

Results SimID.2765202

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Disclaimer

**This report has been auto-generated using paraprobe-autoreporter.
It is the responsibility of the author to check the validity and correctness of these results!**

1 paraprobe-transcoder

Here is place for tool-specific comments.

The dataset contains 13114038 ions in total.

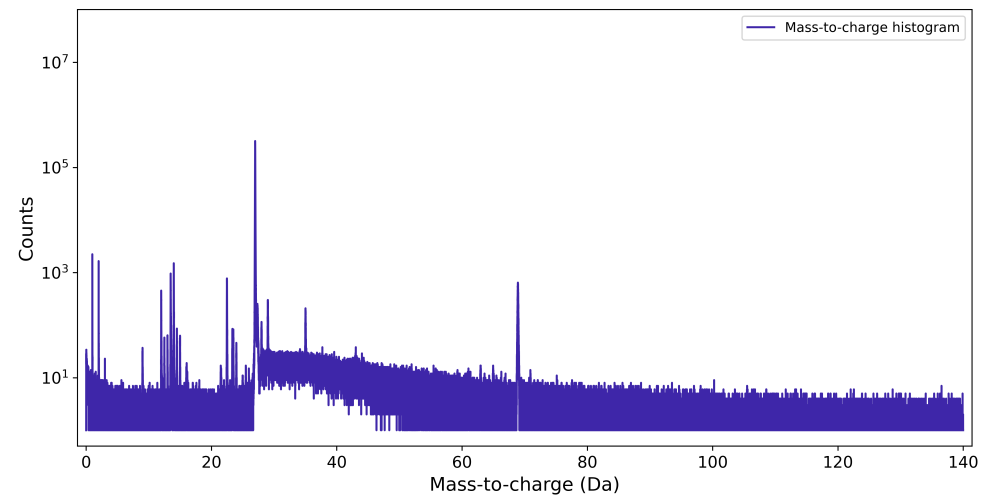
Table 1: Which XML settings were used for paraprobe-transcoder?

| Keyword | Value | Unit | Description |
|-----------------|-------------------|------|-------------|
| Inputfile | R76_27652-v02.pos | | |
| TranscodingMode | 1 | | |

2 paraprobe-ranger

Table 2: What is the composition of the dataset, i.e. how many ions with particular ion type labelled?

| unknown | Al | Sc | Si | Mg | H: | C: | O: | Xe | AlO: | ScH: | AlH: | Total |
|---------|----------|-------|-------|-------|-------|-----|------|-----|-------|------|-------|----------|
| 740067 | 12227563 | 27429 | 44233 | 15563 | 14446 | 221 | 1605 | 891 | 15602 | 3182 | 23236 | 13114038 |



(a)

Figure 1: What is the mass-to-charge histogram/diagram of the entire dataset?

Table 3: Which XML settings were used for paraprobe-ranger?

| Keyword | Value | Unit | Description |
|-----------------|-------------------|------|-------------|
| Inputfile | R76_27652-v02.pos | | |
| TranscodingMode | 1 | | |

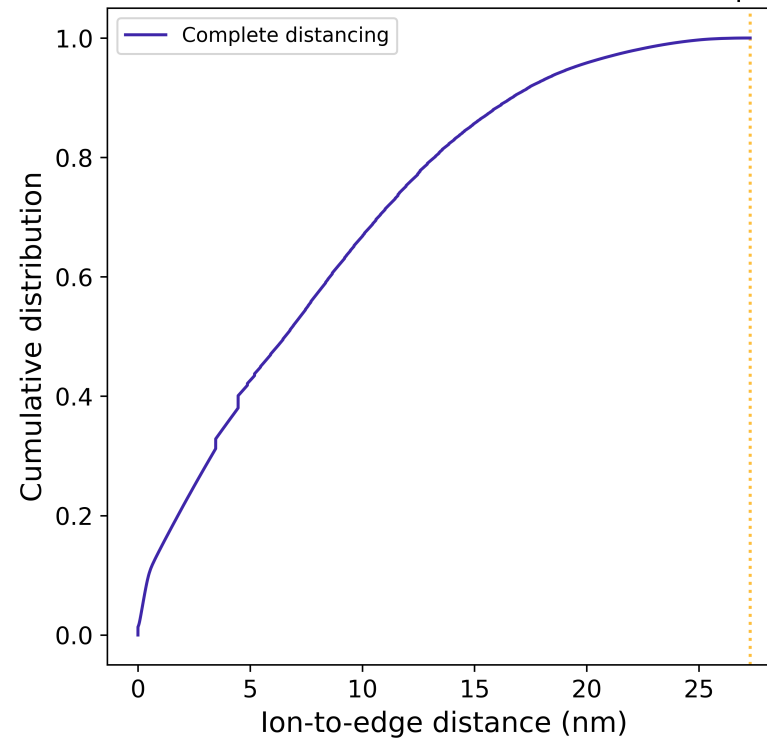
3 paraprobe-surfacer

4 paraprobe-tessellator

5 paraprobe-spatstat

6 paraprobe-dbscan

PARAPROBE.Surfacer.Results.SimID.2765202.h5 α -shape, $\alpha = 1.175$



(a)

Figure 2: How many ions are so and so far away from the dataset edge?

