Mathematical modelling simulation of nanotheranostics induced hyperthermia and heat diffusion simulation in water medium.

Final Project Report.

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Aim:

Mathematical modelling simulation of nanotheranostics induced hyperthermia and heat diffusion simulation in water medium.

Theory:

- Local surface plasmon resonance [LSPR] effect is induced by stimulating the nanoparticle with laser light irradiation.

- Mie scattering theory helps to mathematically analyze the absorbtion cross section of the nanoparticle.

- FDTD theory derives the absorbed power of laser irradiation into the nanoparticle.

- Heat diffusion is devised based on fourier heat diffusion algorithm with a boundary condition of constant temperature to emulate the human body temperature in macroscopic scale.

Mathatical derivations are described in detail on the attachement named as Algorithm_derivation.

Objective:

- Create crystal structure of nanoparticle with experimentally defined lattice structure.

- Prepare the codes based on the algorithm derived for LSPR and analyze the result with nanoparicles of different nature.

- Prepare the codes for Heat diffusion based on Derived algorithm and run the simulation.

- Analyze the Results of respective experiments.

Softwares Required:

- Charmm_GUI.

- Jupyter Notebook and python.

- Tecplot_360.

- Spyder_ GUI.

Sample Nanoparticle used on study:

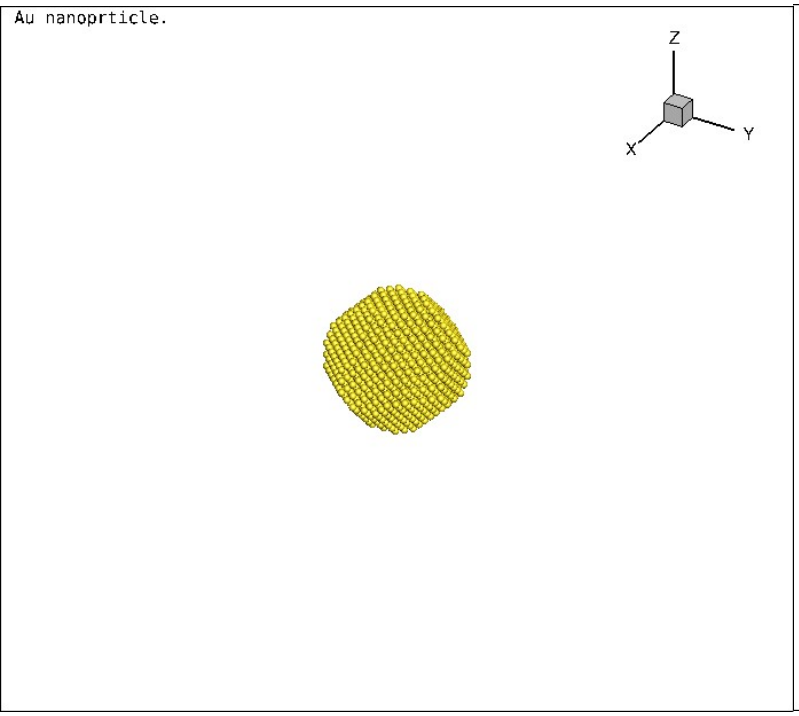
Material: Gold Nanoparticle.
Size: 2nm, 5nm, 10nm, 15nm,20nm.
Medium: Water.

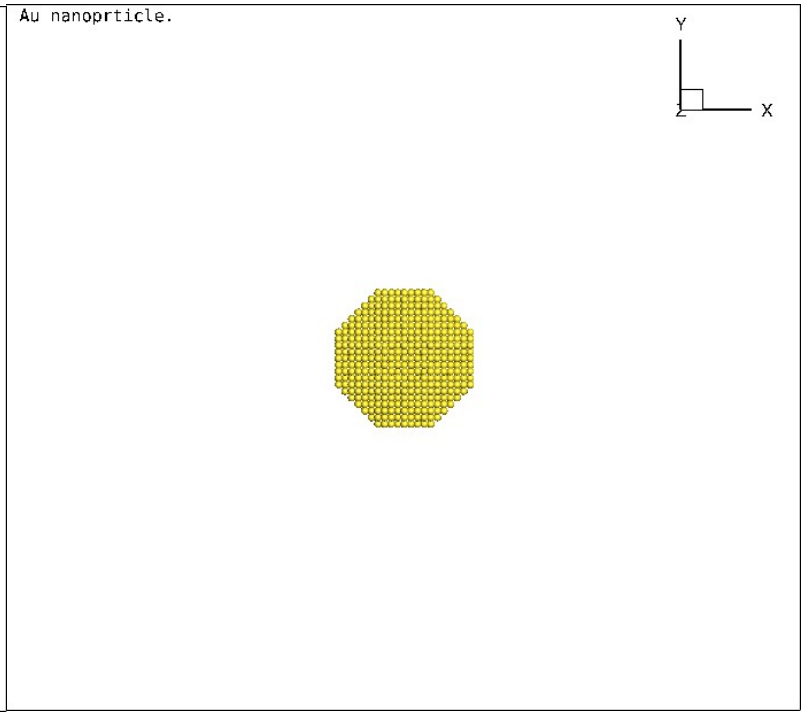
Results:

Crystal Generation:

Lattice Structure of Au Nanoparticle:

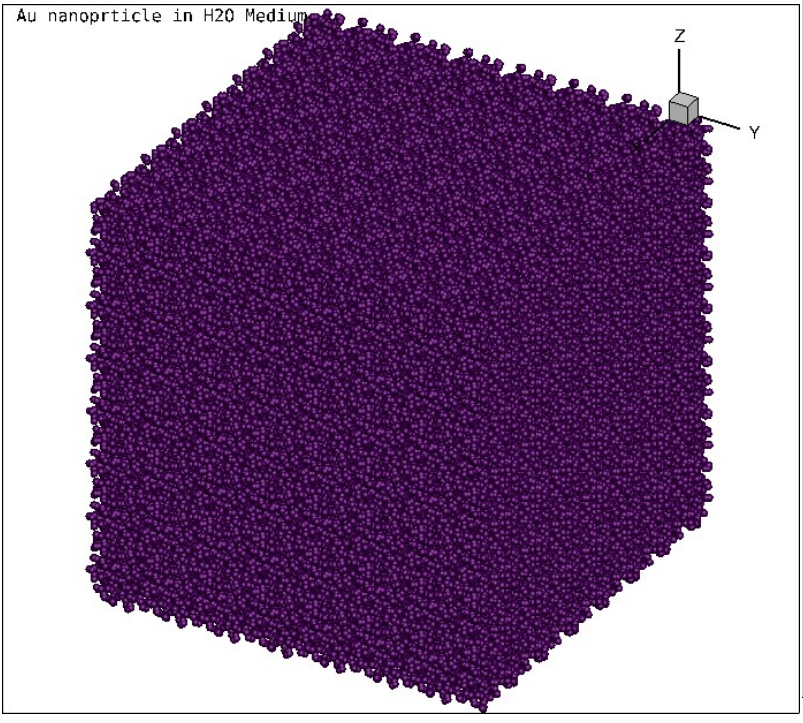
Wulff Construction. [100-110-111]

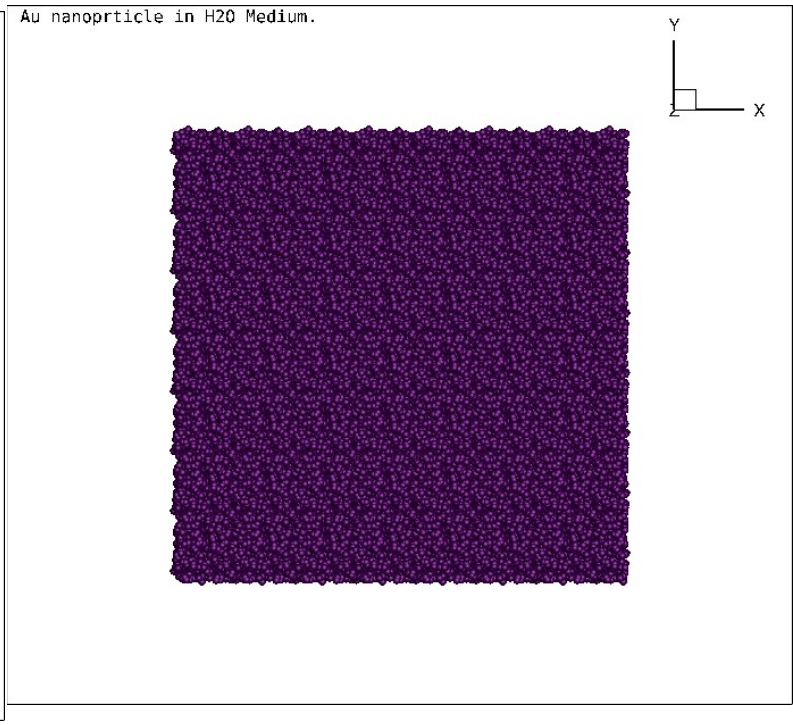




Lattice Structure of complete system:

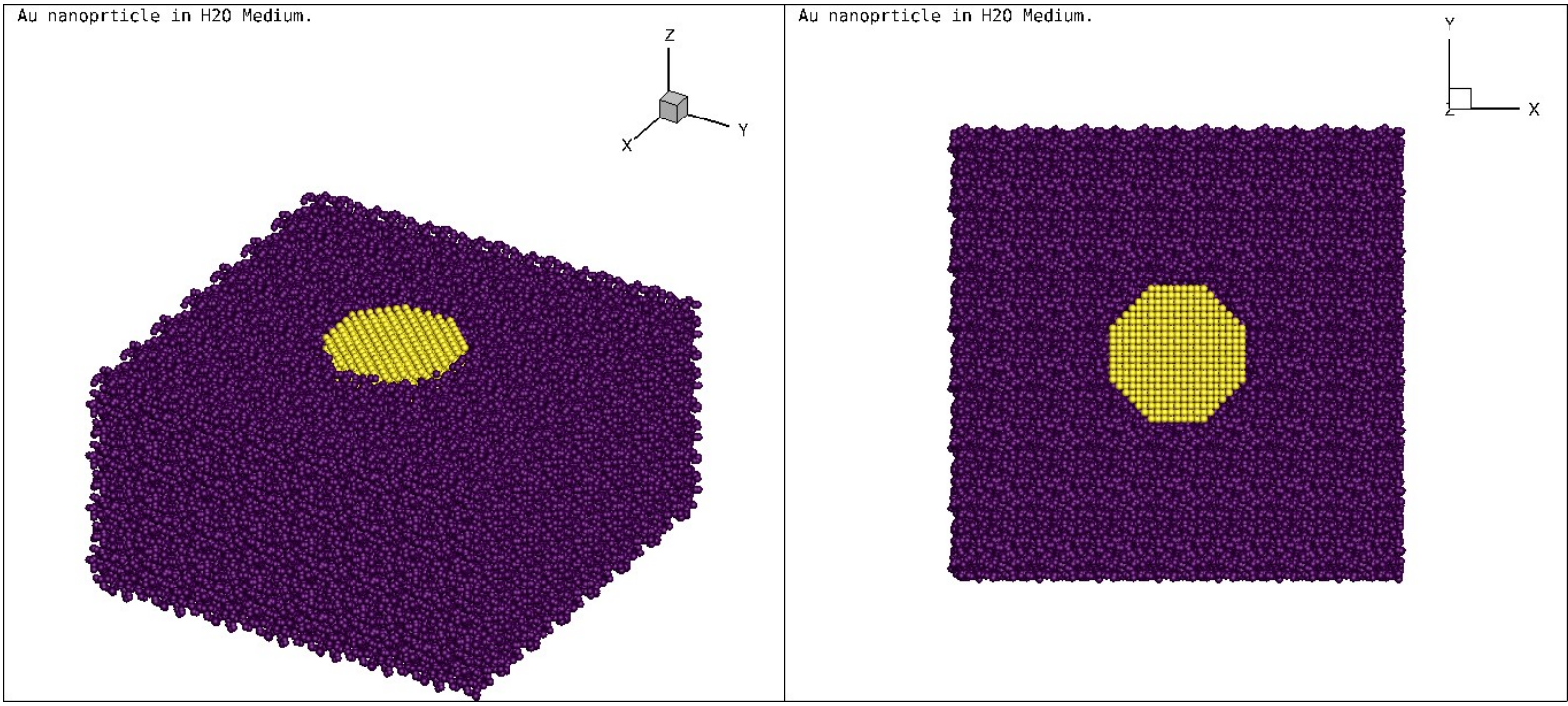
[Water molecules (Tip3) and Au Nps]





Lattice Structure of complete system:

[Placement Au Nps in water medium]

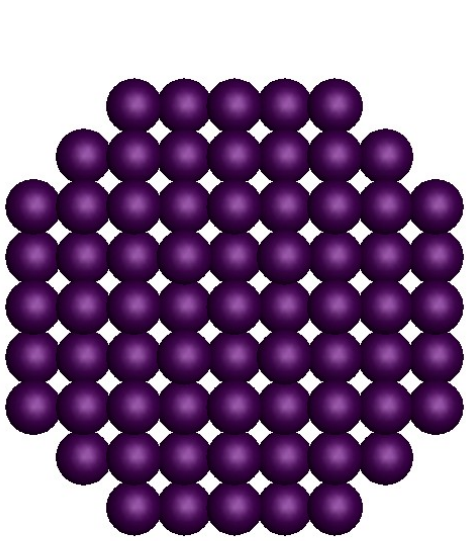


[Nanoparticle- Yellow Colour ; Water medium – Violet Colour]

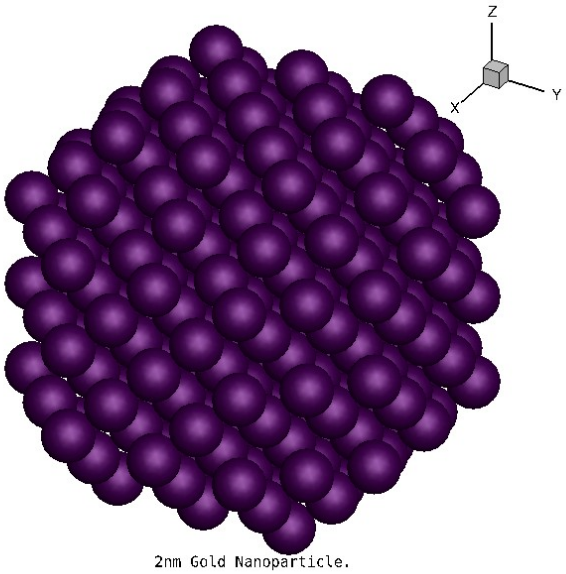
Specification of crystal used for final study:

- **Size of Nanoparticle** : 4nm
- **Size of complete crystal** : 14nm
- **Note** : Nanoparticle is placed in the middle of the crystal [5nm from the edge of the crystal]

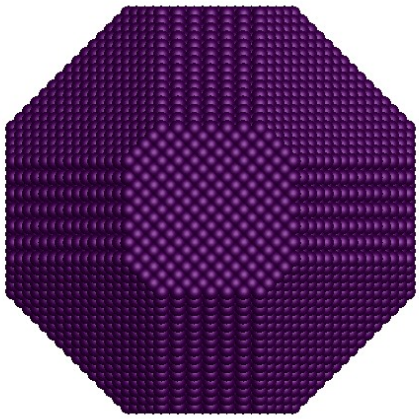
Size Variants:



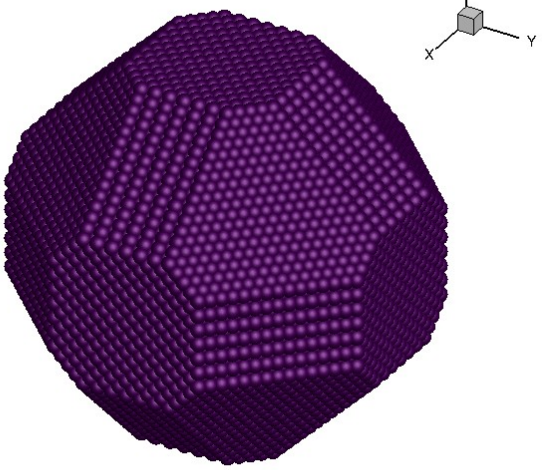
2nm Gold Nanoparticle.



