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MOSE

Molecular Optical Simulation Environment

User Manual

Version 2.3

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Catalogue

1 About MOSE

The functions of MOSE and its application areas will be introduced in this chapter. Compared to the previous version, the new version has made great improvements to meet the requirements of the users.

1.1 Introduction

Optical molecular imaging using near-infrared light is very useful to study the development and changes of disease in the biomedical field. Over the past twenty years, optical molecular imaging has attracted more and more attention and made progress with a series of breakthroughs.

The imaging technologies can be divided into two groups: the first is the two-dimensional (2D) planar imaging, and the second is the three-dimensional (3D) tomographic imaging, such as diffuse optical tomography (DOT), fluorescence molecular tomography (FMT), and bioluminescence tomography (BLT). The forward problem of tomographic imaging is to study the light propagation and the inverse problem is to reconstruct the optical properties of the inner tissues or the light sources. There are three distinct technology domains for optical tomography, which are the continuous wave (CW), the time-domain (TD) and the frequency-domain (FD). Each has distinct advantages and disadvantages, and the selection of the appropriate technology depends on the specific application. In order to realize high-fidelity in small-animal imaging, non-contact imaging approaches in free-space were introduced recently compared to the traditional method using light-guiding fibers. Although non-contact imaging has become mainstream, it needs to consider the procedure of light propagation in free-space and makes light propagation research in this medium more difficult.

Molecular Optical Simulation Environment (MOSE) is a simulation platform for optical molecular imaging research co-developed by Xidian University, Institute of Automation, Chinese Academy of Sciences, China and Virginia Tech–Wake Forest University School of Biomedical Engineering & Sciences, USA. MOSE is featured by implementing the simulation of near-infrared light propagation both in a medium with complicated shapes (such as a mouse) and in free-space. Up until now, MOSE has accomplished simulation of light propagation both in a medium and in free-space under CW, TD, and FD, thus it is a powerful tool to solve the forward problems in DOT, FMT, and BLT. This manual will help users learn how to use MOSE, and more detailed information will be introduced in the following sections. The solution of the inverse problem remains under investigation and will be added in a future version.

1.2 New Features

Compared to the previous version 2.2, the updates for version 2.3 are as follows:
1. Add support to the simulation of fiber-optic endoscope at the inner tissue.
2. Add some new parameters and the version of the parameter file has been updated to 2.3.

The latest version still supports the older versions of the parameter file.

3. Change the way of output of the detector result under CW simulation. First, output the result of the plane detector, followed by the result of fiber detector.
4. Fix the errors of the simulation property input dialog.
5. Fix some other errors, enhance the stability of the software to run, and improve the efficiency of the algorithm.

1.3 Feature List of Version 2.3

1. Support three kinds of forward simulations in optical molecular imaging: BLT, DOT, and FMT. The simulation algorithms are based on the MC method.
2. Support three kinds of simulation modes: CW, TD, and FD.
3. Support the description of the medium with a regular shape (ellipse, rectangle) under 2D, regular shape (ellipsoid, cylinder, cube) under 3D and irregular shape (the boundary is described by a triangle mesh; for example, data in PLY, OFF, SURF, MESH, and AM formats), and it's helpful for the users to implement the MC simulation under a complex medium.
4. Support the simulation of light propagation in free-space to the panel detector (such as CCD) under CW. The algorithm is based on the theory of pinhole imaging and Lambert's cosine law.
5. Support the simulation of light propagation in medium to the fiber-endoscopic detector under CW.
6. Support the function of mapping the 2D detection results from a multi-angle to the 3D surface of the complex medium.
7. Support Windows and Linux systems.
8. Support multi-thread optical simulation using the OpenMP API.
9. Absorption results can be saved as photon absorption or photon flux density.
10. Support threshold extraction of the medical image data. Users can extract the boundaries of different organs based on the threshold setting (the data can be used in the MC simulation).
11. Support simplification of the trianglar mesh, where it can reduce the mesh number effectively.
12. Support boundary extraction of the tetrahedral mesh.
13. A rich image display mainly includes:
    1) The display properties of the tissues can be set independently, including color, transparency, solid/wireframe display, and whether or not to use a display.
    2) There are two ways to show simulation results (absorption and transmittance results): Point rendering-based and surface rendering-based.
    3) It can display multiple layers (parallel to the XY, YZ or XZ plane) of the absorption results simultaneously which is helpful for users to quickly analyze the simulation results.
14. Support the input and output of the parameter and result files under various types of simulation. All of the files are managed by the project file (.MSE).
15. Add Plane Detector and Fiber Detector.

1.4 Install and Uninstall

System requirements: Windows 2000/XP/Vista/7 or Ubuntu 10.04/10.10.

Install: Download the latest version of MOSE from http://www.mosetm.net. MOSE is green software, no installation is required, and it can be used directly after decompression. User needs to choose the correct version (32-Bit or 64-Bit) according to the system.

Uninstall: Since MOSE is green software, you can uninstall it after deleting the folder of MOSE directly.

2 Detailed Specification

This chapter will conduct a more detailed description of use, including four sections: project, optical molecular imaging, 2D-3D energy mapping and image processing.

2.1 Project

In MOSE, all functions are managed independently by the project. At present, MOSE contains three project types: optical molecular imaging, 2D-3D energy mapping and image processing. These three project types have different functions respectively as follows:

1. Optical Molecular Imaging: Contains three types of forward simulation of optical molecular imaging such as: BLT, FMT, and DOT.
2. 2D-3D Energy Mapping: Contains the function of mapping the 2D detection results captured by CCD to the 3D surface of the heterogeneous medium.
3. Image Processing: Contains threshold extraction of raw CT data, mesh simplification and boundary extraction of the tetrahedral mesh.

As shown in Figure 1, there are two options including 'New Project' or 'Open Project,' which can be chosen after MOSE is started.

New Project: Build a new project object, as shown in Figure 2. The purpose of building the project is to facilitate unified management of the data related to the simulation. Each individual project corresponds to a separate folder. Project name and project path are set freely by the users.

After clicking OK, a project folder in the project path will be generated. The folder contains a project file (suffix .mpj). Please do not modify the project file to avoid unknown errors.