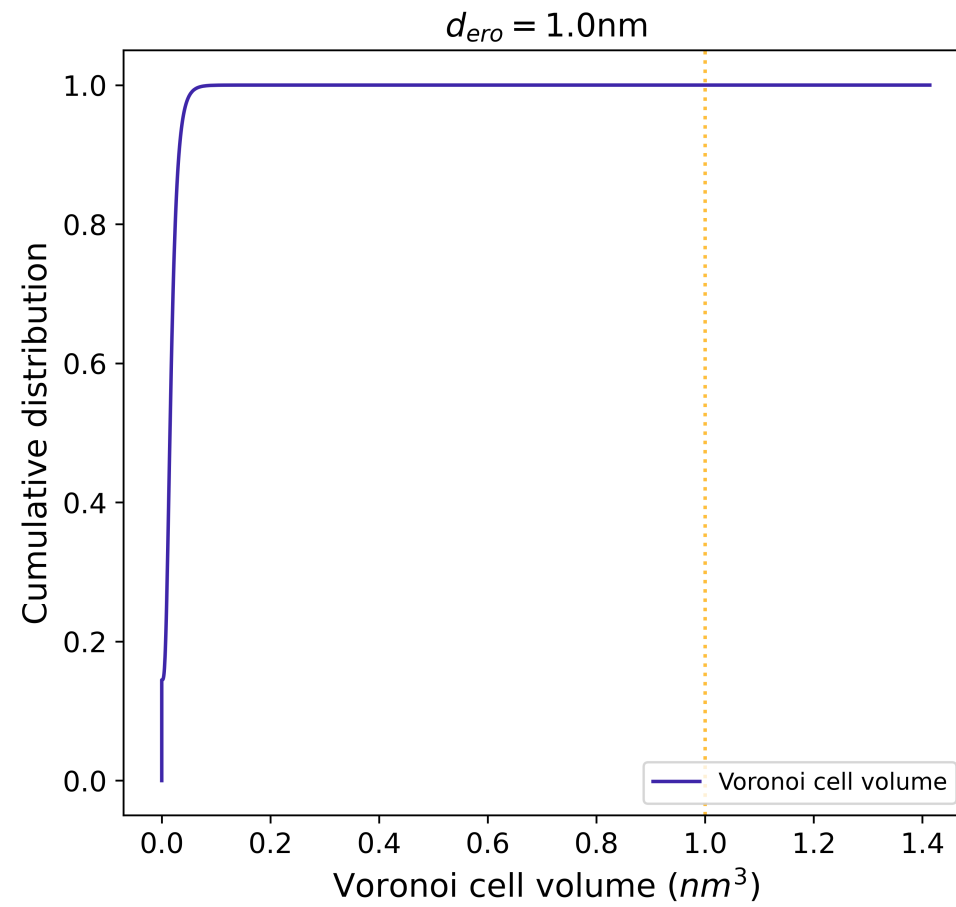
7 Profiling

Table 4: Which XML settings were used for paraprobe-surfacers?

| Keyword | Value | Unit | Description |
|-------------------------|---|-------------|--------------------|
| AdvDistanceBinWidthIncr | 1 | nm | |
| AdvDistanceBinWidthMax | 1 | nm | |
| AdvDistanceBinWidthMin | 1 | nm | |
| AdvIonPruneBinWidthIncr | 1 | nm | |
| AdvIonPruneBinWidthMax | 1 | nm | |
| AdvIonPruneBinWidthMin | 1 | nm | |
| AlphaShapeAlphaValue | 0 | | |
| DistancingMode | 1 | | |
| DistancingRadiusMax | 0 | nm | |
| InputfileReconstruction | PARAPROBE.Transcoder.Results.SimID.2765202.h5 | | |
| RequeryingThreshold | 0 | | |
| SurfacingMode | 1 | | |

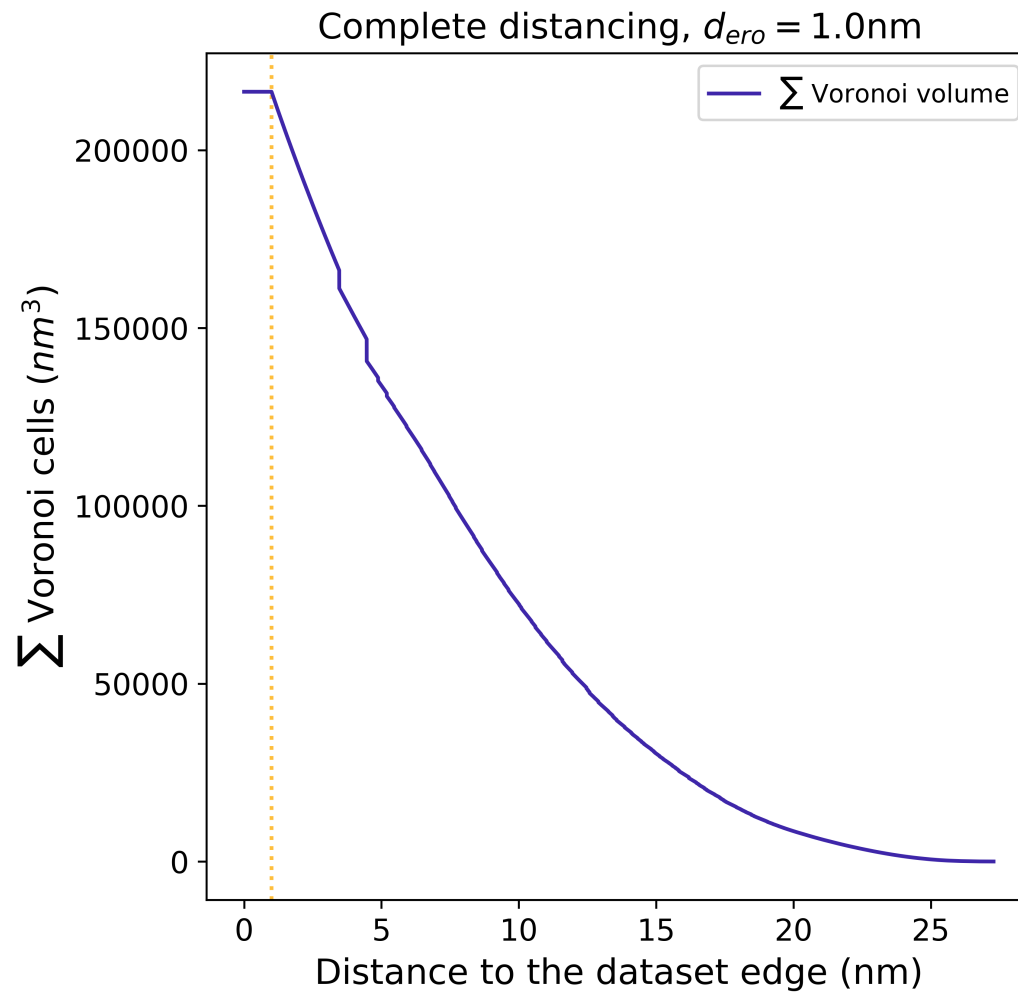
Table 5: Which XML settings were used for paraprobe-tessellator?

