA DEFINITIONS				
	non-bonded	bond stretching	angle bending	torsion
CarbonDioxide	O,C02 C,C02 O,C02			

# 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]	4.7559
Timing @ End [ms]	4.77855
Total physical memory @ End [GB]	6.9719 GiB
Total physical memory @ End [GB]	6.94076 GiB
ENSEMBLE AVERAGES	
Average from cycle	2001
Average to cycle	4000

## Evaluation Times

### Define Grid

## Show Information

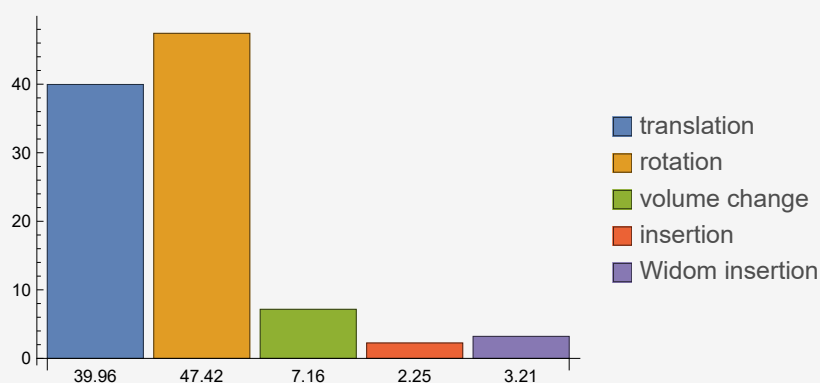
```
ShowEvalTimesCode
ShowEvalTimesPhases
NormalizedTiming[]
markShowCell[EvaluationCell[]];
```

CODE PARTS					
Part	Time / total	$t_{avr}$ / ms	$t_{acc}$ / ms	$t_{rejDu}$ / ms	$t_{rejOv}$ / ms
Translation	2h 15min 50s	1.81133	2.04369	1.68854	0.579444
Rotation	2h 41min 12s	2.14955	2.27762	1.93597	0.842394
Volume Change	0h 24min 20s	365.024	365.354	364.67	–
Insertion	0h 7min 38s	1.52313	6.57159	2.03049	0.789485
Widom	0h 10min 54s	1.30871	1.30871	–	–

SIMULATION PHASES		
Part	Time / total	Time Fraction
Warm-Up Cycles	0h 32min 58s	6.668%
Equilibration Cycles	3h 50min 14s	46.55%
Production Cycles	3h 51min 21s	46.78%
Trial Move Execution	5h 39min 56s	68.74%
Tail Correction	2h 31min 21s	30.6%
Documentation	0h 1min 27s	0.3%
Other	0h 1min 48s	0.37%
Total	8h 14min 33s	

Normalized Timing	$t'_{avr}$	$t'_{acc}$	$t'_{rejeDu}$	$t'_{rejeOv}$	$t'$ per succ. move
Translation	0.886	1.00	0.826	0.284	1.75
Rotation	1.05	1.11	0.947	0.412	1.67
Volume Change	179.	179.	178.	–	345.
Insertion	0.745	3.22	0.994	0.386	43.2
Widom	0.640	0.640	–	–	0.640