Open Project: Open an existing project object, including various data generated by the simulation as shown in Figure 3.
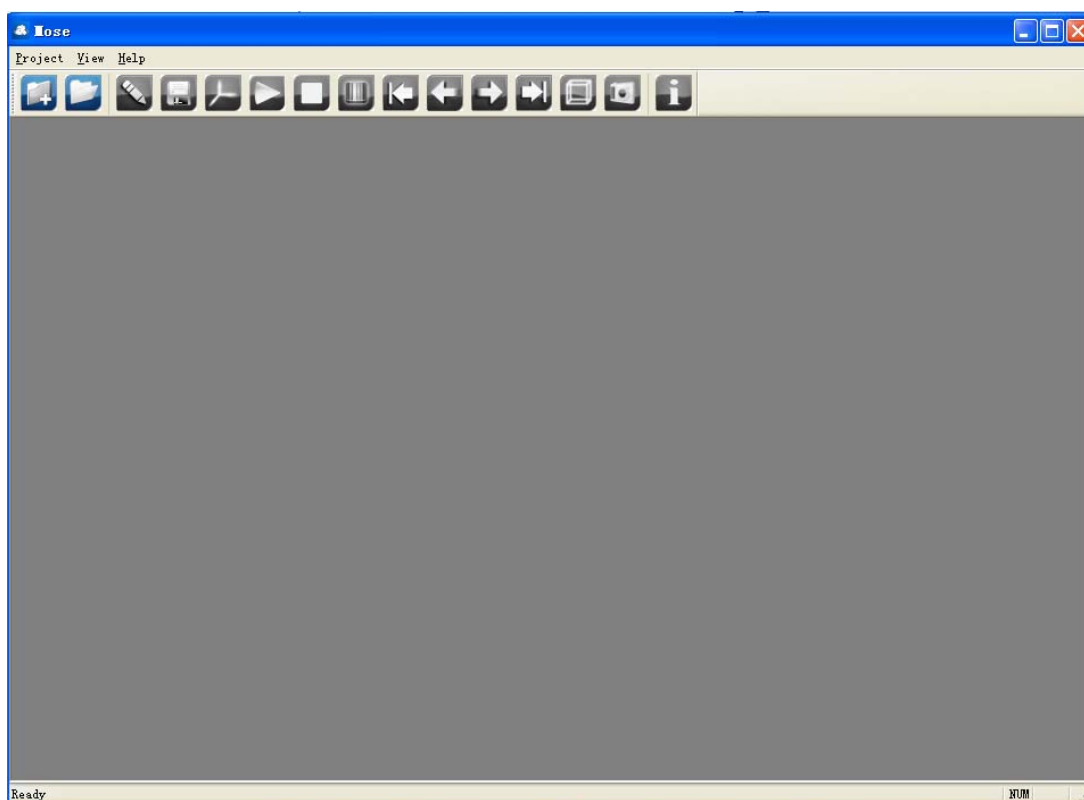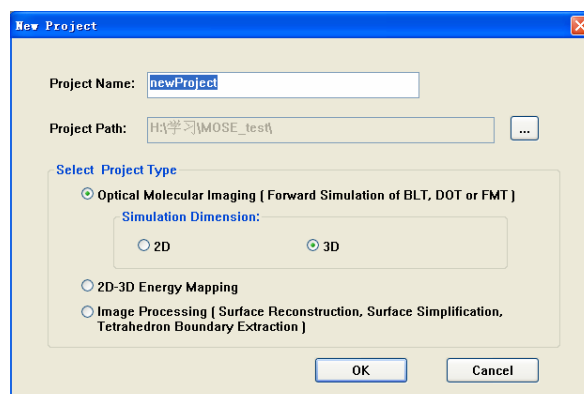
Figure 1 Start MOSE.
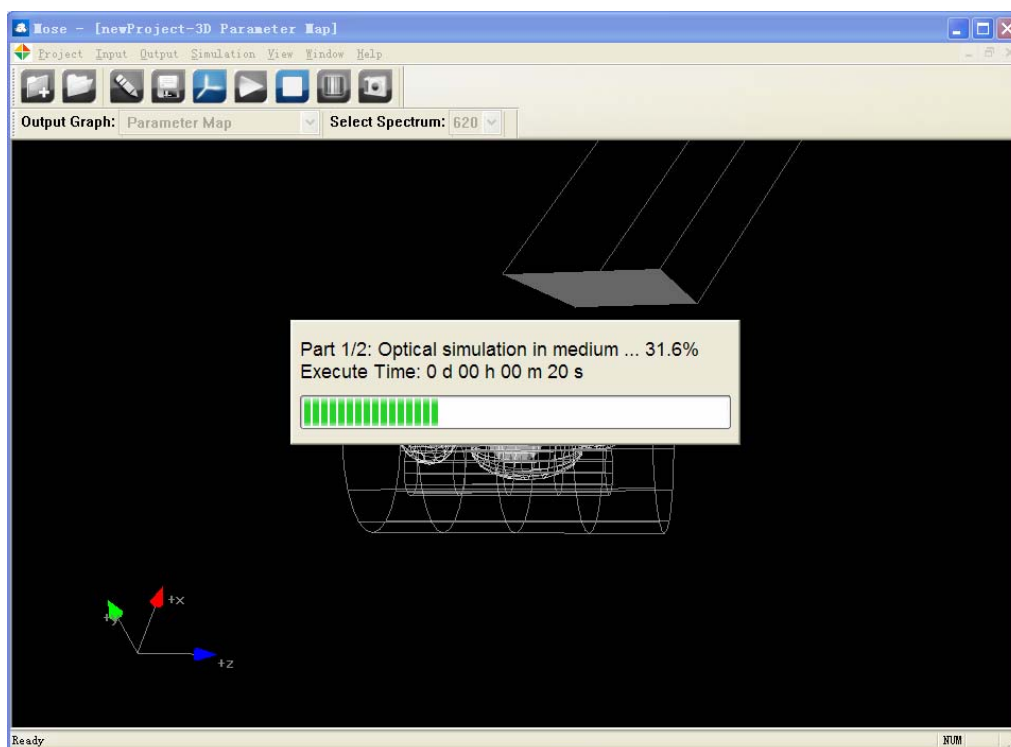

Figure 2 Build a new project.

Figure 3 Open a project.

2.2 Optical Molecular Imaging

2.2.1 Introduction of the Interface

The window interface of the optical molecular imaging project is shown in Figure 4.
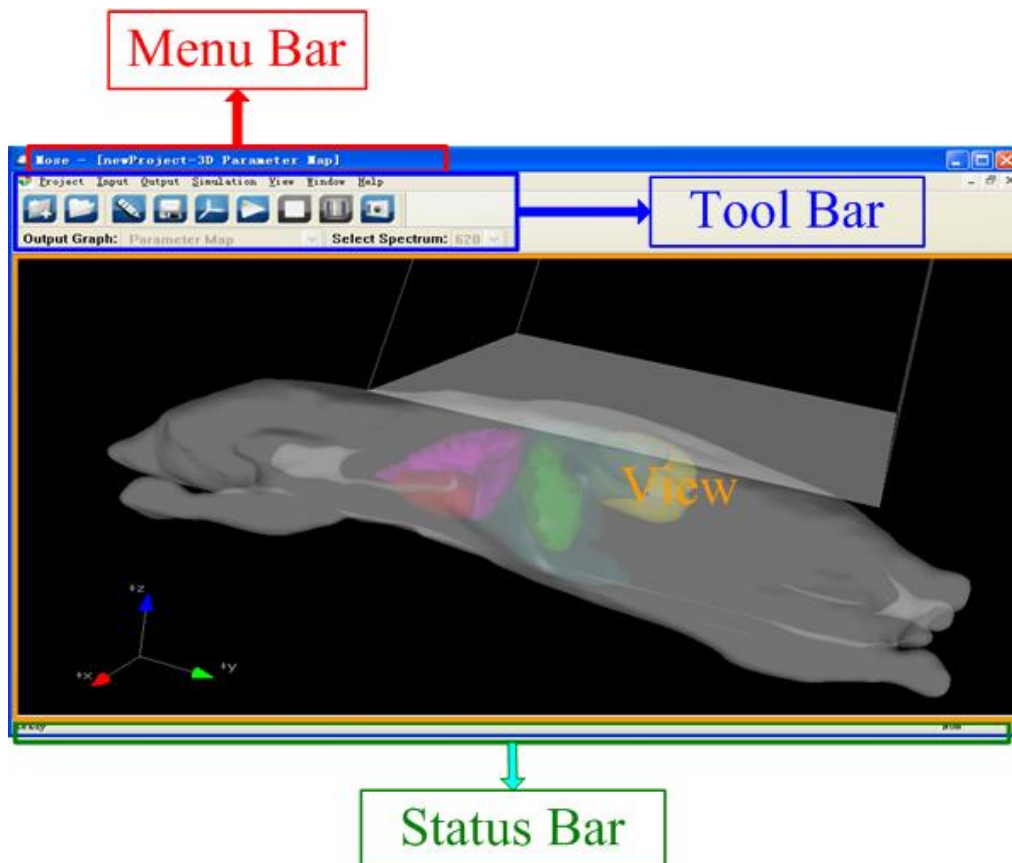
Figure 4 Main interface of MOSE.

