

# Simulation Report: sims4\_kmdcm\_water\_k289

water.2000.heat.dcd  
water.2000.equi.dcd

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	7062.000000	7062.000000	7062.0	7062.000000	7062.000000	7062.000000	7062.000000	7062.000000	7062.000000C
mean	3439.010354	-21769.546489	0.0	408.651402	289.037771	-16344.773347	21513.271100	58397.171340	-365.180765
std	143.577002	331.320764	0.0	286.042722	18.235603	760.305245	549.775238	6701.446165	1157.491111
min	3018.058230	-25088.512700	0.0	0.000000	61.525350	-22641.676890	20362.195790	52966.000000	-5318.421340
25%	3334.811670	-21935.438093	0.0	88.300000	287.461515	-16701.099002	20739.383830	53918.250000	-1167.041508
50%	3461.508575	-21796.865700	0.0	424.100000	290.118585	-16601.212460	21778.657430	54230.000000	-330.554420
75%	3541.074263	-21559.209190	0.0	659.550000	294.218577	-15317.591608	21860.481840	68921.000000	437.684845
max	4072.983730	-20926.176450	0.0	894.800000	307.044530	-15316.644200	24925.828760	68921.000000	3448.681300

## Simulation runs

	dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT
vdw	count	2000.000000	600.000000	1500.000000	1500.000000	1462.000000
	mean	3282.374866	3480.446853	3484.402798	3520.433279	3506.169057
	std	139.155887	89.596995	84.283309	88.180577	82.760659
	min	3018.058230	3228.955390	3220.675310	3250.726930	3225.430390
	25%	3205.140050	3420.401778	3429.697045	3462.297180	3451.844090
	50%	3261.406780	3486.192835	3485.379570	3520.881930	3503.086710
	75%	3322.163610	3540.414082	3546.130962	3580.566930	3562.380175
	max	4072.983730	3748.110840	3729.326160	3828.045870	3753.937280
elec	count	2000.000000	600.000000	1500.000000	1500.000000	1462.000000
	mean	-21527.363483	-21903.233219	-21823.083411	-21898.662160	-21858.585534
	std	494.545896	204.059238	134.909602	149.345512	147.114316
	min	-25088.512700	-22411.339930	-22228.756330	-22375.401970	-22327.797200
	25%	-21526.173010	-22058.858790	-21908.048530	-21997.371508	-21964.716370
	50%	-21437.502295	-21903.316940	-21821.482190	-21905.862110	-21861.156225
	75%	-21323.533450	-21761.046453	-21735.592850	-21799.720635	-21758.878863
	max	-20926.176450	-21419.460740	-21361.448310	-21446.661230	-21366.518140
volume	count	2000.000000	600.000000	1500.000000	1500.000000	1462.000000
	mean	68921.000000	55813.836667	53939.193333	54120.744667	54022.308482
	std	0.000000	3144.901525	337.230325	342.035428	267.964500

dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT
<b>min</b>	68921.000000	53100.000000	52966.000000	53070.000000	53263.000000
<b>25%</b>	68921.000000	53879.750000	53728.750000	53907.750000	53847.500000
<b>50%</b>	68921.000000	54268.000000	53951.000000	54162.000000	54022.000000
<b>75%</b>	68921.000000	56764.500000	54175.000000	54368.250000	54209.250000
<b>max</b>	68921.000000	68921.000000	55131.000000	55066.000000	54770.000000
<b>temp</b>	<b>count</b>	2000.000000	600.000000	1500.000000	1500.000000
	<b>mean</b>	289.197784	288.894683	289.029310	288.882012
	<b>std</b>	33.920202	3.005293	3.069704	3.029424
	<b>min</b>	61.525350	280.614620	278.645650	278.601910
	<b>25%</b>	294.830560	286.917660	286.950475	286.808430
	<b>50%</b>	297.951645	288.980270	289.082310	288.915510
	<b>75%</b>	300.347352	290.854068	291.108162	290.798603
	<b>max</b>	307.044530	302.409570	299.185880	299.008300

