Simulation Report: sims4_mdcm_water_k300

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

	vdw	elec	user	time	temp	tot	energy	volume	pressi
count	7395.000000	7395.000000	7395.0	7395.000000	7395.000000	7395.000000	7395.000000	7395.000000	7395.000000
mean	965.255484	-14436.355101	0.0	431.548560	297.281029	-11097.897532	16413.799064	58050.942123	-281.992017
std	125.164920	470.071630	0.0	298.769049	18.801839	765.688573	470.397352	6657.407978	1074.292673
min	735.356770	-19820.069470	0.0	0.000000	55.365740	-19650.214700	15761.092860	52947.000000	-4303.989080
25%	909.360855	-14454.874670	0.0	92.450000	297.486735	-11193.415130	16129.825550	53831.000000	-996.341880
50%	950.920650	-14378.431400	0.0	446.400000	299.591090	-11109.089070	16479.203810	54090.000000	-284.837680
75%	994.319090	-14296.472860	0.0	692.800000	301.710980	-10791.798425	16549.034035	68921.000000	477.704665
max	2089.505130	-13963.159060	0.0	939.200000	311.154860	-10553.044550	21868.281480	68921.000000	3504.639960

Simulation runs

	dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT	5: DYNA RESTRT CPT
vdw	**count**	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	295.000000
	mean	1006.739417	949.780959	955.400322	948.698835	948.417374	935.396953
	std	213.514434	60.047808	59.594836	62.819472	59.976836	60.695583
	min	775.465620	770.889510	752.103350	763.170110	774.514850	735.356770
	25%	911.947475	909.863280	914.170915	905.468922	905.527970	902.042820
	50%	953.549840	950.192145	956.511670	949.463810	945.239390	939.937340
	75%	1002.656680	987.879248	994.863210	992.461335	990.595327	972.266820
	max	2089.505130	1126.452000	1153.723050	1155.657500	1162.224290	1094.664670
elec	**count**	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	295.000000
	mean	-14659.510018	-14364.289652	-14360.300978	-14349.603526	-14352.227652	-14325.606480
	std	845.880756	109.329561	106.786465	120.086683	105.425777	117.755435
	min	-19820.069470	-14668.152980	-14766.200760	-14734.124400	-14720.787960	-14690.451010
	25%	-14508.688590	-14438.088935	-14431.353208	-14432.745955	-14426.079770	-14419.865810
	50%	-14438.291830	-14365.551115	-14362.494610	-14347.701950	-14354.327200	-14320.268700
	75%	-14369.164360	-14293.989090	-14280.243335	-14267.032180	-14277.721990	-14252.986465
	max	-14130.315370	-14015.580020	-14061.870220	-13963.159060	-14070.581500	-13997.927390
volume	**count**	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	295.000000
	mean	68921.000000	54594.065000	53933.400000	53960.912000	53961.318667	53914.684746
	std	0.000000	2298.945208	288.524904	278.939685	290.688968	327.550753

	dyna	0: DYNA STRT VERL	1: DYNA RESTRT CPT	2: DYNA RESTRT CPT	3: DYNA RESTRT CPT	4: DYNA RESTRT CPT	5: DYNA RESTRT CPT
	min	68921.000000	52989.000000	53105.000000	53157.000000	53076.000000	52947.000000
	25%	68921.000000	53763.000000	53733.750000	53778.750000	53757.000000	53692.000000
	50%	68921.000000	53966.000000	53921.000000	53944.500000	53958.500000	53886.000000
	75%	68921.000000	54247.000000	54126.250000	54139.000000	54159.250000	54177.000000
	max	68921.000000	68921.000000	54678.000000	54944.000000	54782.000000	54673.000000
temp	**count**	2000.000000	600.000000	1500.000000	1500.000000	1500.000000	295.000000
	mean	289.943747	299.860609	300.022716	300.055947	300.015688	299.823121
	std	34.727992	2.921437	3.240143	3.237289	3.250012	3.183725
	min	55.365740	291.000160	290.362740	286.593070	289.192770	288.385700
	25%	296.694035	297.857832	297.858313	297.823323	297.818720	297.590185
	50%	298.520940	299.910700	300.154230	300.052975	300.039955	299.672510
	75%	300.327495	301.679458	302.319813	302.200013	302.281420	302.201865
	max	311.154860	308.898550	309.464150	310.471360	309.391510	307.266910

Densities

density 1: 867.0796999463153 kilogram / meter ** 3

density 2: 1094.6244797854856 kilogram / meter ** 3

density 3: 1108.03324099723 kilogram / meter ** 3

density 4: 1107.4683096534766 kilogram / meter ** 3

density 5: 1107.4599634814952 kilogram / meter ** 3

density 6: 1108.4178694877128 kilogram / meter ** 3

temp. 1: 289.94374725999995

temp. 2: 299.8606093833334

temp. 3: 300.02271604000003

temp. 4: 300.05594736666666

temp. 5: 300.01568814

temp. 6: 299.82312118644063

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:165: DeprecationWarning: DCDReader currently makes independent timesteps by copying self.ts while other readers update self.ts inplace. This behavior will be changed in 3.0 to be the same as other readers. 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)