| Keyword | Value | Unit | Description |
|-------------------------|---|-------------|--------------------|
| CellErosionDistance | 1 | nm | |
| GuardZoneFactor | 5 | | |
| IOCellNeighbors | 0 | | |
| IOCellProfiling | 1 | | |
| IOCellShape | 0 | | |
| IOCellVolume | 1 | | |
| InputfileDistances | PARAPROBE.Surfacers.Results.SimID.2765202.h5 | | |
| InputfilePSE | PARAPROBE.PeriodicTableOfElements.xml | | |
| InputfileReconstruction | PARAPROBE.Transcoder.Results.SimID.2765202.h5 | | |
| IonsPerBlock | 5 | | |
| SpatialSplittingMethod | 0 | | |



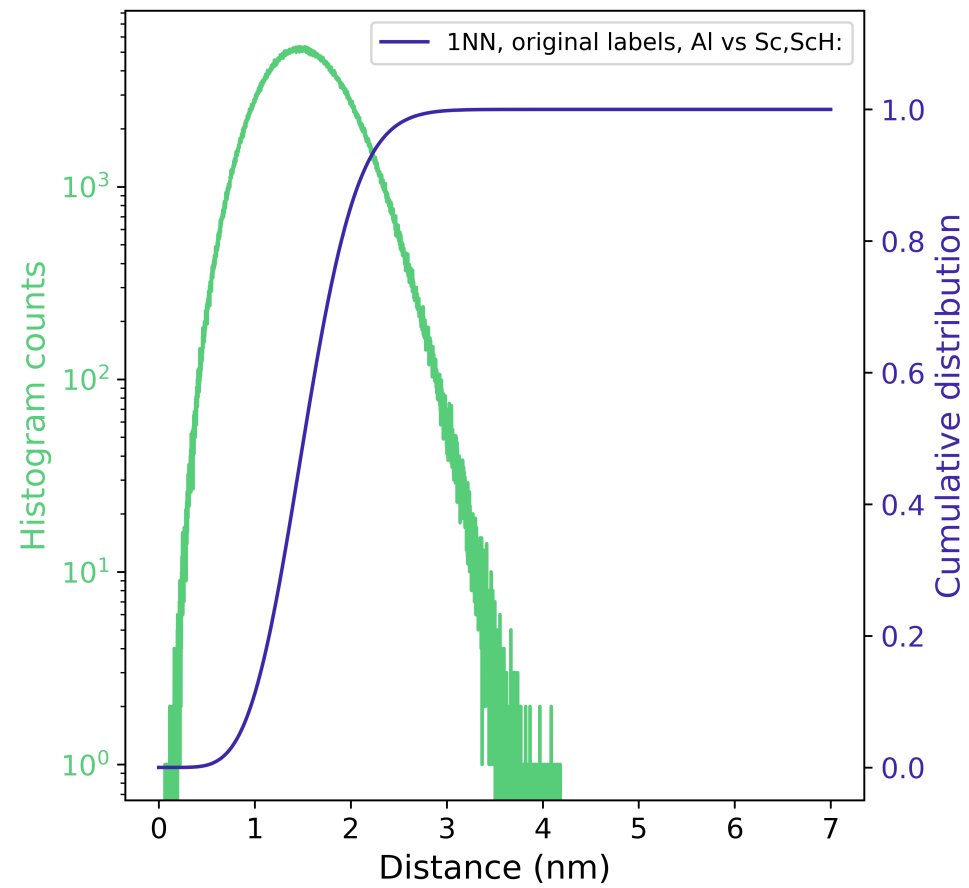
(a)

Figure 3: What is the distribution of volume for the Voronoi cells?