## Densities

density 1: 867.0796999463153 kilogram / meter \*\* 3

density 2: 1070.7022410392738 kilogram / meter \*\* 3

density 3: 1107.9142328046185 kilogram / meter \*\* 3

density 4: 1104.1976670510703 kilogram / meter \*\* 3

density 5: 1106.2096692967002 kilogram / meter \*\* 3

temp. 1: 289.19778405

temp. 2: 288.89468266666665

temp. 3: 289.02931011333334

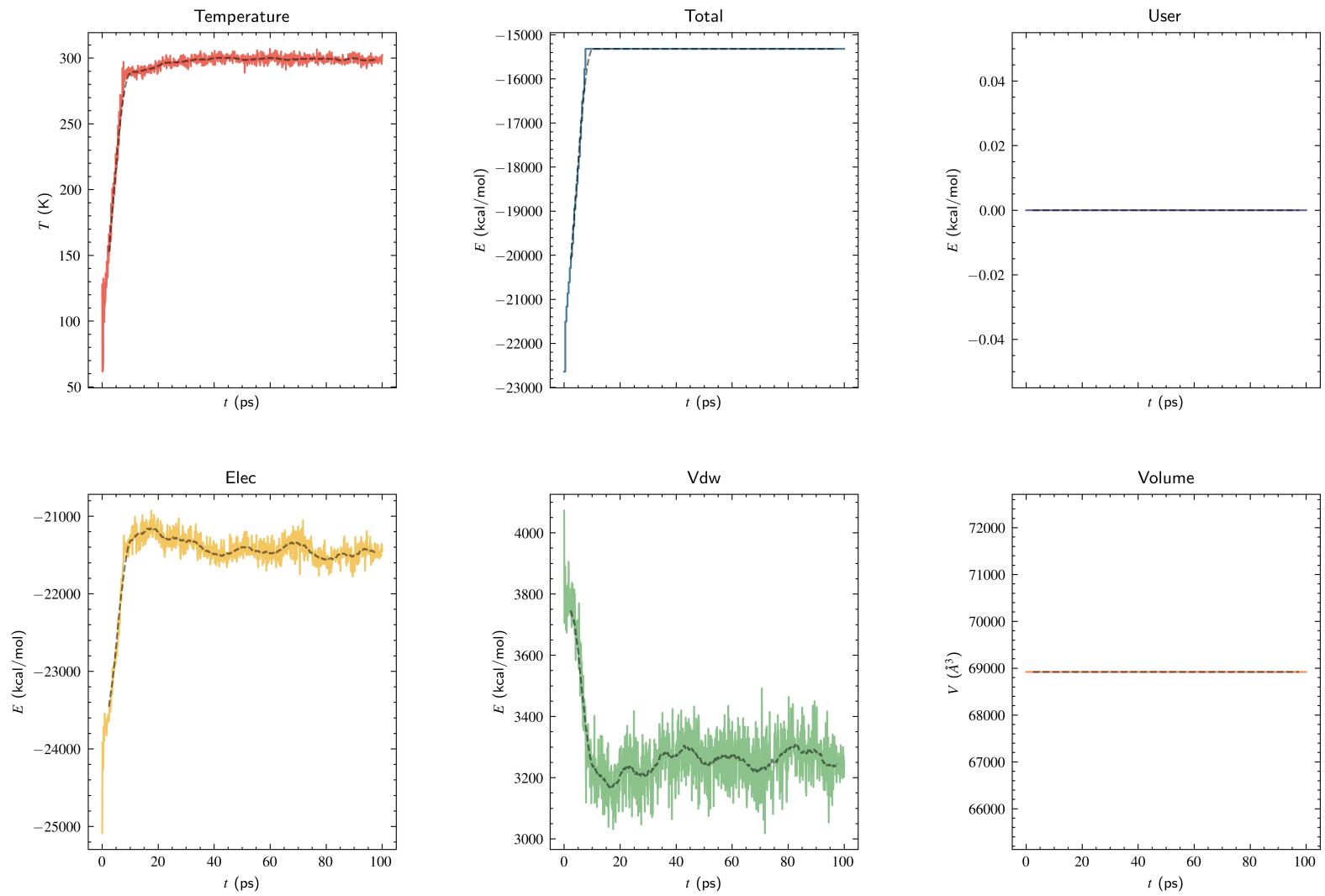
temp. 4: 288.88201202000005

temp. 5: 289.04608528043775

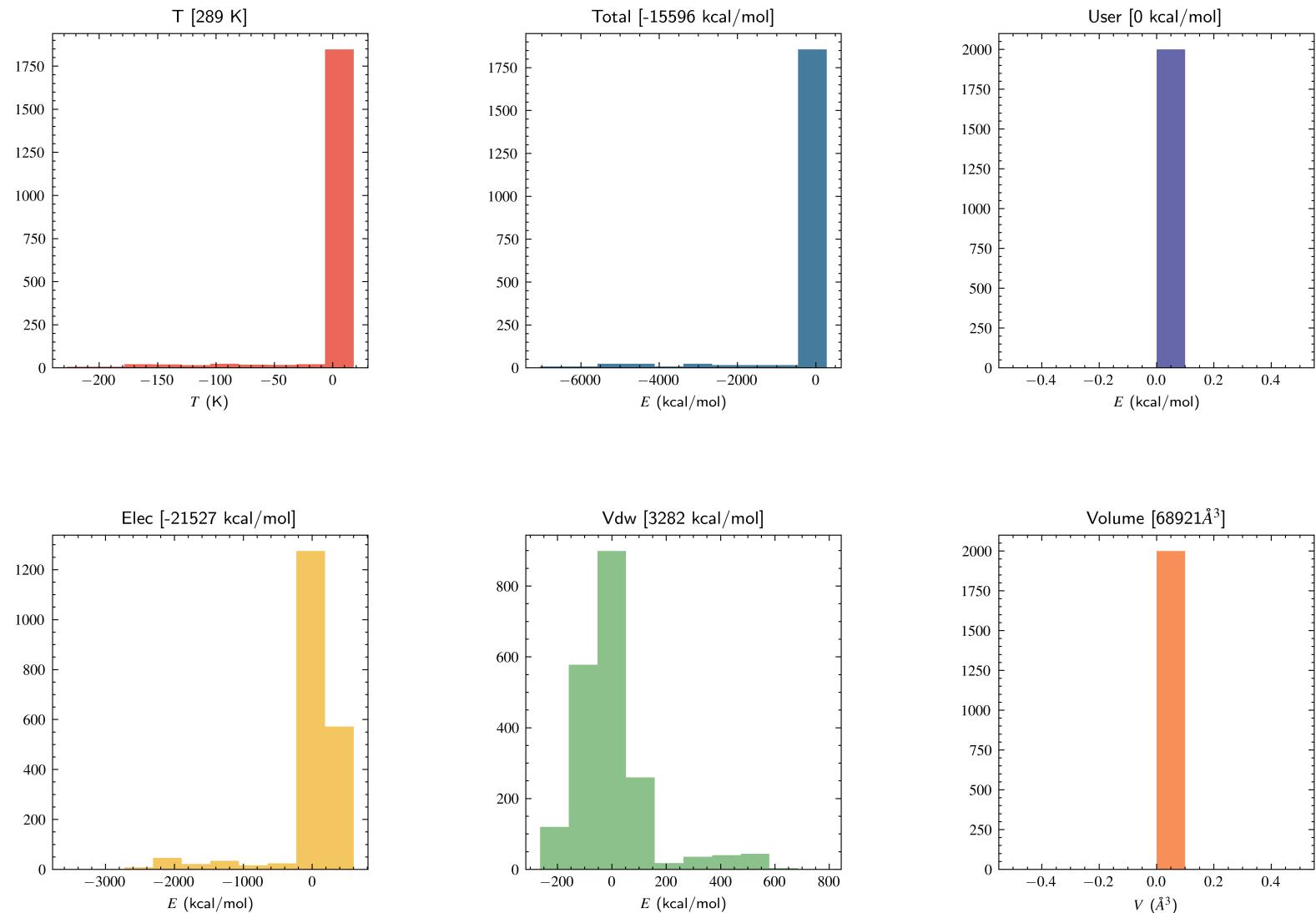
plotting

```
['2: DYNA RESTRT CPT', '0: DYNA STRT VERL', '4: DYNA RESTRT CPT', '3: DYNA RESTRT CPT', '1: DYNA RES  
TRT CPT']
```

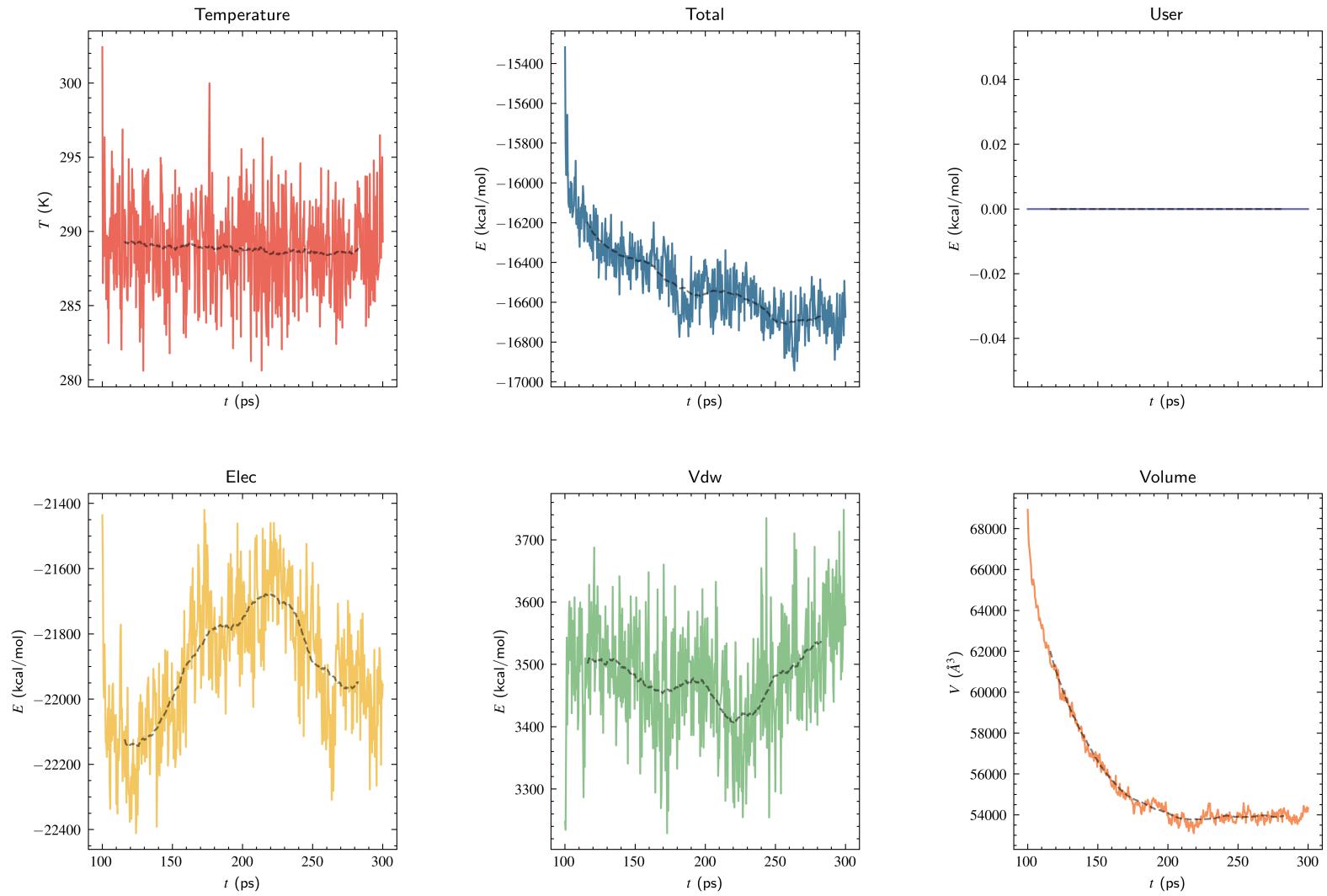
\_home\_boittier\_pc当地\_sims4\_kmdcm\_water\_k289\_dynamics.log  
0: DYNA STRT VERL [100.0 ps]



