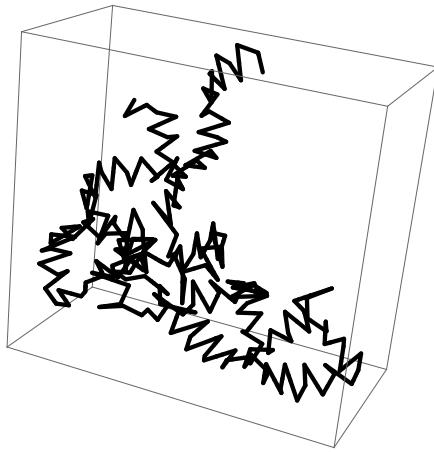


```

pdb = Import[NotebookDirectory[] <> "temp.xyz", "Table"];
(*import the molecule PDB*)
Graphics3D[{Thickness[0.01], Line[pdb]}]

```

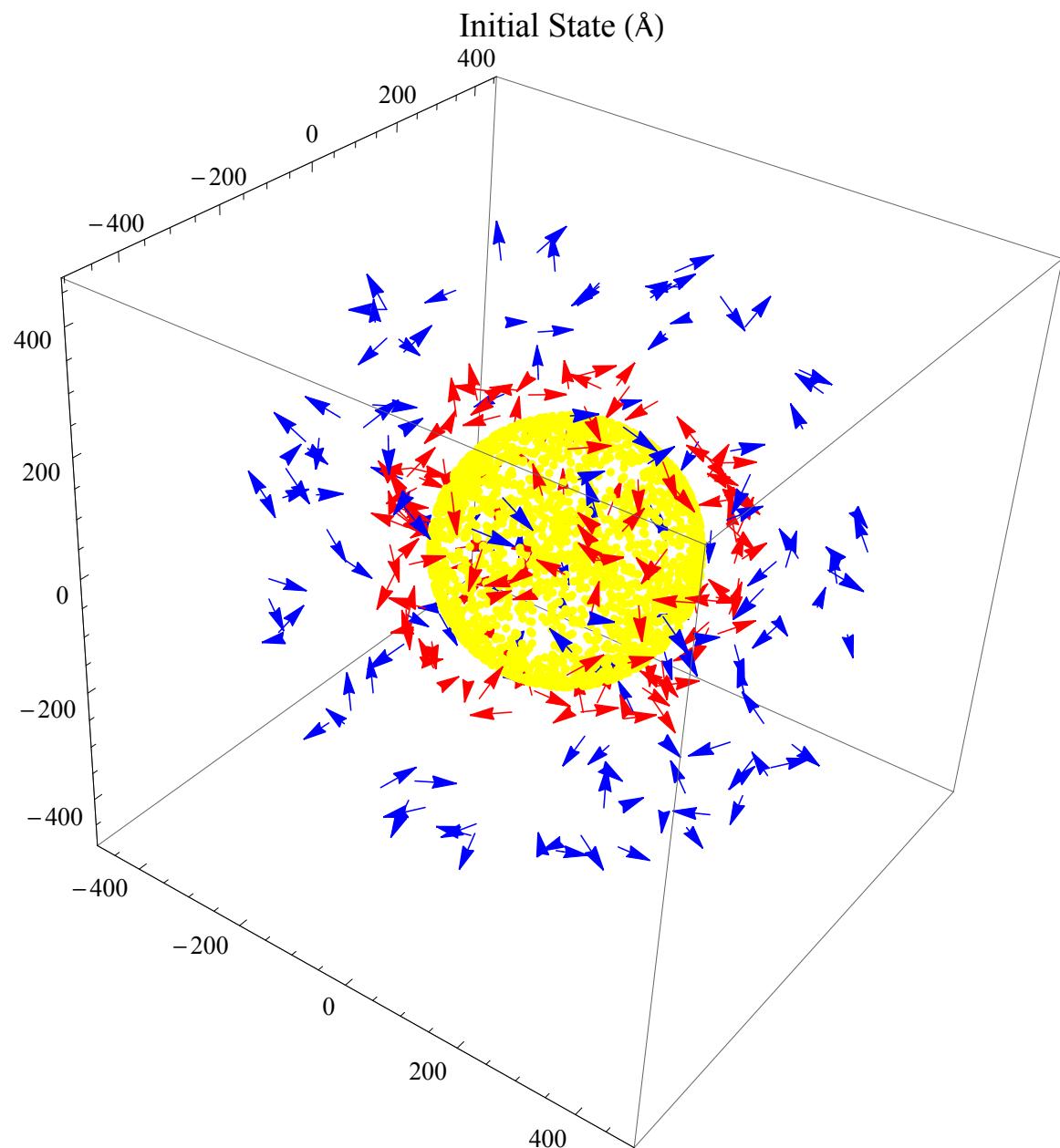


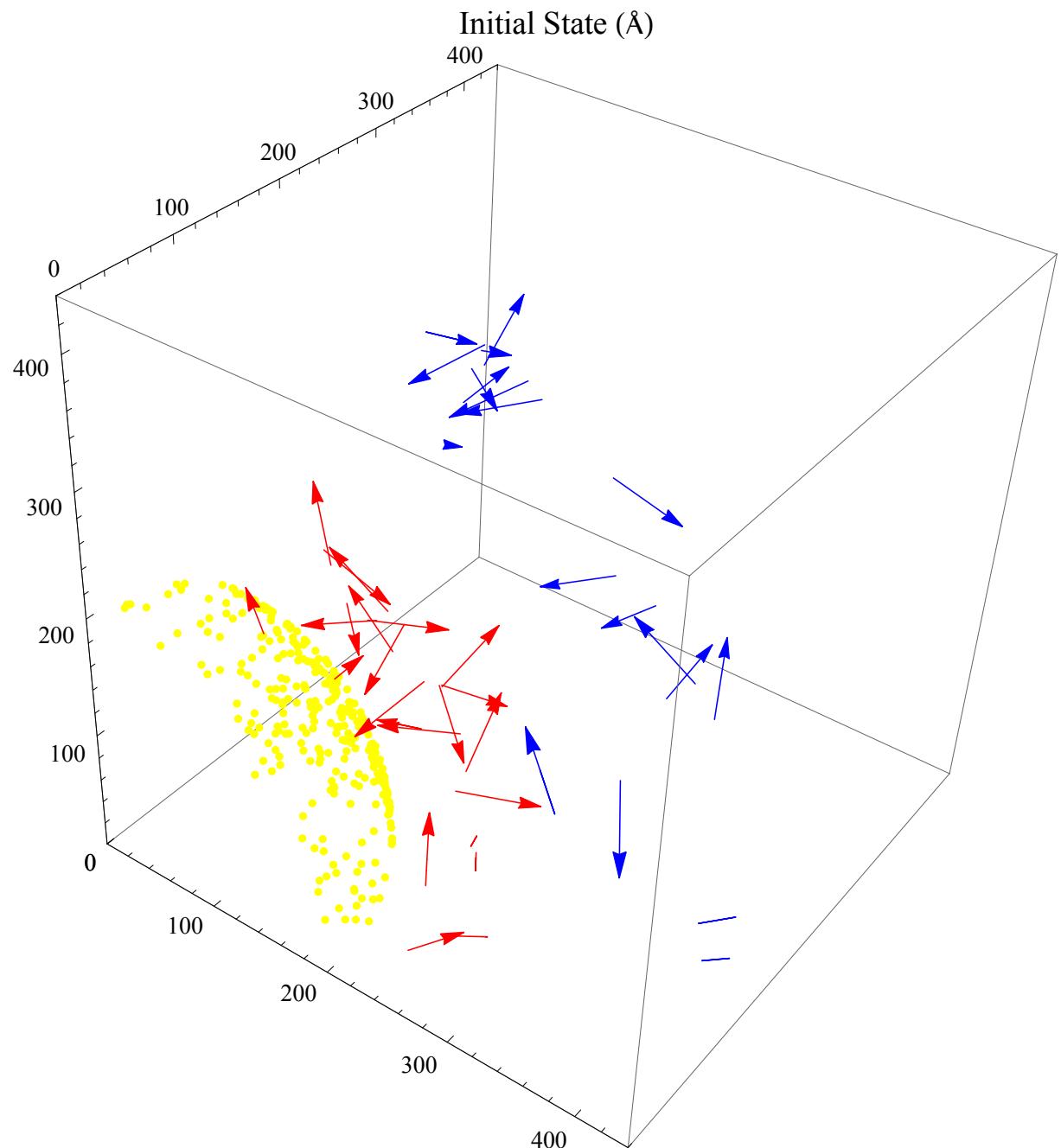
```

AuR = 1.46; (*gold atom radius*)
NpR = 200; (*nano particle radius*)
MoL = 60; (*molecule's longest length*)
BoxL = 4 MoL; (*simulation box size*)
NpSurf = 4 π NpR2; (*nano particle surface area*)
Print["Nanoparticle surface bead number: ", AuN = Round[NpSurf / AuR2 / 100]]
(*gold atom number*)