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



## Calculations

## Visual Check

### Show Boxes

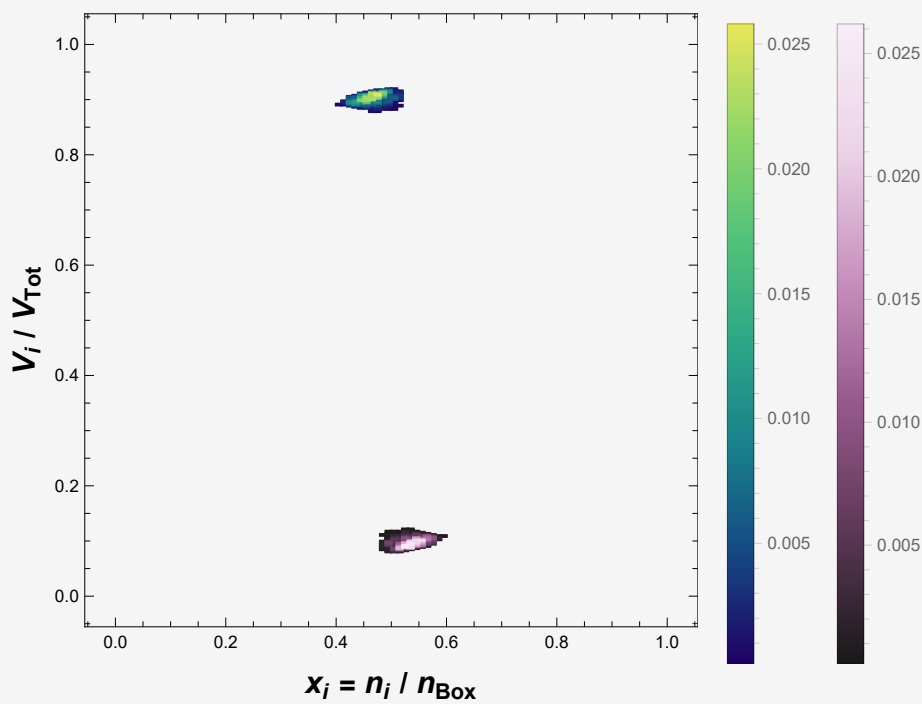
### Probability Plot

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

```

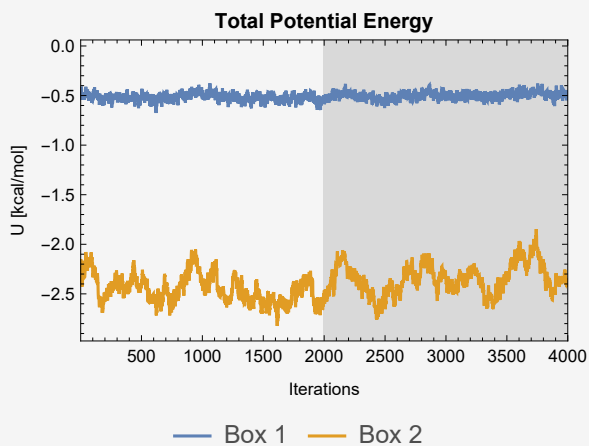
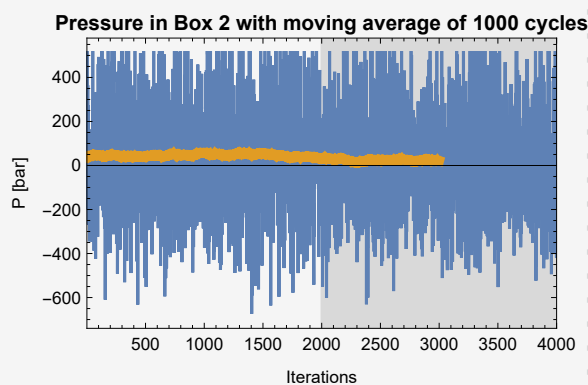
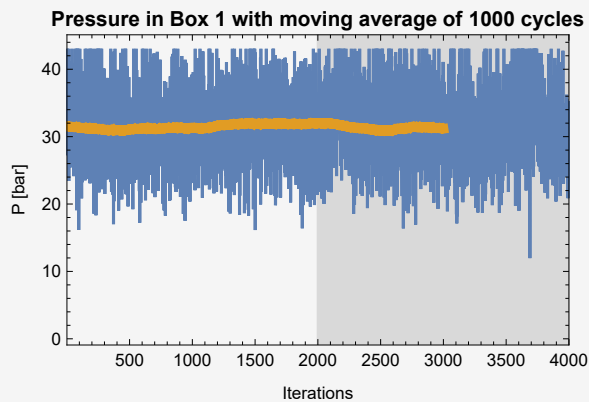
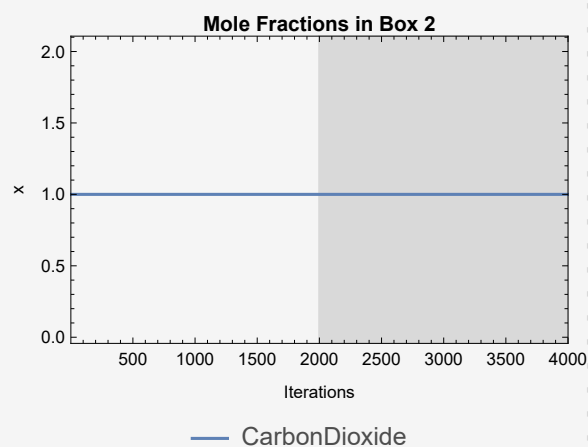
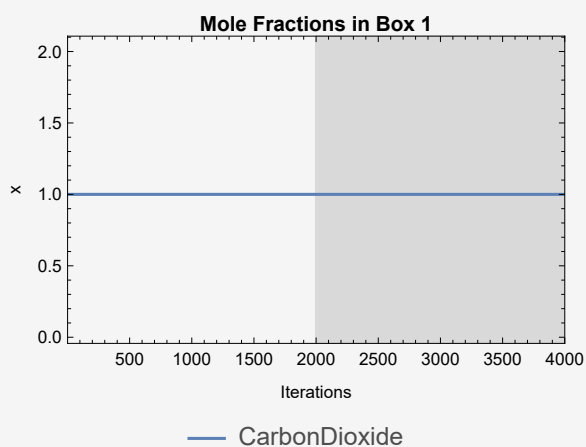
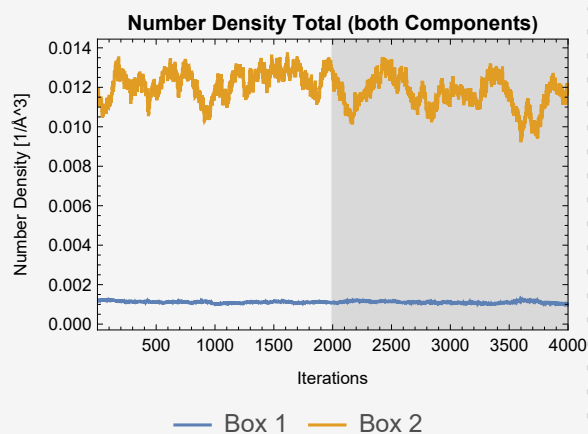
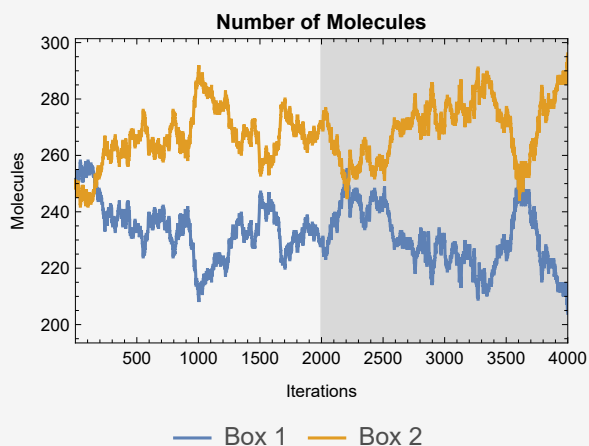
## Values

