Manual of the NP array heating simulator application

Brief description:

The NP array heating simulation APP is a standalone, Matlab-based application. Based on the analytical solution, the APP can calculate the temperature profile of a single spherical nanoparticle (NP) during transient heating with a constant heating power[1,2]. This APP can generate 2D, 3D and spherical NP array and calculate the temperature profile of NP array heating via superposition method[3,4]. The APP can save results as Matlab data file, and plot temperature profile automatically.

In this manual, we introduce how to calculate the temperature profile of NP array heating simulator, how to set up the parameters and discuss the accuracy of the results.

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Manual:

1. **Basics:**
The basic function of this APP is simply to set input parameters and calculate (Fig. 1.1). It is notable that, once the APP is activated, the APP will automatically set reasonable initial values to all necessary values, users need to change them based on the specific problem.

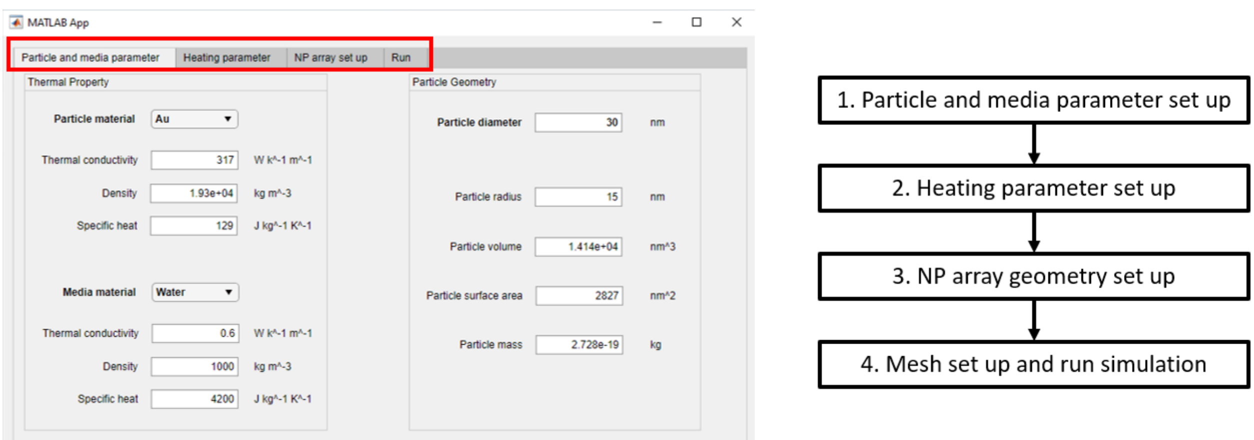


Figure 1.1

2. **Particle and media parameter set up:**
In the “Particle and media parameter” part (Fig. 2.1), we need to set the thermal properties (thermal conductivity, density, specific heat) of the particle and media.

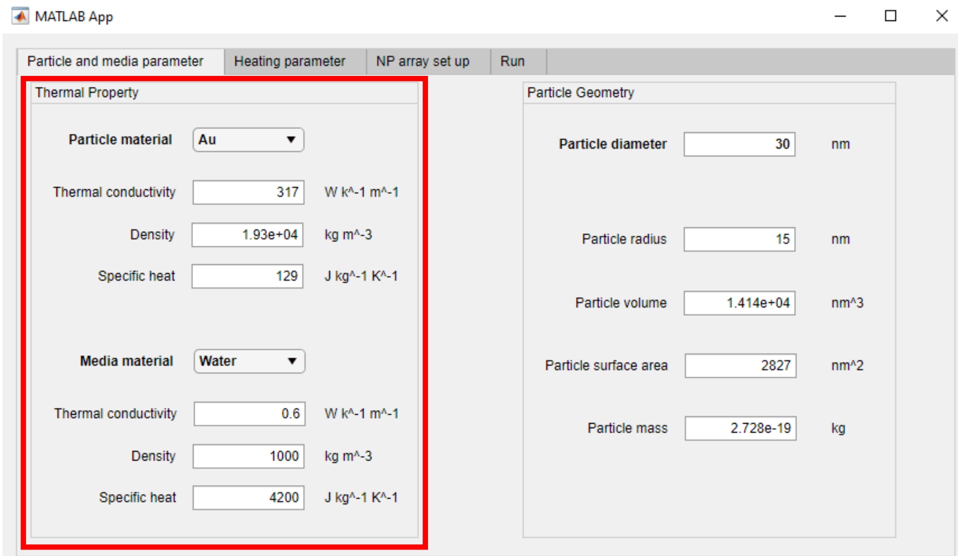


Figure 2.1

There are two methods to set up the thermal properties, the first method is to choose the material (Fig. 2.2), and the APP will automatically set the properties of that materials.