Print["molecule number: ", MoN = Round[NpSurf / MoL2]] (*molecule chain number*)
Print["molecule bead number: ", MoN * 221] (*total bead number in molecules*)
positive = {{0, NpR + 4 MoL}, {0, NpR + 4 MoL}, {0, NpR + 4 MoL}};
(*the range for positive (x,y,z)*)
c = RandomReal[{-1, 1}, 3]
coord[seed_] := c / EuclideanDistance[c, {0, 0, 0}];
(*generate random (x,y,z) coordinates on sphere*)
model[NpR_, AuN_, MoL_, r1_, MoN1_, r2_, MoN2_, region_] := (
  points[r_, n_, c_] := ListPointPlot3D[Table[r coord[0], {i, n}], PlotStyle -> c];
  (*generate nano particle*)
  vectors[r_, l_, n_, c_] :=
    Graphics3D[Table[c0 = coord[1]; c1 = coord[2];
      {c, Arrowheads[{0.02}], Arrow[{r c0, r c0 + l c1}]}, {i, n}]];
  (*generate random oriented arrows*)
  Magnify@Show[vectors[r2, MoL, MoN2, Blue], vectors[r1, MoL, MoN1, Red],
    points[NpR, AuN, Yellow], BoxRatios -> Automatic, Axes -> True,
    PlotLabel -> "Initial State (Å)", PlotRange -> region]
  (*function to show conformation*)
)
model[NpR, AuN, MoL, NpR + MoL, MoN, NpR + 4 MoL, MoN, All] (*all*)
model[NpR, AuN, MoL, NpR + MoL, MoN, NpR + 4 MoL, MoN, positive]
(*only the positive coordinates*)

