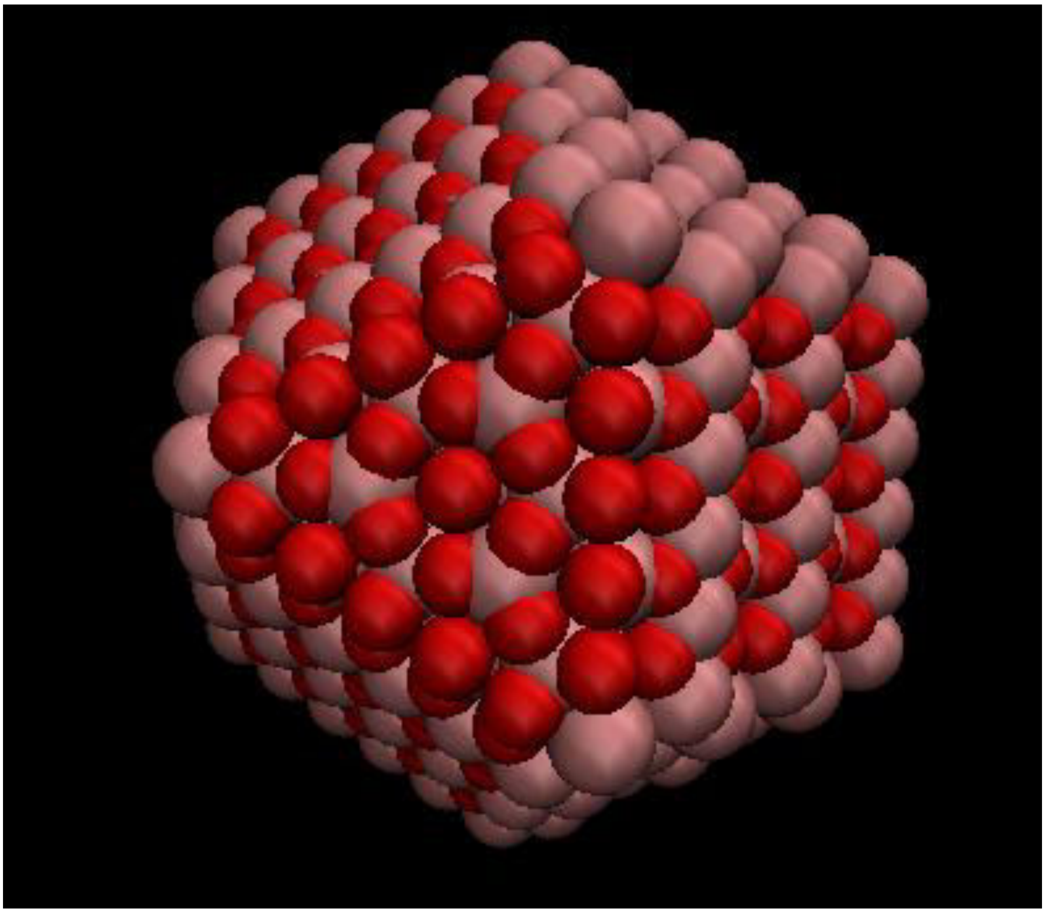
NANO-Crystal : A Web Server for the creation of Nanoparticles for modeling and simulation



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http://83.212.102.179/NanoCrystal/Nano_Spherical/

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1 Introduction

Nanoparticles (NPs) as drug delivery systems have shown significant promise in cancer treatment, where they are used to improve the biodistribution of cancer drugs. Thus, nanoparticles need to be designed with optimal size and surface characteristics in order to decrease side effects and drug toxicity while maximizing treatment impact. Computational approaches assist researchers in this design by modeling nanoparticles to systematize how MNP attributes affect their interaction with cell components as well as with their drug loading. A limiting factor in such modeling studies by the wider scientific community is the absence of a tool that constructs the morphology of nanoparticles. NANO-Crystal is a web-based tool, which constructs spherical nanoparticles of a given radius defined by the user. Apart from the creation of the spherical nanoparticles, we have already developed code that constructs crystal nanoparticles, which is going to be released as an update in NANO-Crystal within 2017. This computational toolbox computes the macroscopic morphology of any periodic crystal by forming different shapes based on Miller indices and is able to make a link between macroscopic morphology and atomistic structure for a periodic crystal, which is a valuable tool for scientists.