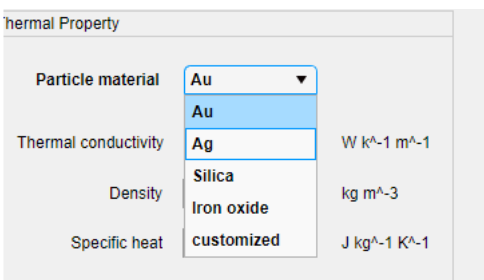


Figure 2.2

The second method is to input the thermal properties. Select 'customized' material, and input the properties (Fig. 2.3). Please note the dimensions for the properties, and the specific heat refers to specific heat under constant pressure (C_p).

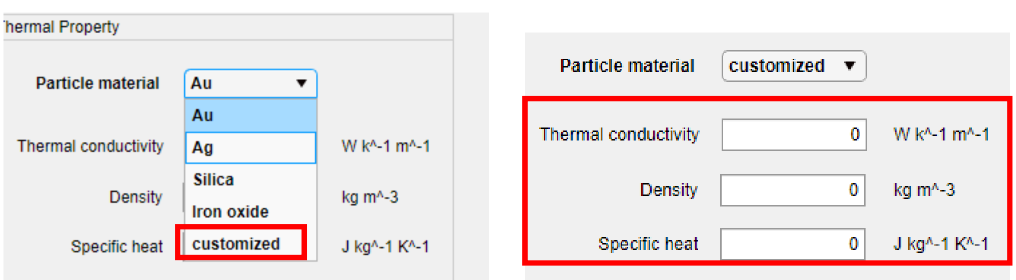


Figure 2.3

Next, we need to set the size of the Particle (Fig. 2.4). This APP can only calculate spherical nano particles, once the diameter of the particle is set, the APP automatically calculate the radius, volume, surface area, mass per particle.

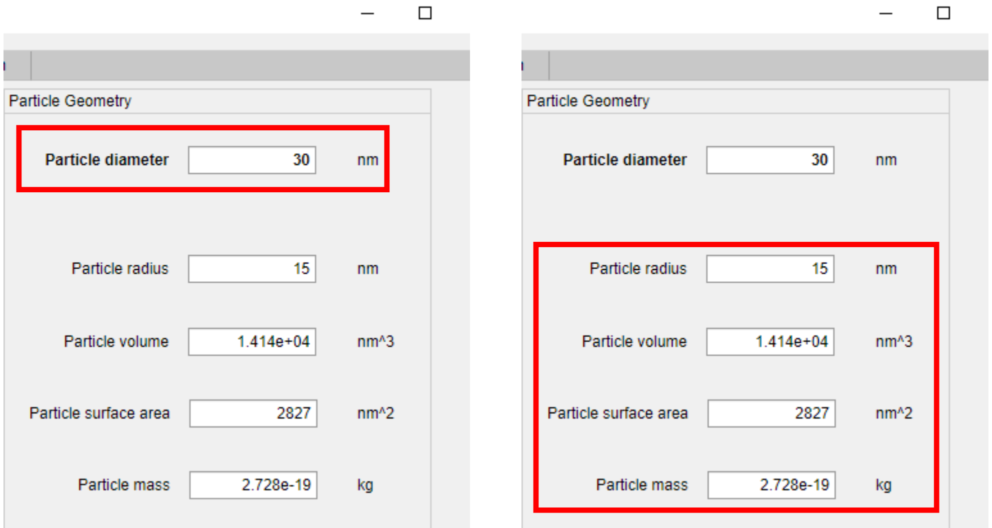


Figure 2.4

3. Heating parameter set-up:

We consider the heating power (g) as a constant in terms of time during the heating duration. (Fig. 3.1). And the heating duration can be set easily.