```

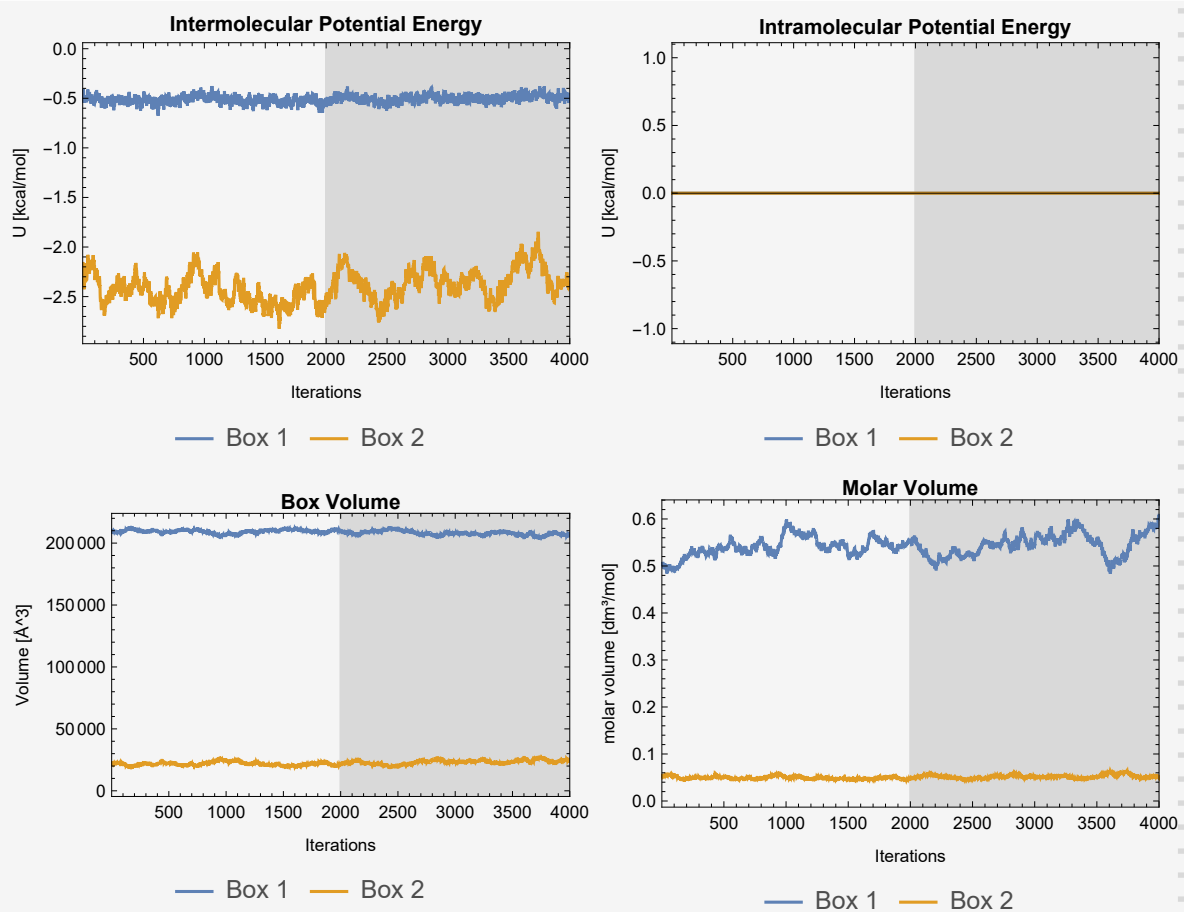
plotValuesGrid = Grid[{
  {plotNumOfMolecules,plotDensityTotal},
  {plotMoleFractions1,plotMoleFractions2},
  {plotPressure1,plotPressure2},
  {plotTotalEnergy},
  {plotInterEnergy,plotIntraEnergy},
  {plotVolume,plotMolarVolume}
},Alignment→Center, ItemSize→Scaled[0.5]]