2 Theoretical Background

2.1 Methodology

Mathematically, a sphere is defined as the set of points in three-dimensional space that are all at the same distance r from a given point.
First of all, the volume of the nanoparticle and the smaller sphere is computed. In three dimensions, the volume inside a sphere is derived to be:

$$V = \frac{4}{3}\pi r^3$$

According to the Kepler conjecture (Hales T, 2005), which is a mathematical conjecture about sphere packing in three-dimensional Euclidean space, no arrangement of equally sized spheres with a greater average density than that of the face-centered cubic and hexagonal close packing can be formed. The density of these arrangements is around 74.05%, and that percentage is used in our study for the validation of the number of smaller spheres packed at the surface of the bigger nanosphere computed with our implementation.

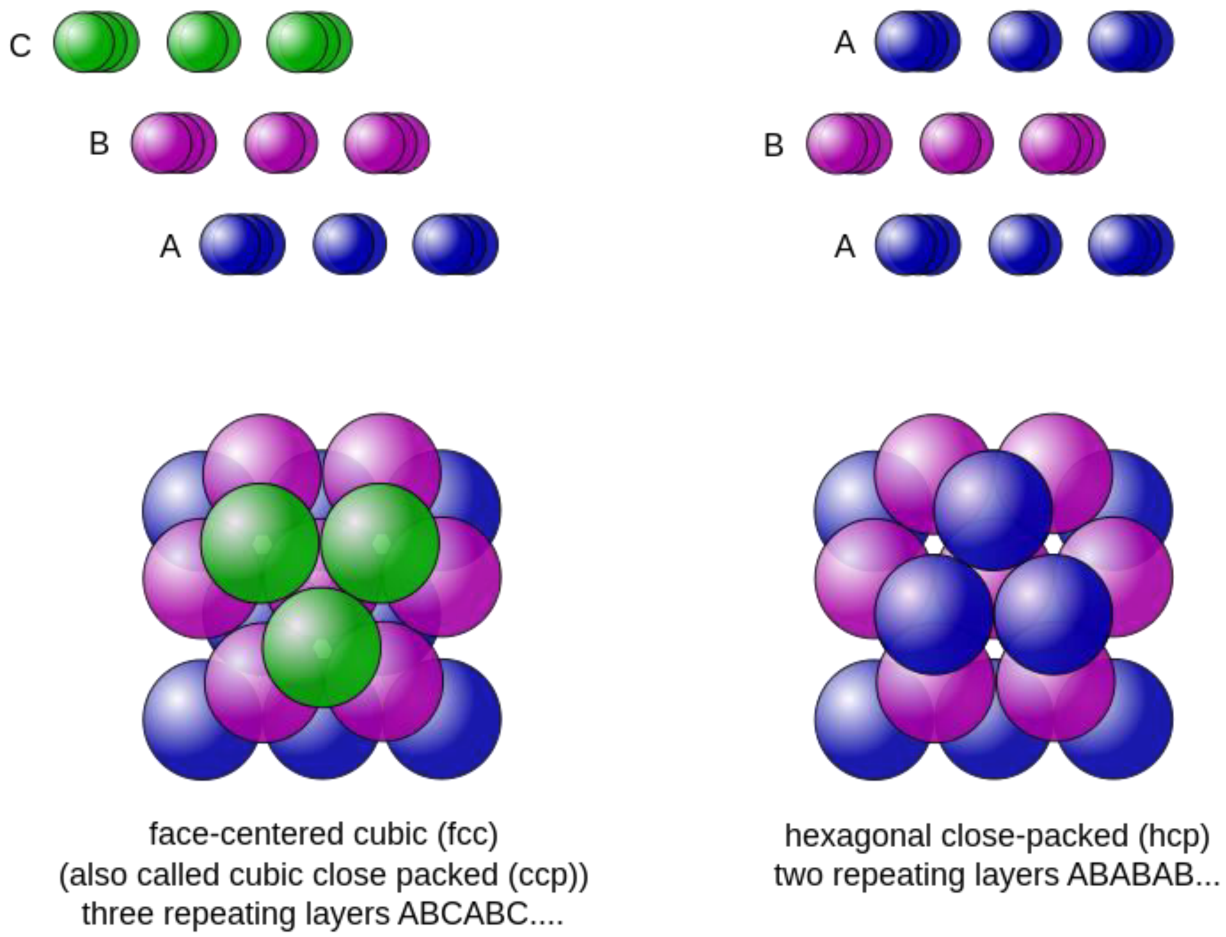

C
B
A
A
B
A
face-centered cubic (fcc)
(also called cubic close packed (ccp))
three repeating layers ABCABC....
hexagonal close-packed (hcp)
two repeating layers ABABAB...