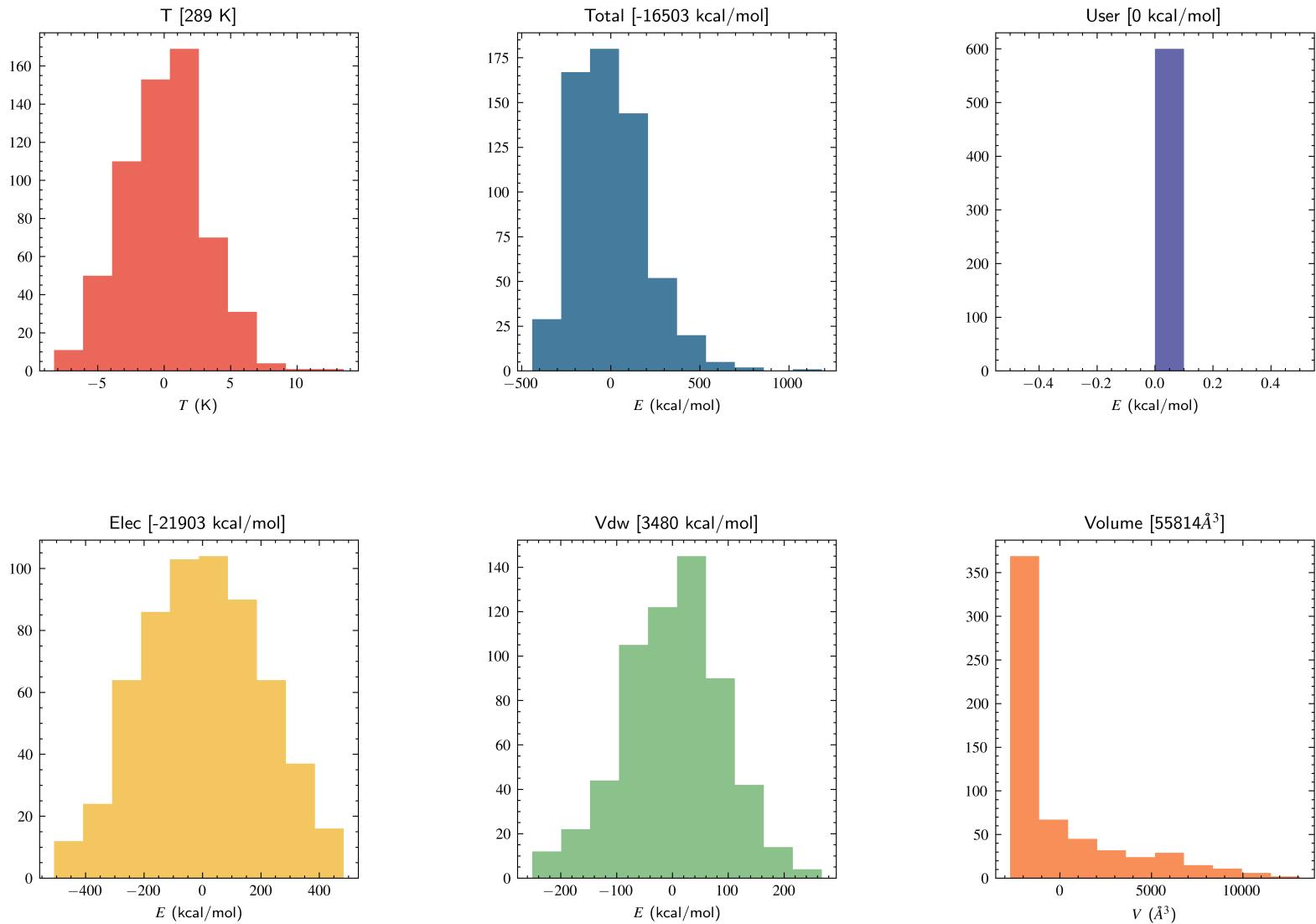
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k289\_dynamics.log  
0: DYNA STRT VERL [100.0 ps]



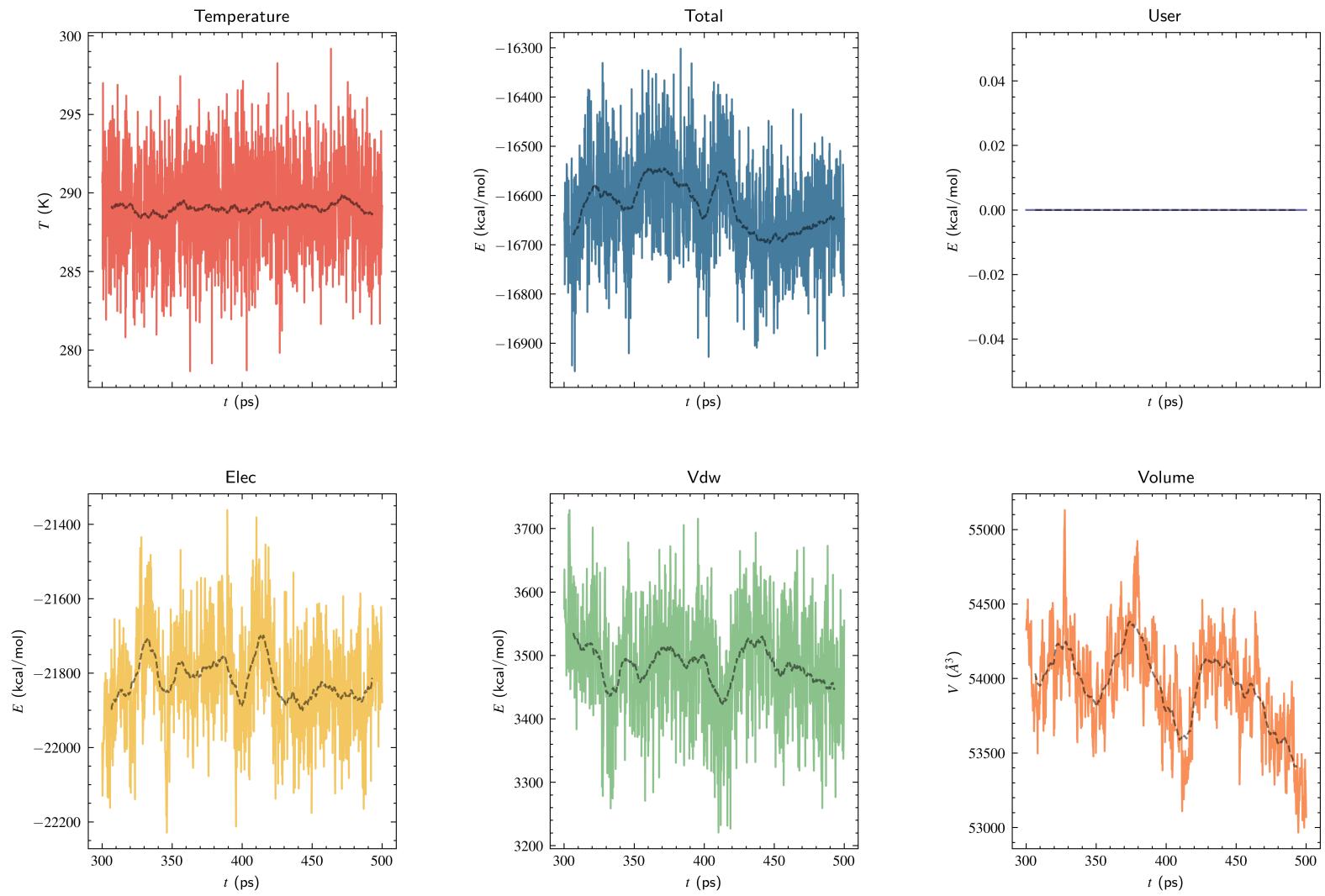
\_home\_boittier\_pc当地\_sims4\_kmdcm\_water\_k289\_dynamics.log  
1: DYNA RESTRT CPT [200.0 ps]



