

# 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_3_EthErr-Me2ndV_FS_23000@ T210K@P26.5bar_n500_PANSwap

panBinarySwaps	True	boxSpecificVolumeLimits	True
panExchangeSpecies	1	speciesSwapProbabilityMode	autoSwap
trialMoveAdoption	acceptedPerCycle	speciesSwapProbability	$\{\frac{1}{2}, \frac{1}{2}\}$
trialMoveAdoptionSetpoint	1	speciesSwapBoundary	1
trialMoveAdoptionBoundary	0.025	speciesSwapWeightIncrease	5
trialMoveAdoptionAvg	10	speciesSwapLive	False
trialMoveScaleMoves	False	widomrOvl	0
trialMoveAdoptionLimit	10	eqAdjAvrCycles	1000
trialMoveSpeciesSepcific	True	-	-
trialMoveAdoptionMaximumSwaps	3000		
trialMoveAdoptionAdaptVolumeChanges	False		
trialMoveLimitsAdoptionMode	numberMoves		
speciesSwapCyclesAdjustment	10		

# 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 Pressure		
Components	Ethane, Methane		
T [K]	210.		
P [bar]	26.5		
	BOX 1	BOX 2	TOTAL
L [Å]	49.0398	29.0715	
V [Å <sup>3</sup> ]	117936.	24570.	142506.
$\rho$ [Molecules/Å <sup>3</sup> ]	$2.1198 \times 10^{-3}$	$1.0175 \times 10^{-2}$	$3.50863 \times 10^{-3}$
v [dm <sup>3</sup> /mol]	0.28409	0.0591855	0.171638
Number of Molecules	250	250	500
Ethane	97	97	194
Methane	153	153	306
Mole Fractions			
Ethane	0.388	0.388	0.388
Methane	0.612	0.612	0.612

SIMULATION DETAILS		
warm-up cycles	2000	
equilibration cycles	6000	
production cycles	15000	
translations per cycle	500	
rotations per cycle	0	
volume changes per cycle	1	
insertions per cycle	1000	
ghost insertions per cycle	125	
total number of moves per cycles	1626	
	BOX 1	BOX 2
cutoff distance [ $\text{\AA}$ ]	24.5	14.5
overlap distance [ $\text{\AA}$ ]	2.88425	2.88425
max translation distance [ $\text{\AA}$ ]		
Ethane	2.	2.
Methane	2.	2.
max rotation angle [rad]		
Ethane	0.436332	0.436332
Methane	0.436332	0.436332
max volume change [ $\text{\AA}^3$ ]	1425.06	1425.06

OPLS-AA DEFINITIONS				
	non-bonded	bond stretching	angle bending	torsion
Ethane	Ethane,Err Ethane,Err			
Methane	Methane,2ndV			

# 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]	4.77695
Timing @ End [ms]	4.69234
Total physical memory @ End [GB]	6.71136 GiB
Total physical memory @ End [GB]	8.45058 GiB
ESEMBLE AVERAGES	
Average from cycle	6001
Average to cycle	21000

## 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	1h 54min 26s	0.597103	0.72909	0.470982	0.313234
Rotation	0h 0min 0s	–	–	–	–
Volume Change	0h 15min 10s	43.3376	42.73	43.9535	–
Insertion	0h 10min 35s	0.734128	2.89447	0.708791	0.462998
Widom	0h 25min 50s	0.590777	0.590777	–	–

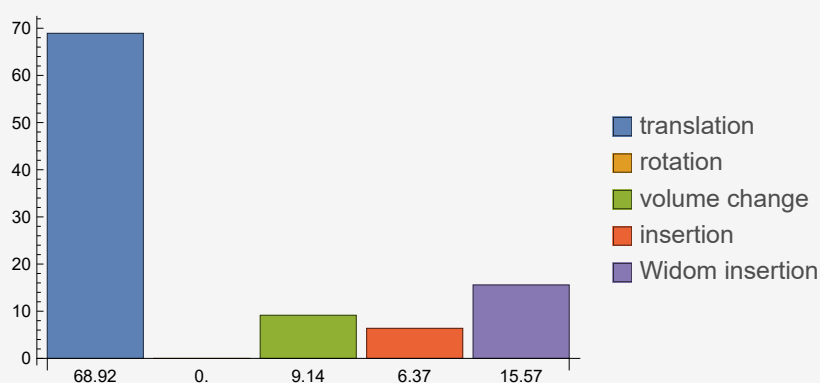
SIMULATION PHASES		
Part	Time / total	Time Fraction
Warm-Up Cycles	0h 10min 8s	4.554%
Equilibration Cycles	1h 3min 57s	28.71%
Production Cycles	2h 28min 41s	66.74%
Trial Move Execution	2h 46min 2s	74.53%
Tail Correction	0h 43min 17s	19.43%
Documentation	0h 11min 6s	4.99%
Other	0h 2min 20s	1.05%
Total	3h 42min 47s	

Normalized Timing	$t'_{avr}$	$t'_{acc}$	$t'_{rejeDu}$	$t'_{rejeOv}$	$t'$ per succ. move
Translation	0.819	1.00	0.646	0.430	1.54
Rotation	–	–	–	–	–
Volume Change	59.4	58.6	60.3	–	118.
Insertion	1.01	3.97	0.972	0.635	16.5
Widom	0.810	0.810	–	–	0.810

ShowEvalTimesBarChart

ExportGraphic["evaluationTimes.pdf", ShowEvalTimesBarChart];

markShowCell[EvaluationCell[]];



