In[1]:=
```
(* +---------------------------------- test_db -------------------------------------+ *)
(* +                                                                                 + *)
(* +           test_db is a consistency check to evaluate the database match, i.e.   + *)
(* +           the match of a given coordination with the database rotation variants + *)
(* +           test_db creates a temperature map for the match of a selected database     + *)
(* +           item against all database items.                                       + *)
(* +           The "lower" the temperature in the map the better the match.            + *)
(* +           It also creates a plot of the best matching database item against     + *)
(* +           the test item. Both should be identical.                               + *)
(* +                                                                                  + *)
(* +           INPUT:  Database file, created with create_db                          + *)
(* +                   Index of the test item                                         + *)
(* +           OUTPUT: Temperature map that shows the distance norm between the      + *)
(* +                   database coordination and the coordination of test item     + *)
(* +                   The output is displayed in the script file.                    + *)
(* +           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                                                    + *)
(* +                                                                                  + *)
(* +           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.                          *)
(* dbDir is a subfolder that holds the database file.                                 *)
(* Please make sure that the folders exist.                                         *)
baseDir = StringJoin[$HomeDirectory, "/Desktop/OrderParameterAnalysis"];
dbDir = "db";
(* dbfileName is name of the database file                  *)
dbfileName = "rotation-database_Fcc_50_1.db";
(* testitem is the index of the database to test against the database               *)
testitem = 1;
(* +-------------------------------------------------------------------------------  + *)
(* +-------------------------- END-- USER INPUT ------------------------------------+ *)
(* +-------------------------------------------------------------------------------- + *)
```

In[5]:=

```
(* Load the database file and the datafile *)
DBfile = StringJoin[baseDir, "/", dbDir, "/", dbfileName];
ModelDB =.;
ModelDB = Get[DBfile];
coordination = Length[ModelDB[[1, 3]]];
NDBItems = Length[ModelDB[[All, 1]]];
```

In[10]:=

```
(* QuickDistance is a module that calculates the distance norm between two coordination vectors *)
QuickDistance[model_, nlist_] := Block[{SortedEntry = {}, tmplist = model, selected = {}, x = {}},
   (* - init *)
  Clear[EuclDist];
  EuclDist = 0;
  (* - analyse / extract numeric data *)
  For[k = 1, k <= coordination, k++,
   x = Nearest[tmplist → Automatic, nlist[[k]], 1];
   selected = N[tmplist[[x[[1]]]]];
   AppendTo[SortedEntry, selected]; tmplist = Drop[tmplist, x]
  ];
  EuclDist = EuclideanDistance[nlist, SortedEntry];
 ]
```

In[11]:=
```
(* GetDistMeas calculates the distance norm to the closest model item in the DB *)
(* *)
(* Returns a global variable: Dist, type: list *)
(* Dist = {atomnr, DBindex,{angle,angle,distance}} *)
(* Example: *)
(* In:   GetDistMeas[41]; Dist *)
(* Out: {41,256,{π/5,π/10,0.468556698631839}} *)
GetDistMeas[atomindex_] := Block[{DistMap = {}},
  Clear[Dist];
  Dist = {};
  (* *)
  (* Create a distance map *)
  (* Here we need permutations because the list of nearest neighbours is not sorted *)
  (* Finding the minimum over all possible permutations is the right way to go, yet very slow *)
  (* therefore we sort the list of data base model atoms *)
  (* for each atom in the neighbour list we search for the closest in the model *)
  (* note that this gives the minimum euclidian distance is achieced only if model and neighbour list are close *)
  (* there might be a solution with a better compromise if the match is not close *)
  neighbours = q[atomindex]
    For[ind = 1, ind ≤ Length[ModelDB], ind++, QuickDistance[ModelDB[[ind, 3]], neighbours]; AppendTo[
      DistMap, {ModelDB[[ind, 2, 1]], ModelDB[[ind, 2, 2]], EuclDist}]];
  WhereMin = Ordering[DistMap[[All, 3]], 1];
  Dist = {atomindex, WhereMin[[1]], DistMap[[WhereMin]][[1]]};
 ]
```

In[12]:=
```
(* Pick the DB element testitem for mapping *)

q = ModelDB[[testitem, 3]];
ListPointPlot3D[q, BoxRatios → {1, 1, 1}, PlotStyle → PointSize[0.1],
  PlotStyle → Directive[Purple, Specularity[White, 50]], PlotRange → {{-1.1, 1.1}, {-1.1, 1.1}, {-1.1, 1.1}}];
```