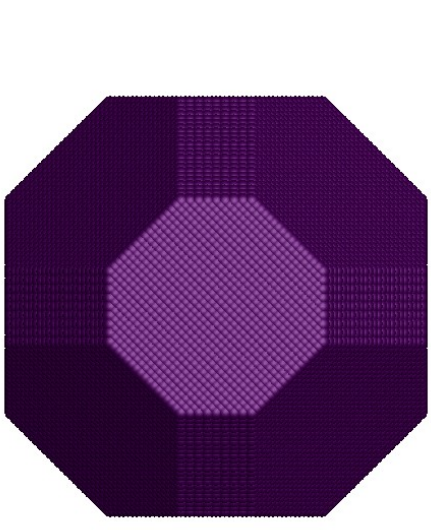
2nm Gold Nanoparticle.



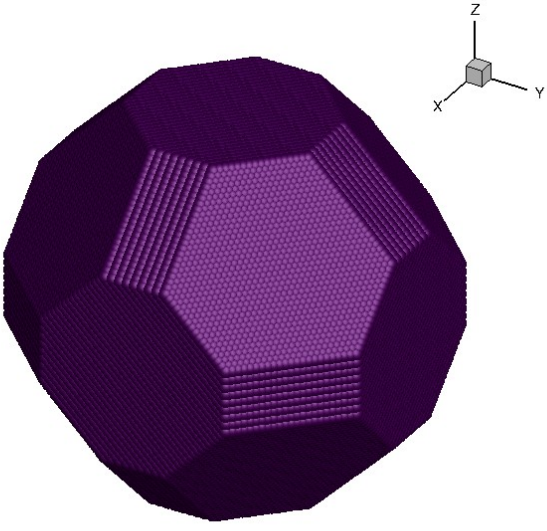
5nm Gold Nanoparticle.



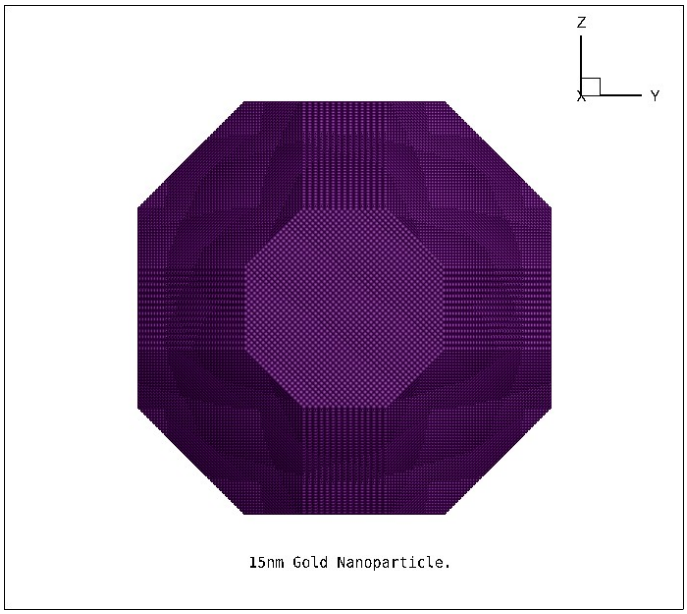
5nm Gold Nanoparticle.