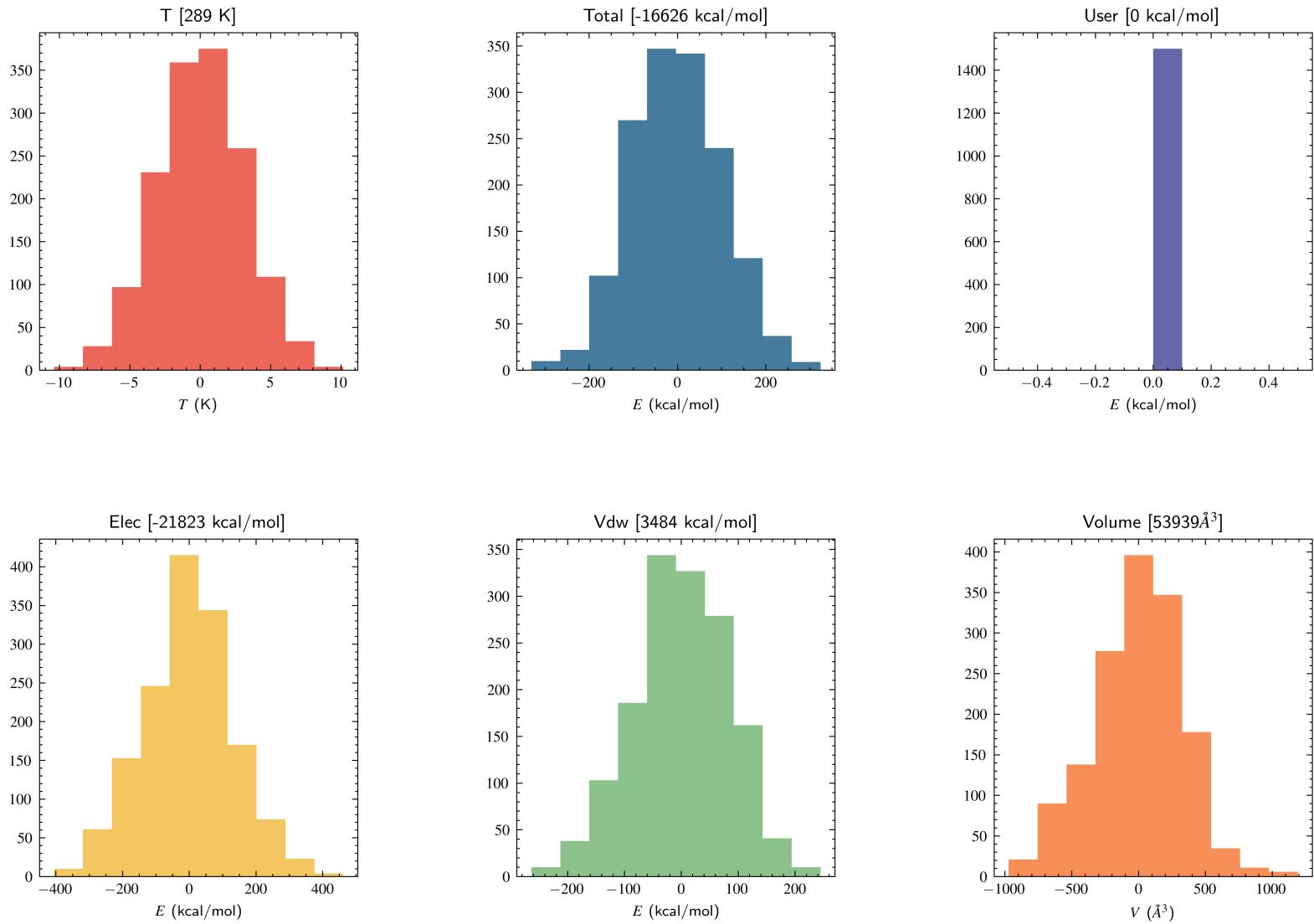
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k289\_dynamics.log  
1: DYNA RESTRT CPT [200.0 ps]