## Calculations

## Visual Check

### Show Boxes

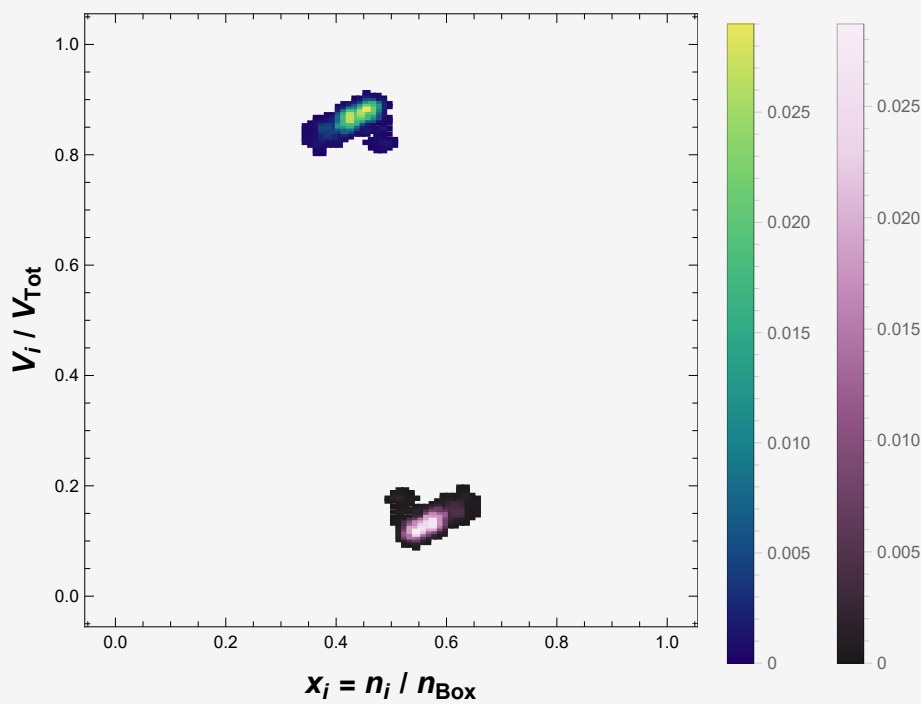
### Probability Plot

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

```

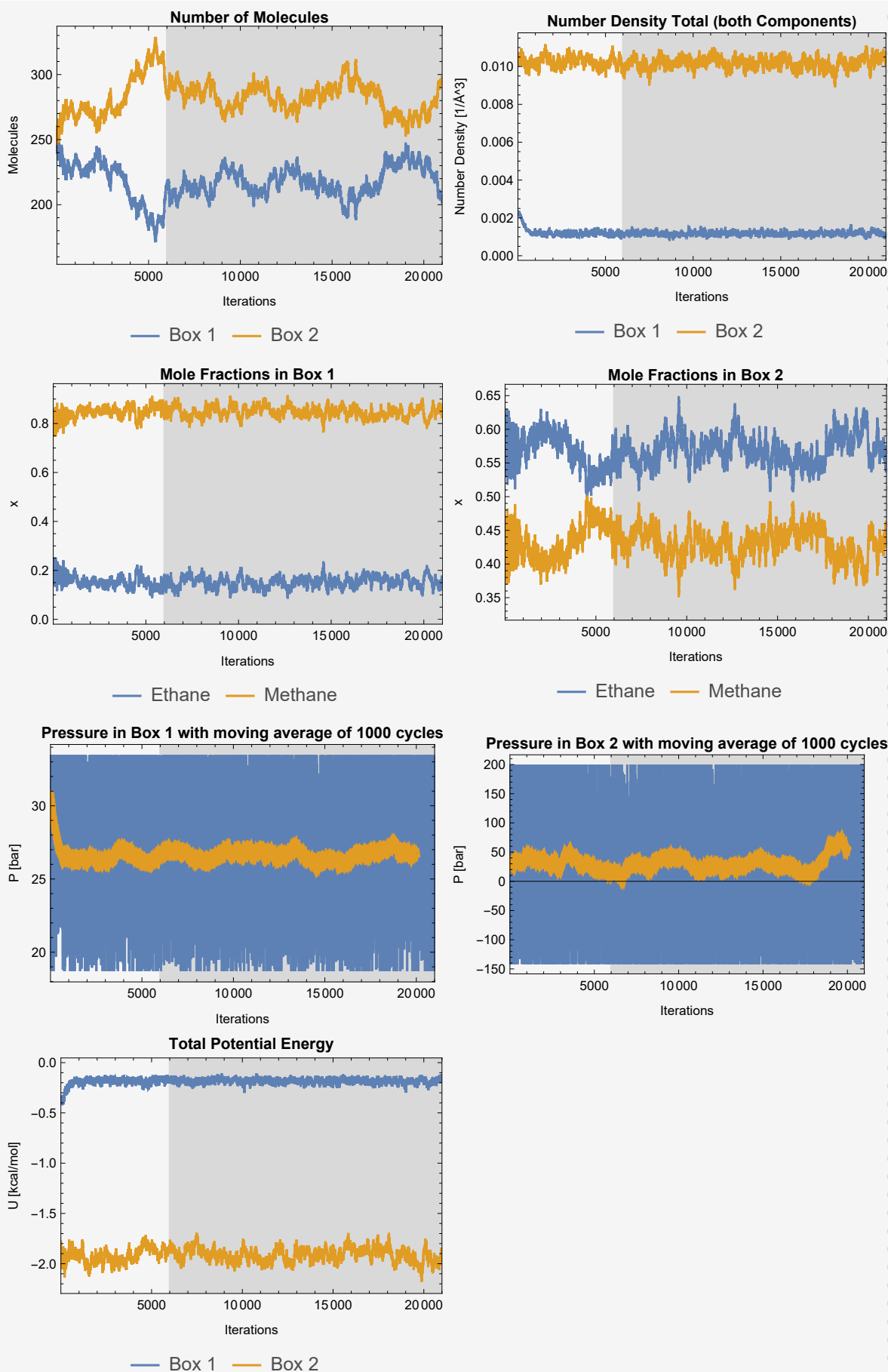
## Values

```

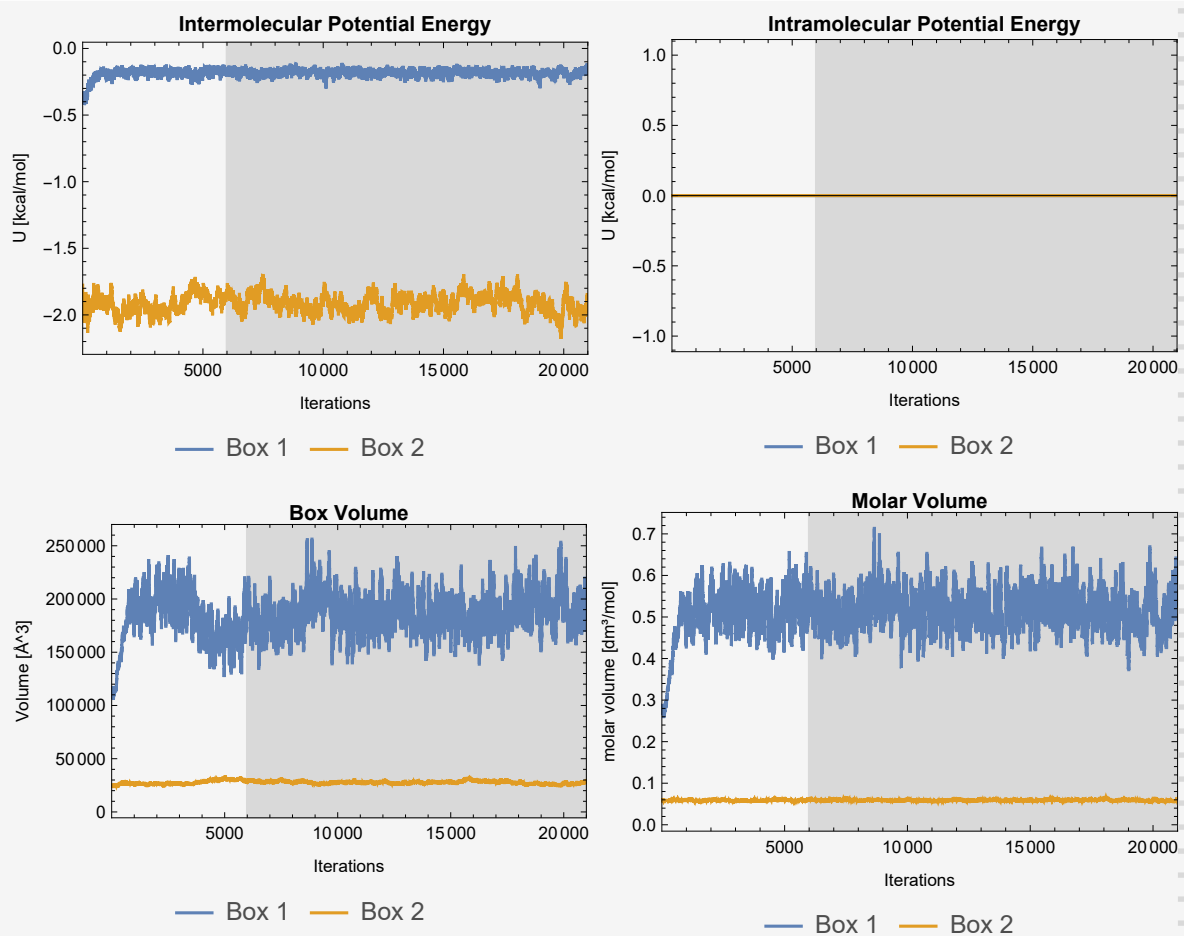
plotValuesGrid = Grid[{
  {plotNumOfMolecules,plotDensityTotal},
  {plotMoleFractions1,plotMoleFractions2},
  {plotPressure1,plotPressure2},
  {plotTotalEnergy},
  {plotInterEnergy,plotIntraEnergy},
  {plotVolume,plotMolarVolume}
},Alignment→Center, ItemSize→Scaled[0.5]]

