

Guide to Model Sediment Data Files

There are four sets of text files available for the 76 packings produced by the cooperative rearrangement algorithm and summarized in Table 1 (see end of this document).

1. Listing of sphere centers and radii for each packing

Folder name: Packing Coordinates

File names in this set are of the form “Coordinates_PackingNN.txt” where NN indicates the number of the packing in Table 1. For example the file named “Coordinates_Packing12.txt” contains data pertaining to the 12th packing. Each file contains four columns. The first 3 columns contain the X-, Y- and Z-coordinates of the sphere centers respectively and the fourth column contains the radius of the corresponding spheres. The coordinates are in the same arbitrary but self-consistent units used to report grain sizes. The ID number for each sphere is the row number on which the data of that specific sphere appears. This ID number is used to refer to the spheres in the Delaunay tessellation (see next file type).

Example: the first ten lines of Coordinates_Packing1.txt are shown below.

2.9510300e+001	2.1302500e+001	4.0295900e+001	2.2783500e+000
5.3711700e+001	1.2861000e+001	4.3209600e+001	2.2168100e+000
6.6300900e+001	6.5553900e+001	1.8227200e+001	2.1118800e+000
9.6867900e+000	6.1662900e+000	2.9074100e+001	2.2594700e+000
2.4610100e+001	2.4928900e+001	1.6943900e+001	2.1263300e+000
1.3072500e+001	2.2058300e+001	1.2149000e+001	2.1046600e+000
5.0956900e+001	3.7340800e+001	2.4290000e+000	2.3653800e+000
7.0123200e+000	4.4366600e+001	2.6550400e+001	2.1209200e+000
2.5703100e+001	1.4560700e+001	6.3361000e+001	2.1258700e+000
6.6219300e+001	3.4782600e+001	5.1609200e+001	2.1561500e+000

Thus Sphere 1 in this packing has radius 2.27835 and its center is located at (29.5103, 21.3025, 40.2959).

2. Listing of sphere IDs corresponding to Delaunay tessellation for each packing

Folder name: Tessellation Matrices

File names in this set are of the form “Tes_Matrix_PackNN.txt” where NN indicates the number of the packing in Table 1. Each file contains four columns. Each row in this text file represents a Delaunay cell. The four numbers listed on each row indicate the IDs of the spheres that make up a Delaunay cell. The ID number for each Delaunay cell is the row number on which the data of that specific Delaunay cell appears. This ID number is used to refer to the Delaunay cells in the topology file (see next file type).

Example: the first ten lines of Tes_Matrix_Pack1.txt are shown below.

2.8910000e+003	3.2660000e+003	2.5230000e+003	4.8480000e+003
2.4040000e+003	4.3260000e+003	1.2230000e+003	2.5280000e+003
3.3540000e+003	1.2910000e+003	3.9550000e+003	4.9920000e+003

1.7380000e+003	4.8110000e+003	7.0900000e+002	4.4200000e+002
6.6900000e+002	1.3730000e+003	3.8360000e+003	4.5170000e+003
6.3000000e+001	3.4640000e+003	4.6450000e+003	1.7090000e+003
1.2460000e+003	3.4640000e+003	4.6450000e+003	1.7090000e+003
1.2460000e+003	2.1210000e+003	3.4640000e+003	1.7090000e+003
2.8360000e+003	2.8910000e+003	3.2660000e+003	2.5230000e+003
4.3630000e+003	3.5390000e+003	4.5110000e+003	2.5380000e+003

Thus the first Delaunay cell corresponds to Spheres 2891, 3266, 2523 and 4848. By inspecting the corresponding lines of the `Coordinates_Packing1.txt` file, we could determine the spatial location of each corner of this tetrahedron, and thus the radii of each pore throat in this cell. Note that Cells 6 and 7 both contain Spheres 3464, 4645 and 1709. This means that Cells 6 and 7 will be neighbors (see next file type). Similarly, Cell 1 and Cell 9 have three spheres in common, namely 2891, 3266 and 2523.

3. Listing of network topology (which cells in the above file are the neighbors of each cell)

Folder name: Neighbor Identification

File names in this set are of the form “Neighbors_Matrix_PackNN.txt” where NN indicates the number of the packing in Table 1. Each file contains four columns. Each row corresponds to one cell in the tessellation. Each column contains the ID number of a cell that neighbors the given cell. There are four columns, because all cells are tetrahedral and therefore have four neighbors. Though the packings are periodic, this listing treats the packing as though it were finite and limited to the cubic domain used by the cooperative rearrangement algorithm. Thus cells on the outer face of the packing will have fewer than four neighbors *within* the packing. The exterior face(s) of these cells are assigned a neighbor index of zero (0).