```

Nanoparticle surface bead number: 2358
molecule number: 140
molecule bead number: 30 940





```

divide[dθ_] := (*Divide the sphere surface
  "uniformly" in term of "solid angle" with points*)
ANGcoords = Append[Prepend[Flatten[Table[
  Table[{ϕ, θ}, {ϕ, 0, 2 π - 2 π/Round@2 π Sin[θ]/dθ, 2 π/Round@2 π Sin[θ]/dθ}], {θ, dθ, Pi - dθ, dθ}], 1], {0, 0}], {0, π}];

(*a combination of (ϕ,θ) to divide the sphere. they will be
 replaced with actual simulation boxes*)
Print["Box Needed: ", BoxN = Length[ANGcoords] / 2];
(*only need to show the front face*)
XYZcoords = Table[θ = a[[2]]; ϕ = a[[1]];
  (*derive the (x,y,z) coordinates from (r,ϕ,θ)*)
  NpR {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {a, ANGcoords}];
Magnify@Column[{ListPlot[ANGcoords, AspectRatio → Automatic, Frame → True,
  FrameLabel → {"ϕ", "θ"}, PlotLabel → "(ϕ, θ) coordinates", ImageSize → 300],
  ListPointPlot3D[Table[XYZcoords[[i]], {i, Length[XYZcoords]}],
  ColorFunction → "Rainbow", BoxRatios → Automatic, AxesLabel → {"x", "y", "z"},
  PlotLabel → "Division Points on Sphere", ImageSize → 300]}]]]

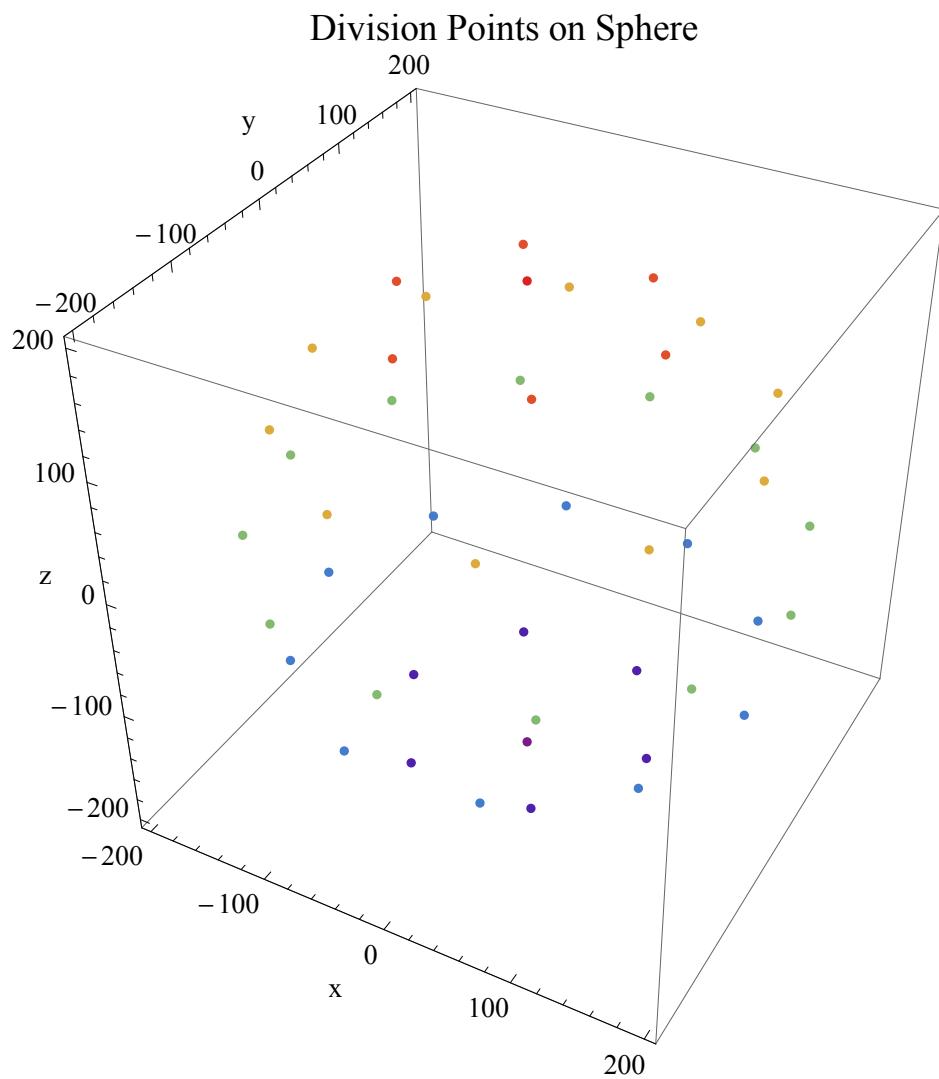