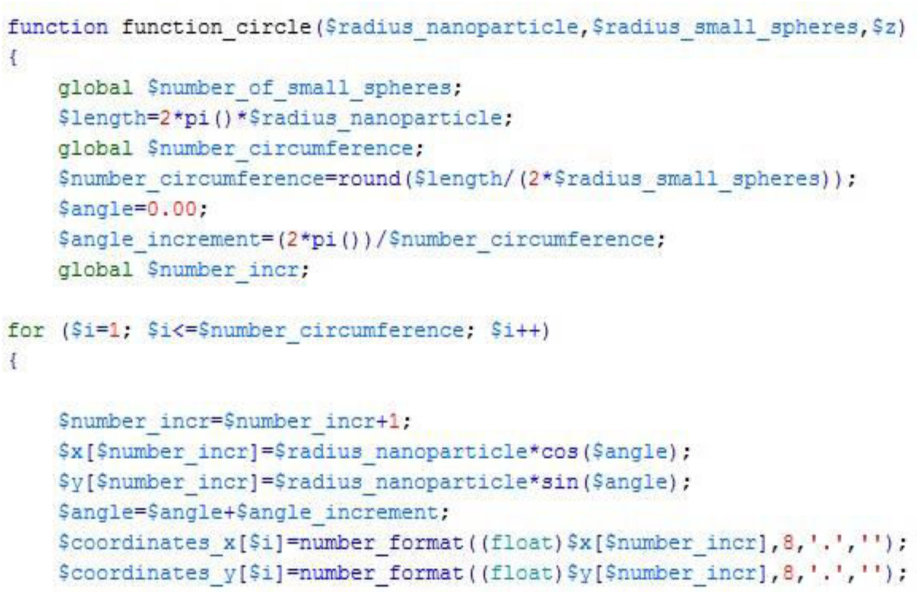
Figure 1: Representation of face-centered cubic packing (left) and hexagonal close packing (right).

The spheres are considered to be of identical size and non-overlapping. This arrangement in the three-dimensional Euclidean space is called packing. Our consideration is to find an arrangement in which the spheres fill as large a proportion of the space as possible. That proportion is the density of the arrangement. For equal spheres in three dimensions the densest packing uses approximately 74% of the volume. A random packing of equal spheres generally has a density around 64%.

2.2 Used Functions

Function circle

That function computes the Cartesian coordinates of the spheres that fit at the circumference of the bigger sphere.



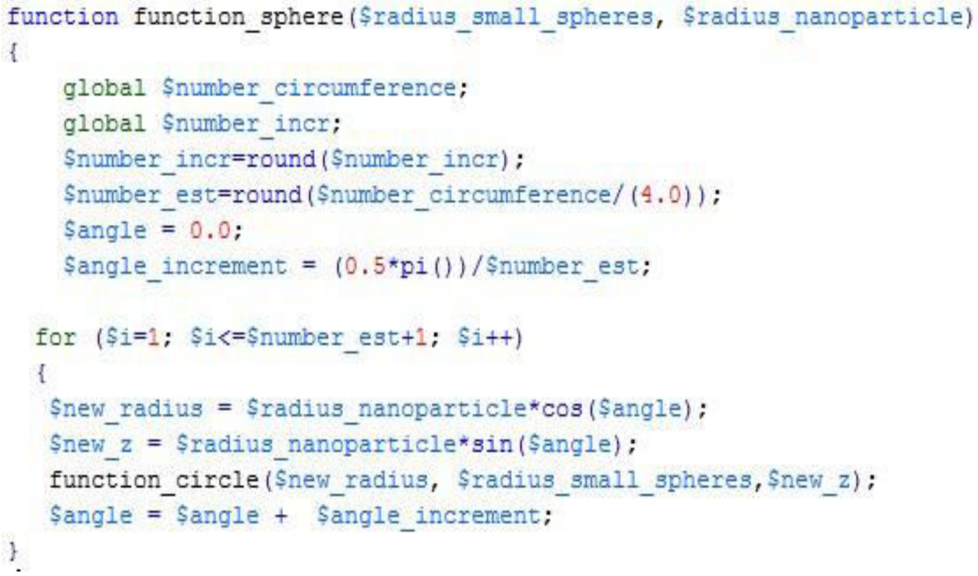
```
function function_circle($radius_nanoparticle,$radius_small_spheres,$z)
{
    global $number_of_small_spheres;
    $length=2*pi()*$radius_nanoparticle;
    global $number_circumference;
    $number_circumference=round($length/(2*$radius_small_spheres));
    $angle=0.00;
    $angle_increment=(2*pi())/$number_circumference;
    global $number_incr;

for ($i=1; $i<=$number_circumference; $i++)
{

    $number_incr=$number_incr+1;
    $x[$number_incr]=$radius_nanoparticle*cos($angle);
    $y[$number_incr]=$radius_nanoparticle*sin($angle);
    $angle=$angle+$angle_increment;
    $coordinates_x[$i]=number_format((float)$x[$number_incr],8,'.','');
    $coordinates_y[$i]=number_format((float)$y[$number_incr],8,'.','');
```