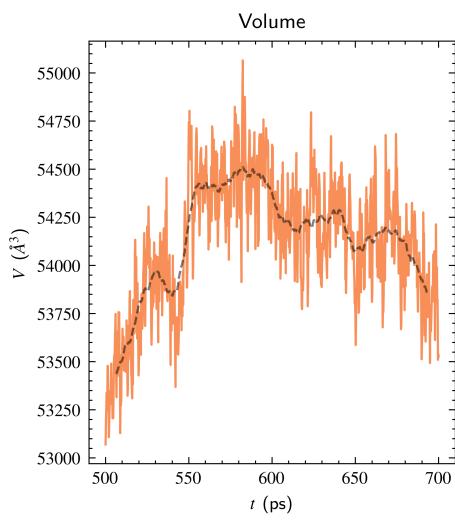
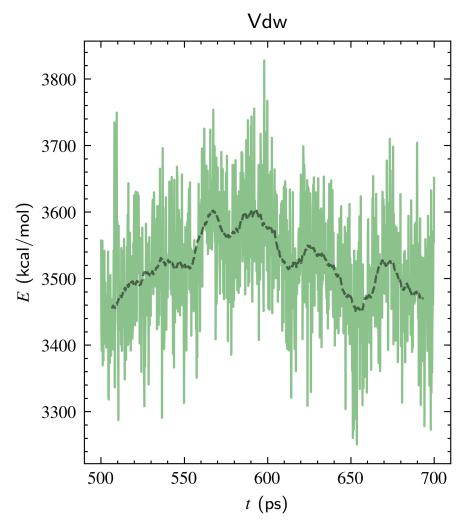
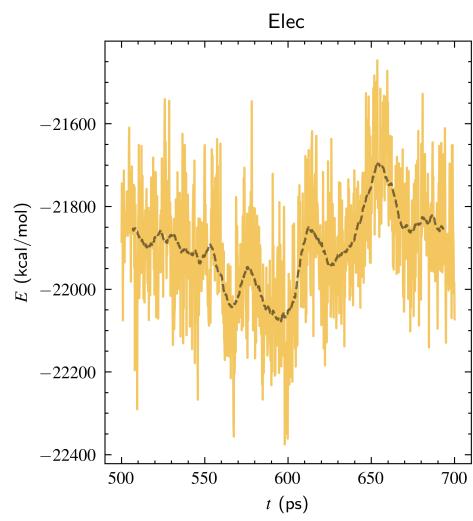
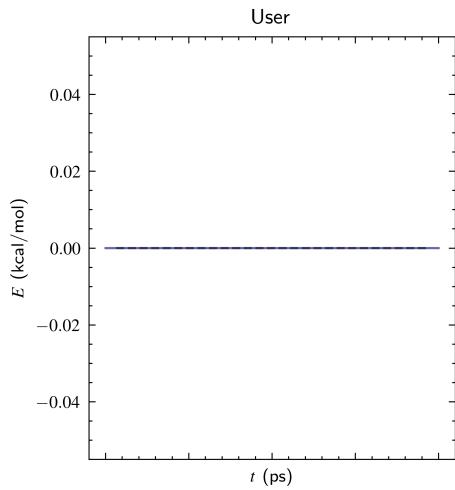
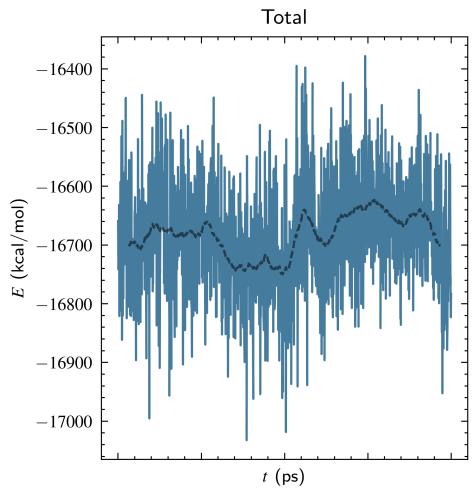
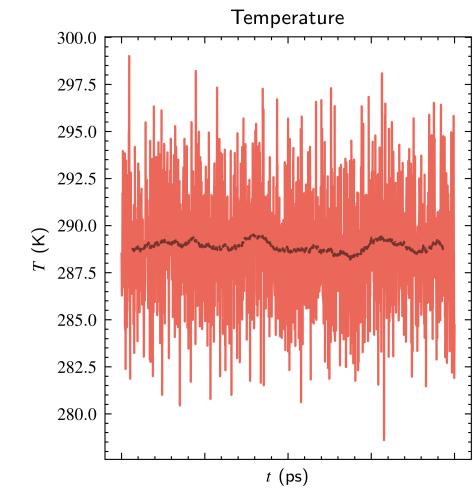
\_home\_boittier\_pc当地\_sims4\_kmdcm\_water\_k289\_dynamics.log  
2: DYNA RESTRT CPT [200.0 ps]



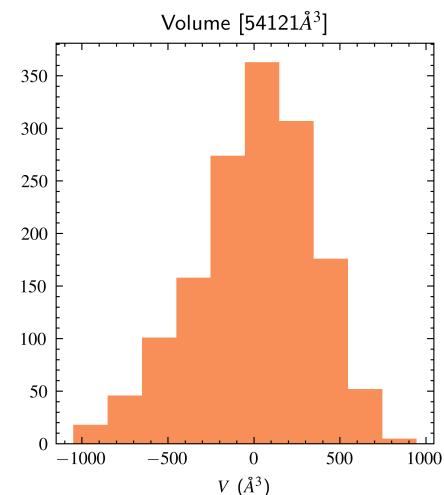
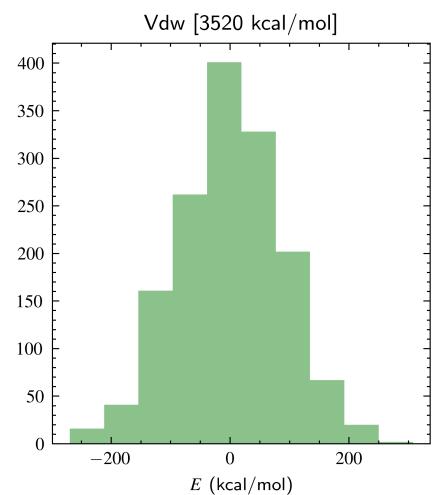
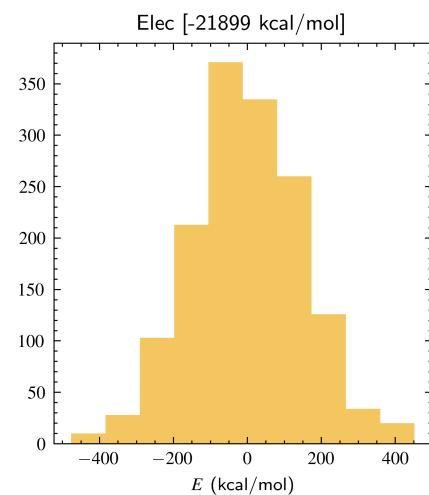
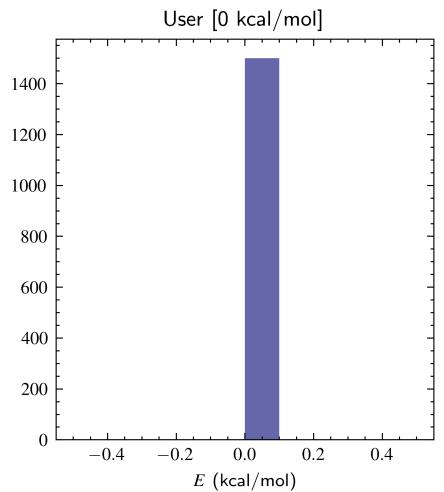
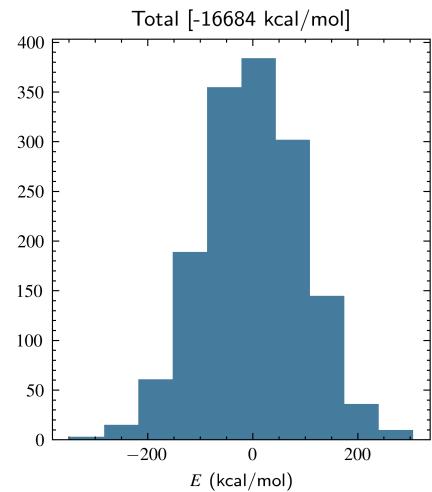
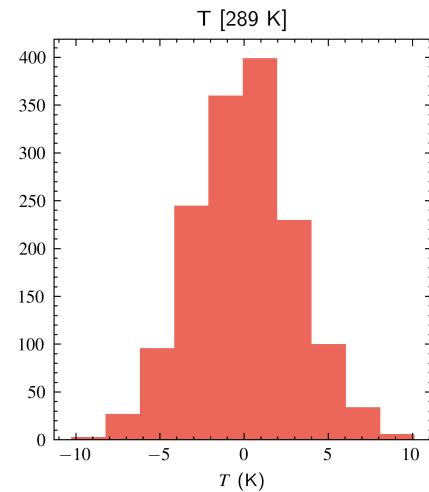
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2: DYNA RESTRT CPT [200.0 ps]



