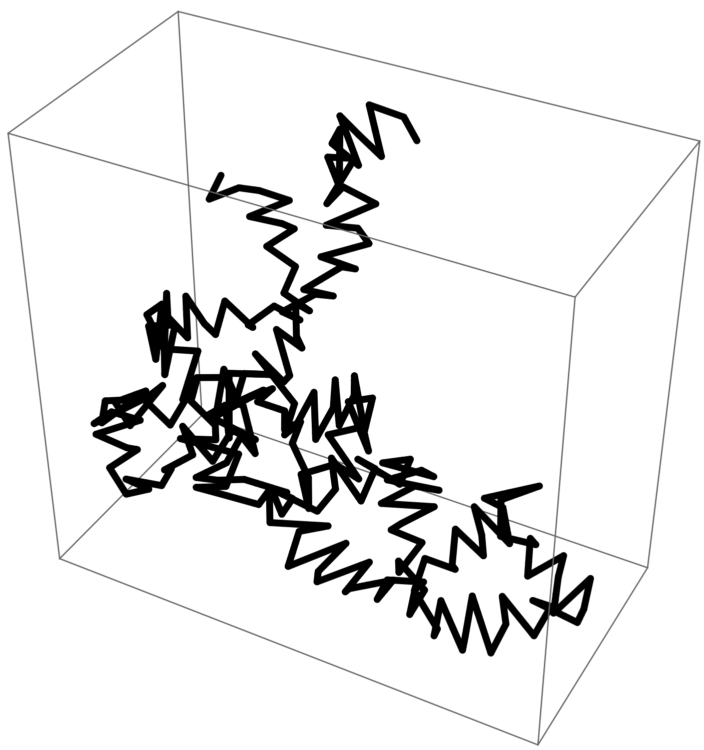
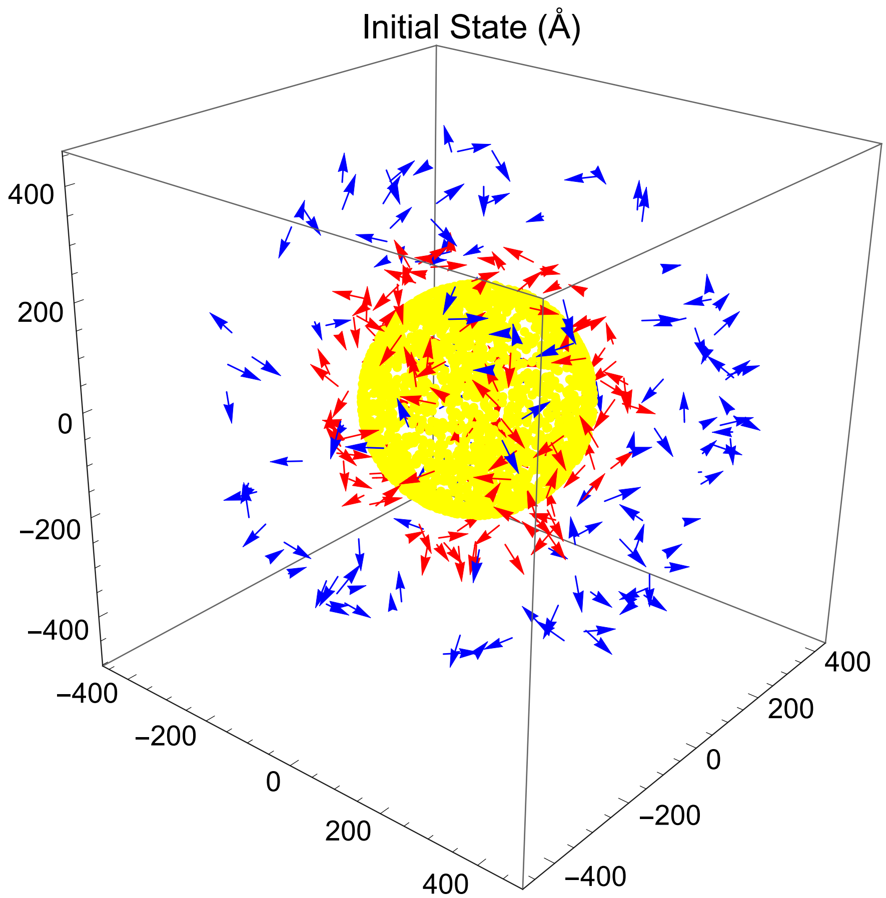
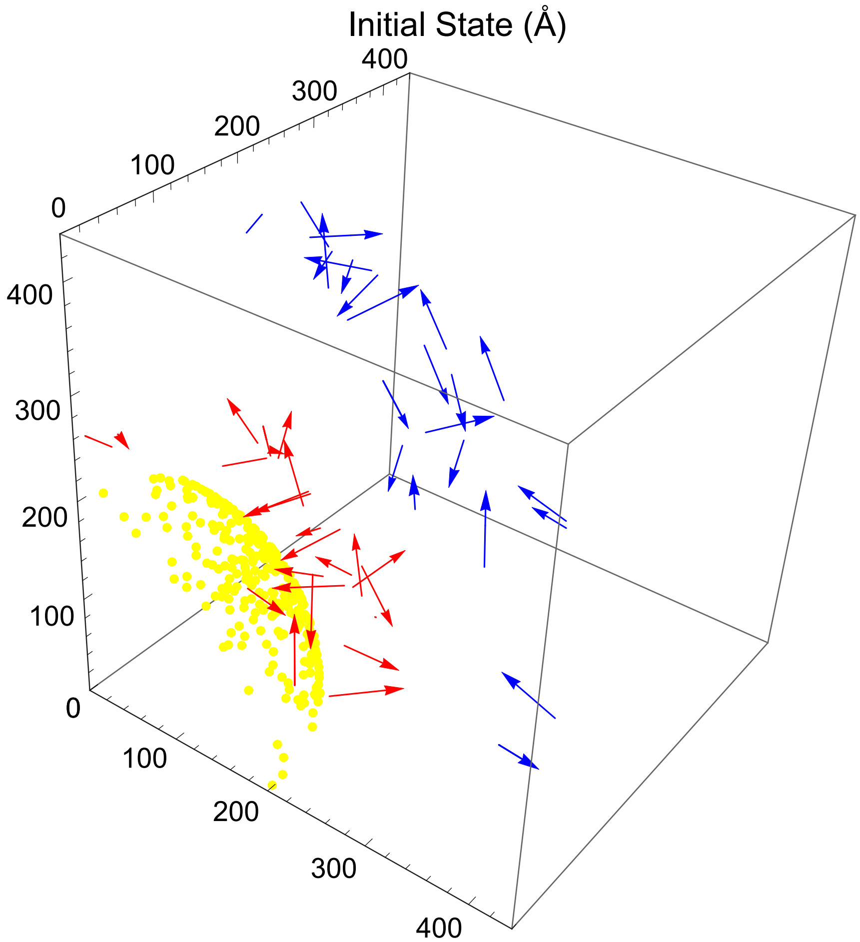
```
pdb = Import[NotebookDirectory[] <> "fmet_coords.xyz", "Table"];
(*import the molecule PDB*)
Graphics3D[{Thickness[0.01], Line[pdb]}]
```