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

```





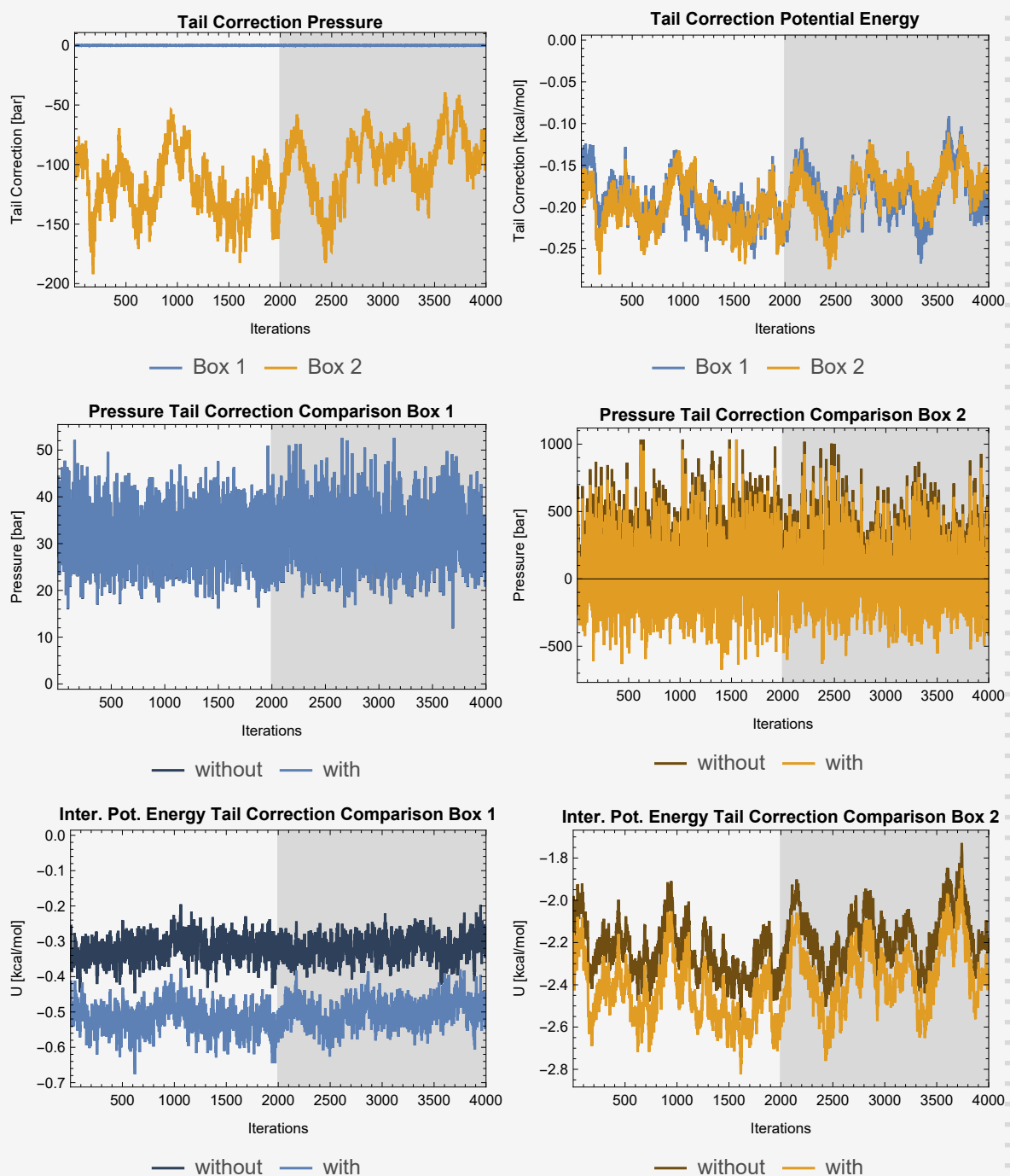


## Tail Corrections

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

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

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



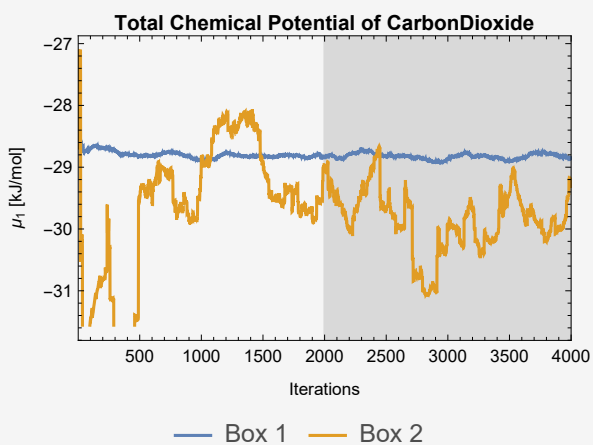
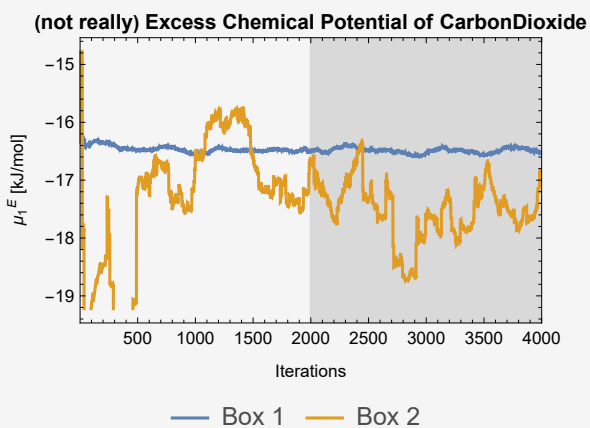
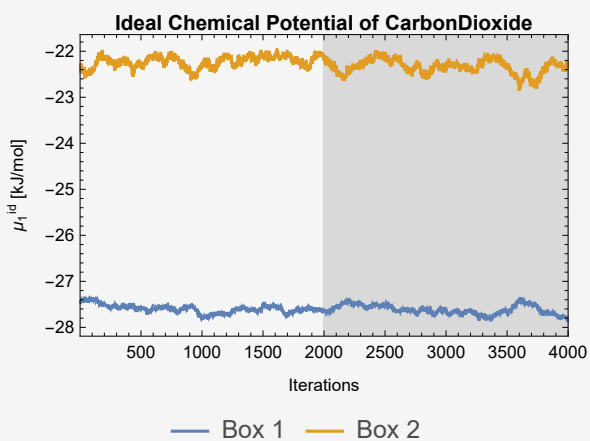
## Chemical Potentials