Figure 2: Function circle of 'Spherical Coordinates Tool'.

Given the radius of the nanoparticle, the circle circumference is computed (= pi* diameter = 2*pi*radius). Dividing the above with the smaller spheres diameter, the number of spheres that fit at the sphere circumference is computed. An angle increment is then defined, allowing to the non-overlapping smaller spheres to be placed at the circumference of the nanoparticle. Polar coordinates are computed and converted to Cartesian coordinates (Equations in Figure 4(i)).

Function sphere

That function computes the Cartesian coordinates of the spheres that fit on the surface of the bigger sphere.



```
function function_sphere($radius_small_spheres, $radius_nanoparticle)
{
    global $number_circumference;
    global $number_incr;
    $number_incr=round($number_incr);
    $number_est=round($number_circumference/(4.0));
    $angle = 0.0;
    $angle_increment = (0.5*pi())/$number_est;

  for ($i=1; $i<=$number_est+1; $i++)
  {
   $new_radius = $radius_nanoparticle*cos($angle);
   $new_z = $radius_nanoparticle*sin($angle);
   function_circle($new_radius, $radius_small_spheres,$new_z);
   $angle = $angle +  $angle_increment;
}
```

Figure 3: Function sphere of 'Spherical Coordinates tool'.

Similarly, an angle increment is defined in each spherical quadrant and the function circle is called with parameters such that the Spherical coordinates can be computed (Figure 4(ii)) and converted again to Cartesian coordinates.

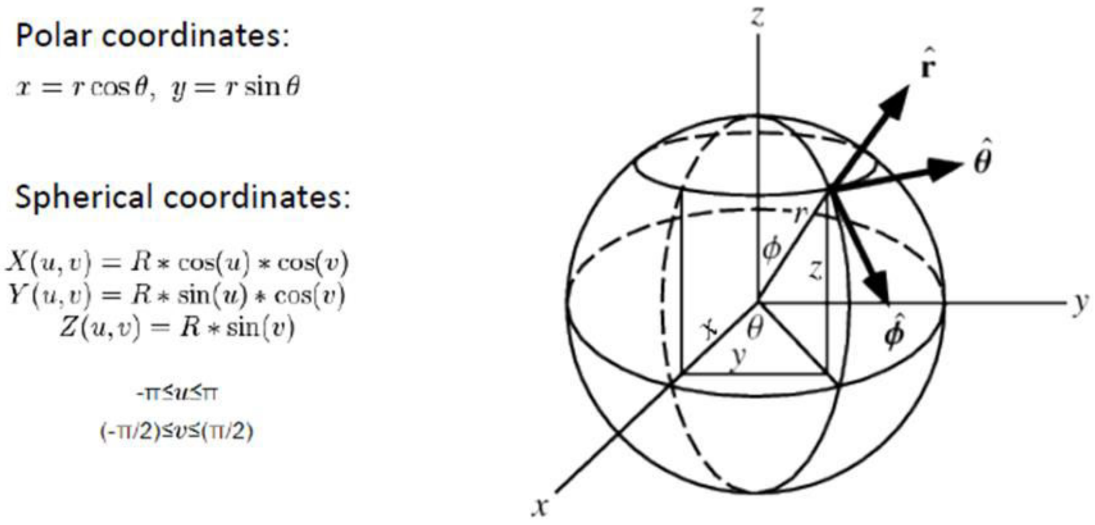


Figure 4: Equations of i) Polar coordinates and ii) Spherical coordinates.

