```
(* +---------------------------------- 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 = "Au-crystal.cel";
(* +---------------------------------------------------------------------------------+ *)
(* +-------------------------- END USER INPUT --------------------------------------+ *)
(* +---------------------------------------------------------------------------------+ *)
```

```
out
```

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

```
/Users/lothar/Desktop/diOPA/data/Au-crystal.cel
```

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

```
/Users/lothar/Desktop/diOPA/out/Au-crystal_PCF
```

```
/Users/lothar/Desktop/diOPA/out/Au-crystal_PCF.log
```

```
(* define plot parameters                                              *)
binwidth = 0.1;
range = {0, 8};
```

```
(* +-------------------------------------------------------------------------------------------------------------------------------------------------------------------+ *)
(*                                                                                                                                                                   *)
(* 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/Au-crystal.cel"

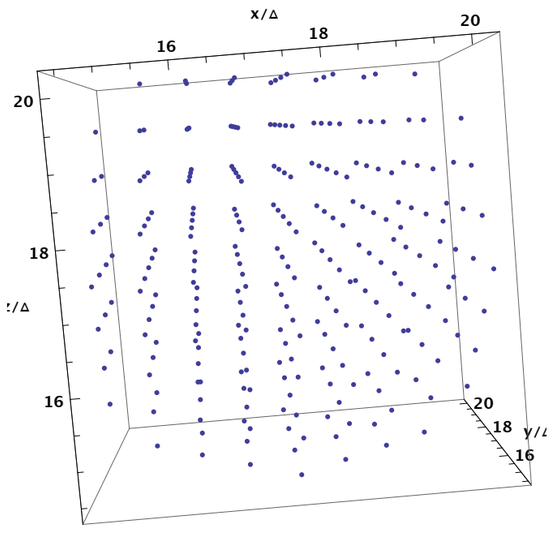
- OUTPUT (celdims) dimensions (a,b,c) [nm]: {34.655, 34.655, 34.655}

- OUTPUT (celangs) axes angles (α,β,γ) [deg]: {90., 90., 90.}

- OUTPUT (natoms) number of atoms : 260

- OUTPUT (celatms[[1]]) first atom : {Au, 0.4428, 0.495314, 0.584261, 1., 0.005, 0.1, 0.1, 0.1}

- OUTPUT (celatms[[260]]) last atom : {Au, 0.5572, 0.504686, 0.415739, 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 : {{14.4074, 20.2476}, {14.4051, 20.2499}, {14.4074, 20.2476}}

- BoundingBox Volume : 199.346

- Axes Position : {14.4074, 14.4051, 14.4074}

1.30426

```
PCFMap[q, binwidth, density]
```

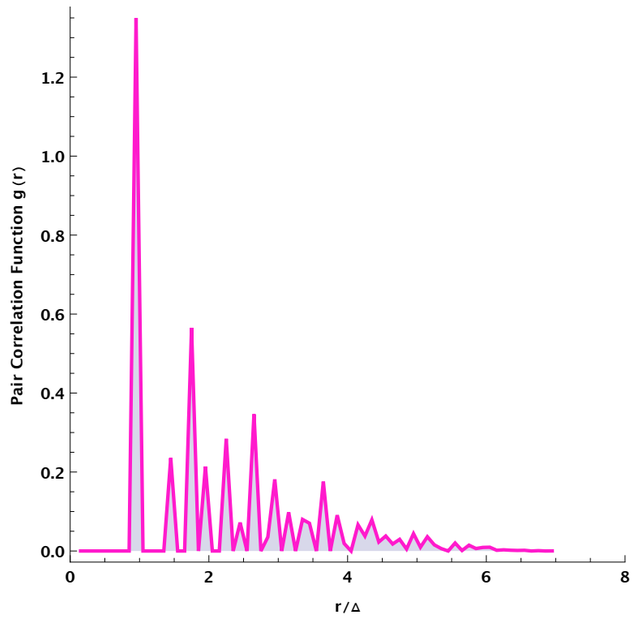
- Minimum distance : 0.

- Maximum distance : 7.06618

- Bin width : 0.1

- NPairs : 33 800

```
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/Au-crystal_PCF.png

```
Close[logfile];

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