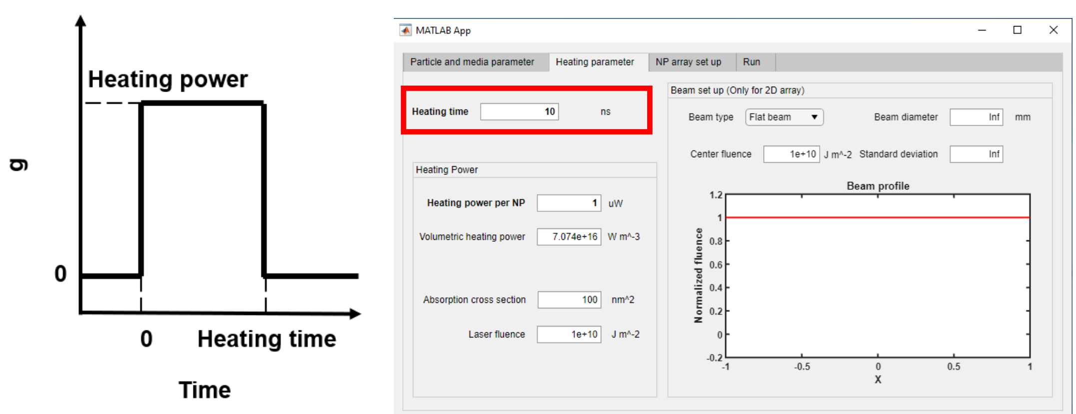


Figure 3.1

There are three methods to set the heating power (g) (Fig. 3.2). The first one is to set the heating power per NP [W], the second method is to set the volumetric heating power [W/m^3], the last method is to set Absorption cross section (C_{abs}) and the Laser fluence (F), g=C_{abs}*F.

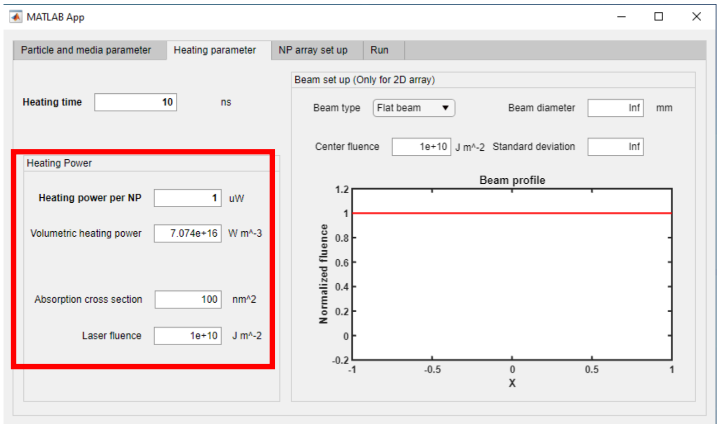


Figure 3.2

For the heating power in terms of space, the APP will automatically set a constant heating power throughout the space, or a flat beam. For 2D nano particle (NP) array, this APP can also calculate heating case with gaussian beam (Fig. 3.3). It should be emphasized that for 3D and SPH NP array, this APP can only calculate heating under flat beam.

Once select Gaussian beam for the Beam type, we can input the center fluence (F_0), Beam diameter, and Standard deviation (sg). The heating power (g) is calculated by: $g(x) = F_0*C_{abs}*\exp(-(x/sg)^2/2)$.

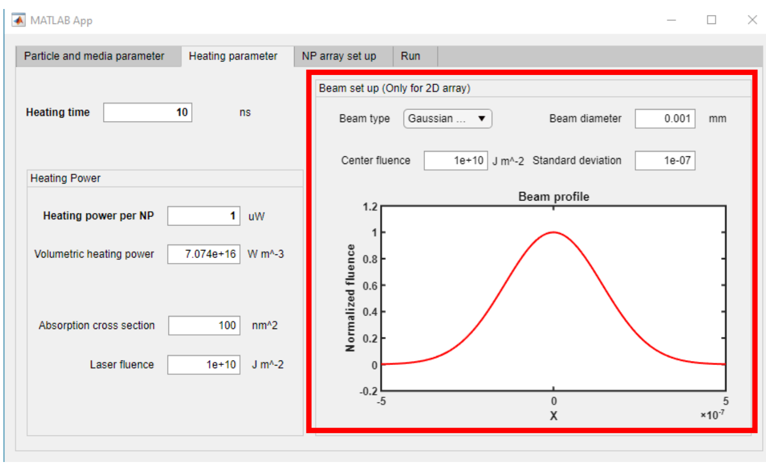


Fig. 3.3

4. NP array set-up:

This APP can generate 3 types of NP arrays, the 2D array, 3D array, and SPH array.