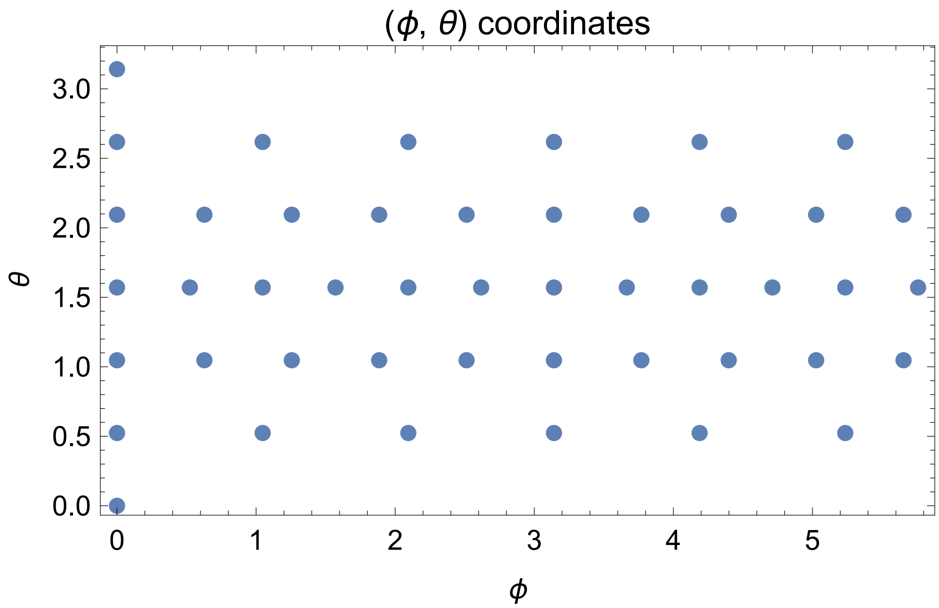
```
AuR = 1.46; (*gold atom radius*)
NpR = 200; (*nano particle radius*)
MoL = 60; (*molecule's longest length*)
BoxL = 4 MoL; (*simulation box size*)
NpSurf = 4 π NpR^2; (*nano particle suface area*)
Print["Nanoparticle surface bead number: ", AuN = Round[NpSurf / AuR^2 / 100]]
(*gold atom number*)
Print["molecule number: ", MoN = Round[NpSurf / MoL^2]] (*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)*)
coord[seed_] := (c = RandomReal[{-1, 1}, 3]) / 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
```

