```
(* +---------------------------------- evaluate_pcf.nb ----------------------------+ *)
(* +                                                                                + *)
(* +           evaluate_pcf.nb calculates the pair correlation function for a       + *)
(* +           data set with xyz coordinates.                                       + *)
(* +                                                                                + *)
(* +                                                                                + *)
(* +           INPUT:  xyz coodinates of the cluster                                + *)
(* +           OUTPUT: graph with the pair correlation function                     + *)
(* +           USAGE:  (1) Delete All Output (from the 'Cell' menu)                 + *)
(* +                   (2) Fill the section between 'BEGIN USER INPUT' and          + *)
(* +                      'END USER INPUT'                                          + *)
(* +                   (3) Evaluate Notebook (from the'Evaluate' menu)              + *)
(* +           DEPENDENCIES: None                                                  + *)
(* +           NOTES:  Boundary effect are not take care of. The pair correlation   + *)
(* +                   function may therefore not converge to 1 for infinite        + *)
(* +                   distance. This is expected for finite size clusters and      + *)
(* +                   not a bug.                                                   + *)
(* +                                                                                + *)
(* +           AUTHOR:  L. Houben, Weizmann Institute of Science                    + *)
(* +                    lothar.houben(at)weizmann.ac.il                             + *)
(* +           COPYRIGHT: This software is licensed under the GNU GENERAL PUBLIC    + *)
(* +                    LICENSE Version 3                                         + *)
(* +                                                                                + *)
(* +--------------------------------------------------------------------------------+ *)
(* +-------------------------- BEGIN USER INPUT ------------------------------------+ *)
(* +--------------------------------------------------------------------------------+ *)
(* baseDir is the base folder for program input and output.                          *)
(* dataDir is a subfolder that holds the data file.                                 *)
(* outDir is a subfolder for the program output files.                               *)
(* Please make sure that the folders exist.                                         *)
baseDir = StringJoin[$HomeDirectory, "/Desktop/diOPA"];
dataDir = "data";
outDir = "out"
(* datafileName is name of the data file with the cluster xyz coordinates *)
datafileName = "Ferritin-agglomerate.cel";
(* +--------------------------------------------------------------------------------+ *)
(* +-------------------------- END USER INPUT --------------------------------------+ *)
(* +--------------------------------------------------------------------------------+ *)
```

```
out
```

```
(*  define input files                                                    *)
celfile = StringJoin[baseDir, "/", dataDir, "/", datafileName]
```

```
/Users/lothar/Desktop/diOPA/data/Ferritin-agglomerate.cel
```

```
(*  define output files                                          *)
graphfileprefix = StringJoin[baseDir, "/", outDir, "/", FileBaseName[datafileName], "_PCF"]
logfilename = StringJoin[baseDir, "/", outDir, "/", FileBaseName[datafileName], "_PCF.log"]
```