The interface mainly includes five parts: menu, function button, view area, and status bar.

Menu bar: Menu bar includes all of the basic operations of MOSE, but it mainly includes project operation (new, open, close), parameter input, result output, simulation control (start and stop), graphic display control, operation of display window and so on.

Tool bar: Some commonly used commands are arranged on the toolbar.

View area: Display all of the parameters and results.

Status bar: Show the progress while writing or reading the simulation results.

2.2.1.1 Menu Bar

The upper part of the main interface ranks a list of menus. Each menu has different functions. The following section is the detailed description of each function menu item.

·**Project**

New

Create a new project.

Open

Open an existing project.

Close

Close the current project.

Exit

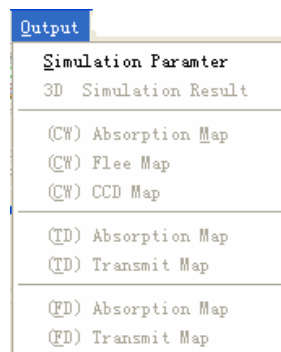Exit MOSE.

·**Input**
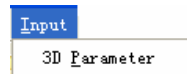
Input
3D Parameter

3D Parameter

Input the simulation parameters into a 3D environment. Please see Chapter 3 for parameter file format.

·**Output**

Output
Simulation Paramter
3D Simulation Result
(CW) Absorption Map
(CW) Flee Map
(CW) CCD Map
(TD) Absorption Map
(TD) Transmit Map
(FD) Absorption Map
(FD) Transmit Map

Simulation Parameter

Output the simulation parameters used in the current simulation to the constructed project folder, where the document suffix is .MSE.

3D Simulation Result

After completing the simulation, output the simulation results to the constructed project folder, including the absorption results, transmission results, and detection results.

(CW) Absorption Map

Display the photon absorption map under CW.

(CW) Transmittance Map

Display the photon transmittance map under CW.

(CW) CCD Map

Display the detection map captured by CCD (this function can only be chosen in 3D CW).

(TD) Absorption Map

Display the photon absorption map under TD.

(TD) Transmit Map
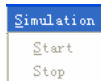
Display the photon transmittance map under TD.

(FD) Absorption Map

Display the photon absorption map under FD (amplitude and phase, respectively).

(FD) Transmit Map

Display the photon transmittance map under FD (amplitude and phase, respectively).

·**Simulation**

Start

Start the simulation.

Stop

Stop the simulation during the simulation process, and the program will return a warning if there is failure.
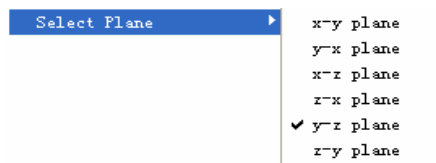
·**View**

Toolbar

Set whether or not you want to display the function button bar.

Status Bar

Set whether or not you want to display the function button bar.

Select Plane

Set the coordinate system of the view, including 'XOY,''YOX ,' 'XOZ,' 'ZOX,' 'YOZ,' and 'ZOY.'

Background Color

Set the background color of the view area. There are three colors to choose from, including black, white, and gray.

Color Bar

There are five options to choose from, as shown in Figure 5, including 'Jet,' 'Autumn,' 'Spring,' 'Hot,' and 'Cool.'
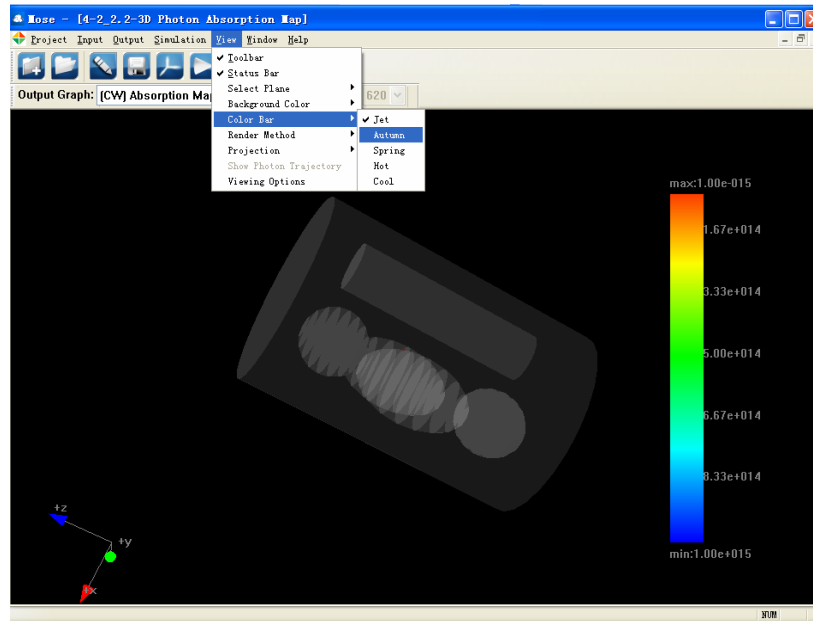
Figure 5 Setting the color bar.

Render Method

The render method includes point-based and face-based options. The point-based one adopts interpolation processing. In the surface-based one, each face has a single color. Figure 6 and 7 shows the effect of the two kinds of render methods.
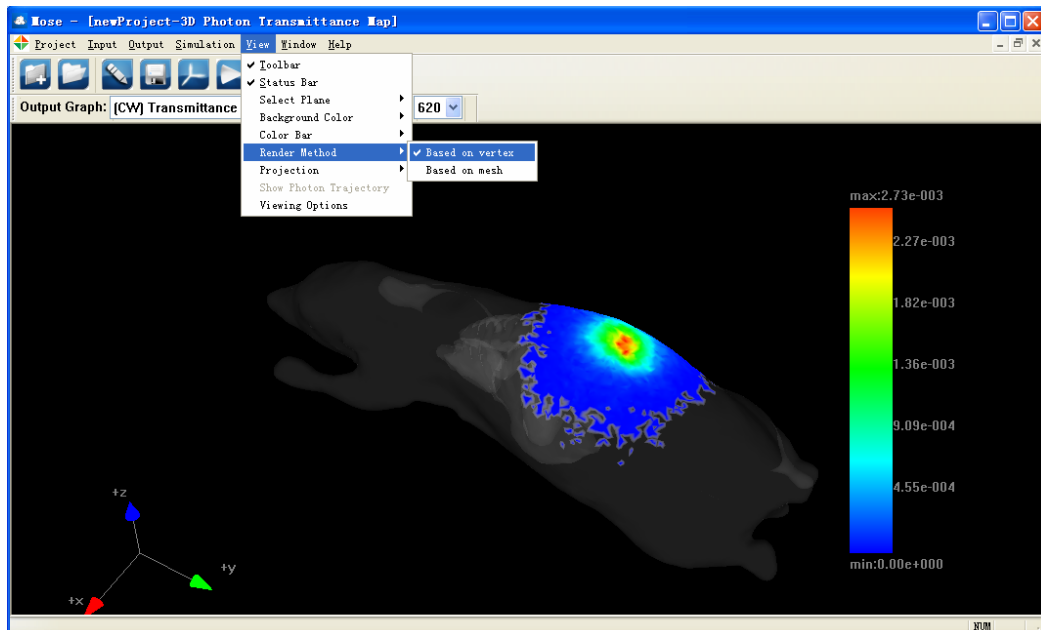

Figure 6 Point-based rendering.