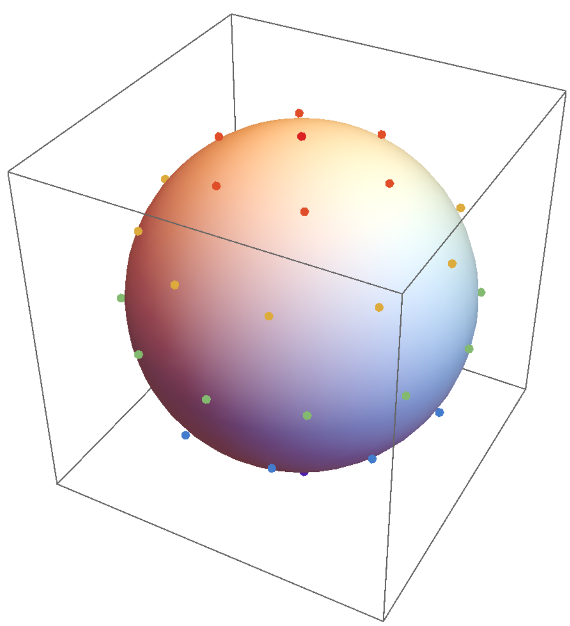

Initial State (Å)
400
200
0
−200
−400
−400
−200
0
200
400
400
200
0
−200
−400


Initial State (Å)
0
100
200
300
400
400
300
200
100
0
100
200
300
400

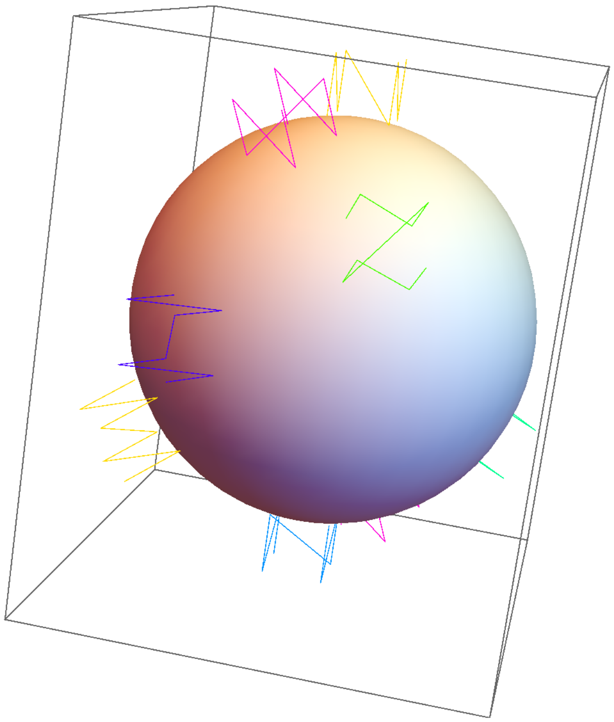
```
In[110]:= divide[dθ_] := ((*Divide the sphere surface
    "uniformly" in term of "solid angle" with points*)
   ANGcoords = Append[Prepend[Flatten[Table[
        Table[{ϕ, θ}, {ϕ, 0, 2 π - 2 π/ Round@(2 π Sin[θ]/dθ), 2 π/ Round@(2 π Sin[θ]/dθ)}],
        {θ, dθ, Pi - dθ, dθ}], 1], {0, 0}], {0, π}];
   (*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],
      Show[Graphics3D[Sphere[{0, 0, 0}, NpR - 5]],
       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 r⃗*)
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[Graphics3D[{Hue[Mod[i, 7] / 7], PointSize[0.02],
    Line[transform @@ Append[Prepend[ANGcoords[[i]], XYZcoords[[i]]],
       (*randomTrans[0,RawCoord]*)2 RawCoord]]}], {i, 1, Length[ANGcoords],
   5(*skip every 5 molecules. for performance purpose*)}],
 PlotRange → All, BoxRatios → Automatic]

Box Needed: 23
```



Out[111]=

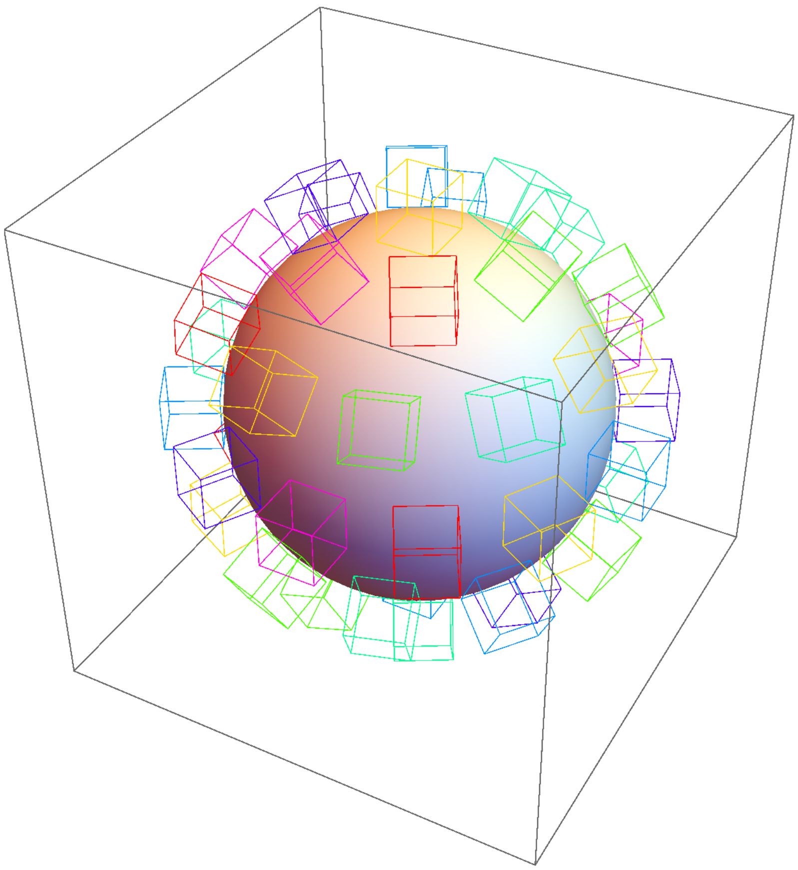


Out[117]=



In[118]:=
```
cube = DeleteCases[
   Flatten[Table[If[EuclideanDistance[RawCoord[[i]], RawCoord[[j]]] == 30,
      {RawCoord[[i]], RawCoord[[j]]}, {}], {i, 8}, {j, 8}], 1], {}];
Show[Graphics3D[Sphere[{0, 0, 0}, NpR]], Table[
  Graphics3D[Table[{Hue[Mod[i, 7] / 7], PointSize[0.02],
     Line[transform @@ Append[Prepend[ANGcoords[[i]], XYZcoords[[i]]],
        (*randomTrans[0,RawCoord]*) 2 cube[[l]]]]}, {l, Length[cube]}]], {i, 1,
   Length[ANGcoords], 1 (*skip every 5 molecules. for performance purpose*)}],
 PlotRange → All, BoxRatios → Automatic]
```