```

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

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

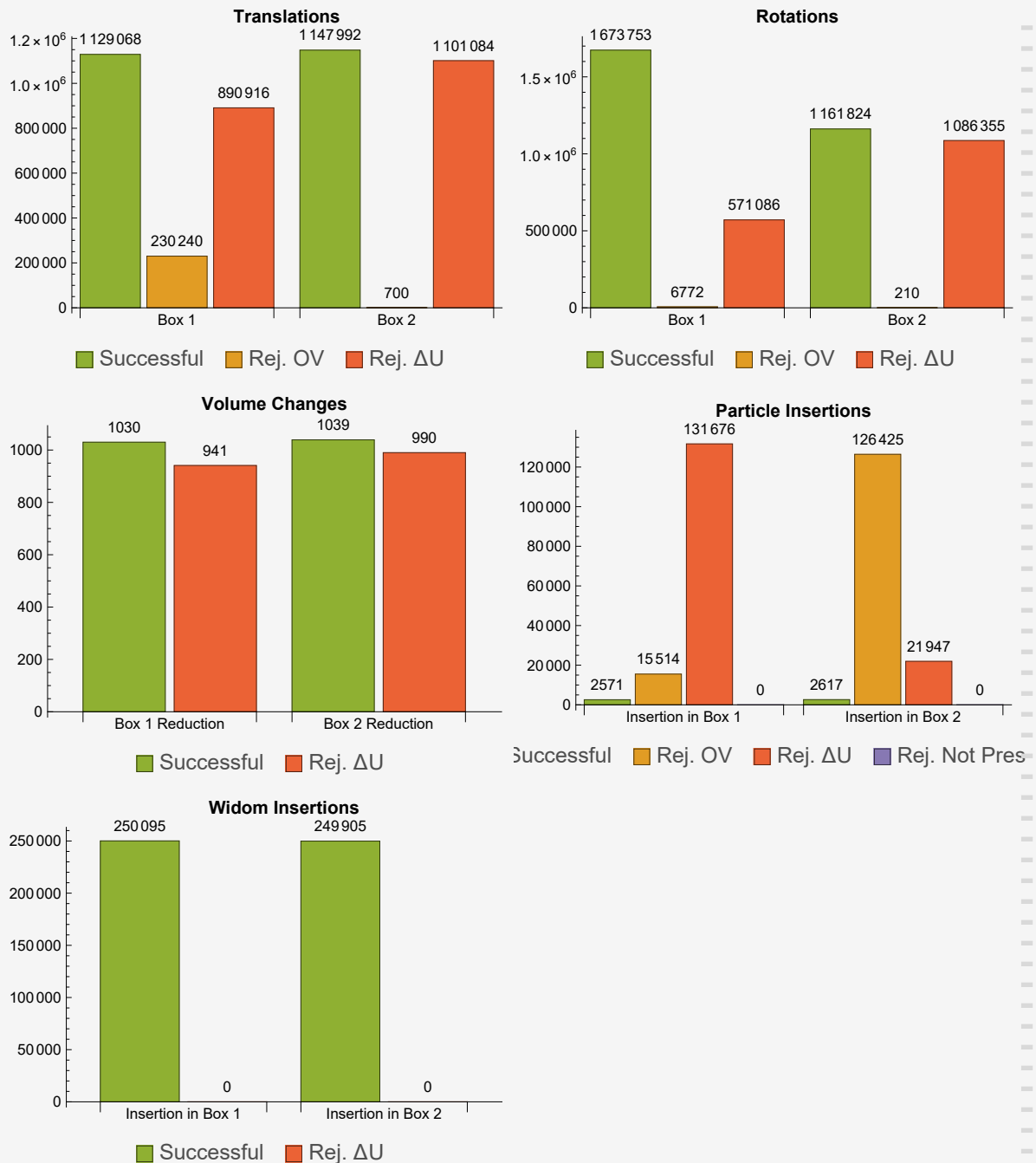
```



## Plot of the Standard Deviation of the molar volume

### Counters

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



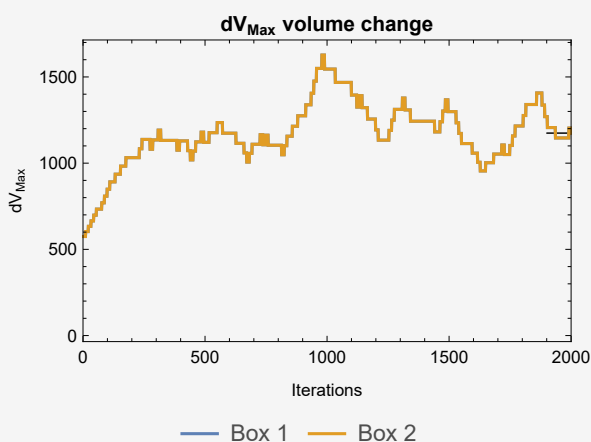
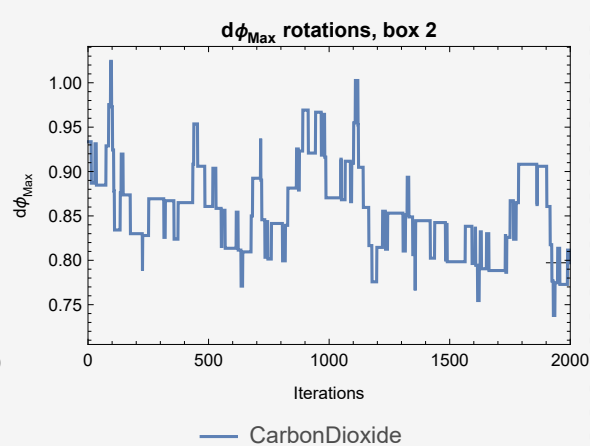
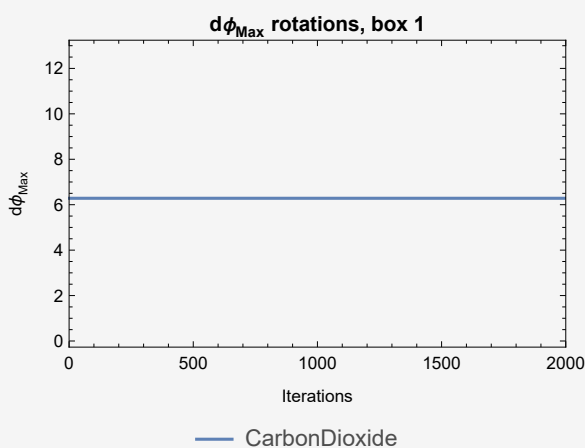
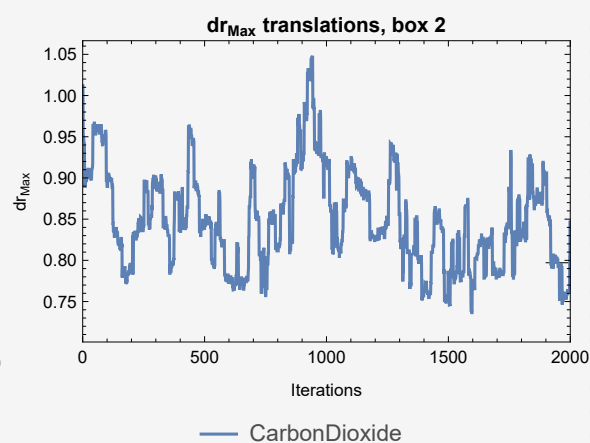
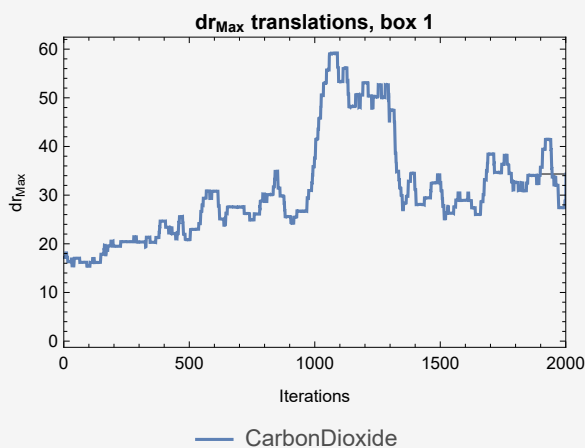
## Species specific Counters