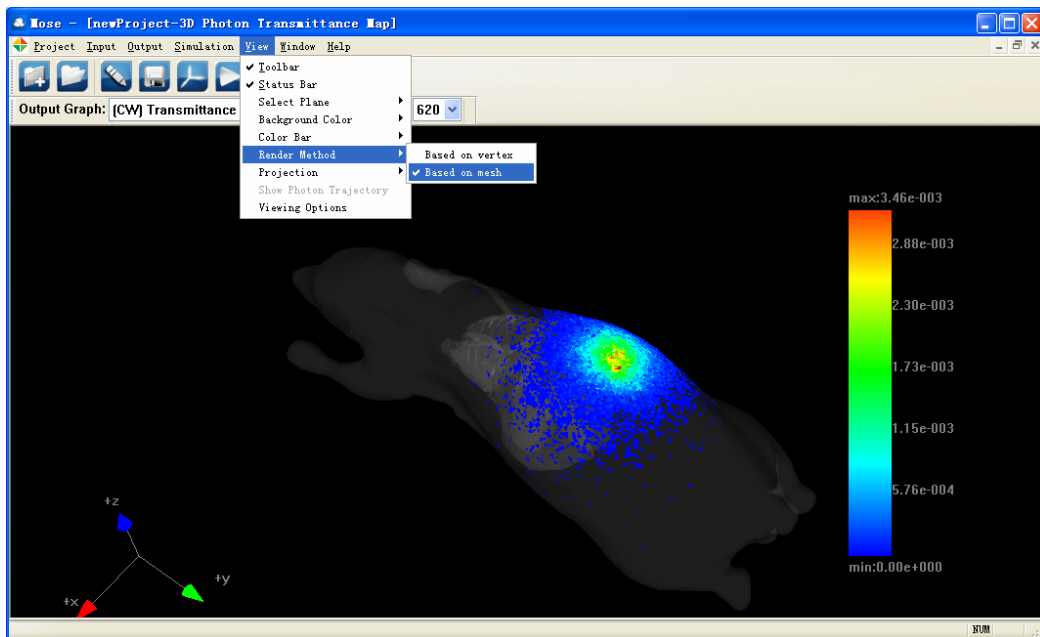9

Figure 7 Surface-based rendering.

Projection

Set the projection method in 3D, including the perspective projection and orthographic projection. The effects are displayed in Figures 8 and 9 respectively.
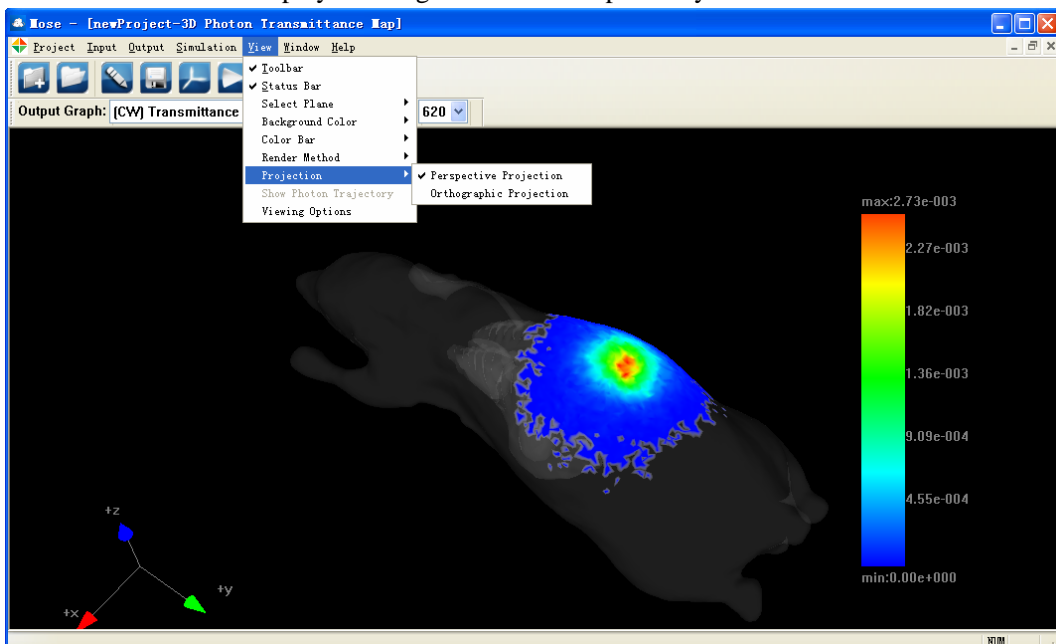

Figure 8 Perspective projection.
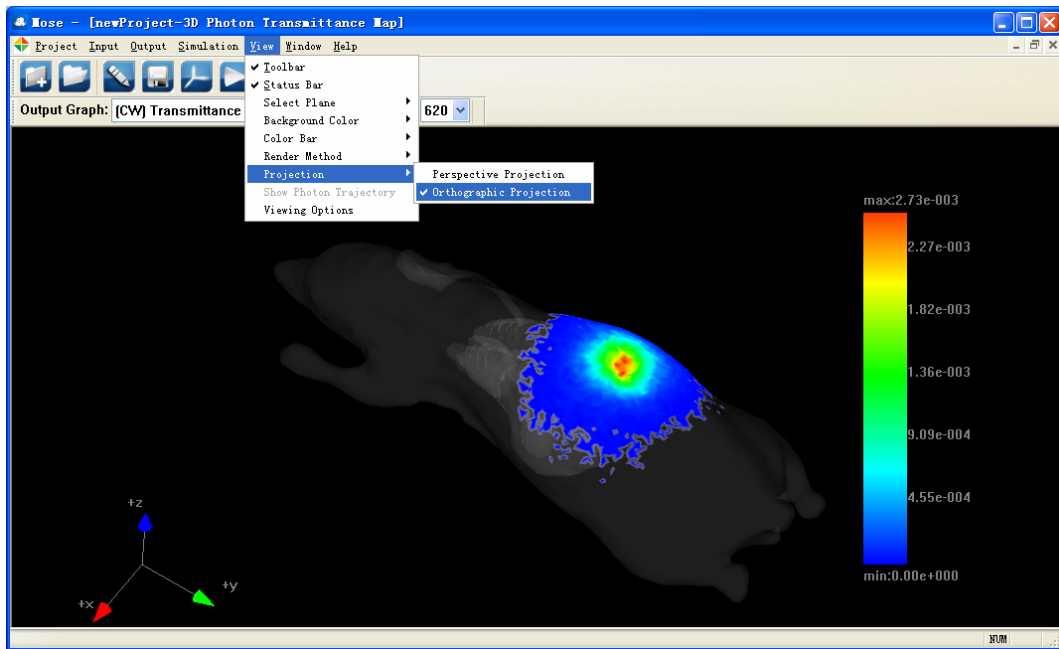
Figure 9 Orthographic projection.

Show Photon Trajectory

Set whether or not to show the photon running path in the process of simulation. After setting it, the view will display the path of each photon running. However, this will largely reduce the simulation speed. Do not suggest users to set this item. The result is displayed in Figure 10.

Figure 10 Show photon trajectory.