/Users/lothar/Desktop/diOPA/out/Ferritin-agglomerate_PCF

/Users/lothar/Desktop/diOPA/out/Ferritin-agglomerate_PCF.log

```
(* define plot parameters                                        *)
binwidth = 0.1;
range = {0, 5};
```

```
(* +-----------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
(*
          *)
(* END PARAMETER
 DEFINITION                                                                                                                     *)
(*
          *)
(* +-----------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
```

```
(* +-----------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
(*
          *)
(* START FUNCTION
 DEFINITION                                                                                                                     *)
(*
          *)
(* +-----------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
```

```
(* ReadCelFile: Function for Reading a celfile *)
(* courtesy of J. Barthel, RWTH-Aachen University, Germany *)
(* Email: ju.barthel-at-fz-juelich.de *)
(* Reads super cell structure data in CEL file format from *)
(* The specified file and stores the information in global arrays: *)
(*   celdims = dimensions of the super-cell  *)
(*   celangs = angles between the super-cell axes  *)
(*   natoms  = number of atoms in the super-cell *)
(*  *)
ReadCelFile[filename_] := Block[{celstrs},
  (* - init *)
  Clear[celdims, celangs, celatms, natoms];
  celdims = {0., 0., 0.}; celangs = {90., 90., 90.}; celatms = {}; natoms = 0;
  (* - read data from file *)
  celstrs = ReadList[filename, "String"];
  (* - analyse / extract numeric data *)
  celdims = Take[ReadList[StringToStream[celstrs[[2]]], "Number"], {2, 4}];
  celangs = Take[ReadList[StringToStream[celstrs[[2]]], "Number"], {5, 7}];
  celatms = Table[
    ReadList[StringToStream[celstrs[[i]]], Join[{"Word"}, Table["Number", {8}]]][[1]]
    , {i, 3, Length[celstrs] - 1}];
  natoms = Length[celatms];
  (* - report *)
  Print["- INPUT  CEL file: ", InputForm[filename]];
  Print["- OUTPUT (celdims) dimensions  (a,b,c)  [nm]: ", celdims];
  Print["- OUTPUT (celangs) axes angles (α,β,γ) [deg]: ", celangs];
  Print["- OUTPUT (natoms)  number of atoms          : ", natoms];
  If[natoms > 0,
   Print["- OUTPUT (celatms[[1]]) first atom          : ", celatms[[1]]];
  ];
  If[natoms > 1,
   Print["- OUTPUT (celatms[[", natoms, "]]) last  atom          : ", celatms[[natoms]]];
  ];
 ]
```

```
(* BoundingBox: Returns box coordinates around the centre *)
(* in a list variable cutoff *)
(* INPUT: xyz_= {{x1,y1,z1},{x2, y2, z2}, ...}  *)
(*        margin = margin size to add               *)
(*                                  *)
(* OUTPUT: bbox ={{xmin-margin,xmax+margin},{ymin-mrgin,ymax+margin}{zmin-margin,zmax+margin}}  *)
BoundingBox[xyz_, margin_] := Block[{tmp},
  (* - init *)
  Clear[bbox];
  bbox = {{0, 0}, {0, 0}, {0, 0}};
  bbox[[1, 1]] = Min[xyz[[All, 1]]] - margin;
  bbox[[2, 1]] = Min[xyz[[All, 2]]] - margin;
  bbox[[3, 1]] = Min[xyz[[All, 3]]] - margin;
  bbox[[1, 2]] = Max[xyz[[All, 1]]] + margin;
  bbox[[2, 2]] = Max[xyz[[All, 2]]] + margin;
  bbox[[3, 2]] = Max[xyz[[All, 3]]] + margin;
  bboxvol = (bbox[[1, 2]] - bbox[[1, 1]]) * (bbox[[2, 2]] - bbox[[2, 1]]) * (bbox[[3, 2]] - bbox[[3, 1]]);
  axespos = {bbox[[1, 1]], bbox[[2, 1]], bbox[[3, 1]]};
  Print["- BoundingBox         : ", bbox];
  Print["- BoundingBox Volume  : ", bboxvol];
  Print["- Axes Position       : ", axespos];
 ]

(* PCFMap *)
(* returns normalized pcf data in a list variable pcff *)
(* INPUT: xyz_= {{x1,y1,z1},{x2, y2, z2}, ...}  *)
(*        bwidth_= bin width                    *)
(* OUTPUT: pcf = list with pcf data             *)
PCFMap[xyz_, bwidth_, dens_] := Block[{distlist = {}, v, kk, jj},
  (* - init *)
  Clear[pcf];
  pcf = {};
  distlist = {};
  distlist = Outer[EuclideanDistance, xyz, Take[xyz, Floor[Length[xyz] / 2]], 1] // Flatten;
  v = BinCounts[distlist, {bwidth, Max[distlist], bwidth}];
  radius = Length[v] * bwidth;
  Print["- Minimum distance       : ", Min[distlist]];
  Print["- Maximum distance       : ", Max[distlist]];
  Print["- Bin width              : ", bwidth];
  Print["- NPairs                 : ", Length[distlist]];
  For[jj = 1, jj ≤ Length[v], {tmpr = (jj - 1) * bwidth; tmpR = tmpr + bwidth; norm = (4 * Pi * ((tmpR * tmpR * tmpR) - (tmpr * tmpr * tmpr)));
    AppendTo[pcf, {(jj + 0.5) * bwidth, v[[jj]] / norm / Length[xyz] / density}]}; jj++];
 ]
```