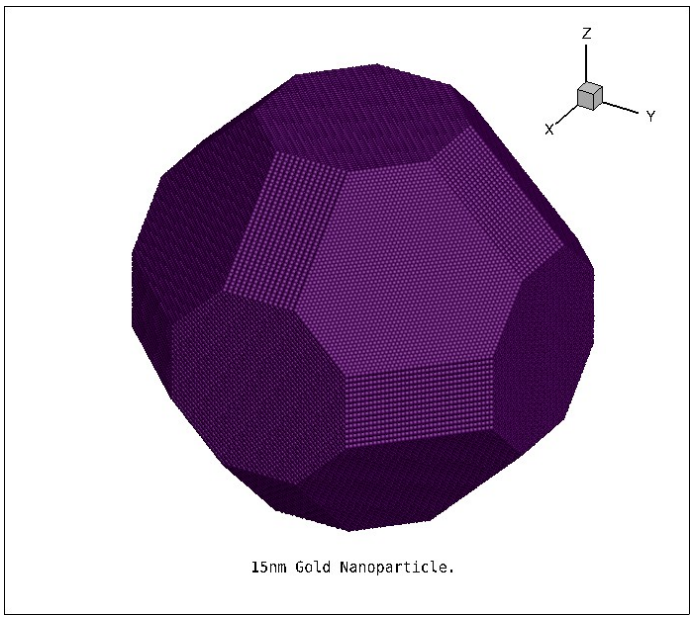


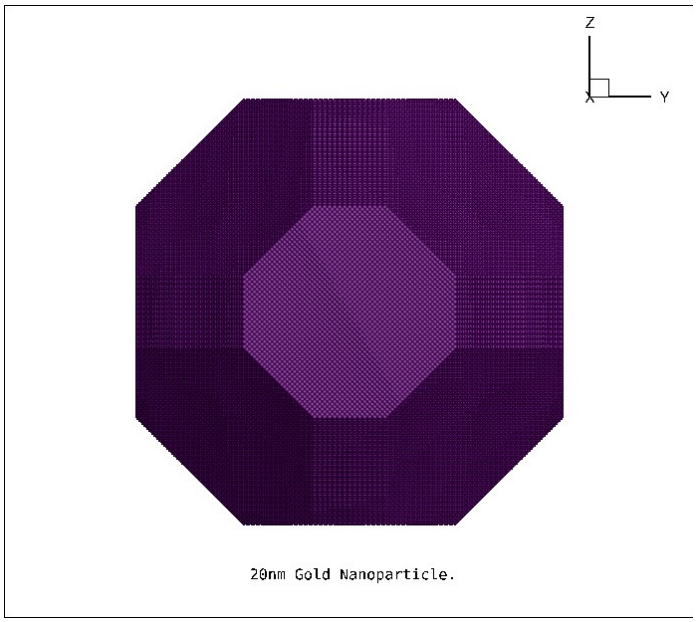
10nm Gold Nanoparticle.

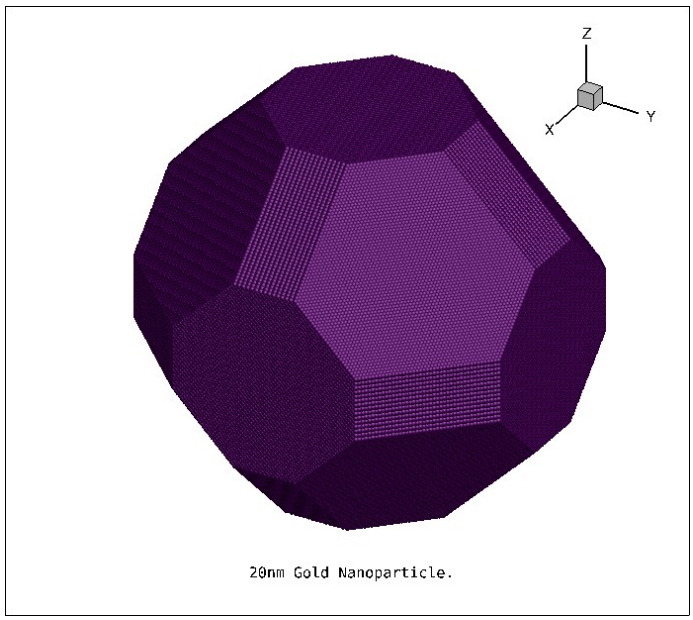


10nm Gold Nanoparticle.

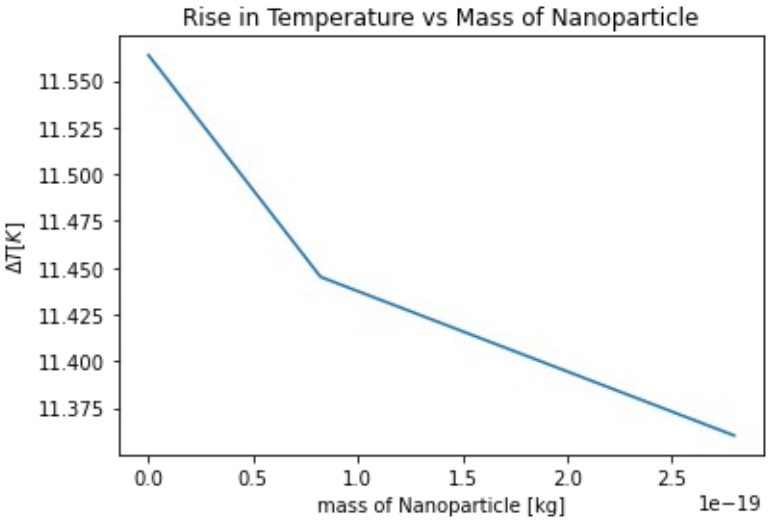


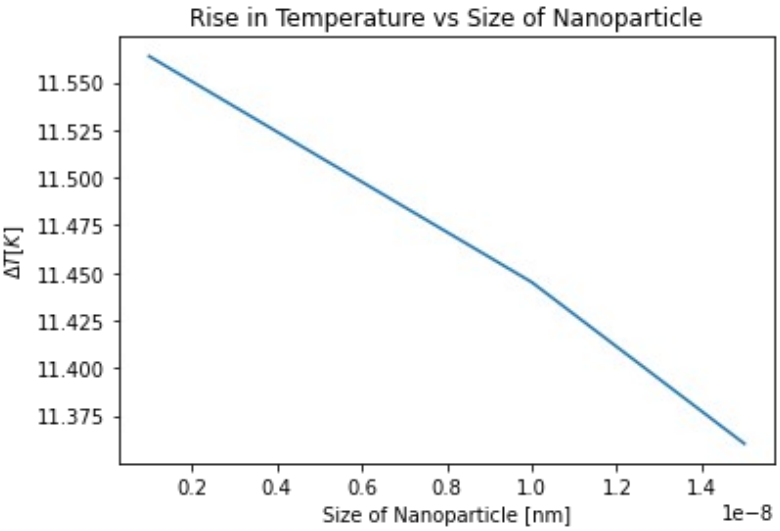






Dependance of size with temperature change:
Material: Gold Nanoparticle.
Size: 2nm, 5nm, 10nm, 15nm, 20nm.