Viewing Options

Set display properties of the medium, the light source and the detector in different types of maps (parameter map, absorption map, and transmittance map), including color, opacity, and show/hide and solid/wireframe as shown in Figures 11 and 12.
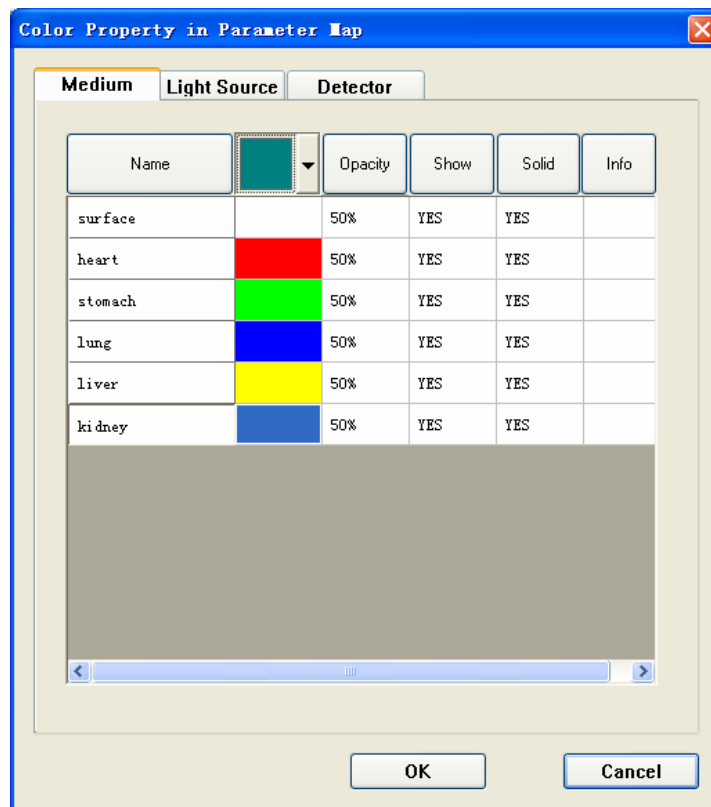
Figure 11 Display properties setting.
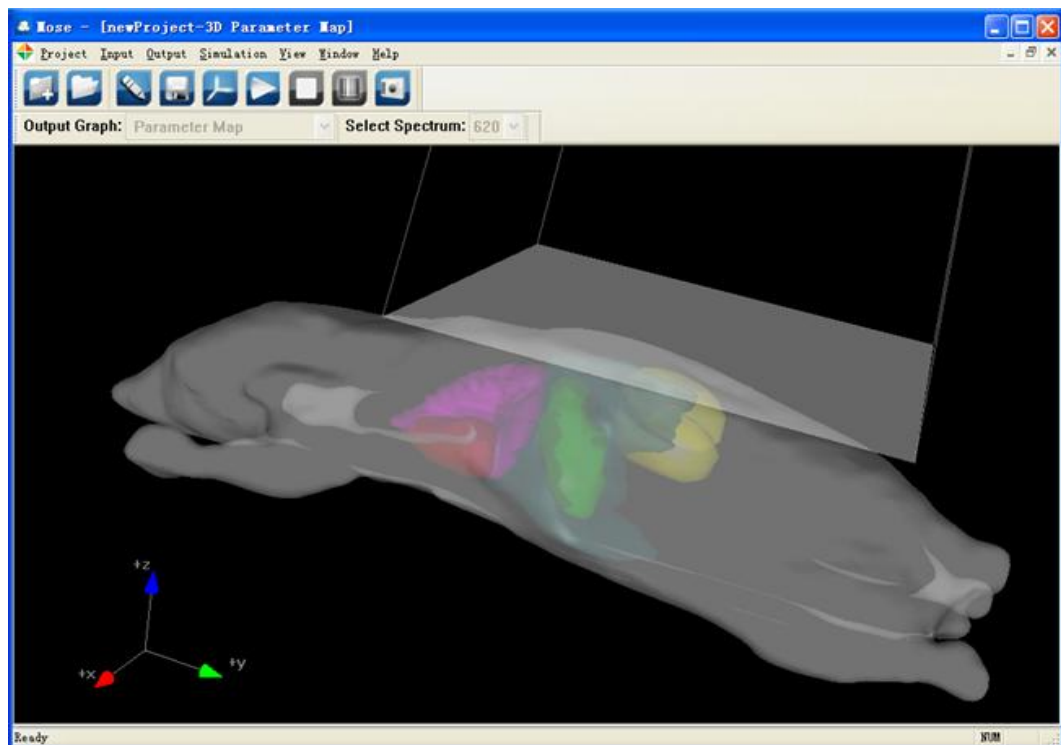
Figure 12 Display properties rendering.
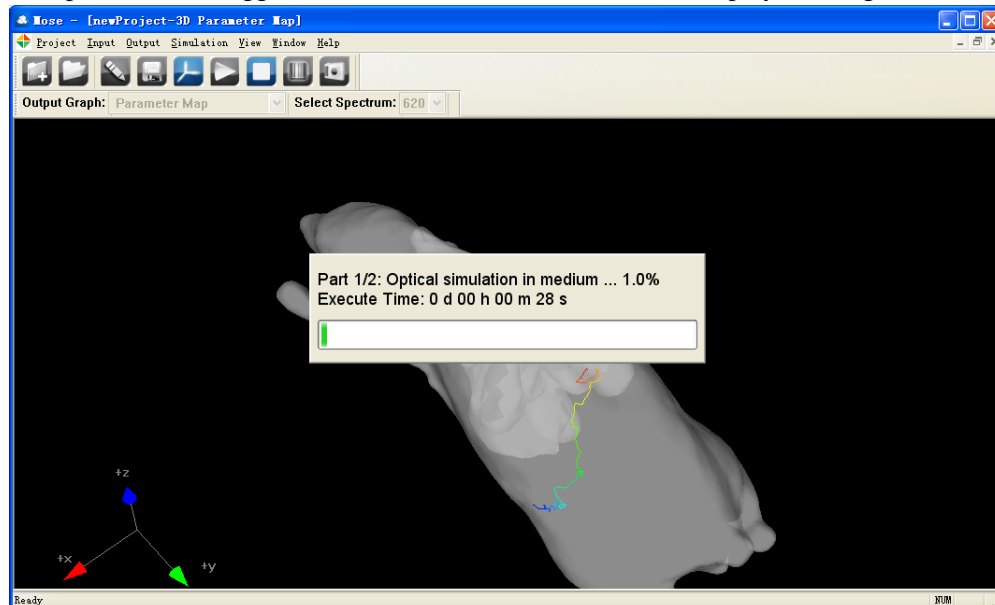
·Window
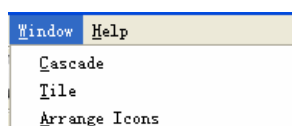
Set the view's layout.

Cascade

View cascade.

Tile

View tile.

Arrange Icons

Arrange Icons.

·Help
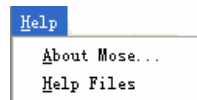
About MOSE

Display the version and copyright information for MOSE.

Help Files

Show the help file for MOSE.

2.2.1.2 Tool Bar

The toolbar is a series of function button combinations, which provides a shortcut method to perform common commands.

Table 1 Description of the toolbar

Icon	Function
	New project
	Open project
	Input parameters
	Save parameters/results
	Reset coordinate axis
	Start simulation
	Stop simulation
	Show/Hide colorbar
	Screenshot

2.2.1.3 View Area

View area is the display area, mainly responsible for displaying the simulation parameters and the simulation results as shown in Figure 13.
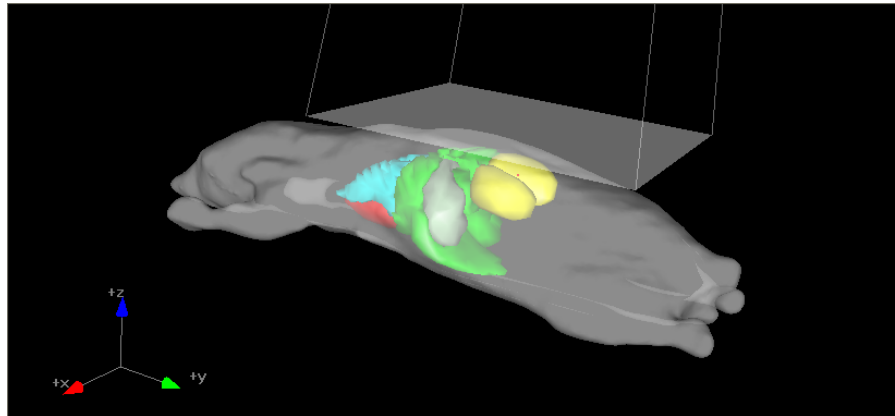
Figure 13 View area.