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

```





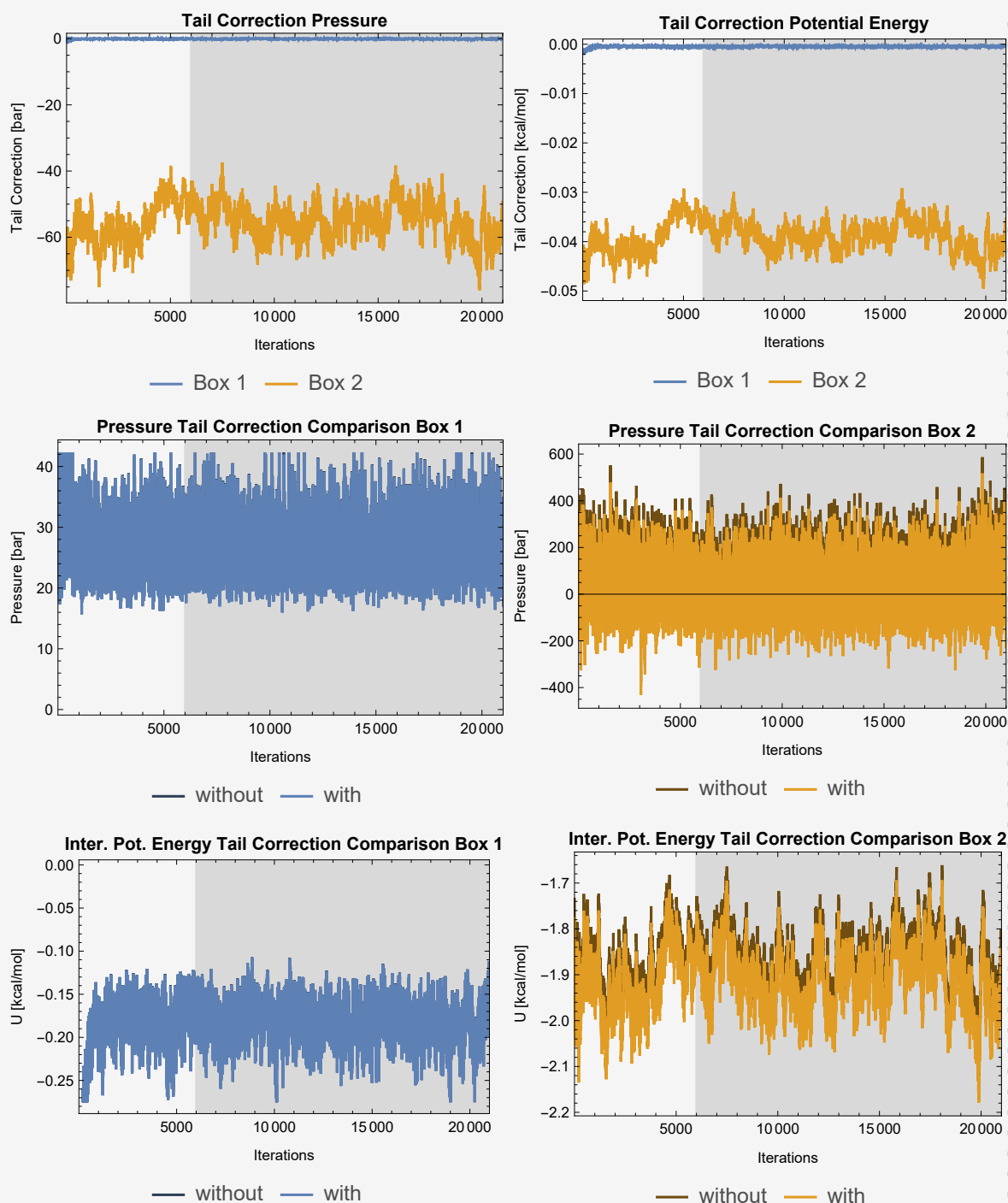


## Tail Corrections

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

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

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



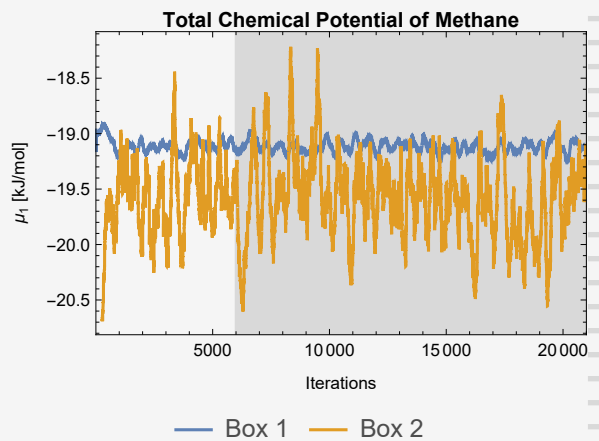
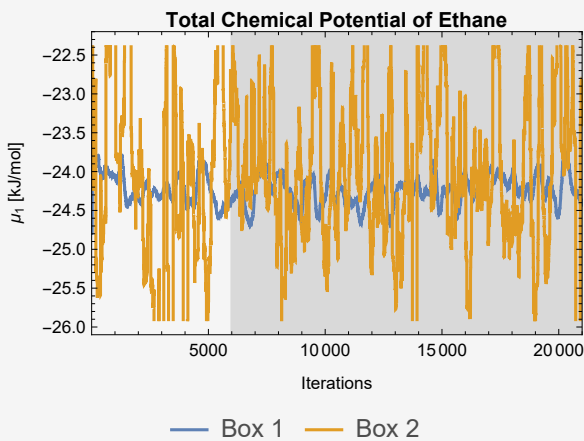
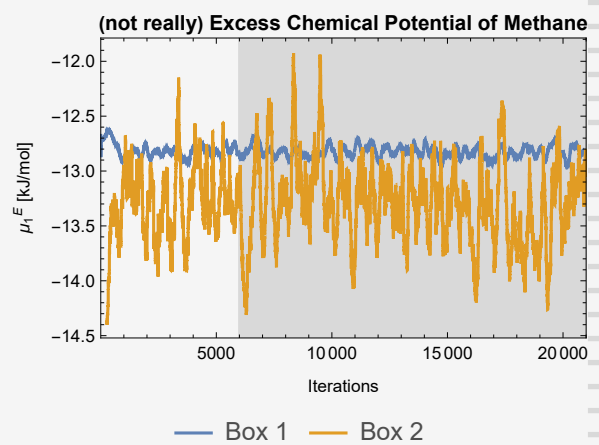
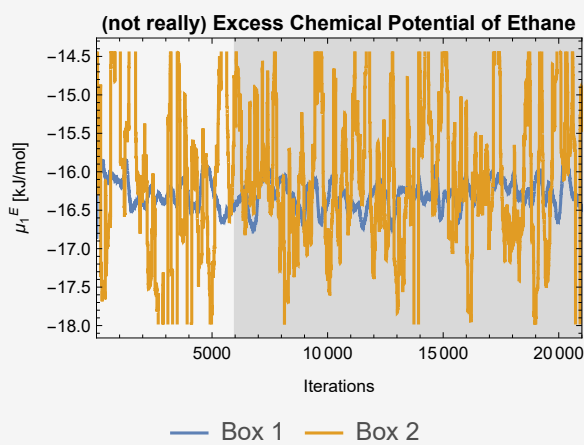
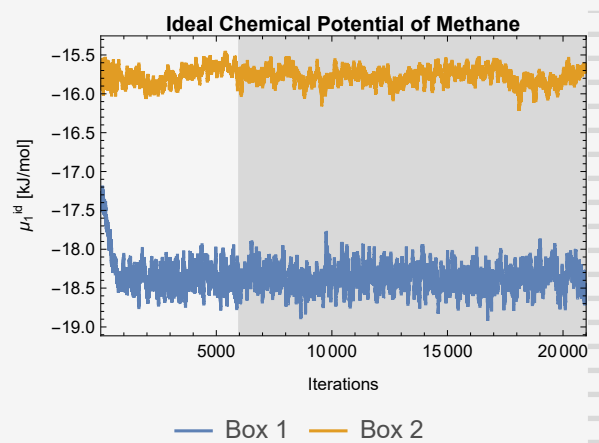
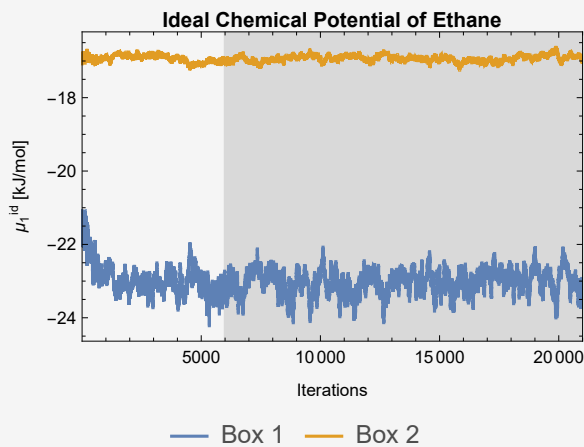
## Chemical Potentials