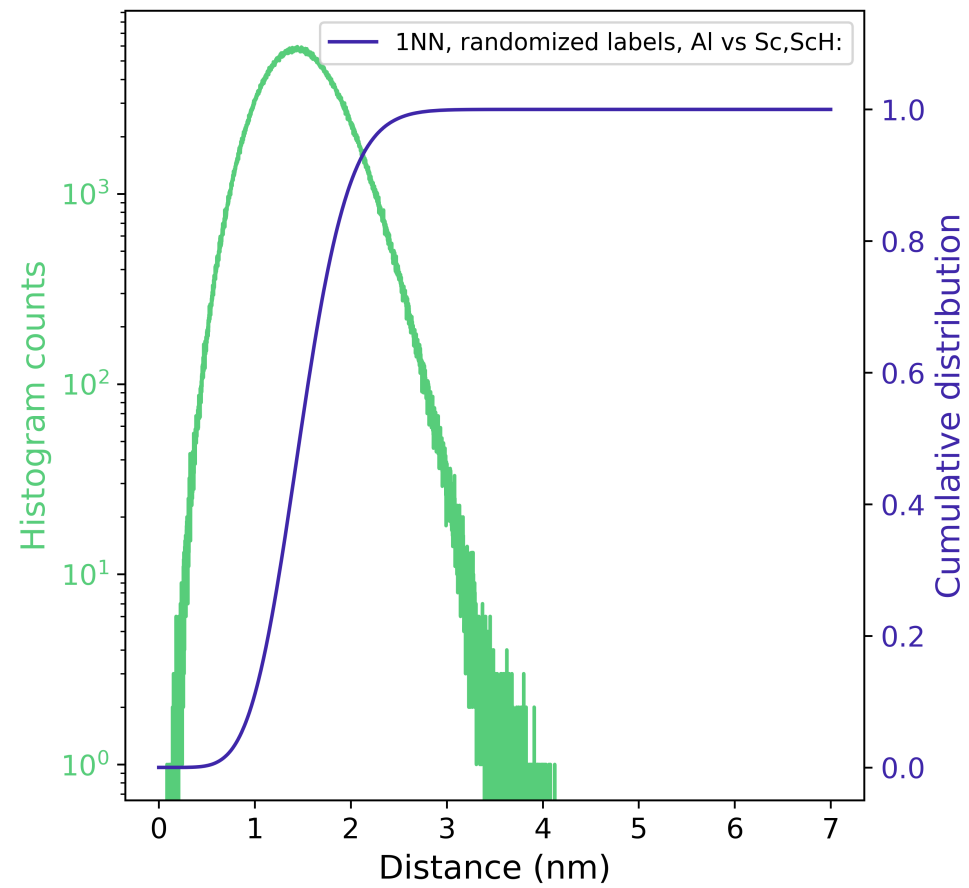
(a)

Figure 4: How much accumulated volume of Voronoi cells remains when successively eroding Voronoi cells from the dataset edge towards the interior?



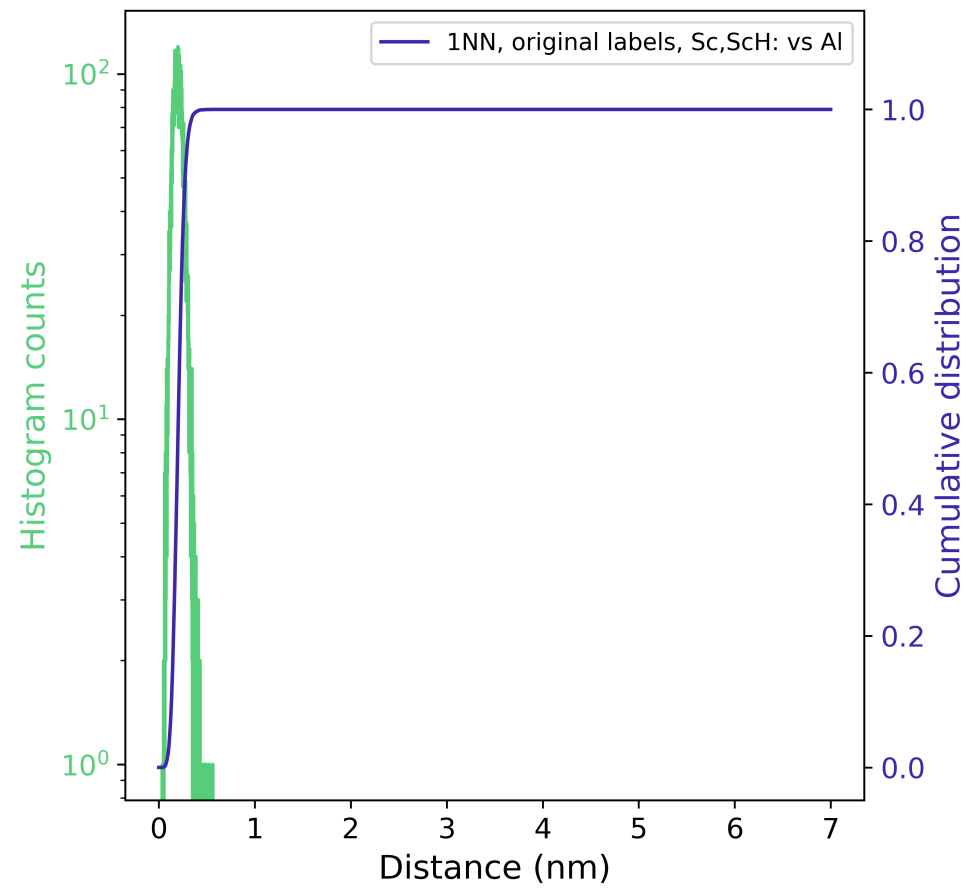
(a)