4.1. 2D NP array set-up:

The set-up of the 2D array is the key to the set-up of the simulation. As shown in Fig. 4.1, the first step is to select the shape of the 2D array. Two shapes are available: Square and Circular.

For Square shape, the 2D array will be cut into a square, and for Circular shape, the 2D arrays will be cut into a circle.

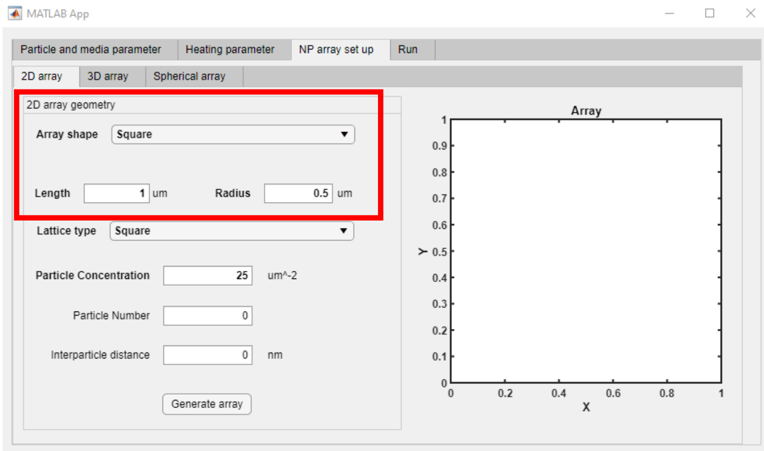


Figure 4.1

Next, we need to set the size of the array. For a square array, we can set the size by inputting the Length, which determines the side length of the array. For a circular array, we can set the size by inputting the Radius of the array.

It is notable that Length as severs as an important parameter is mesh set up, for circular array, the APP will automatically set the Length as 2*Radius.

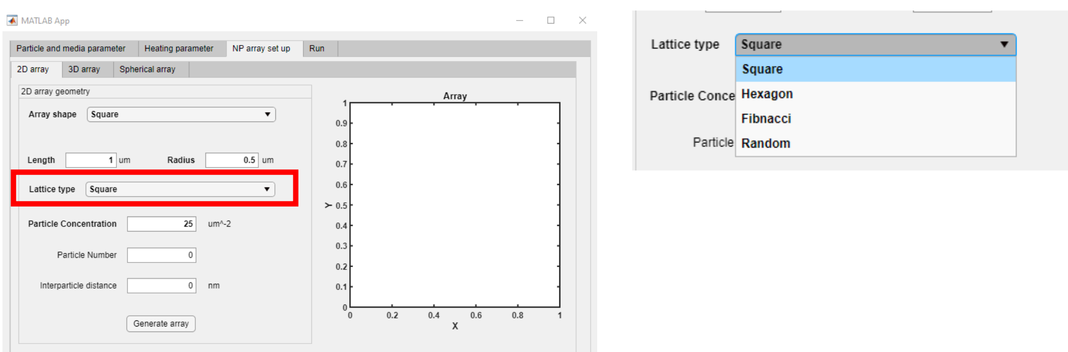
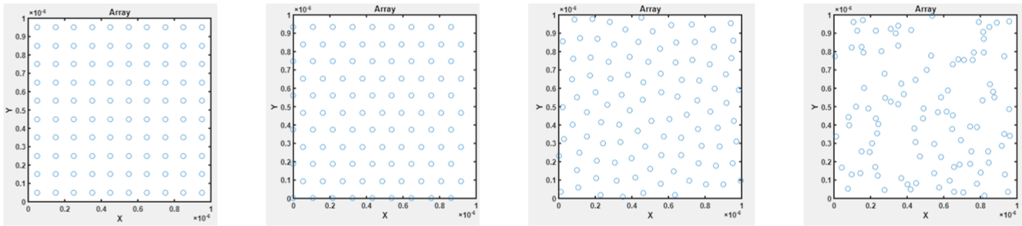


Figure 4.2

After setting the shape and size of the array, we need to select the lattice of the array. There are 4 types of lattice, the sample of the lattices are shown in Figure 4.3:



Square lattice Hexagon lattice Fibonacci lattice Random lattice

Figure 4.3

Next, we need to set the particle concentration. Once the particle concentration is set, we can press the “Generate array” button, the APP will generate the NP array based on our setting, we can check the Particle Number, Interparticle distance and the distribution of the particles (Figure 4.4).