Some operations of the view area have been introduced in the section of the menu bar. In addition, clicking the right, middle and left mouse buttons can operate the rotation, move, and enlarge/reduce operations respectively. The simulation parameters map, photon absorption map, photon transmittance map and photon detection map can be selected from the output menu or output graph on the toolbar as shown in Figure 14.
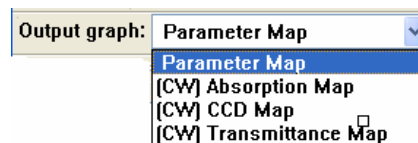
Figure 14 View area operations.

2.2.1.5 Status Bar

The main function of the status bar is to display the progress information while saving or reading the simulation results as shown in Figure 15.
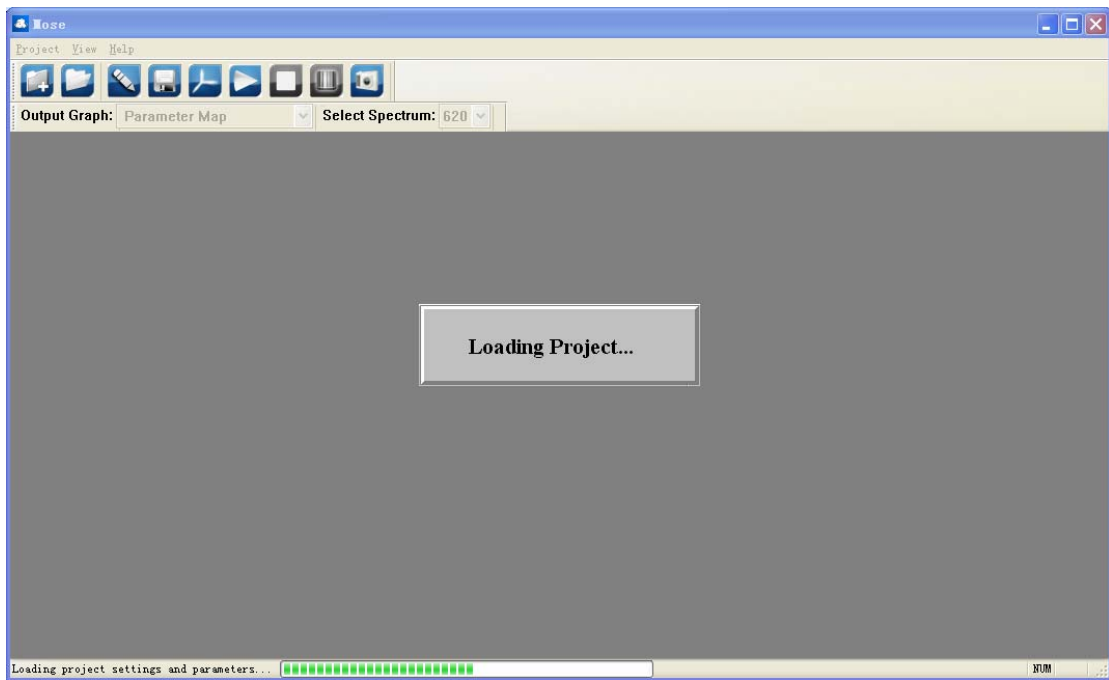
Figure 15 Status bar.

2.2.2 Simulation Example

2.2.2.1 New Project

Users need to choose the optical molecular imaging project and space dimension in the 'New Project' page. For example, Figure 16 shows the interface after users choose the optical molecular imaging project under a 3D environment and click 'OK.'
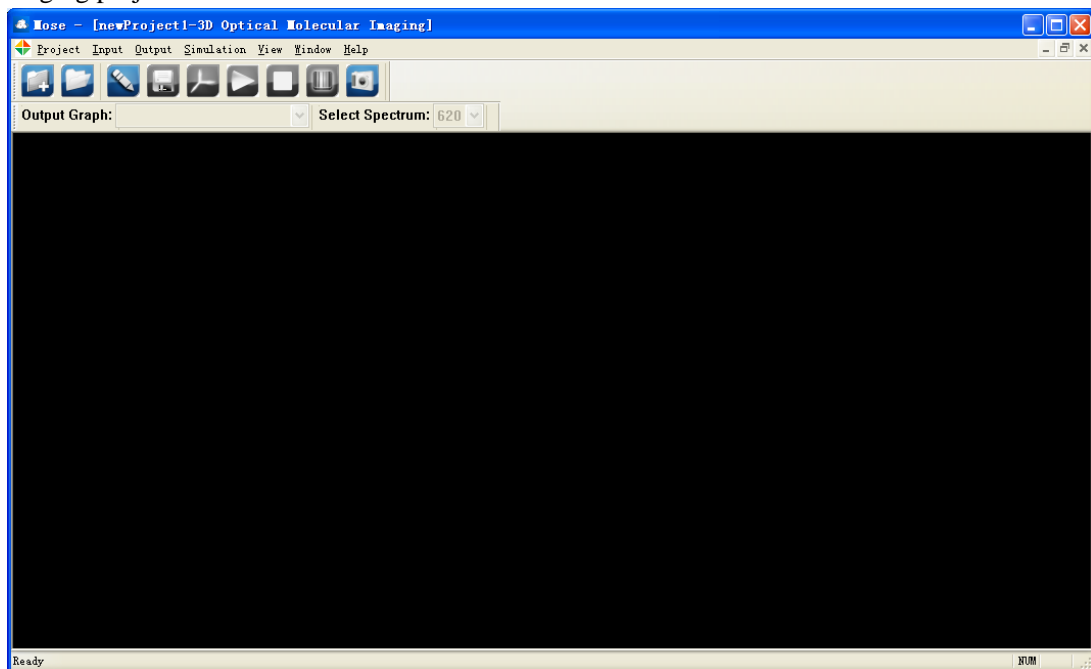
Figure 16 Interface of the optical molecular imaging project under a 3D environment.

2.2.2.2 Input Simulation Parameters

Input parameters have the same steps in both a 2D and 3D environment. We only discuss the 3D environment as an example. Select the '**Input-3D Parameter**,' and the Parameter settings dialog box pops up as shown in Figure 17. The dialog box has four different sub-pages: **Medium**, **Light Source**, **Detector**, and **Simulation Property**. There are two ways to set the simulation parameters: Parameter file input and dialog box input. They are described separately below.