Figure 5: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



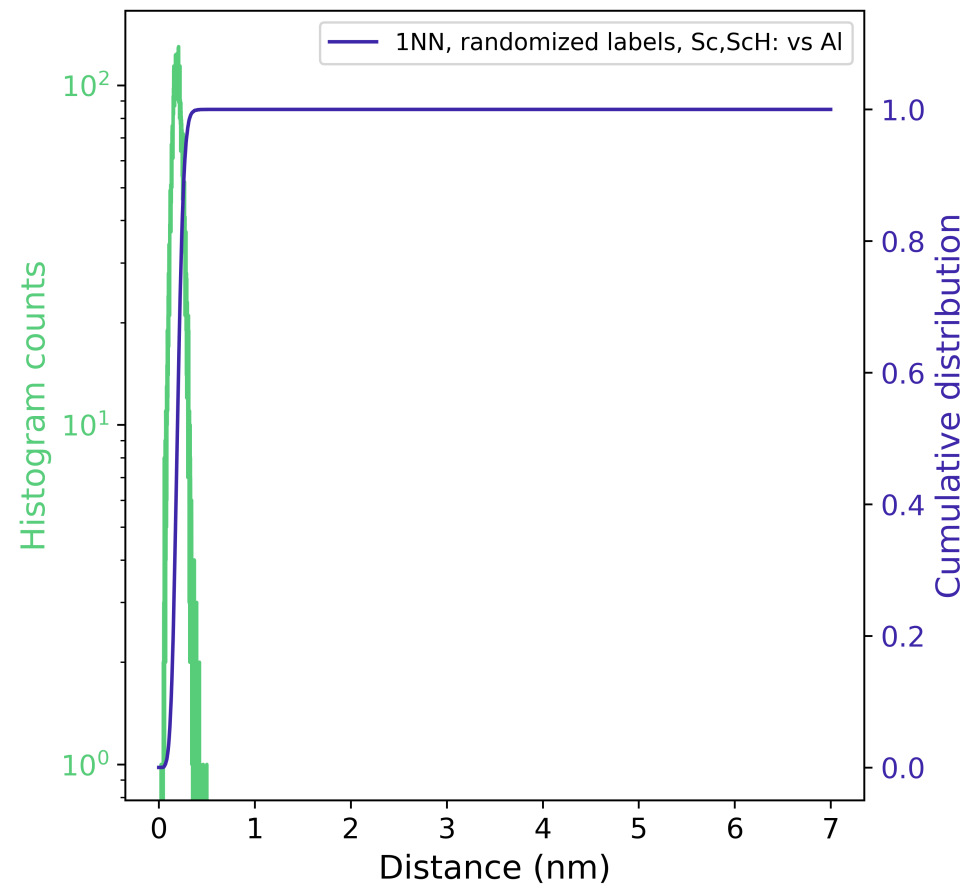
(a)

Figure 6: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



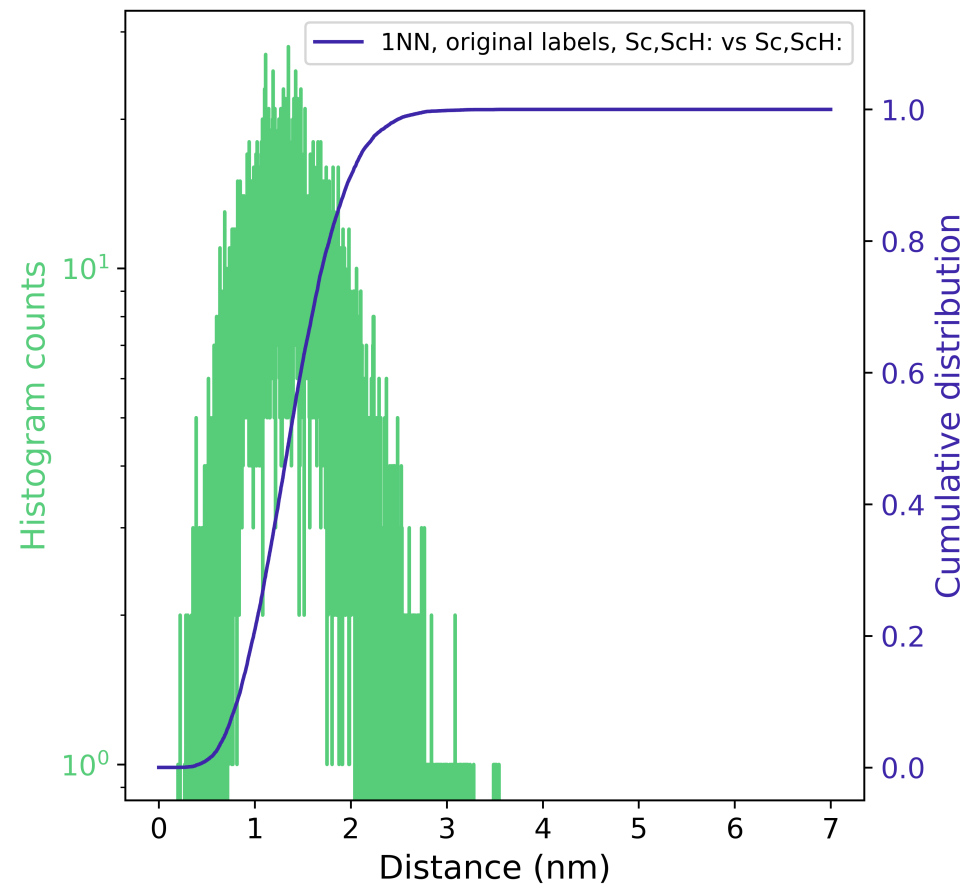
(a)