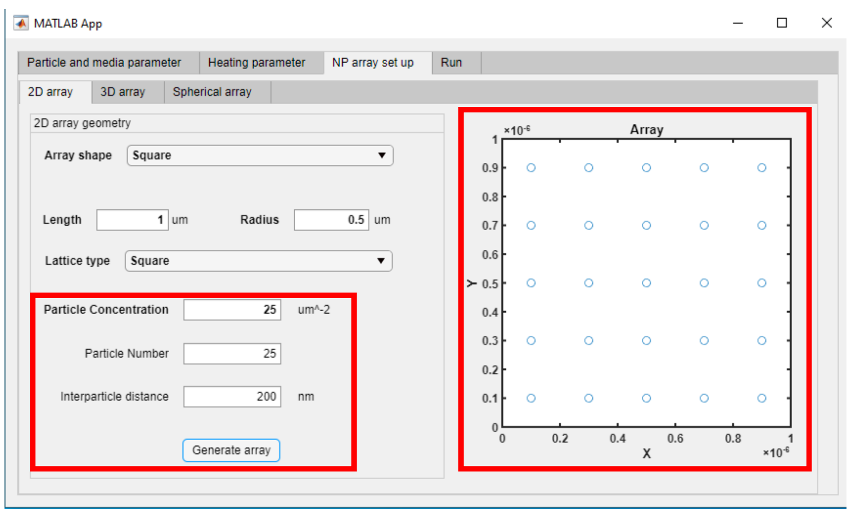


Figure 4.4

It should be noted: 1. The interparticle distance must not be smaller than the size of the particle. 2. Blue circles in the left figure only demonstrate the location of particles, the size of the blue circle does not represent the size of the particle. 3. For a random NP array, the particle concentration cannot be too high, which may result in an infinite loop.

4.2. 3D NP array and SPH NP array set-up:

The setup for 3D and SPH NP array is relatively straightforward. For a 3D array, we need to set the radius of an array and the particle concentration, and the APP will generate a spherical-shaped 3D NP array with a cubic lattice. For the SPH array, we need to set the radius and the particle number, and the APP will generate an NP array along a spherical surface with a Fibonacci lattice.

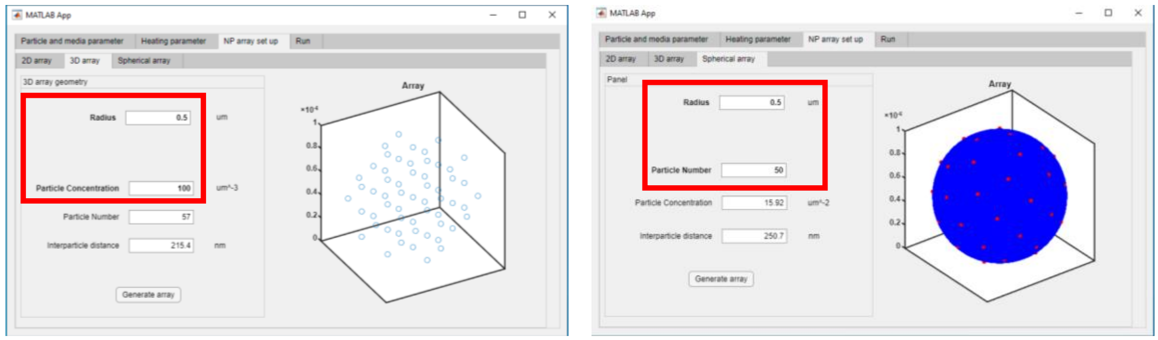


Figure 4.5

Once the parameters are set, we can check the array by pressing the "generate array" button, and we can also check the interparticle distance. For the SPH array, the interparticle distance P is calculate by the following equation:

$$P = \frac{A}{\sqrt{N}}$$

Where A refers to the area of the spherical surface, and N refers to the particle number. **Similarly, the interparticle distance must not be smaller than the NP size.**

5. Mesh set-up and run simulation:

The mesh set-up is highly related to the simulation process. Briefly, this APP will first calculate the temperature profile for single NP with the analytical solution[1,2]. Based on the temperature profile of the single NP heating, the APP will do superposition to get the temperature profile for the NP array[3,4].