NOTE: After updating to version 2.2, the support of the tetrahedral structure data is added, which is propitious to the comparison between MOSE and the finite element method. However, optical simulation only supports the way that a parameter file is inputted, while the medium is constructed by a tetrahedral mesh in version 2.2.
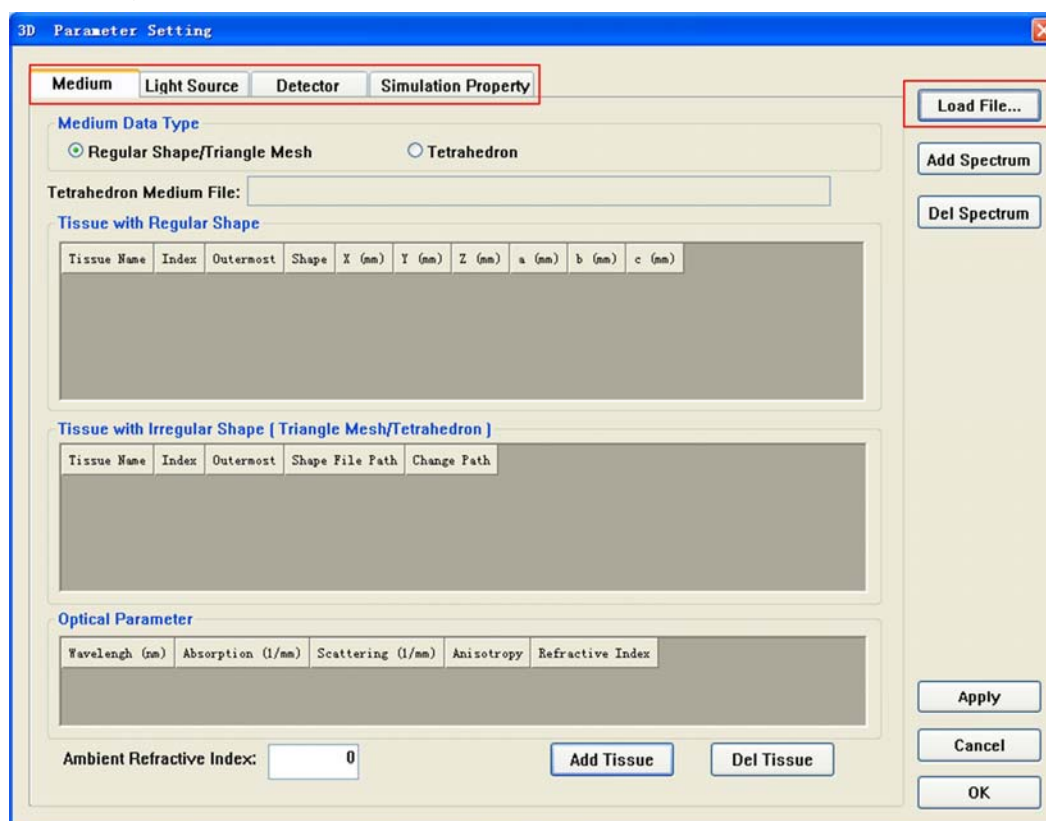
Figure 17 Main interface of the parameter setting.

2.2.2.2.1 Parameter File Input

Click '**Load File**,' import the simulation parameter file from the external shown as Figure 18. MOSE sets a fixed format for the parameter file, while users need to set the parameter file according to the file format requirements. For a specific parameter file format, see Chapter 3. After loading the parameter file, users can still modify the parameters in the '**Parameter Setting**' dialog box.

The page of the medium properties will be different based on the differences in the medium model:

1) After loading the "Independent medium model" (regular shape or triangle mesh), the media properties page is shown in Figure 18(a);

2) After loading the "Integral medium model" (tetrahedral mesh), the media properties page

is shown in Figure 18(b).

(a) Load the "Independent medium model."

(b) Load the "Integral medium model."

Figure 18 Dialog box of loading the parameter file.

2.2.2.2.2 Dialog Box Input

User can also set various simulation parameters through the dialog box interface. The functions of various buttons on each sub-page are described below, including 5 parts: the main interface of the parameter setting, the medium interface, the light source interface, the detector interface and the interface of the simulation properties.

1. Main Interface of the Parameter Setting

Click '**Add spectrum**,' where users can add a new spectrum as shown in Figure 19. Due to the different optical parameters among different spectra, users should enter the optical parameters of the tissues and source parameters corresponding to the new spectrum.

Figure 19 Dialog box of adding a new spectrum.

Click '**Del Spectrum**,' users can delete the selected spectrum shown as Figure 20. Click "OK," and all of the optical parameters of the tissues and the source parameters corresponding to the spectrum will be deleted.

Figure 20 Dialog box of deleting a spectrum.

Click '**Apply**,' and users will save all of the parameters in the interface.

Click '**Cancel**,' and users will quit the '**Parameter Setting**' dialog box without saving the parameters.

Click '**OK**,' and users will save all of the parameters and quit the '**Parameter Setting**' dialog box.

2. Medium Interface

In MOSE, the simulation object is defined as medium, and it consists of a homogeneous medium (contains only one tissue) and heterogeneous medium (contains more than one tissue). Parameters used to define the tissue consist of the shape and optical parameters. The shape can be

regular (2D: rectangle, ellipse; 3D: cube, ellipsoid, cylinder) or irregular (triangle mesh). The optical parameters of the tissue consist of the absorption coefficient, scattering coefficient, anisotropy factor and refractive index.

As shown in Figure 21, the first list in the medium interface displays the parameters of the tissues with regular shapes, the second list in the medium interface displays the parameters of tissues with irregular shapes, and the last list in the medium interface displays the optical parameters of the tissue chosen by users. In addition, the refractive index of the ambient can be set at the bottom of the medium interface (Ambient Refractive Index).
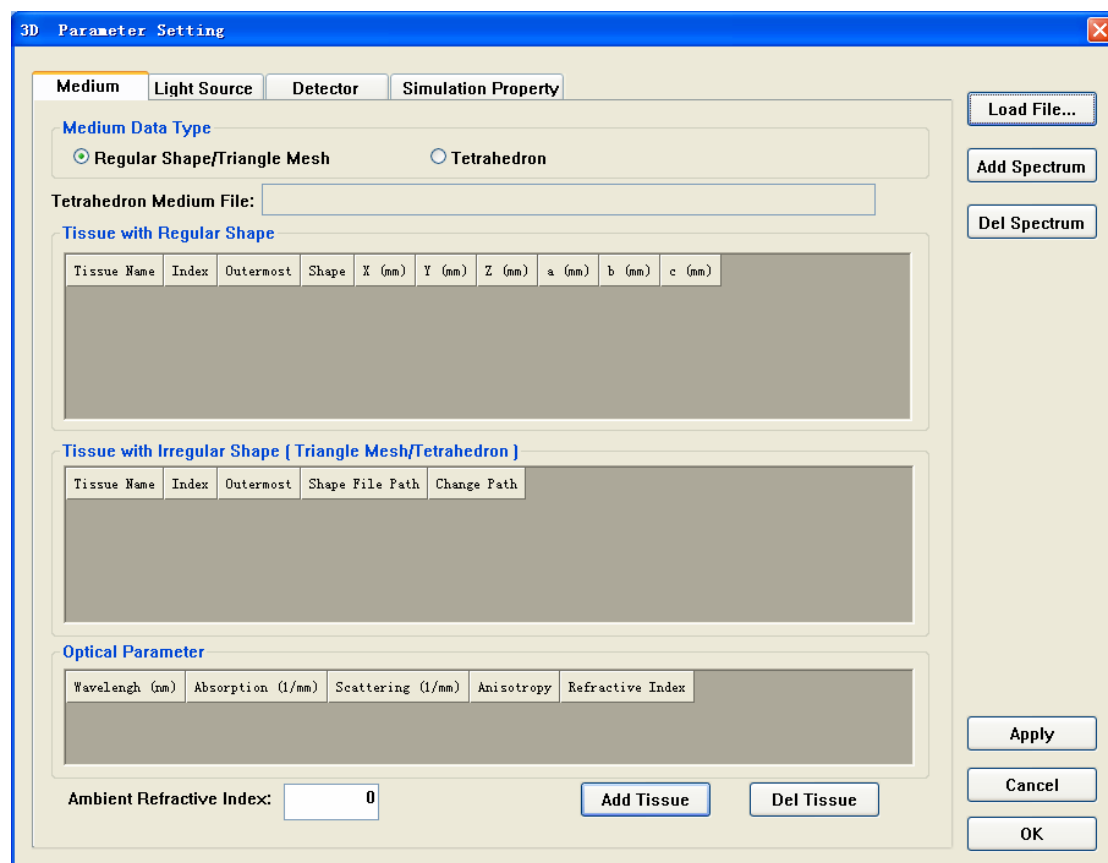
Figure 21 Interface of the setting of the tissue parameters.