Example: the first ten lines of `Neighbors_Matrix_Pack1.txt` are shown below.

9.0000000e+000	1.5300000e+002	0.0000000e+000	0.0000000e+000
1.2000000e+003	3.8980000e+003	3.9410000e+003	3.8130000e+003
1.9750000e+003	8.8300000e+002	0.0000000e+000	0.0000000e+000
2.9000000e+002	1.3110000e+003	4.0350000e+003	8.7830000e+003
1.2400000e+002	1.2200000e+002	5.8490000e+003	0.0000000e+000
7.4500000e+002	7.4800000e+002	3.0400000e+002	7.0000000e+000
2.7220000e+003	1.4300000e+002	8.0000000e+000	6.0000000e+000
6.9680000e+003	7.0000000e+000	2.8850000e+003	3.0300000e+002
1.5400000e+002	2.9100000e+003	2.5000000e+001	1.0000000e+000
1.6000000e+002	7.3600000e+002	4.5000000e+001	2.1762000e+004

Thus the first Delaunay cell has as neighbors Cells 9, 153, 0 and 0. The latter two values mean that the first cell has two faces on the exterior of the packing. The ninth line indicates that Cell 9 has neighbors 154, 2910, 25 and 1. The presence of Cell 1 in this list serves as a consistency check; we have carried out this check on the topology file for every packing. Similarly, Cell 7 is the fourth neighbor of Cell 6, and Cell 6 is the fourth neighbor of Cell 7. To determine the size of the pore throat connecting Cells 6 and 7, one would identify the sphere IDs that are common to the Delaunay cell definitions for Cells 6 and 7 (see previous section). The spatial locations and radii of these spheres can be extracted from the file of coordinates. This information is sufficient to determine the radius of the inscribed circle (and any other geometric information desired), which we use as a measure of the pore throat size (see next file type).

4. Listing of pore throat radii associated with each throat connecting neighboring cells

Folder name: Norm Throat Size Matrices

File names in this set are of the form “Normalized_Pore_Throat_Size_Matrix_PackNN.txt” where NN indicates the number of the packing in Table 1. It includes the normalized pore throat radii associated with each throat connecting neighboring cells throughout the packing. The throat radii in each packing are normalized by the mean sphere radius (see Table 1). Thus the normalization factor differs from packing to packing, but after normalization all quantities involving length are comparable between packings. A radius of -1 indicates a throat that is connected to the exterior of the packing. The treatment of such throats depends on the algorithm to be used for drainage and imbibition. If the actual geometric value is needed, it can be readily extracted from the other three data files as discussed above.

The throat radii file is constructed in exactly the same order as the topology file above. The line number of each row corresponds to the Delaunay cell number. For a given row, the first column contains the radius of the throat connecting the given cell to its first neighbor. (The first neighbor is identified in the corresponding line of the topology file.) The second column contains the radius of the throat connected the given cell to the second neighbor, and so on.

Example: the first ten lines of Normalized_Pore_Throat_Size_Matrix_Pack1.txt are shown below.

```
1.7554545e-001 1.6062099e-001 -1.0000000e+000 -1.0000000e+000
4.2141740e-001 2.5307557e-001 3.0896714e-001 2.4233366e-001
3.7456316e-001 3.7354064e-001 -1.0000000e+000 -1.0000000e+000
3.1531876e-001 2.2893521e-001 3.1233790e-001 3.7145802e-001
1.4884367e-001 1.5176807e-001 4.1038120e-001 -1.0000000e+000
2.6542254e-001 1.6435000e-001 3.7279741e-001 4.1491201e-001
2.7451845e-001 2.0055349e-001 3.8093278e-001 4.1491201e-001
5.3127678e-001 3.8093278e-001 4.2109478e-001 5.0433782e-001
2.2256290e-001 2.2367991e-001 1.7227901e-001 1.7554545e-001
3.6117889e-001 2.8125971e-001 1.7008389e-001 2.9634619e-001
```

Thus the first Delaunay cell has throats of radius $0.175545R$, $0.160621R$ and two throats connected to the exterior of the packing. Here R is the mean radius of spheres in packing No. 1, which is 2.18 (see Table 1). Cell 10 is connected to its neighbors through throats of radius $0.361179R$, $0.28126R$, $0.170084R$ and $0.296346R$. Cell 6 is connected to Cell 7 through a throat of radius $0.414912R$, i.e. through the fourth throat of Cell 6.