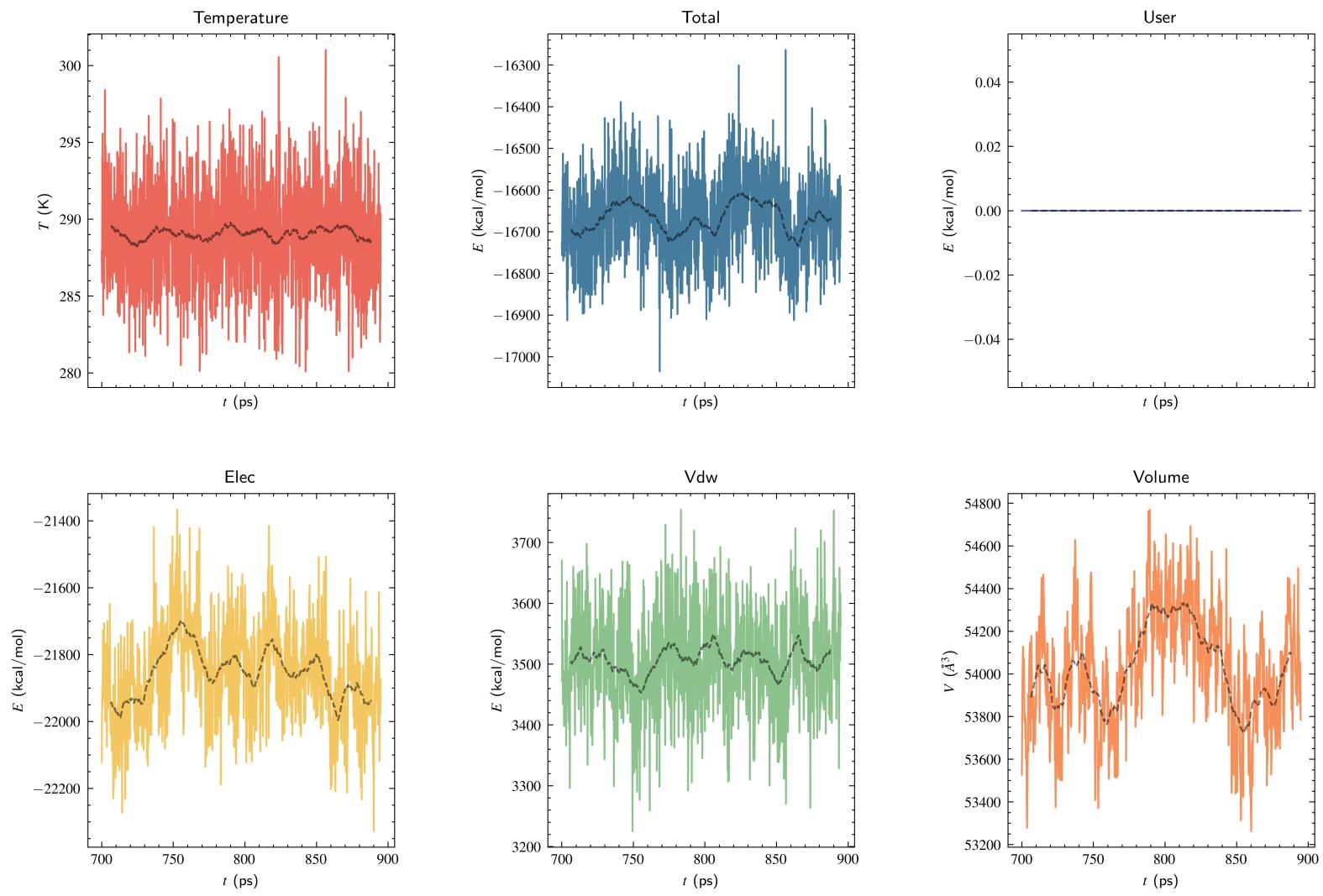
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3: DYNA RESTRT CPT [200.0 ps]



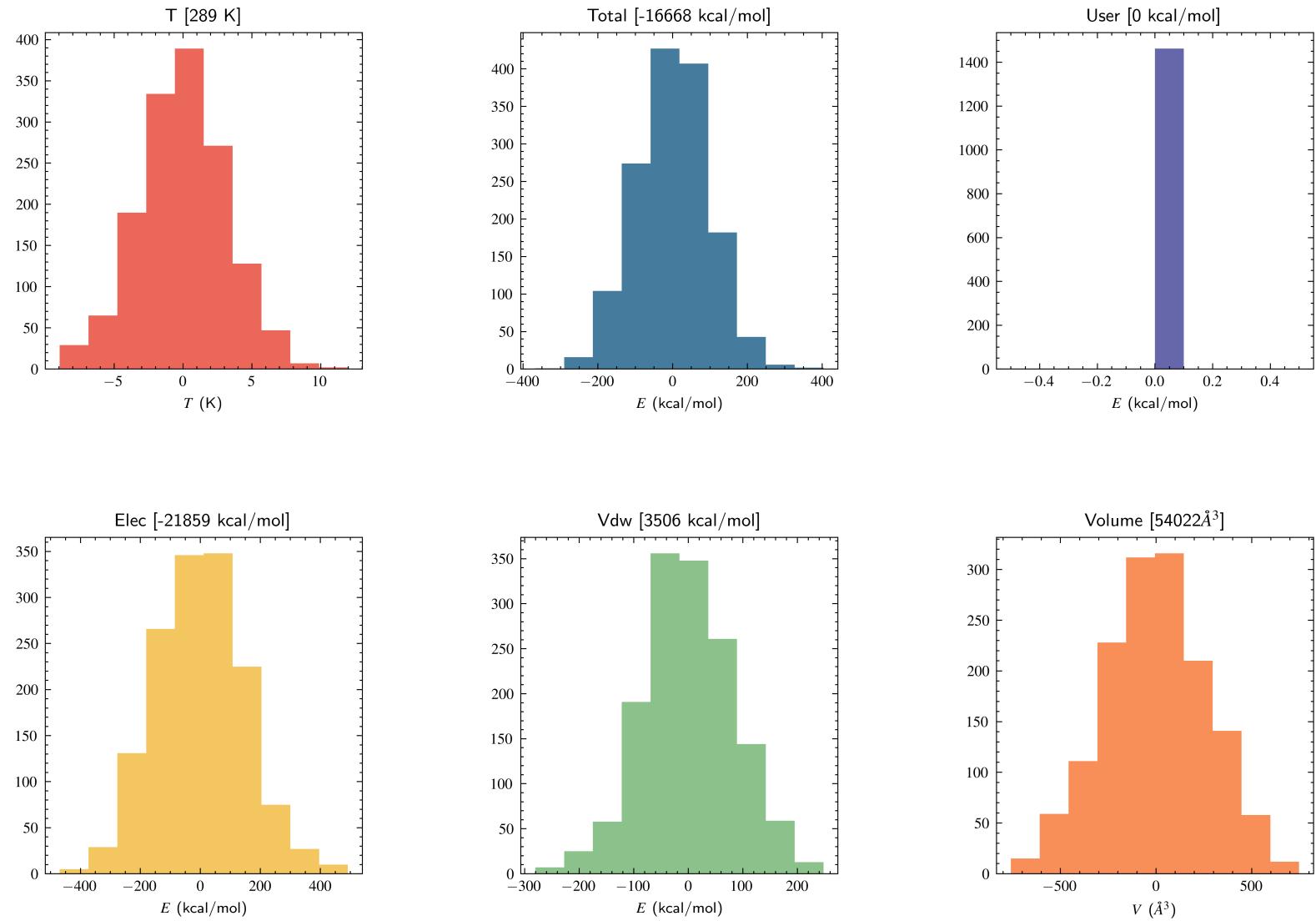
\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k289\_dynamics.log  
3: DYNA RESTRT CPT [200.0 ps]