Figure 7: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



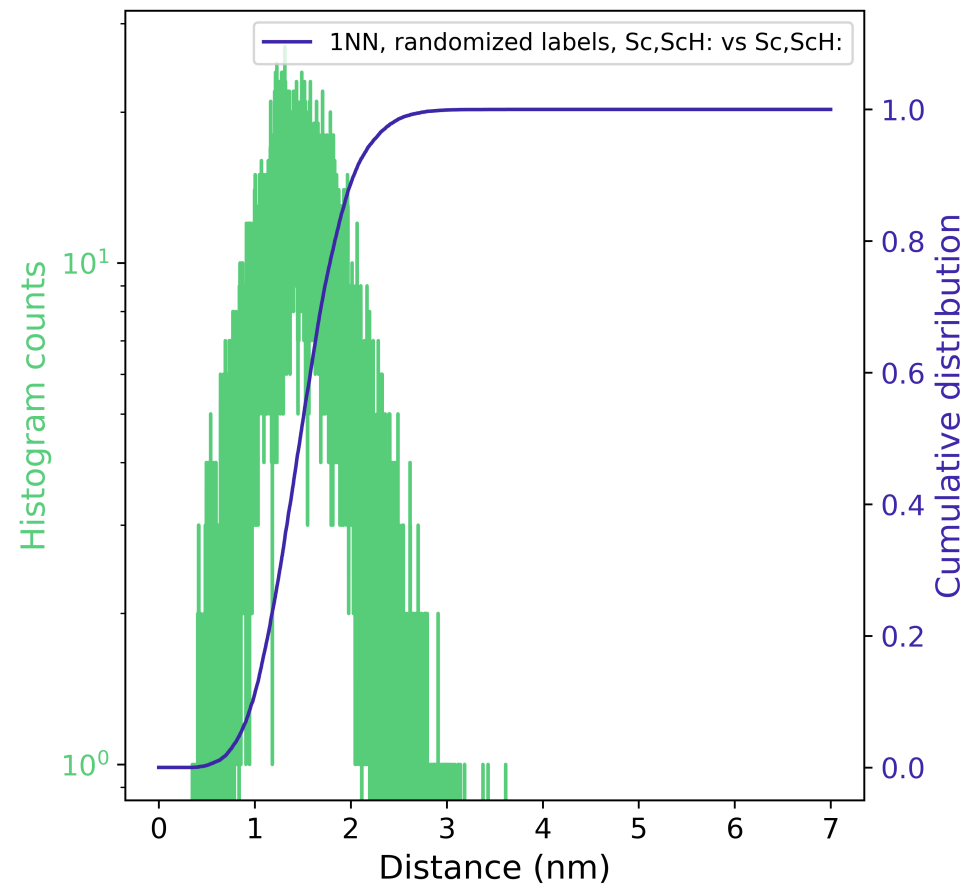
(a)

Figure 8: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



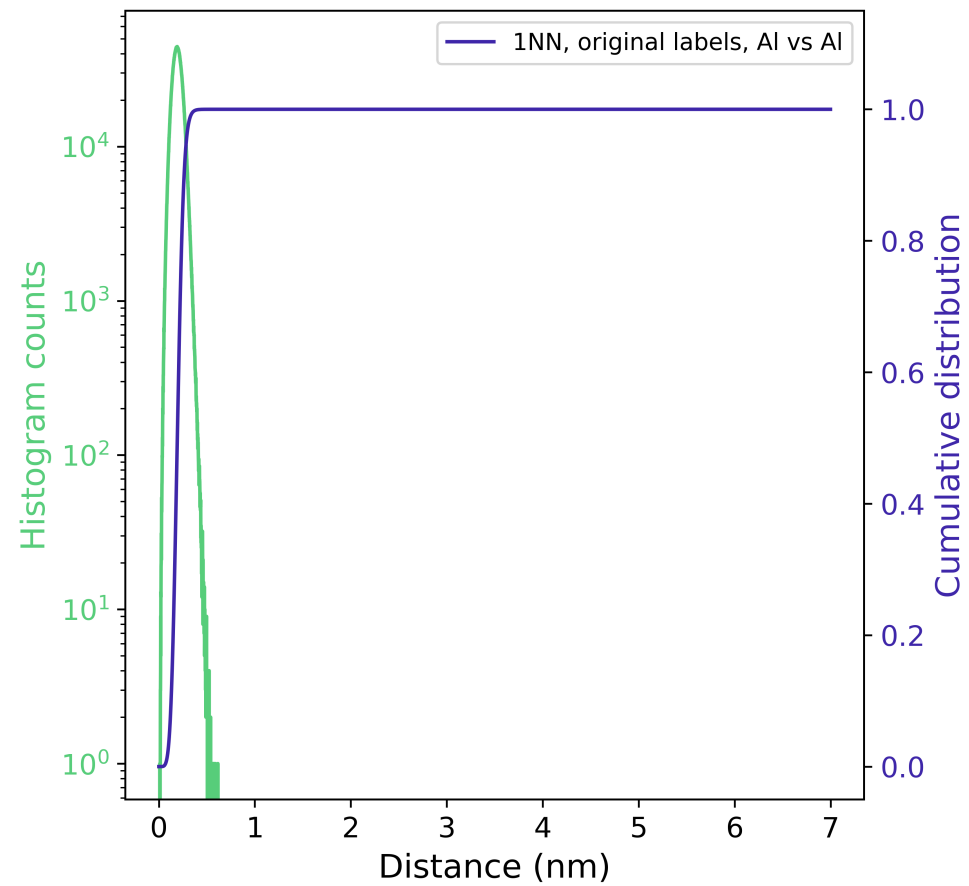
(a)