Table 1. Summary of Properties of Model Sediments

Packing No.	Grain sizes (arbitrary units)				Porosity (fraction)	Sorting Index		Notes*
	Minimum Radius	Maximum radius	Mean radius	Standard deviation		Number fraction basis	Volume or weight fraction basis	
1	0.32	2.58	2.18	0.11	0.37	1.04	1.04	LN
2	1.84	2.64	2.18	0.11	0.36	1.03	1.03	LN
3	1.80	2.60	2.18	0.11	0.37	1.03	1.03	LN
4	0.32	2.59	2.18	0.11	0.35	1.03	1.03	LN
5	1.82	2.52	2.15	0.11	0.41	1.03	1.03	LN
Average	1.22	2.59	2.17	0.11	0.37	1.03	1.03	
6	1.50	3.22	2.17	0.22	0.36	1.07	1.07	LN
7	1.50	3.08	2.16	0.22	0.36	1.07	1.07	LN
8	1.48	2.99	2.17	0.22	0.36	1.07	1.07	LN
9	1.47	3.06	2.16	0.22	0.37	1.07	1.07	LN
Average	1.49	3.09	2.16	0.22	0.36	1.07	1.07	
10	0.96	4.12	2.12	0.42	0.35	1.14	1.14	LN
11	0.93	4.64	2.12	0.43	0.34	1.14	1.14	LN
12	1.07	4.49	2.11	0.42	0.35	1.14	1.14	LN
13	0.99	4.27	2.11	0.43	0.35	1.14	1.14	LN
Average	0.99	4.38	2.11	0.43	0.35	1.14	1.14	
14	4.24E-03	7.05	1.90	0.80	0.32	1.31	1.32	LN
15	3.44E-03	6.44	1.90	0.79	0.35	1.31	1.31	LN
16	3.91E-01	6.38	1.91	0.78	0.33	1.31	1.29	LN
17	7.81E-03	7.01	1.90	0.79	0.32	1.31	1.30	LN
18	1.59E-03	7.62	1.91	0.79	0.32	1.31	1.29	LN
Average	8.17E-02	6.90	1.90	0.79	0.33	1.31	1.30	
19	1.86E-03	11.30	1.31	1.16	0.29	1.72	1.48	LN; Trn
20	2.39E-03	10.16	1.31	1.17	0.25	1.72	1.54	LN; Trn
21	7.85E-03	11.26	1.31	1.15	0.30	1.72	1.53	LN; Trn
22	1.17E-03	11.17	1.30	1.16	0.30	1.69	1.53	LN; Trn
Average	3.32E-03	10.97	1.31	1.16	0.29	1.71	1.52	
23	3.45E-05	11.31	0.69	1.25	0.31	3.11	1.32	LN; Trn
24	1.63E-05	11.19	0.71	1.26	0.30	3.12	1.38	LN; Trn
25	3.80E-05	11.28	0.70	1.25	0.37	3.16	1.30	LN; Trn
26	1.44E-05	12.16	0.72	1.23	0.32	3.07	1.46	LN; Trn
Average	2.58E-05	11.49	0.71	1.25	0.33	3.11	1.37	
27	8.10E-06	18.29	0.30	1.07	0.31	3.63	1.38	LN; Trn
28	2.04E-06	21.32	0.30	1.04	0.29	3.77	1.37	LN; Trn
29	6.94E-06	22.46	0.31	1.04	0.32	3.95	1.41	LN; Trn
Average	5.69E-06	20.69	0.31	1.05	0.31	3.79	1.39	
30	1.24E-03	11.93	1.01	1.20	0.29	2.00	1.50	LN; Trn
31	6.31E-04	11.99	1.04	1.22	0.32	2.00	1.56	LN; Trn
32	5.70E-04	12.34	1.02	1.21	0.30	2.03	1.48	LN; Trn
33	4.21E-05	12.57	1.07	1.22	0.31	1.94	1.51	LN; Trn
34	5.47E-04	11.63	1.03	1.19	0.34	2.01	1.49	LN; Trn
Average	6.06E-04	12.09	1.03	1.21	0.31	2.00	1.51	
35	4.62E-04	9.67	1.63	1.03	0.30	1.51	1.40	LN
36	1.89E-03	9.70	1.61	1.04	0.30	1.50	1.43	LN
37	1.35E-03	9.30	1.59	1.04	0.27	1.49	1.46	LN
38	3.98E-03	9.41	1.60	1.05	0.27	1.51	1.44	LN
Average	1.92E-03	9.52	1.60	1.04	0.29	1.50	1.43	
39	1.97	2.40	2.19	0.07	0.34	1.02	1.02	N
40	1.97	2.41	2.19	0.07	0.35	1.02	1.02	N
41	1.95	2.39	2.17	0.07	0.38	1.02	1.02	N
42	1.97	2.40	2.19	0.07	0.37	1.02	1.02	N
Average	1.97	2.40	2.18	0.07	0.36	1.02	1.02	
43	1.07	3.20	2.14	0.35	0.36	1.12	1.10	N
44	1.07	3.20	2.14	0.35	0.36	1.12	1.10	N
45	1.07	3.20	2.14	0.36	0.35	1.12	1.11	N
46	1.07	3.20	2.14	0.35	0.37	1.12	1.11	N
Average	1.07	3.20	2.14	0.35	0.36	1.12	1.10	