\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k289\_dynamics.log  
4: DYNA RESTRT CPT [194.0 ps]



\_home\_boittier\_pcbach\_sims4\_kmdcm\_water\_k289\_dynamics.log  
 4: DYNA RESTRT CPT [194.0 ps]



## Trajectory info.

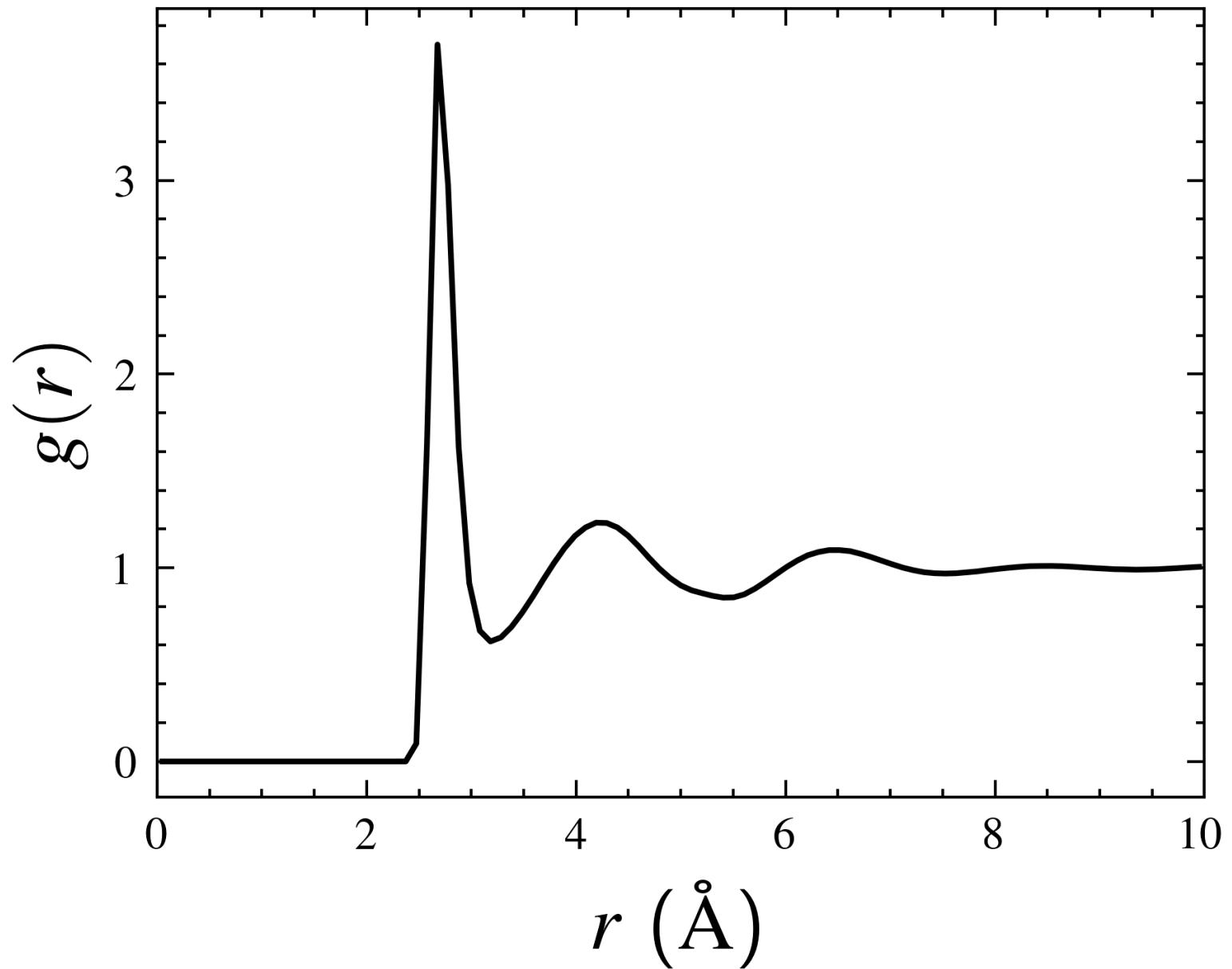
```
<Universe with 6000 atoms>
<ChainReader containing water.2000.dyna.0.dcd, water.2000.dyna.1.dcd with 2000 frames of 6000 atoms>
/home/boittier/miniconda3/envs/pycharmm/lib/python3.8/site-packages/MDAnalysis/coordinates/DCD.py:16
5: DeprecationWarning: DCDReader currently makes independent timesteps by copying self.ts while othe
r readers update self.ts inplace. This behavior will be changed in 3.0 to be the same as other reade
rs. Read more at https://github.com/MDAnalysis/mdanalysis/issues/3889 to learn if this change in beh
avior might affect you.
```

```
warnings.warn("DCDReader currently makes independent timesteps")
```

sim. time : 400 (ps)

```
<AtomGroup [<Atom 1: OH2 of type OT of resname TIP3, resid 1 and segid WAT>, <Atom 4: OH2 of type OT
of resname TIP3, resid 2 and segid WAT>, <Atom 7: OH2 of type OT of resname TIP3, resid 3 and segid
WAT>, ..., <Atom 5992: OH2 of type OT of resname TIP3, resid 1998 and segid WAT>, <Atom 5995: OH2 of
type OT of resname TIP3, resid 1999 and segid WAT>, <Atom 5998: OH2 of type OT of resname TIP3, resi
d 2000 and segid WAT>]>
[2.75626263 4.34641414 6.78464646 8.90484848] [3.7007318 1.23263242 1.09094828 1.00920912]
```