```
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]

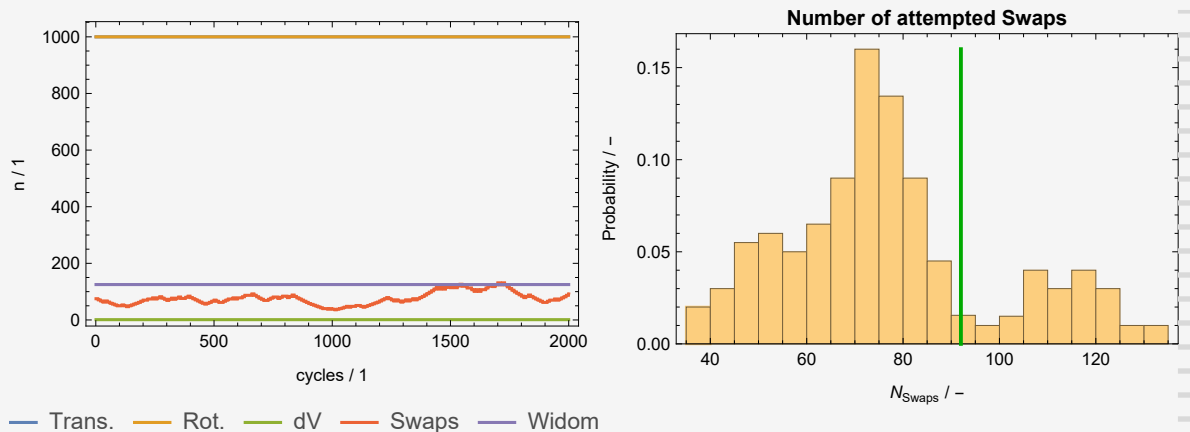
```

## Number of Trial Moves

```

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

```

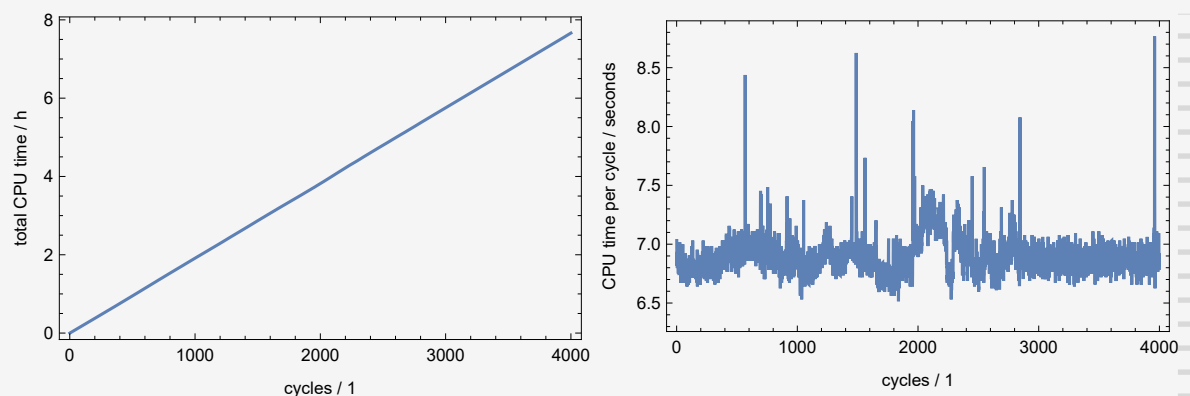


## CPU Time Usage