Figure 9: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



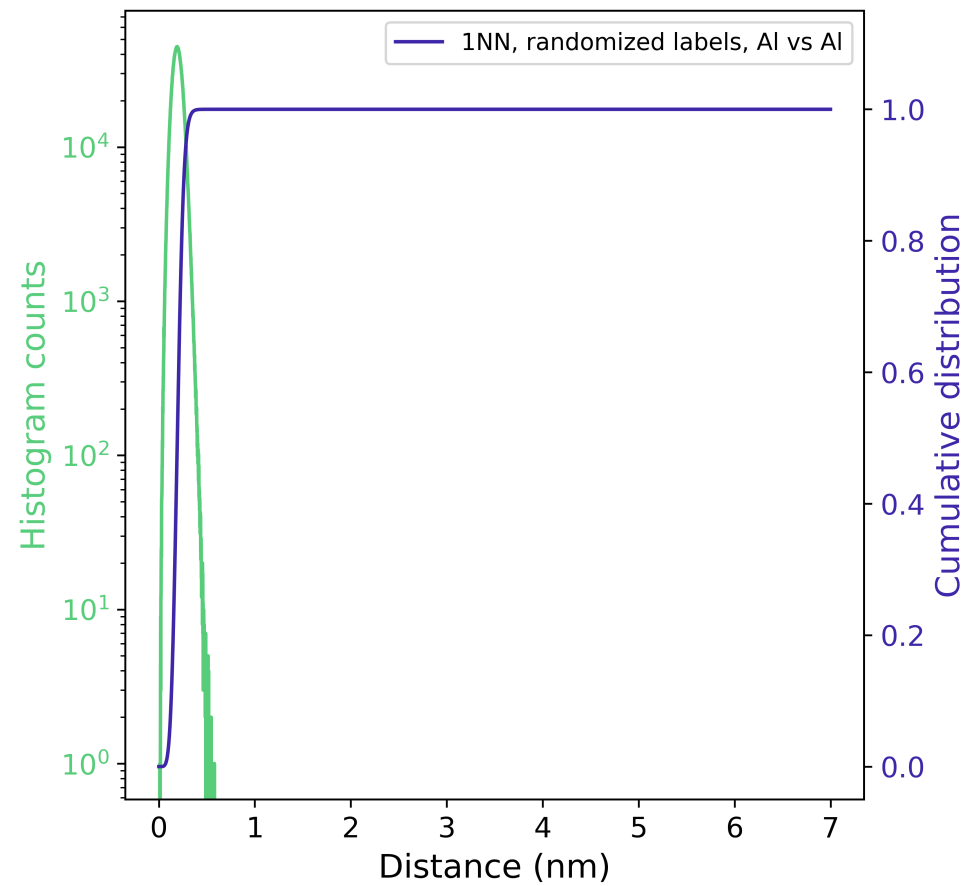
(a)

Figure 10: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?



(a)