# RDF



$MSD$  and  $D$

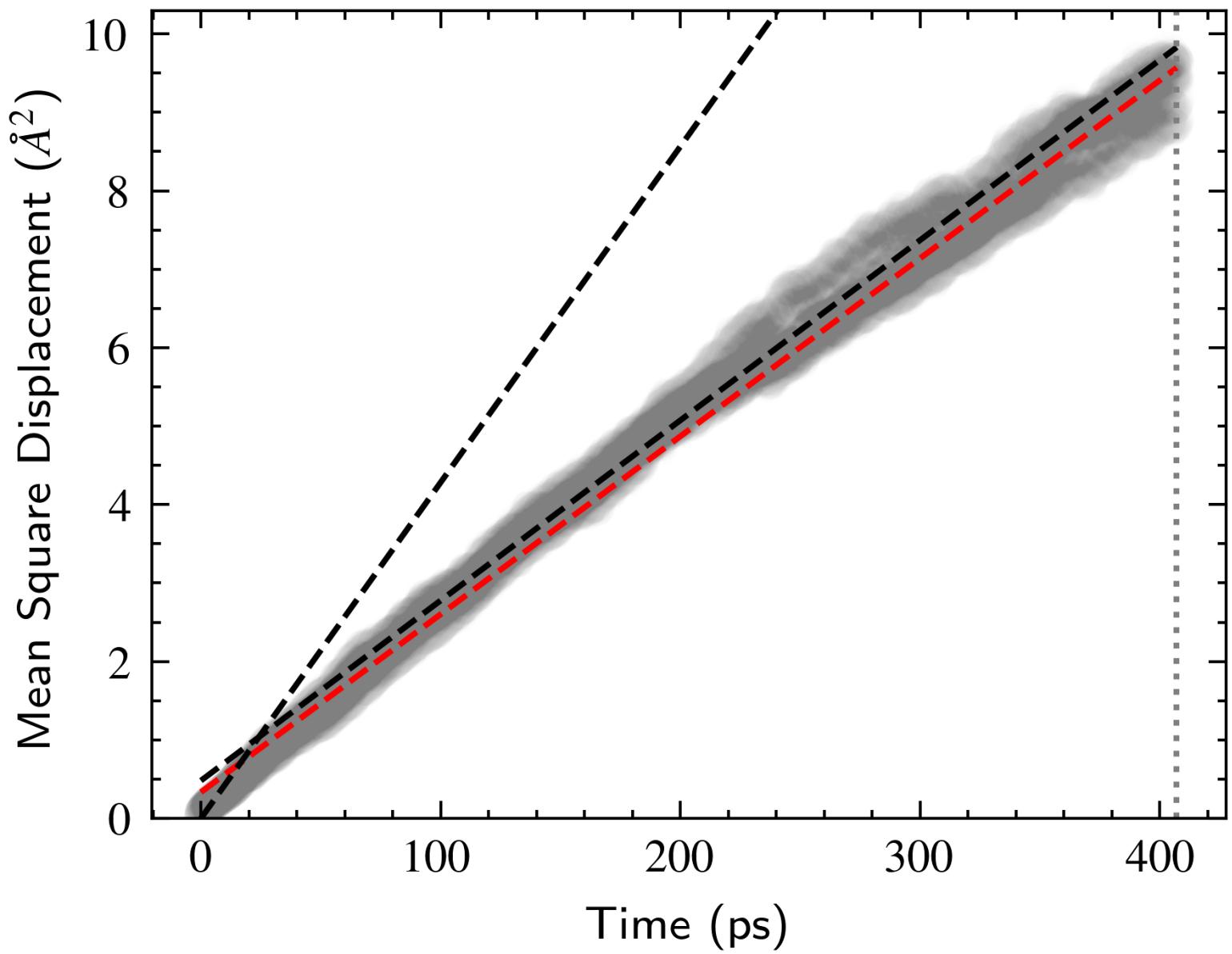
true  $\rho$ : 999

true  $D$ : 1.80e-05

0.0002

407.0166167328458

<Axes: xlabel='Time (ps)', ylabel='Mean Square Displacement (\$\AA^2\$)'>

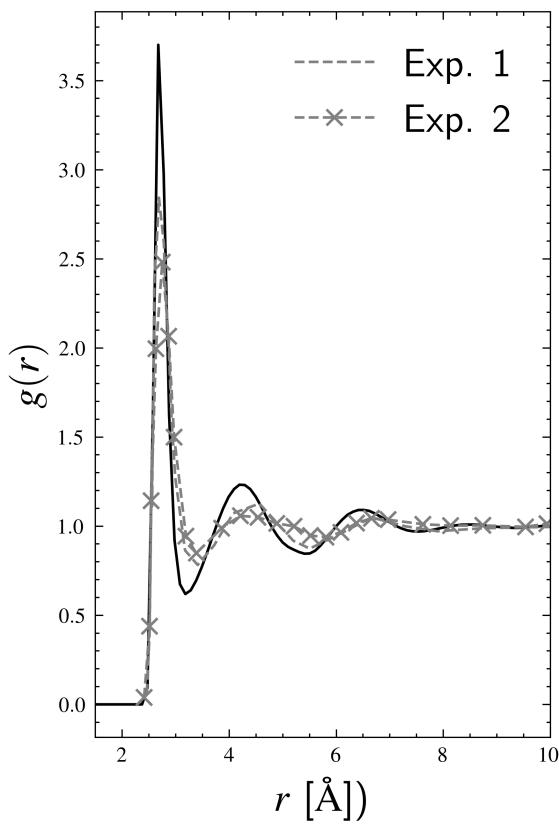


## Structure and Transport

407.0166167328458

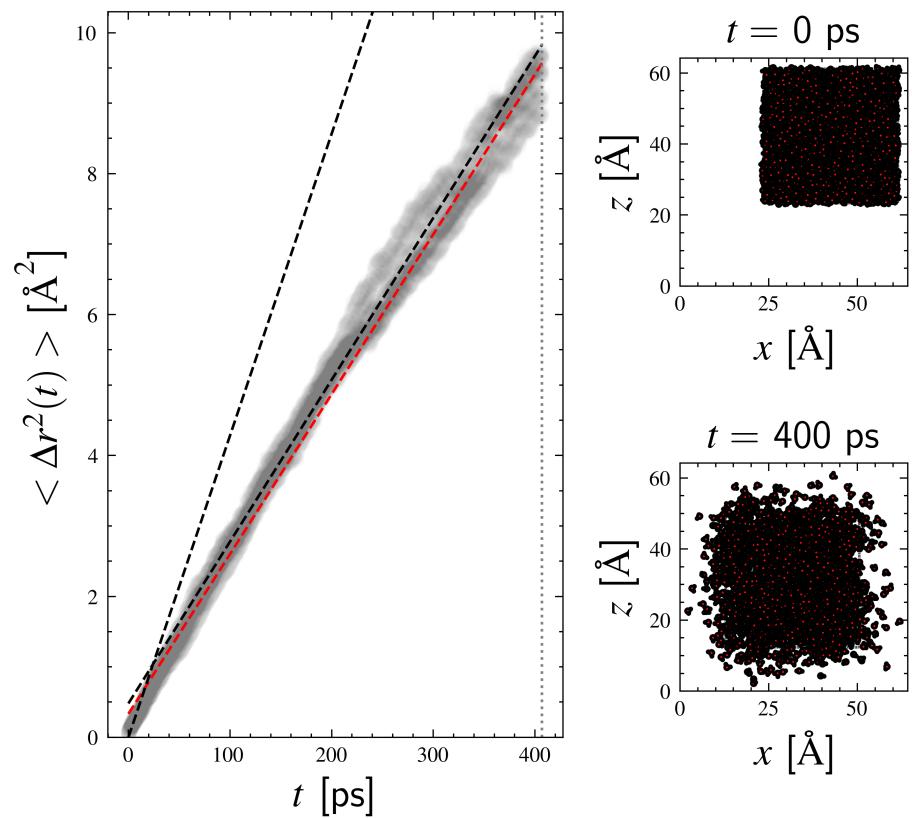
$$\rho = 1097 \text{ [kg/m}^3\text{]} \text{ (error} = 9.9\%\text{)}$$

RDF

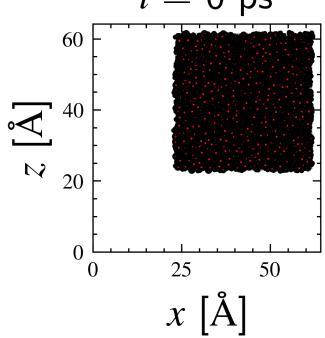


$$D = 0.2 \text{ [10}^{-5} \text{ cm s}^{-1}\text{]} \text{ (error} = -87.0\%\text{)}$$

MSD



$t = 0 \text{ ps}$



$t = 400 \text{ ps}$