3 Description of the Program

3.1 Construction of spherical nanoparticles (Spherical Coordinates tool)

The "Spherical Coordinates tool", which is a web-based tool, is implemented for the construction of spherical nanoparticles of a given radius. More specifically, our goal is to find the number and the Cartesian coordinates of smaller spheres that fit on the surface of the nanoparticle and visualize the output morphology.

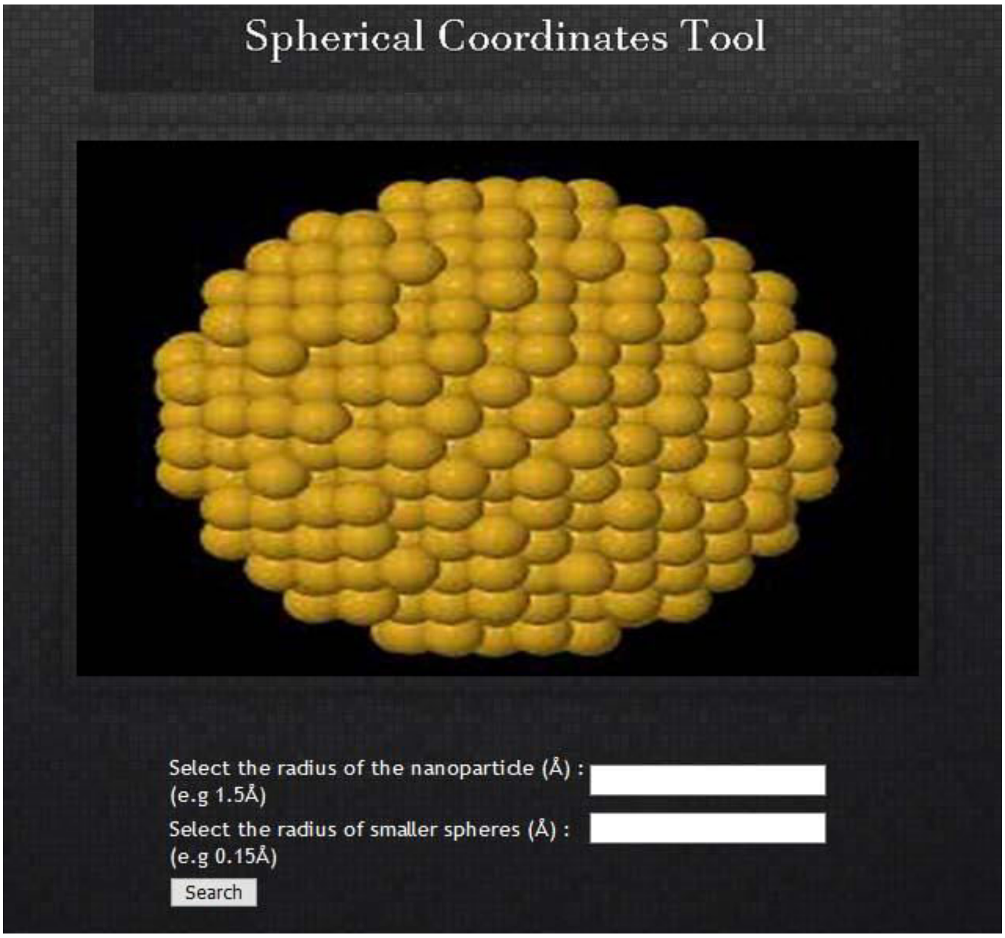

Spherical Coordinates Tool
Select the radius of the nanoparticle (Å) :
(e.g 1.5Å)
Select the radius of smaller spheres (Å) :
(e.g 0.15Å)
Search

Figure 5: Home page of 'Spherical Coordinates Tool'.

