Description

April 29, 2022

This repository contain data presented in *Comparing four hard-sphere approximations for the low-temperature WCA melting line* by Eman Attia, Jeppe C. Dyre and Ulf R. Pedersen (Roskilde University, Denmark). Please write to URP for questions (ulf@urp.dk).

[1]:
```
%ls
```

```
Description.ipynb  clausius_clapeyron.csv
Description.pdf    interface_pinning.csv
```

The CSV file `interface_pinning.csv` contain data of the phase transition line determined using the interface pinning method. The first four columns have the following information

	Description	Symbol	Unit
`T`	Coexistence temperature	T	ε/k_B
`p`	Coexistence pressure	p	ε/σ^3
`rho_l`	Fluid number density	ρ_l	$1/\sigma^3$
`rho_s`	Solid number density	ρ_s	$1/\sigma^3$

The last three columns give the statistical error on p, ρ_l and ρ_s, respectively.

[2]:
```
import pandas as pd
ip = pd.read_csv('interface_pinning.csv')
ip
```

[2]:

	T	p	rho_l	rho_s	p_error	rho_l_error	rho_s_error
0	2.000	31.808648	1.084410	1.151919	0.006594	0.000051	0.000059
1	0.200	2.051686	0.800040	0.873563	0.000329	0.000033	0.000036
2	0.020	0.174944	0.706377	0.778886	0.000047	0.000048	0.000056
3	0.002	0.016687	0.677174	0.747911	0.000003	0.000025	0.000033

The CSV file `clausius_clapeyron.csv` contain data of the phase transition line determined by integration of the Clausius-Clapeyron relation.

The CSV file `interface_pinning.csv` contain data of the phase transition line determined using the interface pinning method. The first six columns have the following information

	Description	Symbol	Unit
`T`	Coexistence temperature	T	ε/k_B
`p`	Coexistence pressure	p	ε/σ^3

	Description	Symbol	Unit
`v_fcc`	Solid specific volume	$1/\rho_s$	σ^3
`v_liquid`	Fluid specific volume	$1/\rho_l$	σ^3
`u_fcc`	Solid potential energy per particle	u_s	ε
`u_liquid`	Fluid potential energy per particle	u_l	ε

The last two columns (`slope0` and `slope1`) are the slopes (f) computed in the first and final step of the trapzodial predictor corrector method.

[3]:
```
cc = pd.read_csv('clausius_clapeyron.csv')
cc
```

[3]:

	T	p	v_fcc	v_liquid	u_fcc	u_liquid	\
0	0.020000	0.174944	1.284030	1.415833	0.005514	0.006344	
1	0.018170	0.158407	1.287121	1.419728	0.004802	0.005520	
2	0.016508	0.143457	1.290724	1.423717	0.004183	0.004802	
3	0.014998	0.129939	1.293907	1.426986	0.003642	0.004174	
4	0.013626	0.117712	1.297073	1.430798	0.003169	0.003629	
..	…	…	…	…	…	…	
99	13.625840	384.288100	0.587939	0.613666	40.318910	43.327680	
100	14.997880	435.519000	0.575172	0.600038	45.274950	48.563760	
101	16.508080	493.495500	0.562600	0.586685	50.792230	54.396050	
102	18.170350	559.105800	0.550200	0.573623	56.944450	60.862380	
103	20.000000	633.309000	0.538068	0.560766	63.798720	68.074010	

	slope0	slope1
0	9.061429	9.015647
1	9.015350	8.971734
2	8.971782	8.930681
3	8.930895	8.892160
4	8.891828	8.854951
..	…	…
99	36.819490	37.858800
100	37.862580	38.917390
101	38.936840	40.003810
102	40.011620	41.100360
103	41.106010	42.231010

[104 rows x 8 columns]