```

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

```



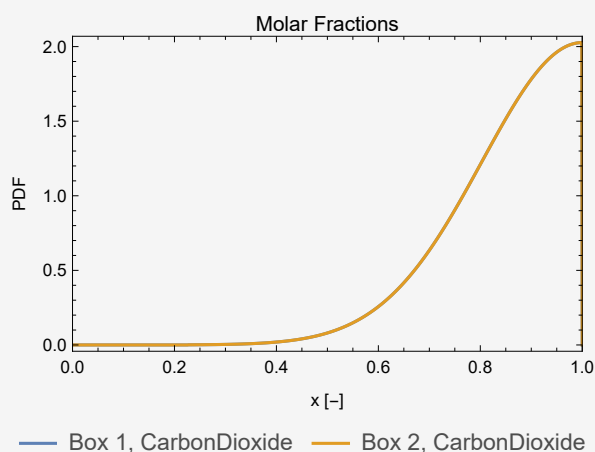
## Ensemble Averages

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

### Density Plots

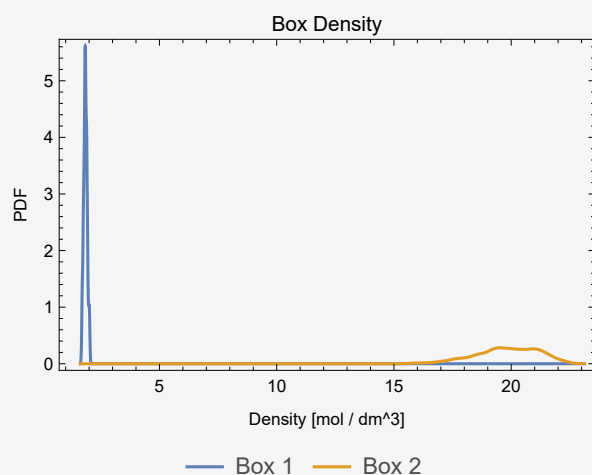
#### Mole Fractions

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



#### Box Densities

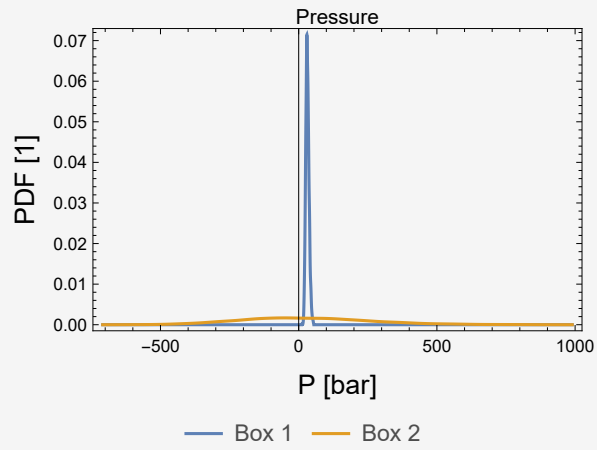
```
ExportGridGraphic[{"densityHistogram", plotDensityHistogram[]}, False];
markShowCell[EvaluationCell[]];
```





## Pressure

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



## Averaged Values

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

AVERAGED VALUES				
averaged from 2001 to 4000				
Box V corresponds to Box 1, Box L corresponds to Box 2				
System	Box V		Box L	
	mean	std	mean	std
T [K]	270.	–	270.	–
v [dm <sup>3</sup> / mol]	0.545357	0.0241468	0.052	0.00367563
rho [mol / dm <sup>3</sup> ]	1.83727	0.081728	19.3237	1.32159
n [1]	230.132	10.6246	269.869	10.6246
<b>Pressure</b>				
P ideal [bar]	41.2451	1.83472	433.8	29.6684
P viral [bar]	–9.71308	5.73791	–310.292	231.263
P tail [bar]	0.0516405	0.0417811	–97.1009	24.9178
P [bar]	31.5836	5.88907	26.4072	233.957
<b>Internal Energy</b>				
U Inter [kcal/mol]	–0.498223	0.0371691	–2.34703	0.153272
U Intra [kcal/mol]	0.	0.	0.	0.
U Total [kcal/mol]	–0.498223	0.0371691	–2.34703	0.153272
<b>Mole Fractions</b>				
CarbonDioxide	1.0000	0	1.0000	0
<b>Ideal <math>\mu</math> [kJ/mol]</b>				
CarbonDioxide	–27.618	0.099621	–22.339	0.15593
<b>Excess <math>\mu</math> [kJ/mol]</b>				
CarbonDioxide	16.489	0.045188	17.525	0.49613
<b>Total <math>\mu</math> [kJ/mol]</b>				
CarbonDioxide	–28.825	0.045188	–29.860	0.49613