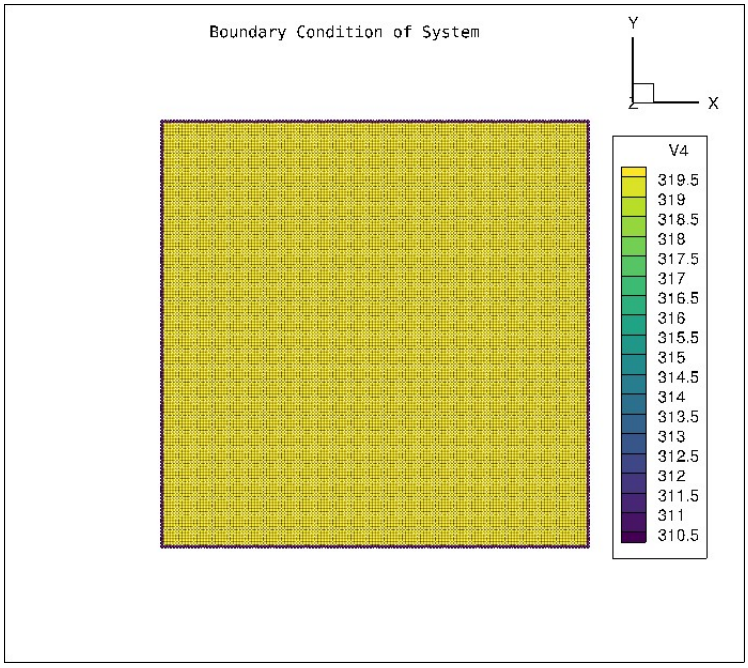


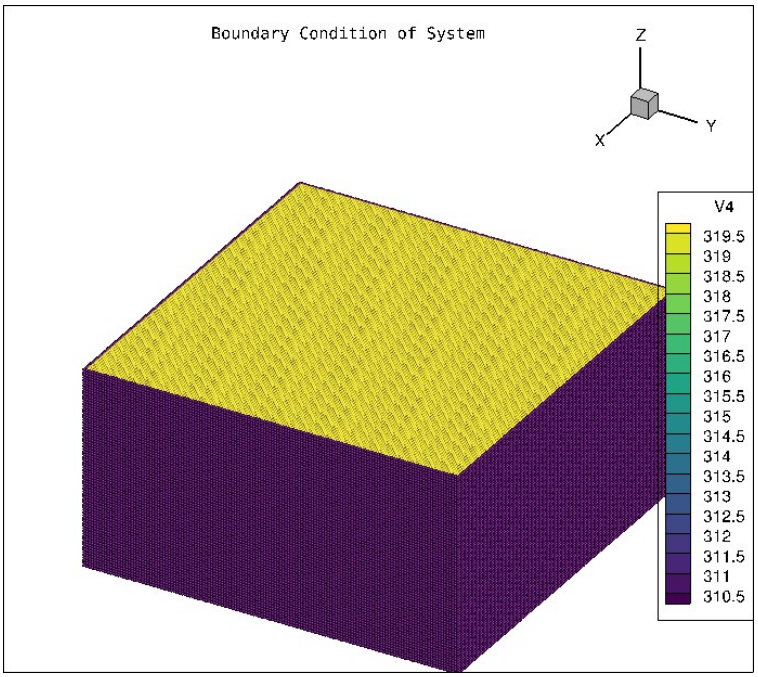
Boundary Condition:

To emulate a human body temperature in macroscopic scale the boundary condition is set at 310.15 K.