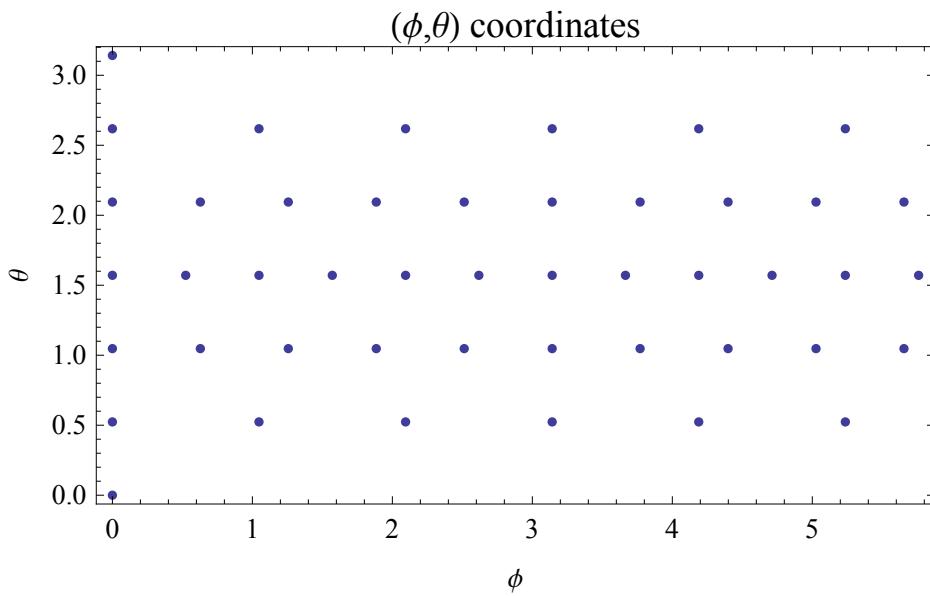
divide[π/6]
cuboid[BoxL_] :=
  Flatten[Table[BoxL {x, y, z}, {x, -1/2, 1/2}, {y, -1/2, 1/2}, {z, 0, 1}], 2];
(*a cubic box with box length*)

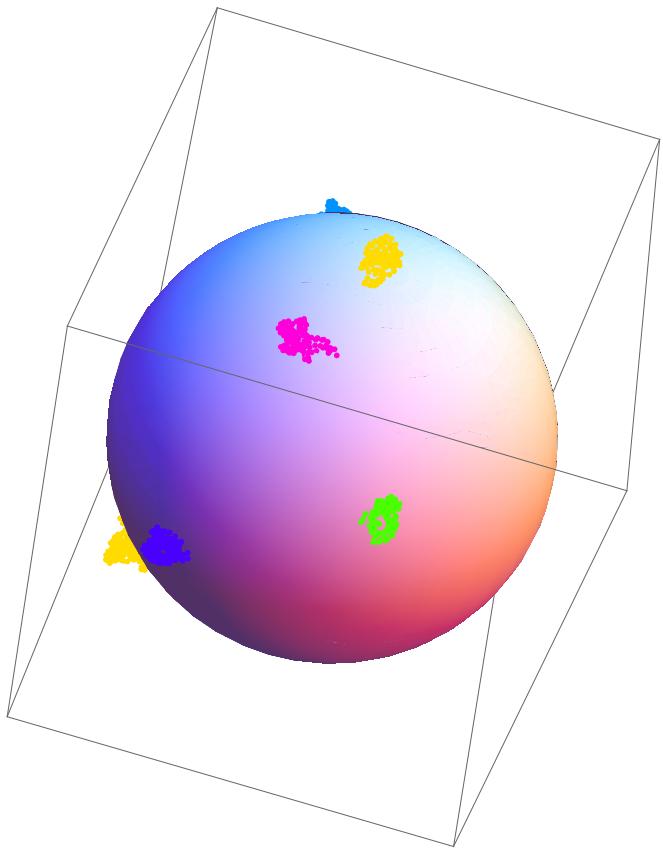
RawCoord = cuboid[MoL / 2]; (*use the cuboid as raw coordinates*)
RawCoord = pdb; (*or use pdb*)
kx = {1, 0, 0}; (*unit vector for XYZ axis*)
ky = {0, 1, 0};
kz = {0, 0, 1};
rm[axis_, α_] := RotationMatrix[α, axis]
(*the rotation matrix for rotating α angle around axis*)
transform[r_, φ_, θ_, RawCoord_] :=
  Table[rm[kz, φ].rm[ky, θ].RawCoord[[i]] + r, {i, Length[RawCoord]}];
(*for all raw coordinates, rotate θ around Y,
then rotate φ around Z. then move along ī*)
randomTrans[r_, RawCoord_] :=
  transform[r, RandomReal[{0, 2 π}], RandomReal[{0, π}], RawCoord];
(*randomly rotate then move*)

Show[Graphics3D[Sphere[{0, 0, 0}, NpR]], Table[ListPointPlot3D[transform @@
  Append[Prepend[ANGcoords[[i]], XYZcoords[[i]]], randomTrans[0, RawCoord]],
  PlotStyle → {Hue[Mod[i, 7] / 7], PointSize[0.02]}], {i, 1, Length[ANGcoords]},
  5 (*skip every 5 molecules. for performance purpose*)}],
  PlotRange → All, BoxRatios → Automatic]