## Reduced Units

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

name	dimensional	unit	critical norm	
T	270.	K	$T_{\text{red}}=T/T_c$	0.888
$p_v$	31.6	bar	$p_{\text{red}}=p/p_c$	0.428
$p_L$	26.4	bar		0.358
$\rho_v$	1.84	mol / dm <sup>3</sup>	$\rho_{\text{red}}=\rho/\rho_c$	0.173
$\rho_L$	19.3	mol / dm <sup>3</sup>		1.82
$\mu_v$	-28.8	kJ / mol	$\mu_{\text{red}}=\mu/\mu_c$	-
$\mu_L$	-29.9	kJ / mol		-

# Comparison & Checks

## Comparison Functions

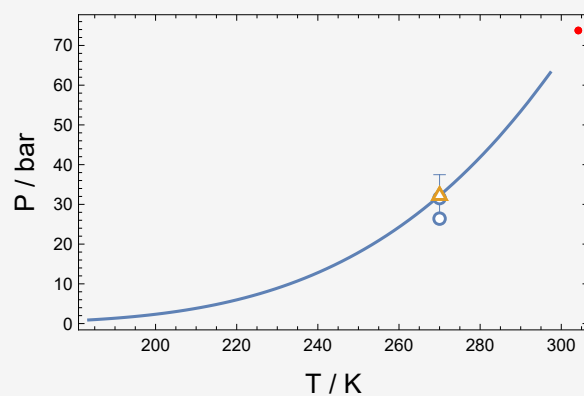
## Equation of State Comparison

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

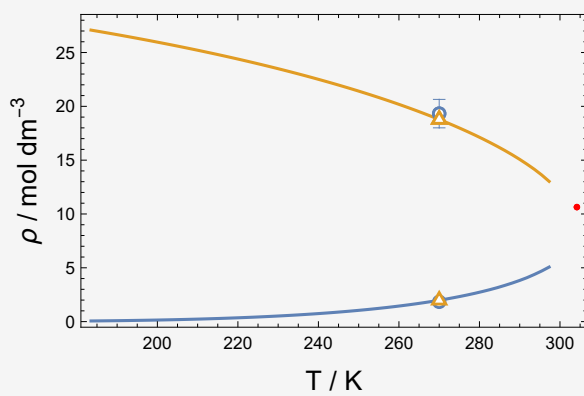
```
EosResultsAssoc = <| |>;
CalculateEosComparison[]; Pause[1];
markShowCell[EvaluationCell[]];
```

SRK Comparison, CarbonDioxide at T = 270 K  
Defintion relative error:  $\text{Abs}[\zeta_{\text{Sim}} - \zeta_{\text{EOS}}] / \zeta_{\text{EOS}}$

	Box V			Box L		
Unit	Sim	SRK-EoS	$\Delta_{\text{rel}} / \%$	Sim	SRK-EoS	$\Delta_{\text{rel}} / \%$
$\rho / \text{mol dm}^{-3}$	1.84	1.98	7.44	19.3	18.8	2.90
P / bar	31.6	32.2	1.94	26.4	32.2	18.0



○ Simulation    △ SRK EOS    ● Critical point



○ Simulation    △ SRK 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 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

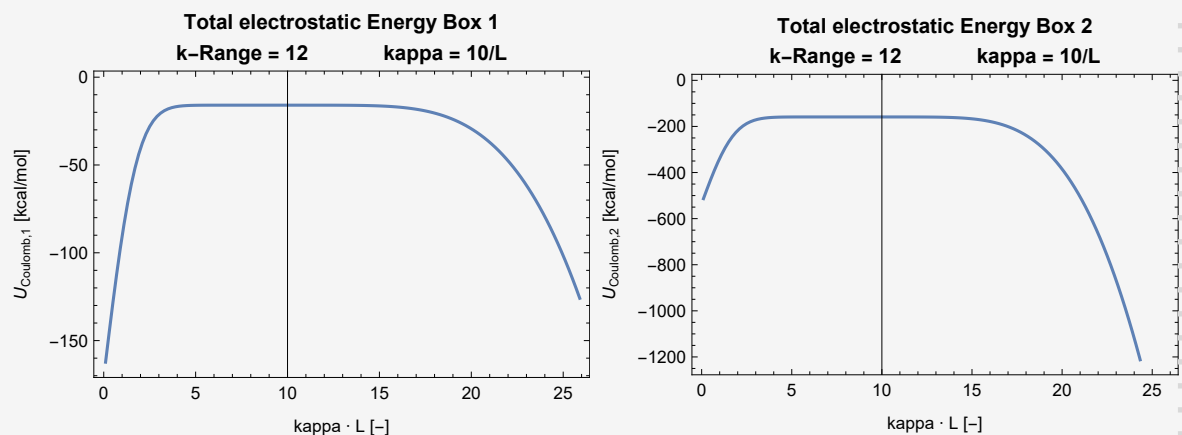
CFC Vlugt

SwapMove Species Choice probabilities

PAN Binary Swaps

## Ewald Electrostatic Long Range Correction

```
If[SameQ[checkGetAssocParameter[custParam, "eLRCMethod"], "Ewald"],
  VisualizeELRCEwald[exportFlag];
  markShowCell[EvaluationCell[]];];
```



## Wolf Electrostatic Long Range Correction

### Custom Evaluations

## Export Analysis Results

## Credits