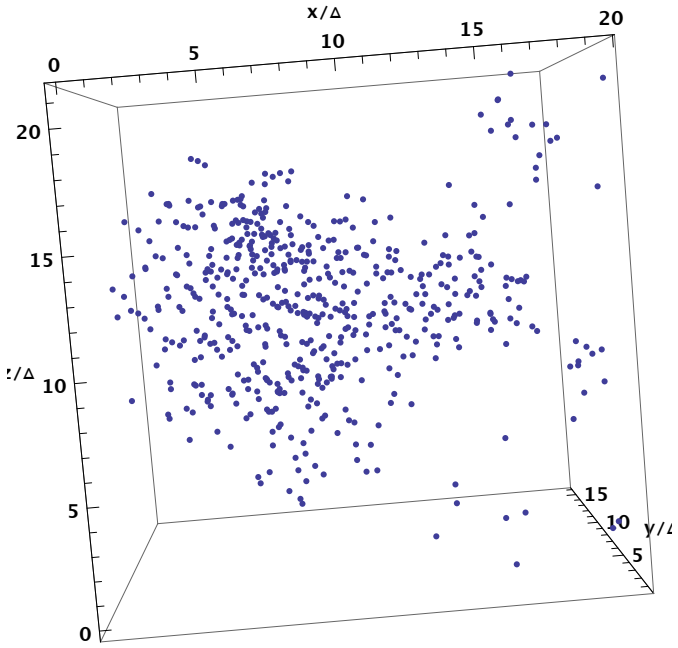
```
(* +------------------------------------------------------------------------------------------------------------------------
                                                  -----------+ *)
(*
          *)
(* END FUNCTION
 DEFINITION                                                                                                   *)
(*
          *)
(* +------------------------------------------------------------------------------------------------------------------------
                                                  -----------+ *)

(* +------------------------------------------------------------------------------------------------------------------------
                                                  -----------+ *)
(*
          *)
(* START
 PROCESSING                                                                                                   *)
(*
          *)
(* +------------------------------------------------------------------------------------------------------------------------
                                                  -----------+ *)

(* Open log file and start logging *)
logfile = OpenWrite[logfilename];
WriteString[logfile, "Filename:", celfile, "\n"];


(* Open data file and plot data *)
ReadCelFile[celfile];
Clear[coordatms, f, q];
(* Extract relative atomcoordinates only *)
coordatms = celatms[[All, {2, 3, 4}]];
(* multiply atom relative coordinates with cell dimensions *)
f[x_] := {celdims[[1]] * x[[1]], celdims[[2]] * x[[2]], celdims[[3]] * x[[3]]}
q = Map[f, coordatms];
(* Plot atoms *)
ListPointPlot3D[q, BoxRatios → {1, 1, 1}, PlotStyle → PointSize[0.01],
 AxesLabel → {"x/Δ", "y/Δ", "z/Δ"}, Lighting → "Neutral", LabelStyle → Directive[Bold]]
```

```
- INPUT  CEL file: "/Users/lothar/Desktop/diOPA/data/Ferritin-agglomerate.cel"
- OUTPUT (celdims) dimensions  (a,b,c)  [nm]: {19.6635, 16.056, 21.3574}
- OUTPUT (celangs) axes angles (α,β,γ) [deg]: {90., 90., 90.}
- OUTPUT (natoms)  number of atoms          : 559
- OUTPUT (celatms[[1]]) first atom          : {Fe, 0., 0.514721, 0.544393, 1., 0.005, 0.1, 0.1, 0.1}
- OUTPUT (celatms[[559]]) last  atom          : {Fe, 1., 0.21619, 0.073572, 1., 0.005, 0.1, 0.1, 0.1}
```




```
WriteString[logfile, "- Number of atoms: ", ToString[Length[q]], "\n"];

BoundingBox[q, 0]
density = Length[q] / bboxvol
```