```

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

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

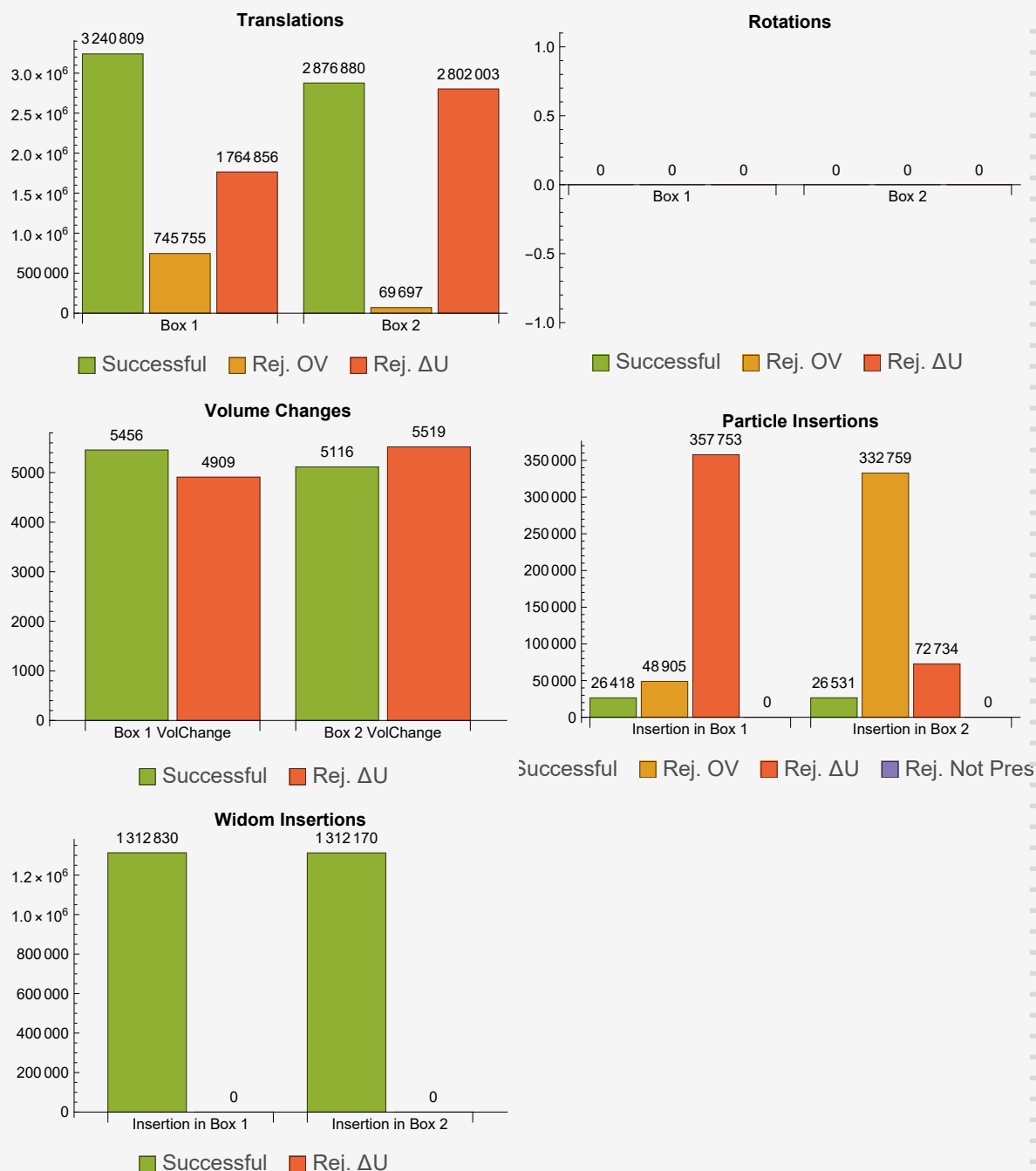
```



## Plot of the Standard Deviation of the molar volume

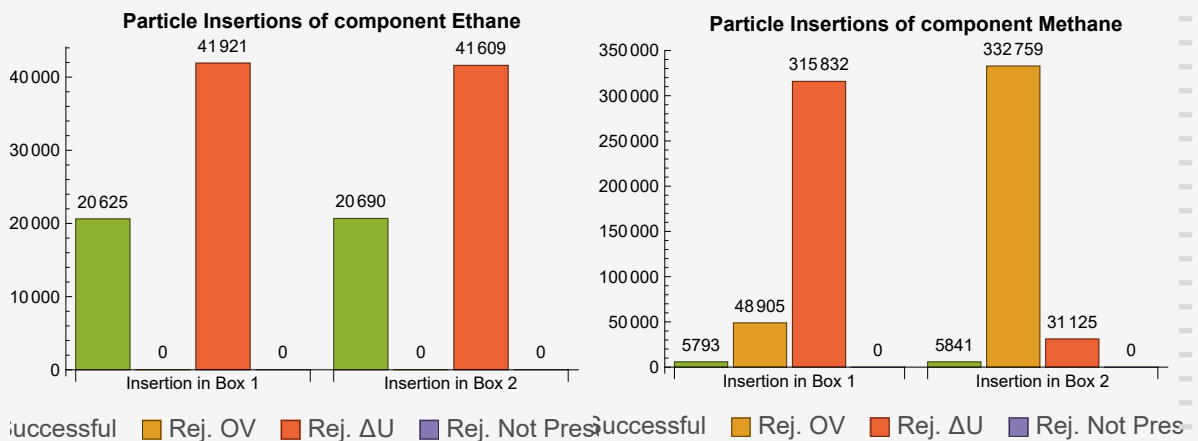
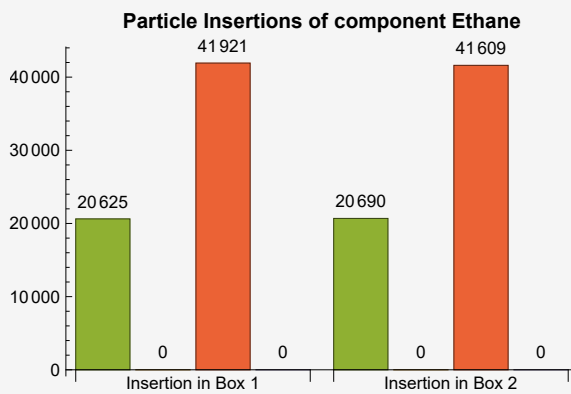
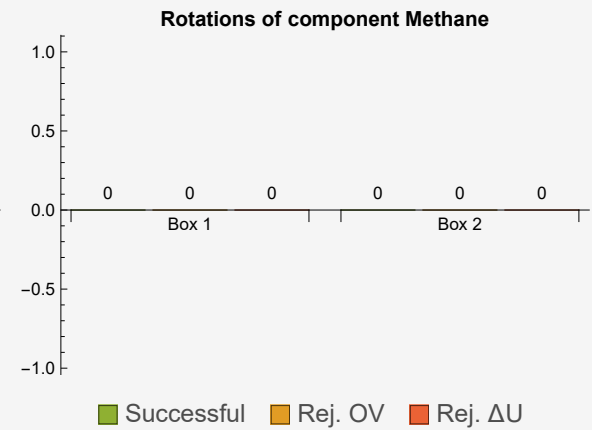
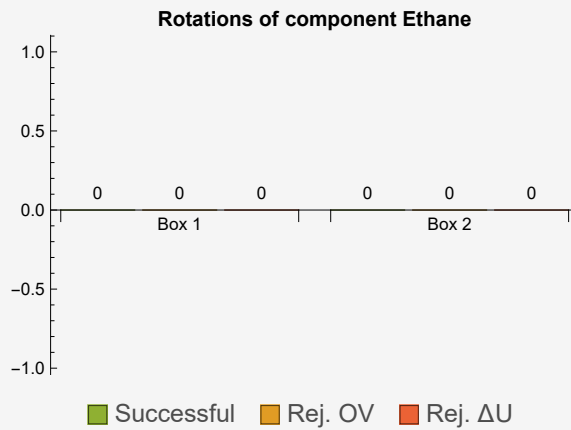
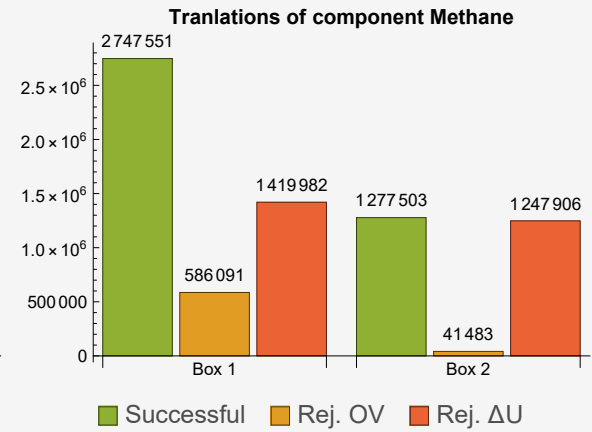
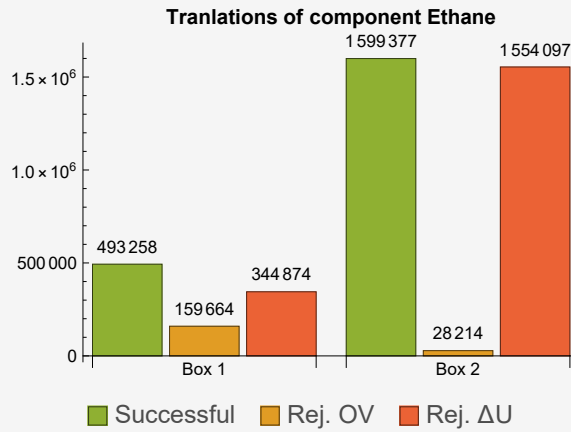
### Counters

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