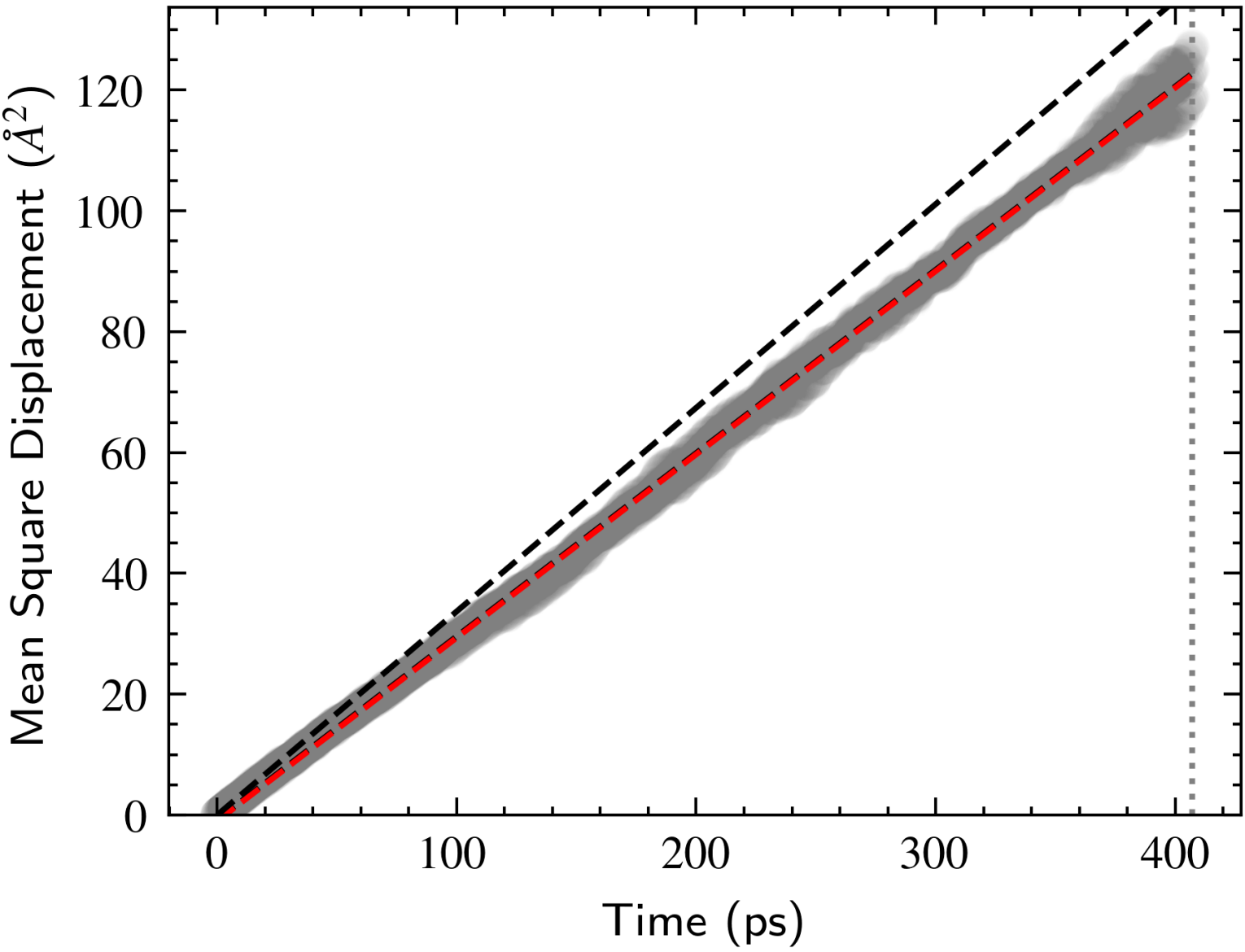
MSD and D

true ρ: 996

true D: 2.41e-05

```
0.0002
```

```
407.0166167328458
<Axes: xlabel='Time (ps)', ylabel='Mean Square Displacement ($\\AA^2$)'>
```

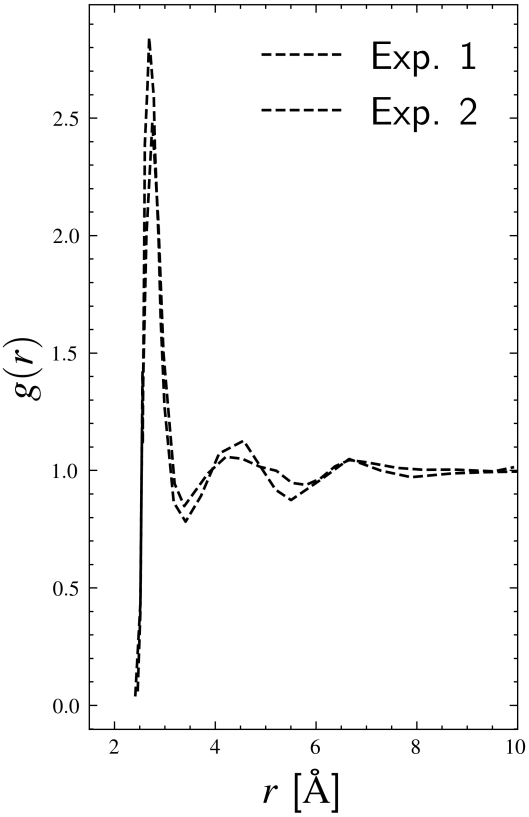


Structure and Transport

407.0166167328458
D:t,s 2.4057702102773286e-05 3.087700905447548
den:t,s 996.1905427677091 1105.20077268108

ρ = 1105 [kg/m^3] (error = 10.9%)

RDF



D = 3.1 [10^{-5} cm s^{-1}] (error = 28.3%)

MSD