5.1. Mesh set-up for single NP calculation:

Based on this process, we need to set the spatial and temporal mesh of the single NP calculation:

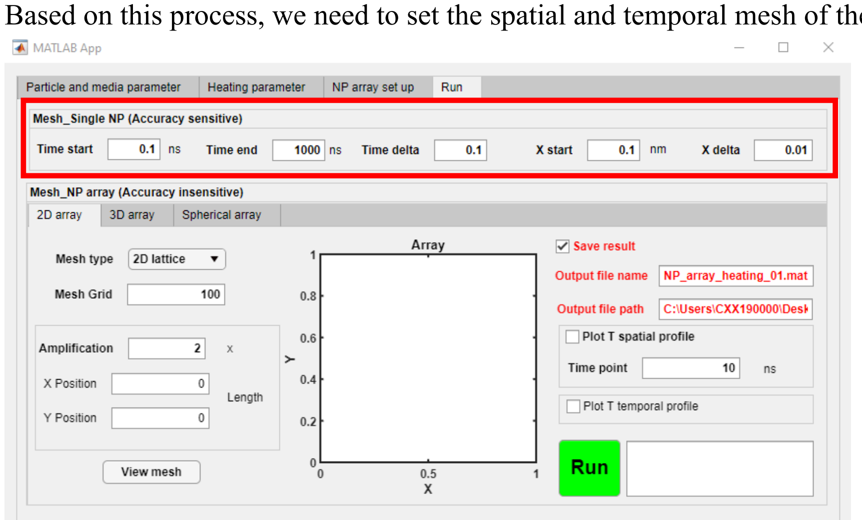


Fig. 5.1

The time start is the temporal starting point. **It should be noted that this APP uses logarithmic temporal mesh for single NP heating, thus the temporal starting point must not be 0.** If mistakenly set the time start as 0, the APP will automatically correct the time start to 0.01 ns in the calculation. The time end is the temporal ending point, **and the time delta is the logarithmic temporal mesh step:**

$$t^{n+1} = t^{n} \times 10^{time\_delta}$$

For the spatial mesh set-up, we need to set the X start, which serves as the spatial starting point. Similar to the temporal mesh, this APP uses a **logarithmic spatial mesh, thus the spatial starting point must not be 0.** If mistakenly set the X start as 0, the APP will automatically correct it to 0.01 nm in the calculation. The APP will automatically set a spatial ending point based on the NP array set-up, **and the X delta is the logarithmic spatial mesh step:**

$$x^{n+1} = x^{n} \times 10^{X\_delta}$$

The mesh for single NP heating can affect the accuracy of the result. The smaller the time-delta and X_delta, the finer the mesh grid, however, it will also take more time for calculation. **Here we recommend time_delta≤0.1 and X_delta≤0.01.**

5.2. Mesh set-up for 2D NP array calculation:

After set up the mesh for single NP calculation, we can set the mesh of superposition. The temporal mesh will be the same as the that of the single NP calculation. We need to set a new spatial mesh for the NP array calculation. First we need to select the mesh type:

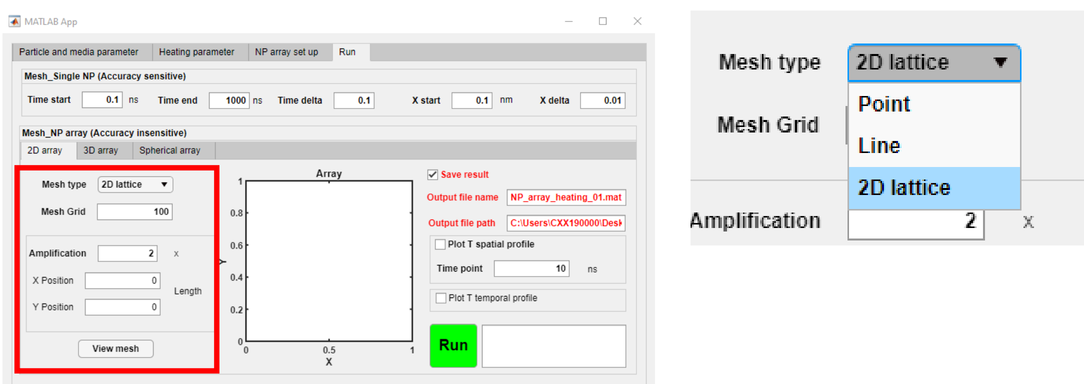


Figure 5.2

There are three types of mesh, the point type refers to a single point, and the result will be the temperature at this point during the heating. The line type refers to a line, and the result will be a temperature profile along this line. The 2D lattice type refers to a square area, the result will be temperature profile in this area.