Figure 11: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

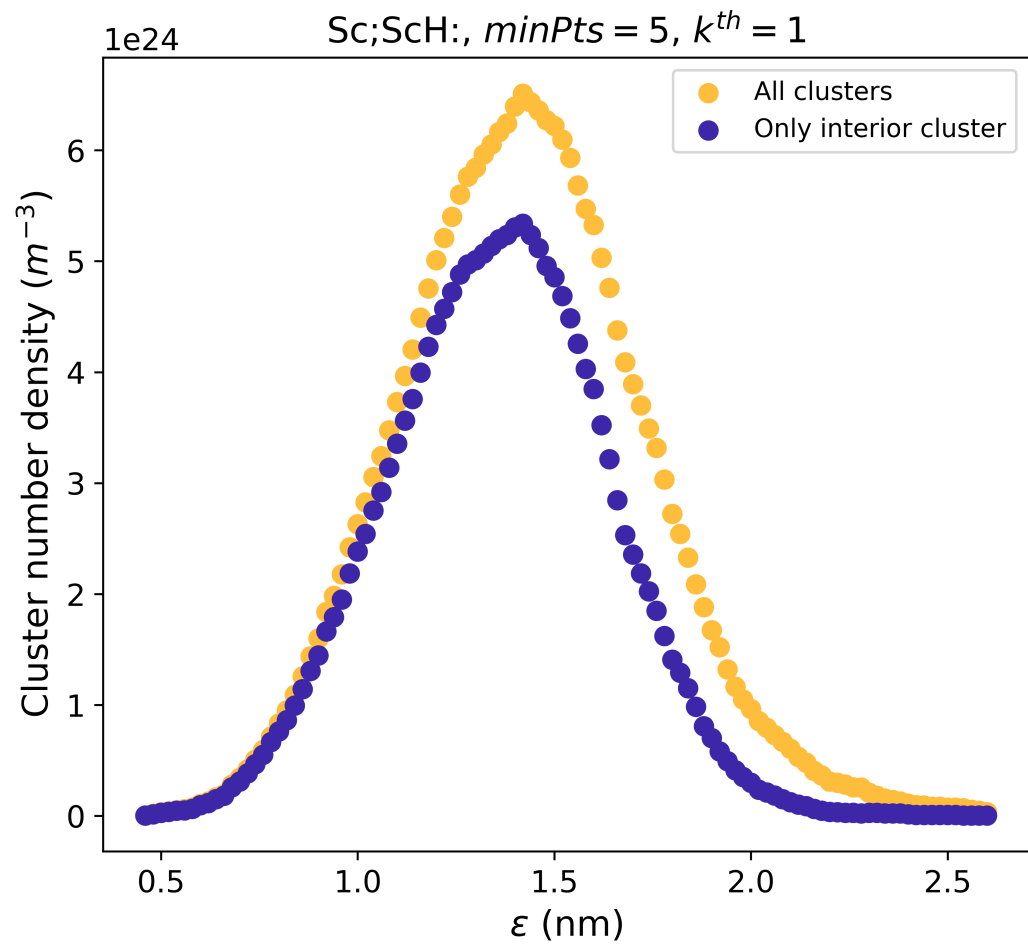


(a)

Figure 12: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

Table 6: Which XML settings were used for paraprobe-spatstat?

| Keyword | Value | Unit | Description |
|---------------------------|---|-------------|--------------------|
| AnalyzeKNN | 1 | | |
| AnalyzeRDF | 1 | | |
| AnalyzeRandomize | 1 | | |
| AnalyzeSDM | 0 | | |
| InputfileHullAndDistances | PARAPROBE.Surfacr.Results.SimID.2765202.h5 | | |
| InputfilePSE | PARAPROBE.PeriodicTableOfElements.xml | | |
| InputfileReconstruction | PARAPROBE.Transcoder.Results.SimID.2765202.h5 | | |
| IontypeCombi0 | Targets;Al;Neighbors;Al | | |
| IontypeCombi1 | Targets;Al;Neighbors;Sc,ScH: | | |
| IontypeCombi2 | Targets;Sc,ScH;;Neighbors;Al | | |
| IontypeCombi3 | Targets;Sc,ScH;;Neighbors;Sc,ScH: | | |
| KOrderForKNN | 1 | | |
| KOrderForSDM | | | |
| MaxSizeCachedResPerNode | 17179869184 | | |
| PRNGType | MT19937 | | |
| PRNGWarmup | 700000 | | |
| PRNGWorldSeed | 18446744073697205938 | | |
| ROIRadiiKNNIncr | 0.001 | nm | |
| ROIRadiiKNNMax | 7 | nm | |
| ROIRadiiKNNMin | 0 | nm | |
| ROIRadiiRDFIncr | 0.001 | nm | |
| ROIRadiiRDFMax | 7 | nm | |
| ROIRadiiRDFMin | 0 | nm | |
| ROIRadiiSDMIncr | 1 | nm | |
| ROIRadiiSDMMax | 0 | nm | |
| ROIRadiiSDMMin | 0 | nm | |
| ROIVolumeInsideOnly | 1 | | |



(a)

Figure 13: What are the number of clusters per unit volume, quantified using high-throughput studies of the DBScan/maximum separation clustering parameter?

Table 7: Which XML settings were used for paraprobe-dbscan?

| Keyword | Value | Unit | Description |
|------------------------------|---|------|-------------|
| ClusteringMethod | 2 | | |
| DBScanEpsilonIncr | 0.02 | nm | |
| DBScanEpsilonMax | 7 | nm | |
| DBScanEpsilonMin | 0.2 | nm | |
| DBScanMinPtsIncr | 1 | | |
| DBScanMinPtsMax | 1 | | |
| DBScanMinPtsMin | 1 | | |
| DatasetEdgeThresholdDistance | 1 | nm | |
| IOStoreClusterIDs | 0 | | |
| IOStoreClusters | 1 | | |
| InputfileHullAndDistances | PARAPROBE.Surfacer.Results.SimID.2765202.h5 | | |
| InputfilePSE | PARAPROBE.PeriodicTableOfElements.xml | | |
| InputfileReconstruction | PARAPROBE.Transcoder.Results.SimID.2765202.h5 | | |
| IontypeCombi0 | Targets;Sc,ScH: | | |
| MaxSepNumberOfIonsIncr | 10 | | |
| MaxSepNumberOfIonsMax | 5 | | |
| MaxSepNumberOfIonsMin | 5 | | |
| MaxSizeCachedResPerNode | 17179869184 | | |

Table 8: How many MPI processes times OpenMP threads respectively were used, and what was the elapsed time for each tool run?

| Toolname | #MPI | #OMP | $t_{elapsed}^{max}$ (s) |
|-------------|------|------|-------------------------|
| Transcoder | 1 | 1 | insignificant |
| Ranger | 1 | 1 | insignificant |
| Surfacer | 1 | 40 | 2233.0 |
| Tessellator | 1 | 40 | 14.0 |
| Spatstat | 1 | 40 | 850.0 |
| DBScan | 1 | 40 | 28.0 |