Table 1. Summary of Properties of Model Sediments (cont.)

Packing No.	Grain sizes (arbitrary units)				Porosity (fraction)	Sorting Index		Notes*
	Minimum Radius	Maximum radius	Mean radius	Standard deviation		Number fraction basis	Volume or weight fraction basis	
47	5.64E-05	4.01	2.01	0.68	0.34	1.27	1.17	N
48	4.20E-05	4.01	2.01	0.66	0.33	1.25	1.17	N
49	3.59E-05	4.03	2.01	0.67	0.34	1.25	1.18	N
50	3.22E-05	4.04	2.02	0.66	0.33	1.25	1.17	N
Average	4.16E-05	4.02	2.01	0.67	0.34	1.26	1.17	
51	1.27E-03	4.59	1.85	0.90	0.32	1.42	1.21	N
52	1.10E-03	4.51	1.85	0.91	0.34	1.42	1.21	N
53	5.94E-04	4.44	1.86	0.89	0.35	1.40	1.21	N
54	2.94E-03	4.59	1.86	0.90	0.32	1.42	1.20	N
Average	1.48E-03	4.53	1.86	0.90	0.33	1.42	1.21	
55	6.34E-04	5.00	1.73	1.04	0.32	1.60	1.23	N
56	3.30E-04	5.06	1.71	1.05	0.31	1.64	1.22	N
57	1.56E-03	5.07	1.71	1.05	0.35	1.62	1.22	N
58	8.76E-04	5.08	1.71	1.05	0.34	1.65	1.23	N
59	1.09E-03	5.01	1.70	1.05	0.33	1.63	1.22	N
Average	8.98E-04	5.04	1.71	1.05	0.33	1.63	1.22	
60	3.81E-03	4.56	1.84	0.91	0.32	1.43	1.21	N
61	4.85E-03	4.82	1.77	1.00	0.31	1.53	1.22	N
62	4.93E-03	4.85	1.76	1.00	0.35	1.53	1.23	N
63	4.47E-04	4.81	1.76	1.00	0.33	1.53	1.22	N
64	2.51E-03	4.82	1.77	0.99	0.33	1.51	1.22	N
65	4.94E-03	4.88	1.76	1.00	0.34	1.54	1.23	N
Average	3.58E-03	4.79	1.78	0.98	0.33	1.51	1.22	
66	3.31E-03	5.36	1.60	1.15	0.33	1.89	1.24	N
67	1.88E-04	5.38	1.61	1.14	0.32	1.85	1.24	N
68	2.30E-03	5.44	1.60	1.15	0.33	1.94	1.23	N
69	2.37E-03	5.43	1.60	1.14	0.33	1.91	1.24	N
70	2.43E-04	5.32	1.59	1.14	0.33	1.90	1.25	N
Average	1.68E-03	5.39	1.60	1.14	0.33	1.90	1.24	
71	2.88E-04	5.46	1.54	1.19	0.33	2.12	1.23	N
72	2.93E-03	5.47	1.53	1.20	0.33	2.20	1.23	N
73	2.86E-04	5.49	1.52	1.20	0.32	2.27	1.24	N
74	2.52E-03	5.64	1.53	1.20	0.33	2.18	1.24	N
75	8.97E-04	5.65	1.53	1.19	0.33	2.13	1.26	N
76	7.35E-04	5.52	1.53	1.20	0.32	2.23	1.24	N
Average	1.28E-03	5.54	1.53	1.20	0.32	2.19	1.24	

LN = log normal distribution of sphere sizes. N = normal distribution of sphere sizes. Trn indicates that the actual distribution of sphere sizes in the packing was truncated.