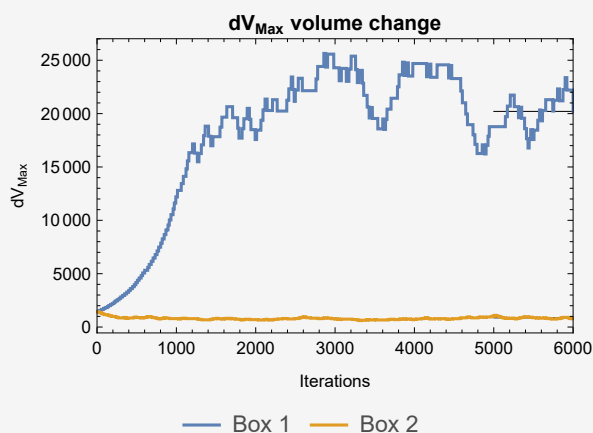
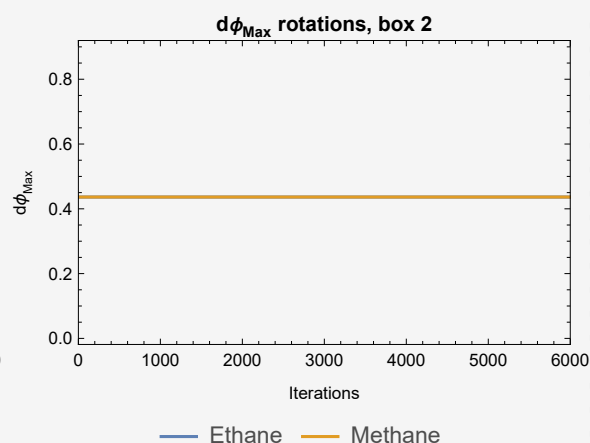
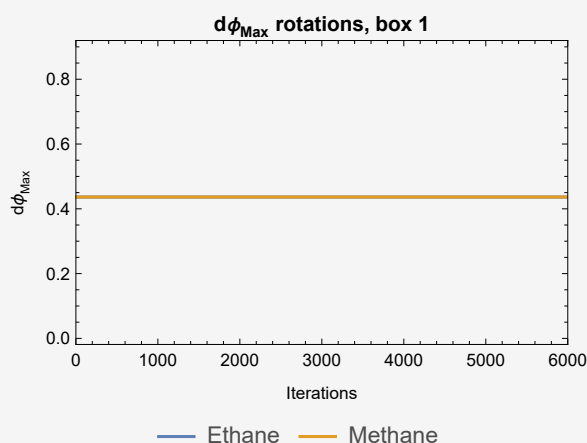
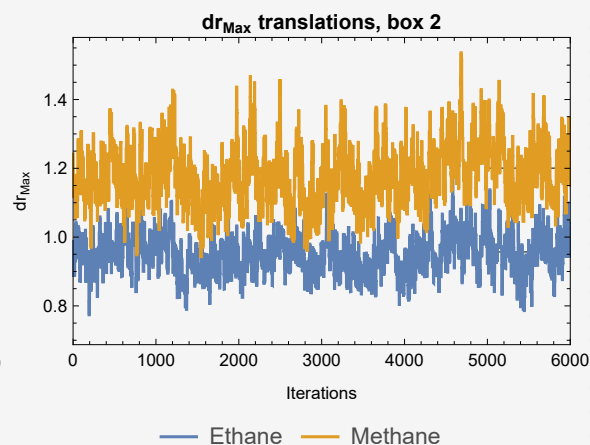
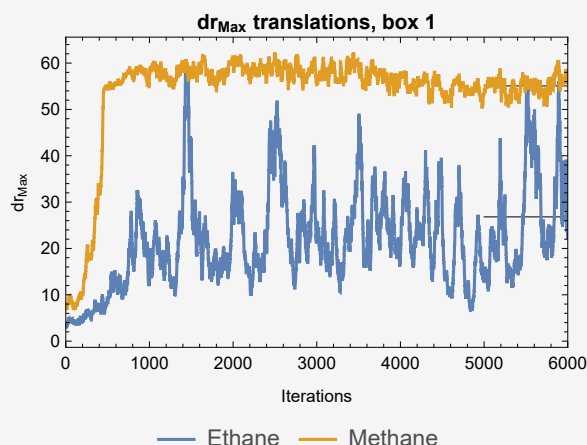
## Species specific Counters

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



## 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]], histo7
, {iCp, Length@system}];

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

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

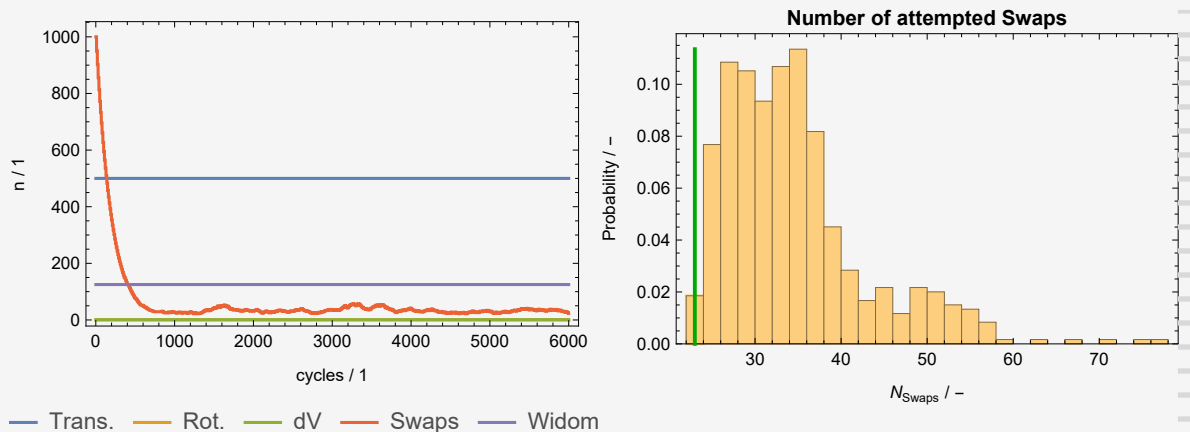
```