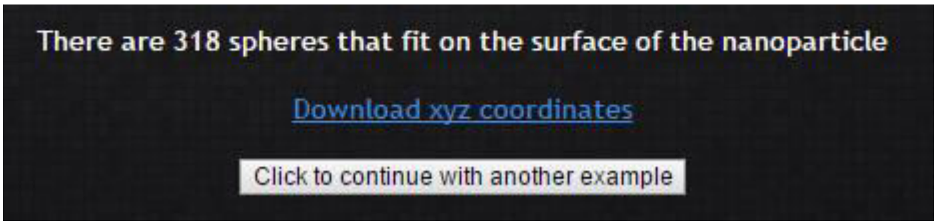
3.2 Program Use

The home page menu (Figure 5), allows two selections for the user:

i) the radius of the nanosphere (Å), and

ii) the radius of smaller spheres (Å), that will cover the surface of the nanoparticle.

The program computes the number of smaller spheres that fit on the bigger surface and the user can download their Cartesian coordinates (output format .xyz).



There are 318 spheres that fit on the surface of the nanoparticle

Figure 6: Home page output for 1.5 Å and 0.15 Å radius of the nanoparticle and the smaller spheres.

3.3 Technologies used

The program code is implemented using PHP server-side scripting language, which is embedded into the HTML and CSS code. JQuery, a cross-platform JavaScript library, is also used. For local host of the webpage tool, the Wamp server is used.

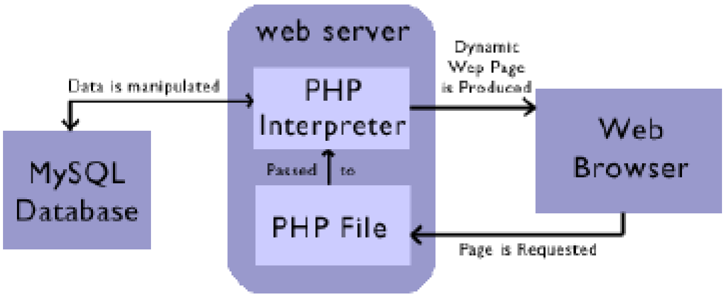


Figure 7: Technologies used for 'Spherical Coordinates tool'.

3.4 Example Results

Radius of the nanoparticle: 1.5 Å
Radius of smaller spheres: 0.15 Å

- There are 317 spheres that fit on the surface of the nanoparticle

Output visualization (.xyz file format):