```

Box Needed: 23





$$\frac{\int_0^{2\pi} \int_0^{\theta_{\text{max}}} r^2 \sin[\theta] d\theta d\phi}{\int_0^{2\pi} \int_0^\pi r^2 \sin[\theta] d\theta d\phi} \quad (*\text{derive the ratio of } \frac{\text{number on section}}{\text{number on sphere}}*)$$

$$\frac{1}{2} (1 - \cos[\theta_{\text{max}}])$$

```

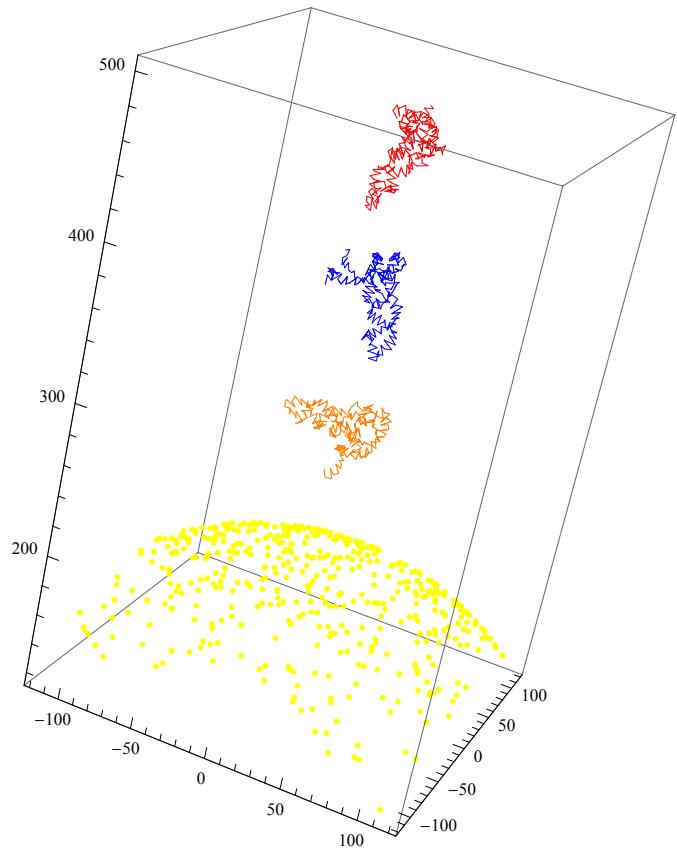
newcoords[r_, n_, l_] := 
$$\left( \begin{array}{l} (*\text{generate random points} \\ \\ \text{on part of the nano particle surface with the same density*}) \\ \\ \theta\text{Range} = \text{ArcSin}\left[\frac{1}{\sqrt{2}} / r\right] \\ \text{Print}\left["\theta \text{ Range:}", N@\frac{\theta\text{Range}}{\pi} * 180\right]; \\ \\ (*\text{the } \theta \text{ angle when the four bottom vertex of box are on sphere*}) \\ \text{PartN} = \text{Round}\left[n \frac{2 \pi r^2 (1 - \text{Cos}[\theta\text{Range}])}{4 \pi r^2}\right]; \\ \\ (*\text{the points needed to fill the partial sphere (round)*}) \\ \{u, v\} = \text{RandomReal}[\{0, 1\}, \{2, \text{PartN}\}]; \\ \\ (*\text{an algorithm to generate random coordinates based on spherical angles*}) \\ \{\phi, \theta\} = \left\{2 \pi u, \text{ArcCos}[2 v - 1] \frac{\theta\text{Range}}{\pi}\right\}; \\ \\ \{x, y, z\} = \{r \text{Sin}[\theta] \text{Cos}[\phi], r \text{Sin}[\theta] \text{Sin}[\phi], r \text{Cos}[\theta]\}; \\ \\ (*\text{derive (x,y,z) coordinates*}) \\ \text{clip} = \text{Transpose}\left[\left\{\text{Clip}\left[x, \frac{1}{2} \{-1, 1\}, \{"out", "out"\}\right], \right.\right. \\ \left.\left. \text{clip}\left[y, \left\{\frac{-1}{2}, \frac{1}{2}\right\}, \{"out", "out"\}\right], z\right\}\right]; \\ \\ \text{squareCoords} = \text{DeleteCases}[\text{Table}[\text{If}[\text{! MemberQ}[\text{clip}[[c]], "out"], \text{clip}[[c]]], \\ \{c, \text{Length}[\text{clip}]\}], \text{Null}]; \\ \\ (*\text{discard the points out of the square from the round partial sphere*}) \\ \text{Print}["Partial surface bead number: ", \text{Length}[\text{squareCoords}]]; \\ \\ (*\text{number of nano particle beads on the partial sphere(square) *}*) \\ \text{squareCoords}
\right)$$

Show[ListPointPlot3D[newcoords[NpR, AuN, BoxL], PlotStyle -> {Yellow, Large}],
Graphics3D[{{Red, Line[randomTrans[{0, 0, NpR + 4.5 MoL}, pdb]]},
{Blue, Line[randomTrans[{0, 0, NpR + 3 MoL}, pdb]]},
{Orange, Line[randomTrans[{0, 0, NpR + 1.5 MoL}, pdb]]}}],
BoxRatios -> Automatic, PlotRange -> All]

```

θ Range:58.0519

Partial surface bead number: 466



$$N @ \frac{\frac{1}{NpR} - \frac{1}{NpR+MoL}}{\frac{1}{NpR}} (*\text{error for potential approximation*})$$

$$N @ \frac{\frac{1}{NpR^2} - \frac{1}{(NpR+MoL)^2}}{\frac{1}{NpR^2}} (*\text{error for force approximation*})$$

0.230769

0.408284