## Number of Trial Moves

```

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

```

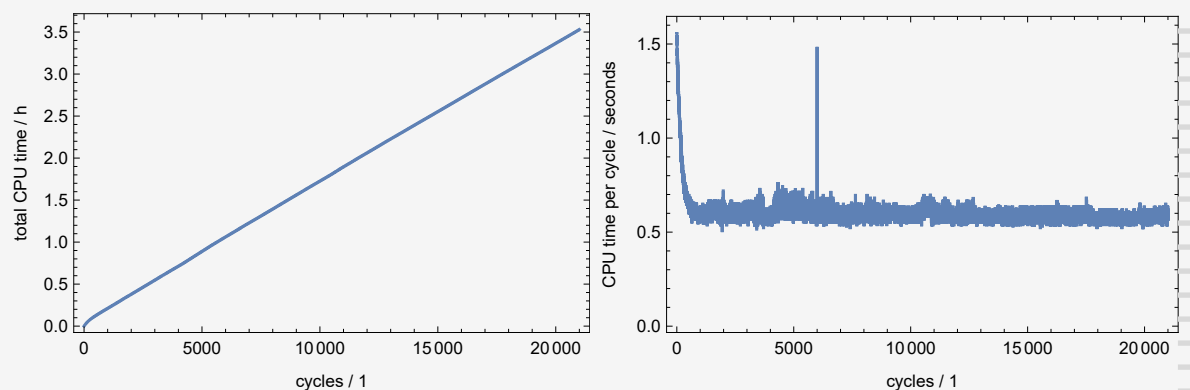


## CPU Time Usage

```

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

```



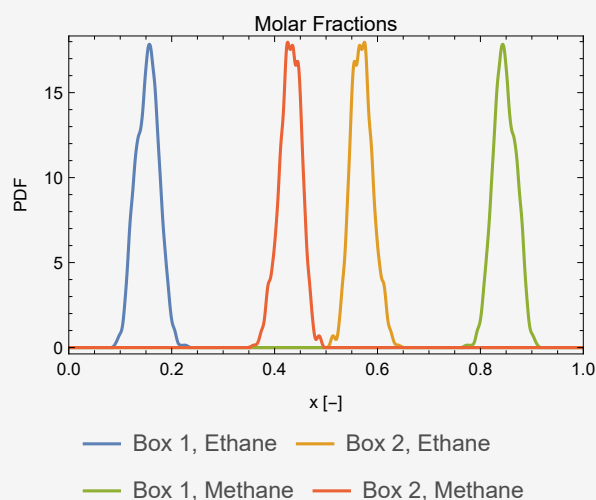
## Ensemble Averages

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

### Density Plots

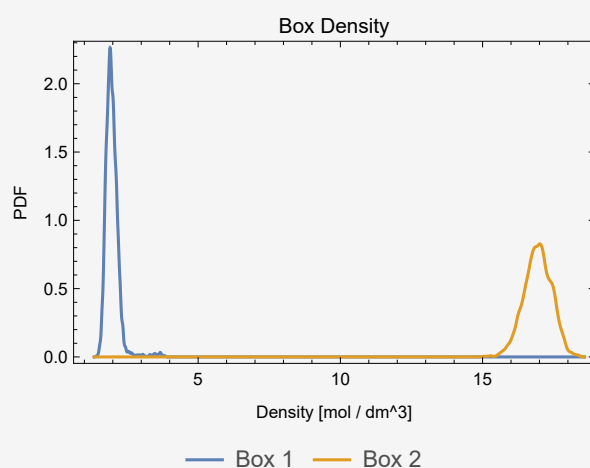
#### Mole Fractions

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



#### Box Densities

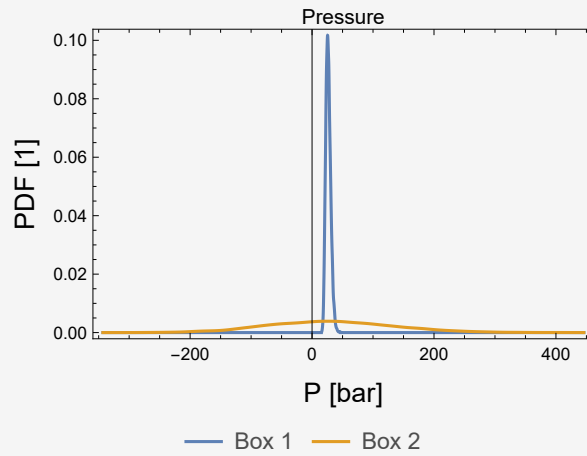
```
ExportGridGraphic[{"densityHistogram", plotDensityHistogram[]}, False];
markShowCell[EvaluationCell[]];
```





## Pressure

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



## Averaged Values

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

<b>AVERAGED VALUES</b> averaged from 6001 to 21000 Box V corresponds to Box 1, Box L corresponds to Box 2				
System	Box V		Box L	
	mean	std	mean	std
T [K]	210.	–	210.	–
v [dm <sup>3</sup> / mol]	0.517147	0.0466	0.0591927	0.00176375
rho [mol / dm <sup>3</sup> ]	1.94949	0.176826	16.9088	0.498591
n [1]	217.753	10.3762	282.247	10.3762
<b>Pressure</b>				
P ideal [bar]	34.0389	3.08745	295.234	8.70558
P viral [bar]	–7.32627	3.94874	–209.548	102.803
P tail [bar]	–0.0760689	0.0212396	–54.9845	5.38833
P [bar]	26.6365	4.06494	30.7014	104.043
<b>Internal Energy</b>				
U Inter [kcal/mol]	–0.181682	0.0234148	–1.91184	0.0687407
U Intra [kcal/mol]	0.	0.	0.	0.
U Total [kcal/mol]	–0.181682	0.0234148	–1.91184	0.0687407
<b>Mole Fractions</b>				
Ethane	0.15286	0.022105	0.56978	0.021442
Methane	0.84714	0.022105	0.43022	0.021442
<b>Ideal <math>\mu</math> [kJ/mol]</b>				
Ethane	–23.025	0.32473	–16.932	0.086158
Methane	–18.371	0.15665	–15.777	0.099010
<b>Excess <math>\mu</math> [kJ/mol]</b>				
Ethane	16.300	0.18440	16.039	1.0642
Methane	12.827	0.050967	13.298	0.36953
<b>Total <math>\mu</math> [kJ/mol]</b>				
Ethane	–24.238	0.18440	–23.978	1.0642
Methane	–19.119	0.050967	–19.590	0.36953

## Reduced Units

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

name	dimensional	unit	critical norm	
T	210.	K	$T_{\text{red}}=T/T_c$	0.688
$p_v$	26.6	bar	$p_{\text{red}}=p/p_c$	0.545
$p_L$	30.7	bar		0.629
$\rho_v$	1.95	mol / dm <sup>3</sup>	$\rho_{\text{red}}=\rho/\rho_c$	0.289
$\rho_L$	16.9	mol / dm <sup>3</sup>		2.50
$\mu_v$	-24.2	kJ / mol	$\mu_{\text{red}}=\mu/\mu_c$	-
$\mu_L$	-24.0	kJ / mol		-

# Comparison & Checks

## Comparison Functions

## Equation of State Comparison

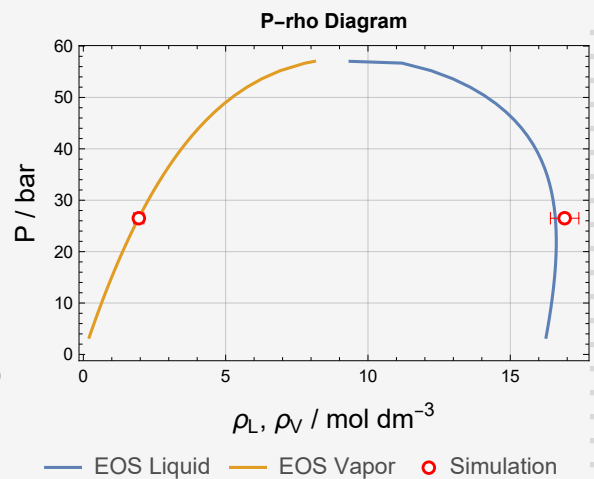
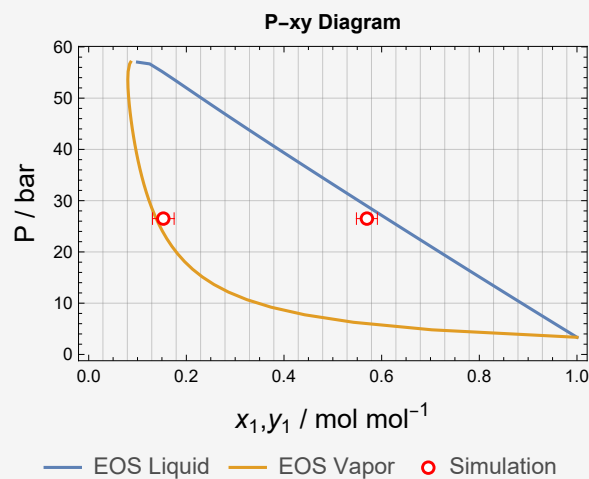
Comparison to a pure LJ EOS (Thol, 2016), a t-PR-LJ EoS (Harismiadis, 1994) or the SRK EoS

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

SRK Comparison, Ethane, Methane at  $T = 210$  K and  $P = 26.5$  bar

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	$\Delta_{\text{rel}} / \%$
$x_1 / [\text{mol/mol}]$	0.153	0.138	10.6	0.570	0.610	6.65
$\rho / \text{mol dm}^{-3}$	1.95	1.94	0.408	16.9	16.6	1.96
$p / \text{bar}$	26.6	26.5	0.515	30.7	26.5	15.9