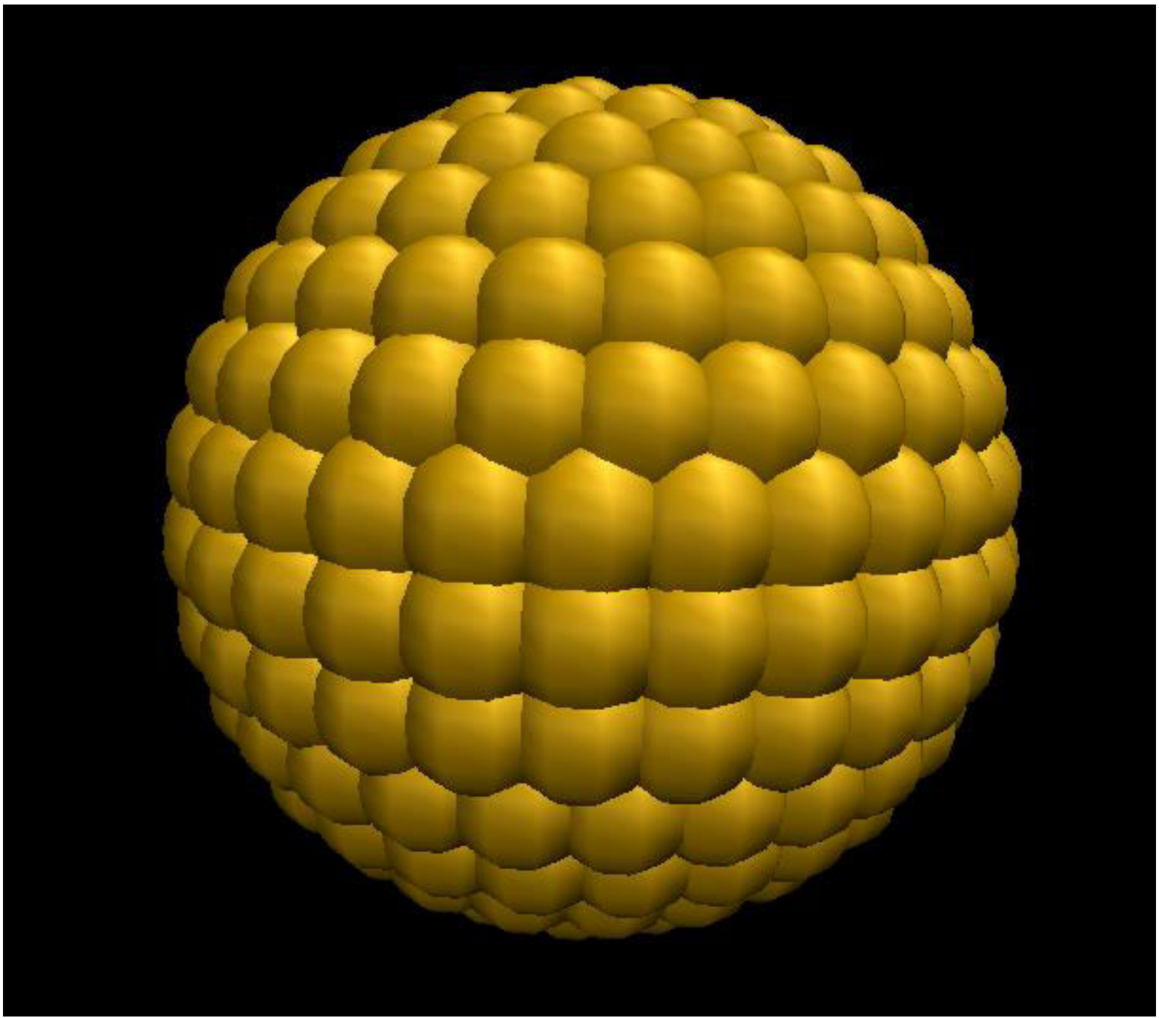
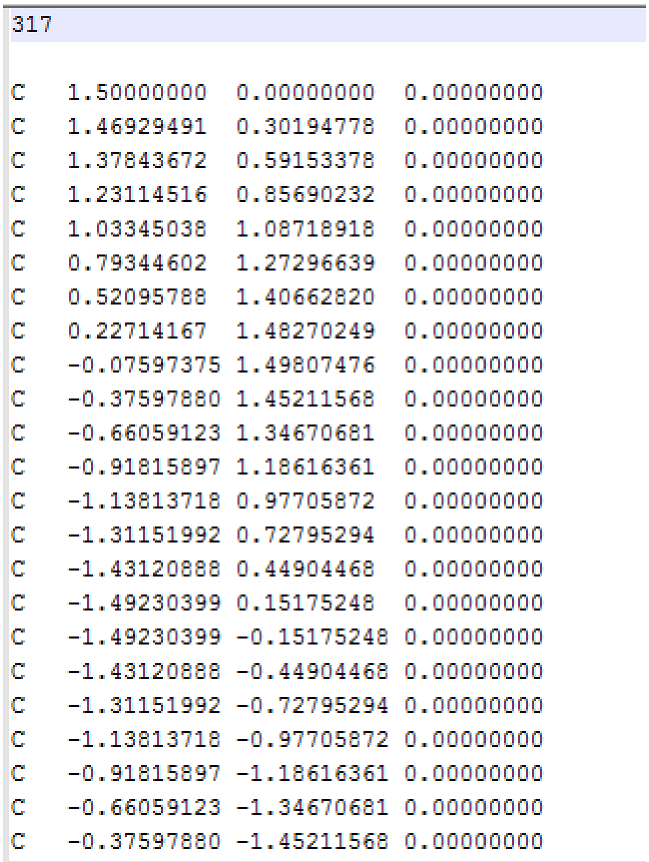


Figure 8: Output visualization of 'Spherical Coordinates tool', 1.5 Å nanoparticle-0.15 Å smaller spheres.



```
317

C   1.50000000  0.00000000  0.00000000
C   1.46929491  0.30194778  0.00000000
C   1.37843672  0.59153378  0.00000000
C   1.23114516  0.85690232  0.00000000
C   1.03345038  1.08718918  0.00000000
C   0.79344602  1.27296639  0.00000000
C   0.52095788  1.40662820  0.00000000
C   0.22714167  1.48270249  0.00000000
C   -0.07597375 1.49807476  0.00000000
C   -0.37597880 1.45211568  0.00000000
C   -0.66059123 1.34670681  0.00000000
C   -0.91815897 1.18616361  0.00000000
C   -1.13813718 0.97705872  0.00000000
C   -1.31151992 0.72795294  0.00000000
C   -1.43120888 0.44904468  0.00000000
C   -1.49230399 0.15175248  0.00000000
C   -1.49230399 -0.15175248 0.00000000
C   -1.43120888 -0.44904468 0.00000000
C   -1.31151992 -0.72795294 0.00000000
C   -1.13813718 -0.97705872 0.00000000
C   -0.91815897 -1.18616361 0.00000000
C   -0.66059123 -1.34670681 0.00000000
C   -0.37597880 -1.45211568 0.00000000
```