Out[119]=



$$\frac{\int_0^{2\pi}\int_0^{theta} r^2\,\mathrm{Sin}[theta]\,\mathrm{d}theta\,\mathrm{d}phi}{\int_0^{2\pi}\int_0^{\pi} r^2\,\mathrm{Sin}[theta]\,\mathrm{d}theta\,\mathrm{d}phi}\ \text{(*derive the ratio of } \frac{\text{number on secion}}{\text{number on sphere}} \text{*)}$$

$$\frac{1}{2}\,(1 - \mathrm{Cos}[theta])$$

```
newcoords[r_, n_, l_] := ((*generate random points
   on part of the nano particle surface with the same density*)
```

$$\mathrm{Print}\left[\text{"}\theta\text{ Range:"}, N@\frac{\theta Range = \mathrm{ArcSin}\left[\frac{1}{\sqrt{2}} \Big/ r\right]}{\pi} * 180\right];$$

```
  (*the θ angle when the four bottom vertex of box are on sphere*)
```

```
PartN = Round[n (2 π r^2 (1 - Cos[θRange]))/(4 π r^2)];
(*the points needed to fill the partial sphere (round)*)
{u, v} = RandomReal[{0, 1}, {2, PartN}];
(*an algorithm to generate random coordinates based on spherical angles*)
{ϕ, θ} = {2 π u, ArcCos[2 v - 1] θRange/π};
{x, y, z} = {r Sin[θ] Cos[ϕ], r Sin[θ] Sin[ϕ], r Cos[θ]};
(*derive (x,y,z) coordinates*)
clip = Transpose[
   {Clip[x, 1/2 {-1, 1}, {"out", "out"}], Clip[y, {-1/2, 1/2}, {"out", "out"}], z}];
squareCoords = DeleteCases[Table[If[! MemberQ[clip[[c]], "out"], clip[[c]]],
    {c, Length[clip]}], Null];
(*discard the points out of the square from the round partial sphere*)
Print["Partial surface bead number: ", Length[squareCoords]];
(*number of nano particle beads on the partial sphere(square) *)
squareCoords

)

Magnify@Show[
  ListPointPlot3D[newcoords[NpR, AuN, BoxL], PlotStyle → {Darker@Yellow, Large}],
  Graphics3D[{{{Red, Line[randomTrans[{MoL, -(√3/3) MoL, NpR + 4.5 MoL}, pdb]]},
    {Red, Line[randomTrans[{-MoL, -(√3/3) MoL, NpR + 4.5 MoL}, pdb]]},
    {Red, Line[randomTrans[{0, (2 √3)/3 MoL, NpR + 4.5 MoL}, pdb]]},
    {Blue, Line[randomTrans[{MoL, (-√3)/3 MoL, NpR + 3 MoL}, pdb]]},
    {Blue, Line[randomTrans[{-MoL, (-√3)/3 MoL, NpR + 3 MoL}, pdb]]},
    {Blue, Line[randomTrans[{0, (2 √3)/3 MoL, NpR + 3 MoL}, pdb]]},
    {Orange, Line[randomTrans[{MoL, (-√3)/3 MoL, NpR + 1.5 MoL}, pdb]]},
    {Orange, Line[randomTrans[{-MoL, (-√3)/3 MoL, NpR + 1.5 MoL}, pdb]]},
    {Orange, Line[randomTrans[{0, (2 √3)/3 MoL, NpR + 1.5 MoL}, pdb]]}}},
```

```
θ Range:58.0519
Partial surface bead number: 444
```

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

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

```
0.230769
0.408284
```