## 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

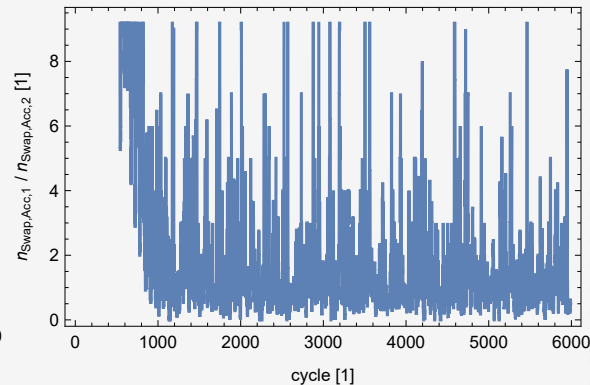
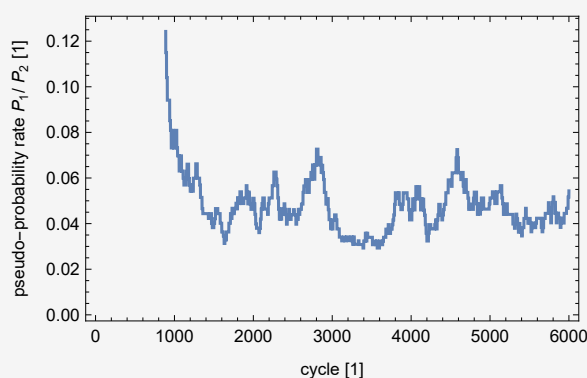
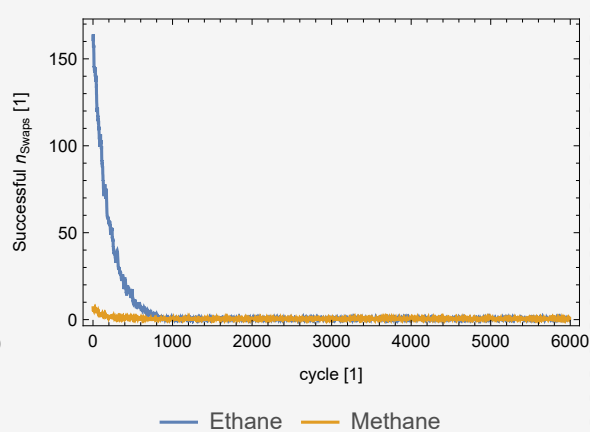
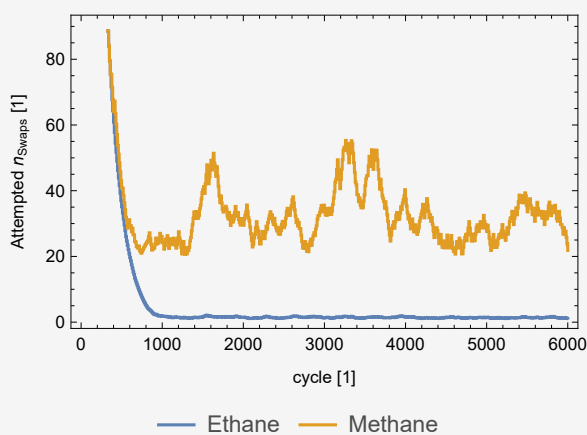
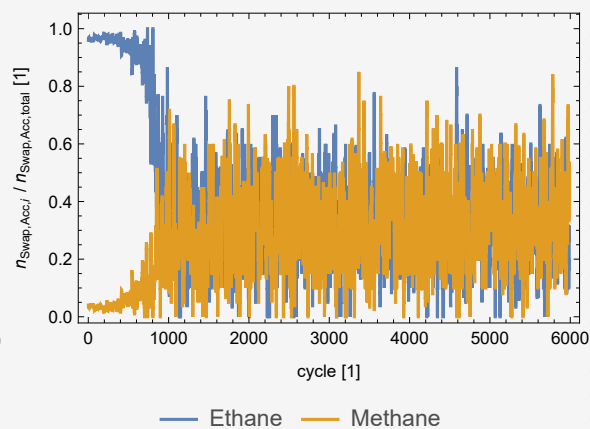
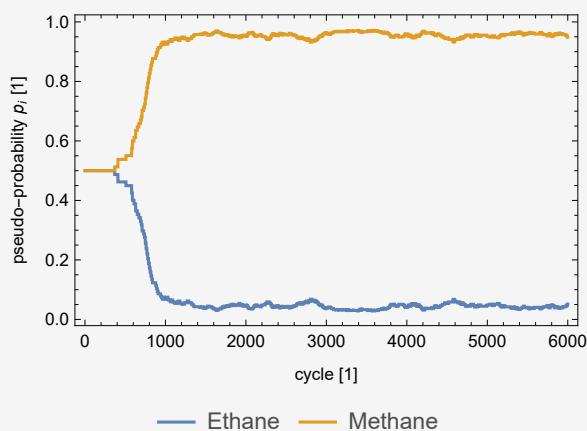
### SwapMove Species Choice probabilities

```
If[Depth@counterInsertAcceptDocu == 3 && KeyExistsQ[custParam,"speciesSwapProbabilityM
VisualizeSMPR[];
If[AnyTrue[{"auto", "autoSwap"},SameQ[checkGetAssocParameter[custParam, "speciesS
(*Print@Grid@speciesSwapProbabilityPlotGrid;*)
VisualizeSwapProbailities[];
];
markShowCell[EvaluationCell[]];];
```

» Swap Move Probability Rate ( $P_1/P_2$ ): 0.0442064

» share Ethane 0.780279

» share Methane 0.219721

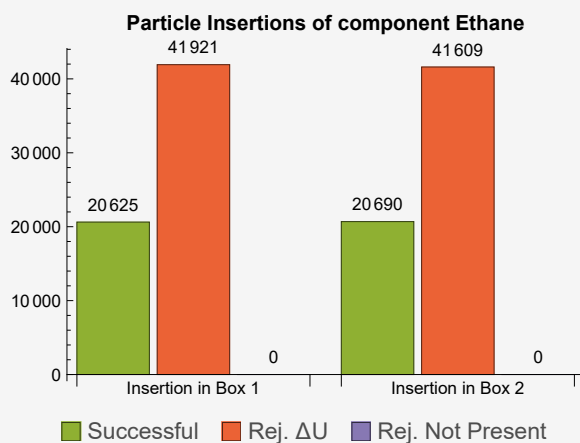


## PAN Binary Swaps

```
If[checkGetAssocParameter[custParam, "panBinarySwaps"],
  panBinarySwaps[(*Export: *) True];
  markShowCell[EvaluationCell[]];];
```

» For component Ethane the pan-binary exchange is used.

PAN Binary Swap Move Timing						
Part	Time / total	$t_{\text{total}}$ / %	$t_{\text{avr}}$ / ms	$t_{\text{acc}}$ / ms	$t_{\text{rejDu}}$ / ms	$t_{\text{rejOv}}$ / ms
Insertion	0h 7min 45s	73.33	1.29866	6.97139	0.599137	0.462998
PAN Binary Swap	0h 2min 49s	26.67	1.35692	1.74644	1.16426	–



Ewald Electrostatic Long Range Correction

Wolf Electrostatic Long Range Correction

Custom Evaluations

---

## Export Analysis Results

---

## Credits