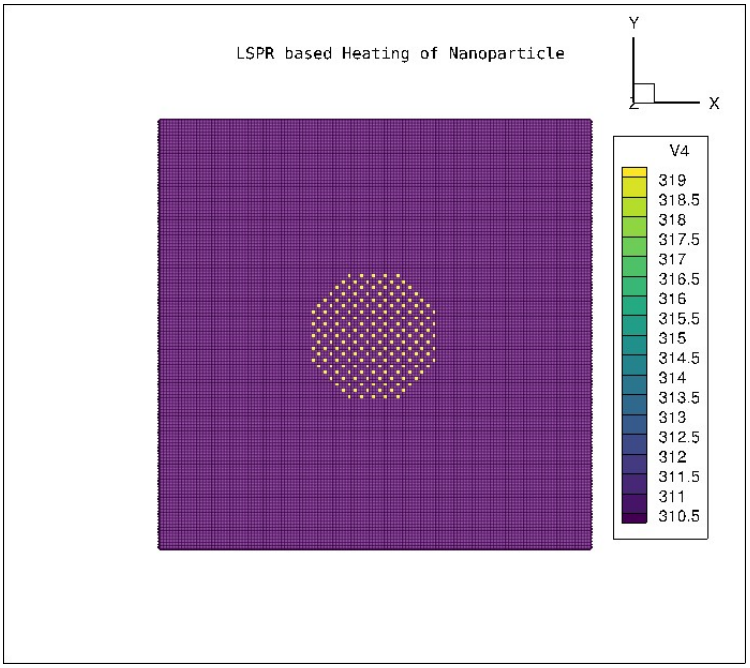
$$T|_{X=L} = T_f$$

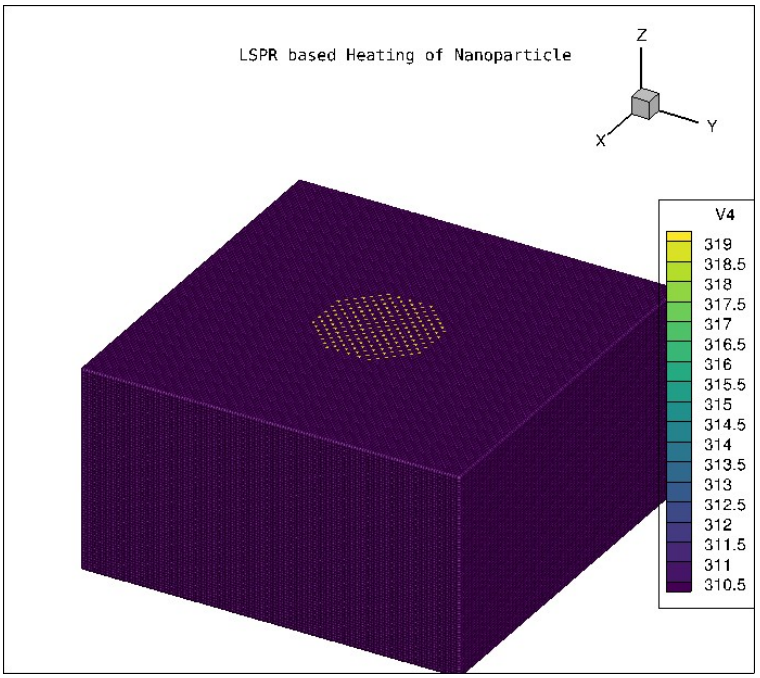
$$T_f = 310.15\ K$$





Heating Of Nanoparticle by laser irradiation:





Heat Diffusion:

Thermal Diffusion Calucluation.

Air medium:

$$\alpha = 1.9494 * 10^{-3}\ A^2/as$$

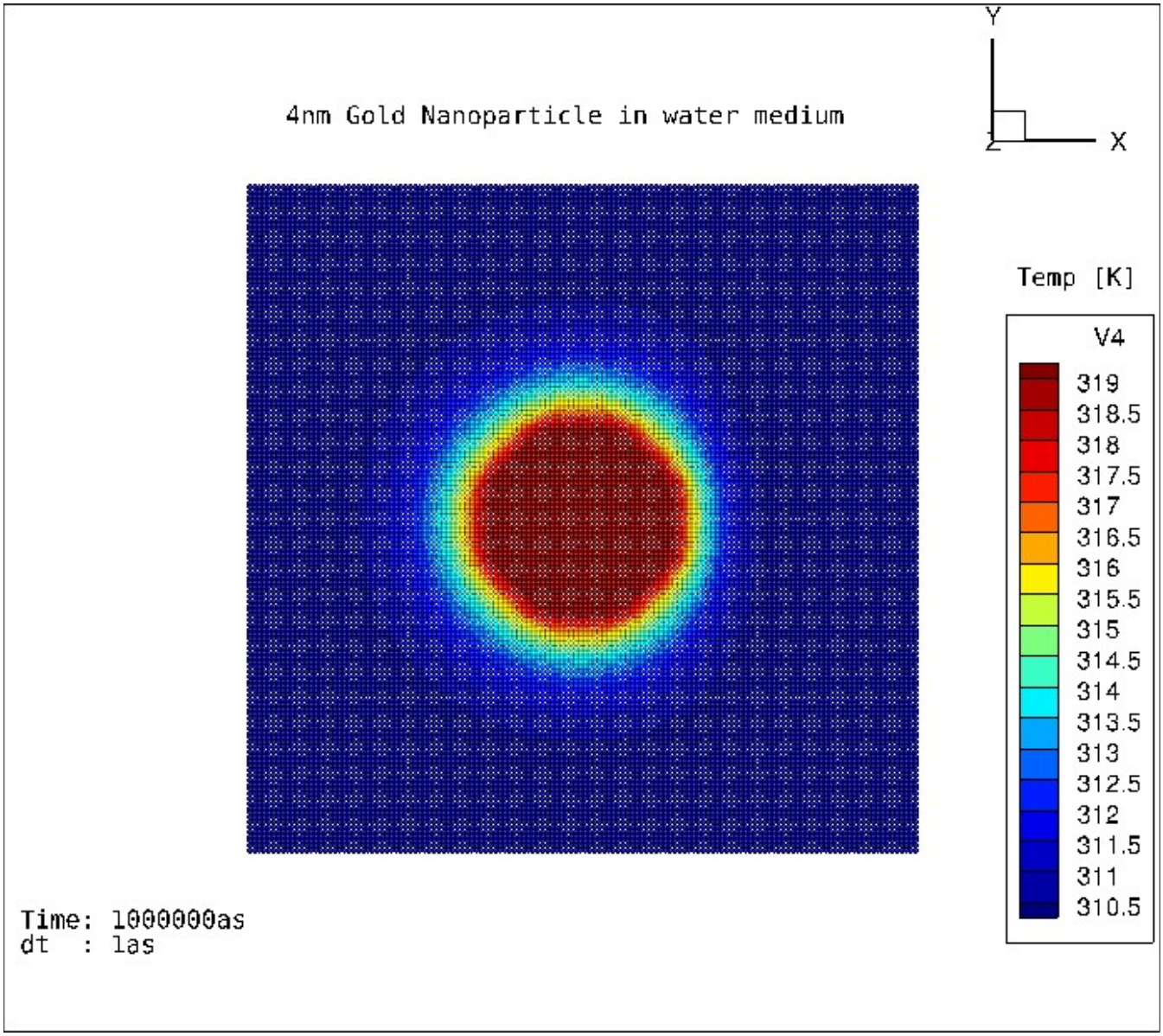
Water medium:

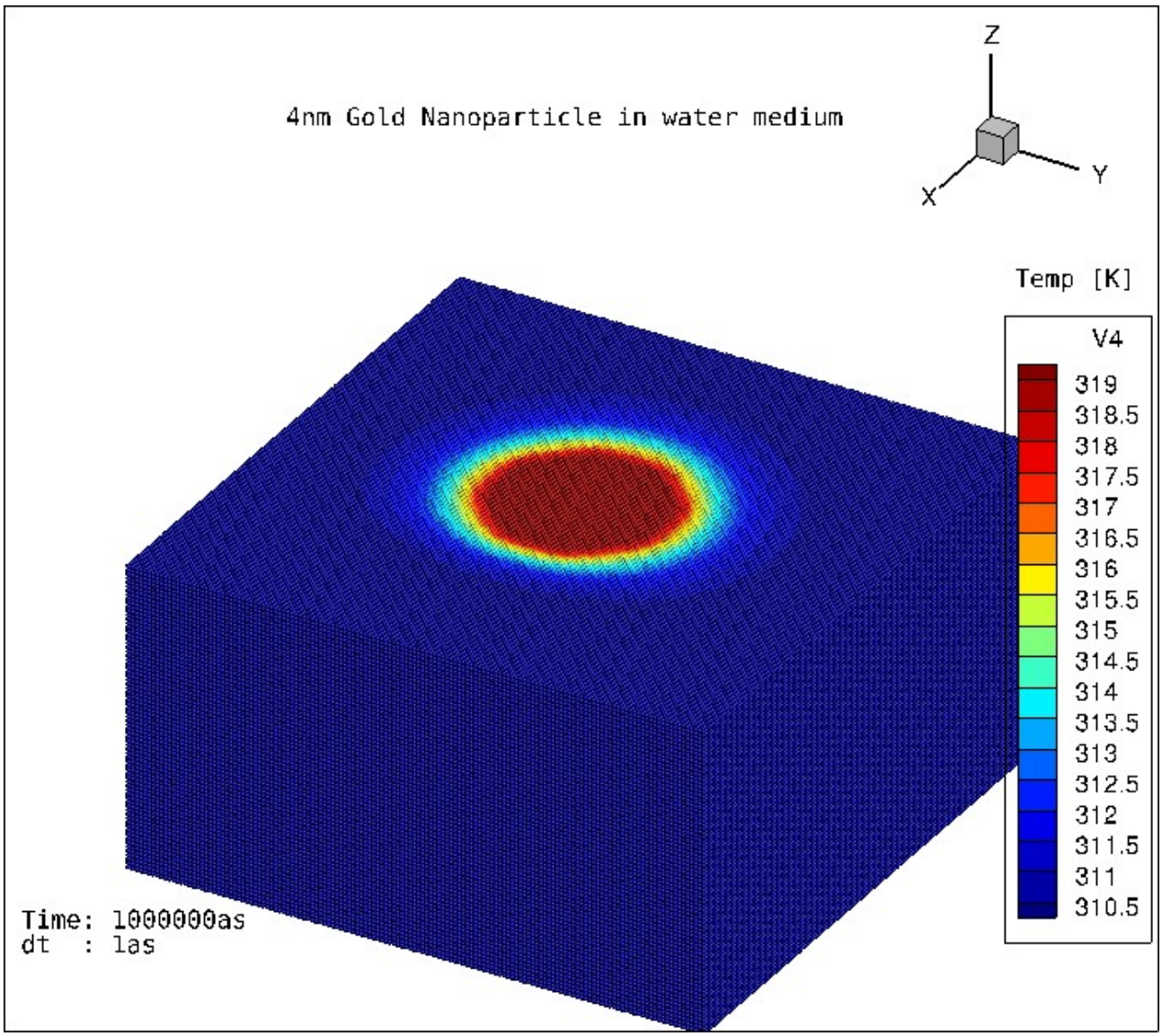
$$\alpha = 1.4555 * 10^{-5}\ A^2/as$$

Gold medium:

$$\alpha = 1.26 * 10^{-2}\ A^2/as$$

[Calculations of thermal diffusion coefficients attached in the name of "Calculations"]





Specification:

nx = ny = nz = 140 + 2[boundary] Angstroms

dx = dy = dz = 1 Angstrom

dt = 1as

T = 1000000as

[Timescaled view of heat diffusion in water medium id attached in video form]

Observation:

- Comparative study of size variants reveals the gradual reduction in tempereature change.
- The timestep is practiced at attosecond scale to satisfy the 'Neumann stability condition'.
- The diffusion is acheived maximum at 1000000as step beyond which the temperature change is neglible to acheive hyperthermia in the surrounding medium.
- The test used 4nm NP to optimize the test by not including large atom clusters from large nanoparticle size.

References:

- Gold nanocrystals with variable index facets as highly effective cathode catalysts for lithium–oxygen batteries.-Dawei Su, Shixue Dou and Guoxiu Wang.
- FDTD simulation of the optical properties for gold nanoparticles.-Lin Cheng, Guixian Zhu, Gannan Liu and Lianqing Zhu.
- Molecular Dynamics Simulation of Heat Transfer from a Gold Nanoparticle to a Water Pool Xiaoling Chen, Antonio Munjiza, Kai Zhang, and Dongsheng Wen.
- Exploring the Structure–Activity Relationship on Platinum Nanoparticles.-Laura Braunwarth, Christoph Jung & Timo Jacob