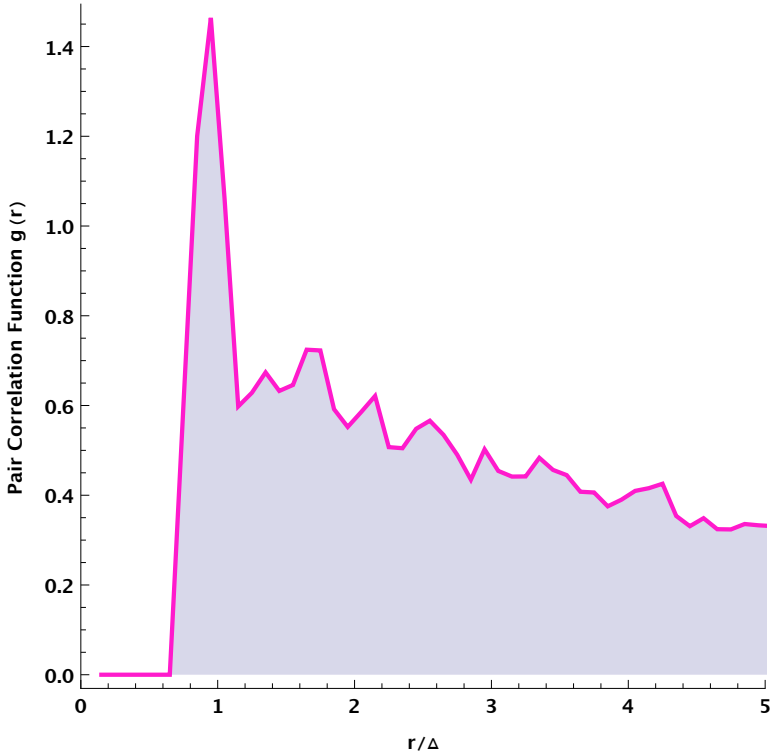
- BoundingBox : {{0., 19.6635}, {0.493642, 16.056}, {0., 21.3429}}
- BoundingBox Volume : 6531.16
- Axes Position : {0., 0.493642, 0.}

0.0855897

PCFMap[q, binwidth, density]

- Minimum distance : 0.
- Maximum distance : 25.0035
- Bin width : 0.1
- NPairs : 155 961

```
pcfplot = ListPlot[pcf, PlotRange → {{range[[1]], range[[2]]}, All}, PlotStyle → {Thick, RGBColor[1., 0.1, 0.8]},
  Filling → Axis, FillingStyle → Automatic, Joined → True, AxesLabel → {"r/Δ", "Pair Correlation Function g(r)"},
  LabelStyle → Directive[Bold], AspectRatio → 1, ImageSize → Medium, Axes → False, Frame → {{True, False}, {True, False}},
  FrameLabel → {{"Pair Correlation Function g(r)", None}, {"r/Δ", None}}, FrameTicks → All]
```



```
goutfile = StringJoin[graphfileprefix, ".png"];
Export[goutfile, pcfplot, "AllowRasterization" → True, ImageResolution → 600]
```

/Users/lothar/Desktop/diOPA/out/Ferritin-agglomerate_PCF.png

```
Close[logfile];
```

```
(* +------------------------------------------------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
(*
*)
(* END
PROCESSING *)
(*
*)
(* +------------------------------------------------------------------------------------------------------------------------------------------------------------------------
-----------+ *)
```