Once the mesh is set, we need to set the mesh grid. The mesh grid is the resolution of the temperature profile. For 2D lattice mesh type, the resolution is $mesh\_grid^2$, for line mesh type, the resolution is $mesh\_grid^1$, and for point mesh type, the resolution is $mesh\_type^0$, i.e. 1.

The mesh grip can significantly affect the time for calculation, thus we need take extra consideration to balance the resolution and calculation time.

The amplification is the ratio of the NP array size to the mesh size (Length/Mesh_size). When amplification =1, the mesh size equals to the NP array size. The amplification can be smaller than 1 but must be lager than 0. For point mesh type, the amplification has no effect on the mesh set-up.

The X position and Y position is the relative deviation of the position of mesh from the center of NP array. For example, if we set X_position=Y_position=0, then the center of the mesh will be at the center of NP array; if X_postion=1, Y_postion=0, then the center of the mesh will be located 1*Length away along the x axis direction from the center of the NP array.
After setting the mesh for NP array, we can preview the NP array and mesh by pressing the "view mesh" button, the NPs (blue circle) and the mesh area (red square for 2D lattice) will be demonstrated (Figure 5.3).

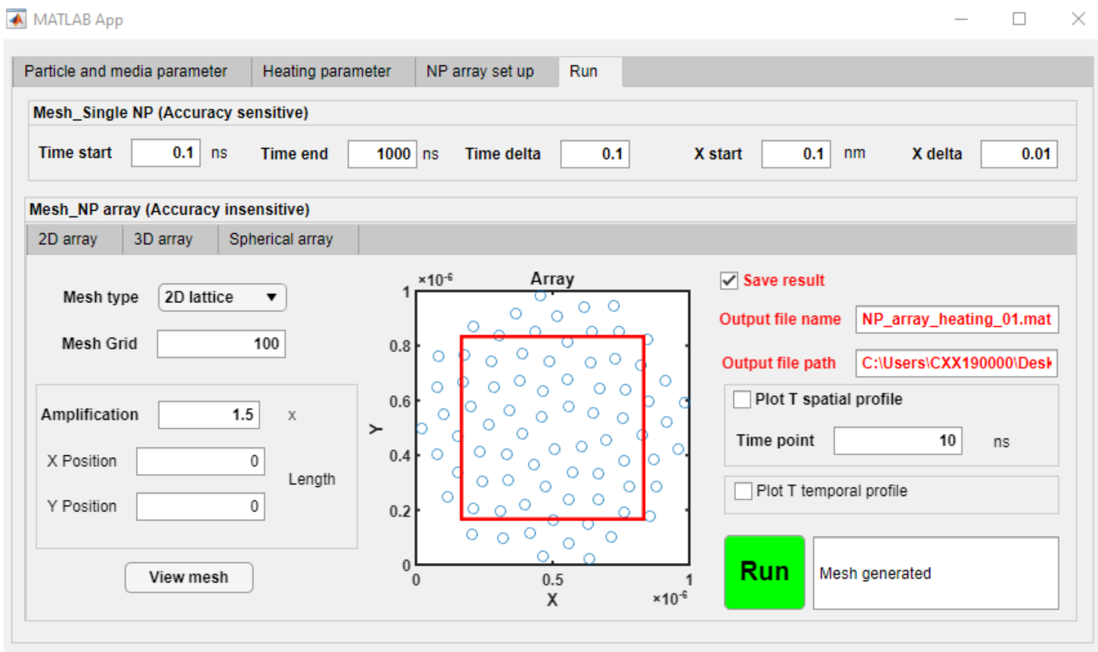


Figure 5.3

5.3. Run simulation and output result:

Once the NP array and mesh are set, we can run simulation and output the result. As shown in figure 5.4, we can select to save the result by checking the box of "save result". We need to input the output file name and the file path, then the APP will save the result as a Matlab data file.