Figure 9: Sample of the xyz output file of 'Spherical Coordinates tool'.

Note that the equation $x^2+y^2+z^2=r^2$ is satisfied by the Cartesian coordinates of the smaller spheres that are packed at the surface of the bigger sphere.

Radius of the nanoparticle: 3 Å
Radius of smaller spheres: 1.5 Å

- There are 14 spheres that fit on the surface of the nanoparticle

Output visualization (.xyz file format):

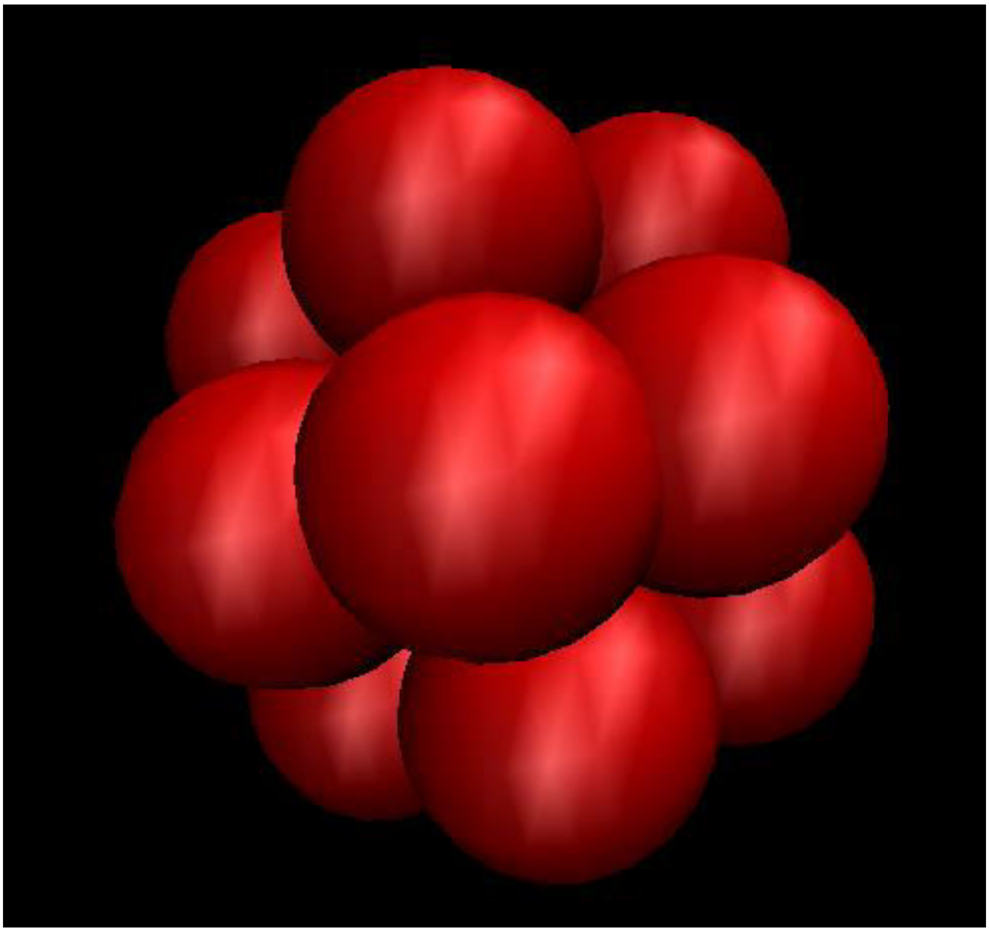


Figure9: Output visualization of 'Spherical Coordinates tool', 3 Å nanoparticle-1.5 Å smaller spheres.