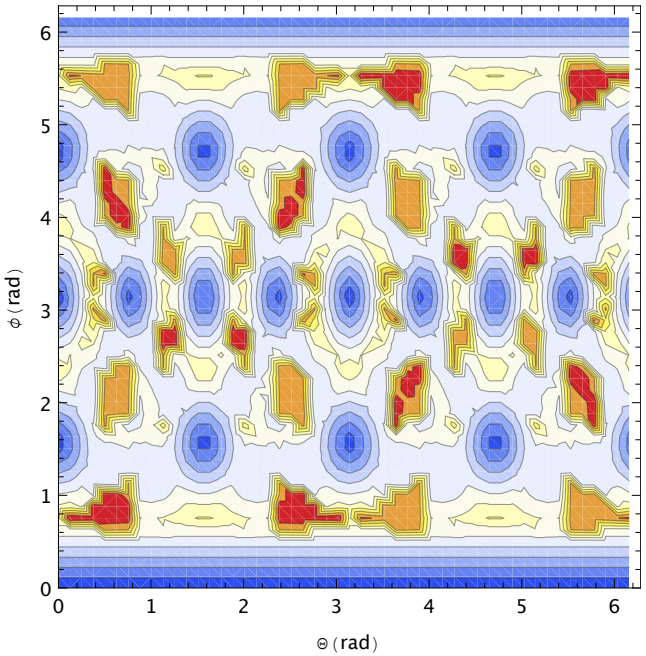
In[14]:=
```
DistMap = {};
For[ind = 1, ind ≤ Length[ModelDB], ind++, QuickDistance[ModelDB[[ind, 3]], q]; AppendTo[
   DistMap, {ModelDB[[ind, 2, 1]], ModelDB[[ind, 2, 2]], EuclDist}]];
```

In[16]:=
```
ColorData["Gradients"]
```

Out[16]=
```
{AlpineColors, Aquamarine, ArmyColors, AtlanticColors, AuroraColors, AvocadoColors, BeachColors, BlueGreenYellow,
 BrassTones, BrightBands, BrownCyanTones, CandyColors, CherryTones, CMYKColors, CoffeeTones, DarkBands, DarkRainbow,
 DarkTerrain, DeepSeaColors, FallColors, FruitPunchColors, FuchsiaTones, GrayTones, GrayYellowTones, GreenBrownTerrain,
 GreenPinkTones, IslandColors, LakeColors, LightTemperatureMap, LightTerrain, MintColors, NeonColors, Pastel, PearlColors,
 PigeonTones, PlumColors, Rainbow, RedBlueTones, RedGreenSplit, RoseColors, RustTones, SandyTerrain, SiennaTones, SolarColors,
 SouthwestColors, StarryNightColors, SunsetColors, TemperatureMap, ThermometerColors, ValentineTones, WatermelonColors}
```

In[17]:=
```
(* Plot distance map vs angular coordinates in a temperature scale *)
xStart = 0;
xEnd = 2 Pi;
yStart = 0;
yEnd = 2 * Pi;
ListContourPlot[DistMap, ColorFunction → ColorData["Temperature"], InterpolationOrder → 3, Contours → 10,
 ColorFunctionScaling → Automatic, PlotRange → {{xStart, xEnd}, {yStart, yEnd}, All}, FrameLabel → {"Θ(rad)", "ϕ(rad)"}]
Print["- INPUT  Database file: ", InputForm[DBfile]];
Print["- Coordination: ", coordination];
Print["- Number of Database items: ", NDBItems];
Print["- Number of Test item: ", testitem];
```

Out[21]=




```
- INPUT  Database file: "/Users/lothar/Desktop/OrderParameterAnalysis/db/rotation-database_Fcc_50_1.db"

- Coordination: 12

- Number of Database items: 2500

- Number of Test item: 1
```

In[26]:=
```
(* Plot of the best matching database item coordination (grey) against the testitem (red) *)
(* Both coordinations should coincide precisely *)
WhereMin = Ordering[DistMap[[All, 3]], 1];
DistMap[[WhereMin]];
plmodel = ListPointPlot3D[{ModelDB[[WhereMin[[1]], 3]]}, BoxRatios → {2, 2, 2}, PlotRange → {{-2, 2}, {-2, 2}, {-2, 2}},
   AxesLabel → {"X", "Y", "Z"}, PlotStyle → Directive[Gray, PointSize[0.1], Opacity[0.5], ViewPoint → {0, 0, Infinity}]];
testmodel = ListPointPlot3D[{q}, BoxRatios → {2, 2, 2},
   PlotStyle → Directive[Red, PointSize[0.05], Opacity[0.5], ViewPoint → {0, 0, Infinity}]];
Show[plmodel, testmodel]
```

Out[30]=