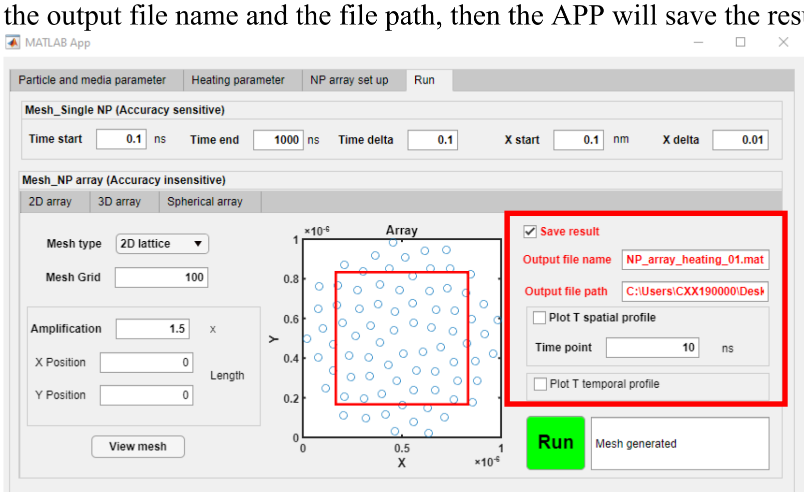


Figure 5.4

The parameters in the result files are:

g: volumetric heating power, W/m^3
laserpulse: the heating duration, s
Mediamaterial: the material of the media
NPmaterials: the material of the particle
T: the temperature profile for the NP array heating
T0: the temperature profile for the single NP heating
time: time mesh
X: the X-direction spatial mesh
Y: the y-direction spatial mesh
Xp: the X-component of the NP coordination
Yp: the Y-component of the NP coordination
Zp: the Z-component of the NP coordination

5.4. Mesh set-up and run simulation for 3D and SPH NP array:
The mesh set-up for 3D and SPH array is relatively straightforward. We need to input the Mesh grid to set the resolution of the result. Here we recommend the Mesh_grid>1000.

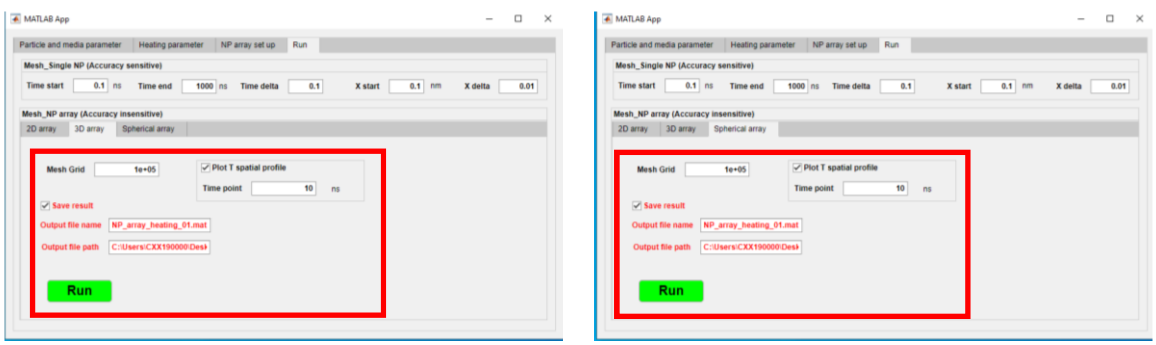


Figure 5.5

reference:

[1] Goldenberg, H., and Tranter, C., 1952, "Heat flow in an infinite medium heated by a sphere," Br. J. Appl. Phys., **3**(9), p. 296.

[2] Kang, P., Xie, C., Fall, O., Randrianalisoa, J., Qin, Z., 2021, "Computational investigation of protein photoinactivation by molecular hyperthermia," J. Biomech. Eng., **143**(3), p. 031004.

[3] Baffou, G., Berto, P., Bermudez Urena, E., Quidant, R., Monneret, S., Polleux, J., and Rigneault, H., 2013, "Photoinduced heating of nanoparticle arrays," ACS Nano, **7**(8), p. 6478.

[4] Xie, C., Qin, Z., 2022, "Spatiotemporal Evolution of Temperature During Transient Heating of Nanoparticle Arrays," J. Heat Transfer, **144**(3), p. 031204.