Table 2 Description of the parameters of a tissue with a regular shape

Tissue Name	The name of the tissue.
Index	The number of the tissue on the tissue list of the medium.
Outermost	Outermost flag: The flag is 'Yes' if the tissue is the outermost one in the tissue list of the medium. The outermost tissue has the largest bounding box and other tissues are inside of it. In the parameter setting of the medium, the outermost tissue must be only one, otherwise the simulation may fail.
Shape	The shape of the tissue may be regular (2D: rectangle, ellipse; 3D: cube, Ellipsoid, cylinder) or irregular (triangle mesh).
X (mm)	The central coordinate of the tissue shape along the X-axis. (**NOTE**: All units of length in MOSE are in millimeters)
Y (mm)	The central coordinate of the tissue shape along the Y-axis.

Z (mm)	The central coordinate of the tissue shape along the Z-axis.
a (mm)	Half of the axis length of the tissue shape along the X-axis. (**NOTE**: half of the axis length has different meanings based on the different shape, so please refer to Figures 63 and 64 in Section 3.2.2)
b (mm)	Half of the axis length of the tissue shape along the Y-axis.
c (mm)	Half of the axis length of the tissue shape along the Z-axis.

Table 3 Description of the parameters of the tissue with irregular shape

Tissue Name	The name of the tissue.
Index	The number of the tissue on the tissue list of the medium.
Outermost	Outermost flag.
Shape File Path	The path of the triangle mesh file used to describe the surface of the tissue. The file format can be PLY/OFF/SURF/MESH.
Change Path	Change the path of the triangle mesh file.

Table 4 Description of the optical parameters of the tissue

Wavelength	The central wavelength of the spectrum.
Absorption	Absorption coefficient.
Scattering	Scattering coefficient.
Anisotropy	Anisotropy factor.
Refractive Index	Refractive index.

Click '**Add Tissue**,' and the selection dialog box '**Shape Type**' will pop up as shown in Figure 22.

Click '**Del Tissue**,' and the shape parameters and optical parameters of the tissue selected in the list will be deleted.

Figure 22 Selection dialog box of the tissue shape

After selecting the type of shape, users will enter the interface shown in Figure 23 or 24. Figure 23 shows the added interface of the tissue with a regular shape, corresponding to Tables 2 and 4. Figure 24 shows the added interface of the tissue with an irregular shape, corresponding to Tables 3 and 4.

Figure 23 Dialog box for adding a tissue with a regular shape.

Figure 24 Dialog box for adding a tissue with an irregular shape.

3. Light Source Interface

The page for setting a light parameter is the same as that for a tissue in a specific structure as shown in Figure 25. The first list displays the parameters corresponding to the light source with a regular shape, the second list displays the parameters corresponding to the light source with an irregular shape, and the last list displays the optical parameters of the light source selected including the photon number, the energy of the spectrum, the excitation wavelength, the quantum yield, absorption factor, and life time (**NOTE**: The last four parameters only belong to the fluorescence in the forward simulation of FMT).
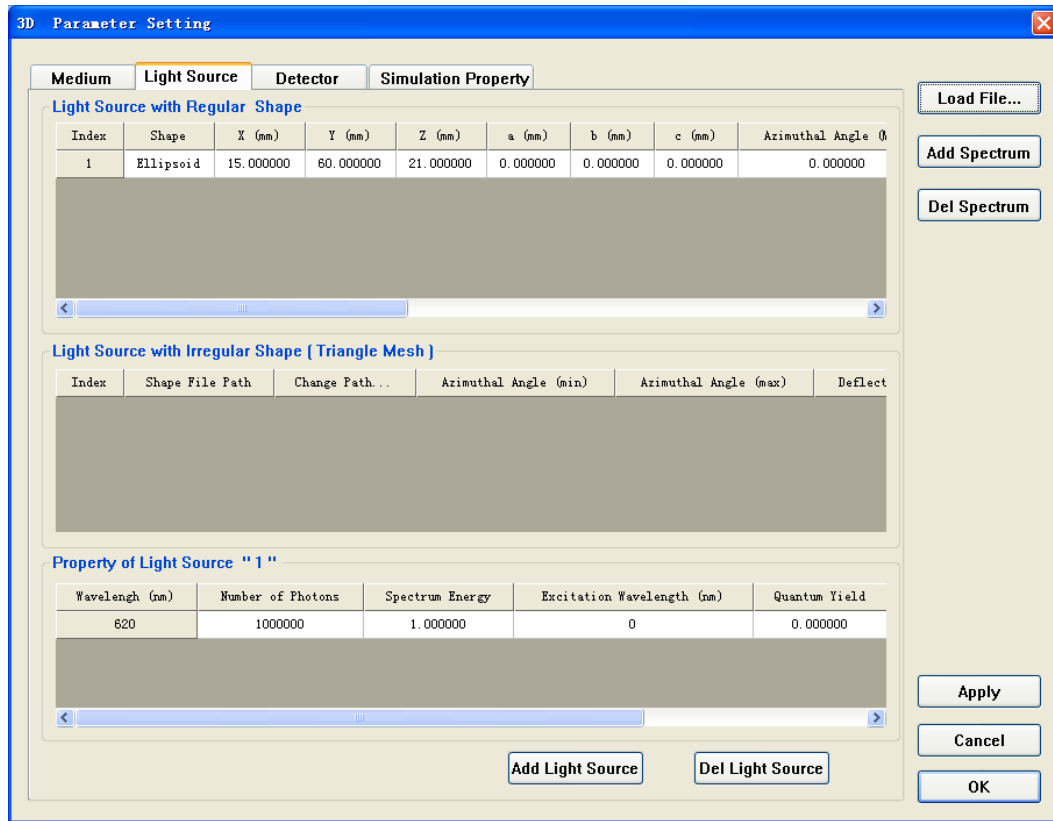
Figure 25 Interface of the setting of the light source parameters.

Table 5 Description of the parameters of the light source with a regular shape

Index	The number of the light source.
Shape	The shape of the light source.
X	The central coordinate of the tissue shape along the X-axis.
Y	The central coordinate of the tissue shape along the Y-axis.
Z	The central coordinate of the tissue shape along the Z-axis.
a	Half of the axis length of the tissue shape along the X-axis.
b	Half of the axis length of the tissue shape along the Y-axis.
c	Half of the axis length of the tissue shape along the Z-axis.
Azimuth Angle (Min)	The minimum azimuth angle of the emitted photon.
Azimuth Angle (Max)	The maximum azimuth angle of the emitted photon.
Deflection Angle (Min)	The minimum deflection angle of the emitted photon.
Deflection Angle (Max)	The maximum deflection angle of the emitted photon.
Internal	Flag: 'YES' means the light source is inside the medium. 'NO' means the light source is outside of the medium.
Solid	Flag: 'YES' means the photon is generated inside the shape or on the boundary of the shape of the light source. 'NO' means the photon is generated on the boundary of the shape.
Specular	Flag: 'YES' means the specular reflectance will happen while the light source is outside of the medium. 'NO' means no specular reflectance.
Luminous Type	Luminous type of the light source. There are four types in the

	latest version of MOSE, including BLT, DOT, FMT Excitation and FMT Emission. The luminous type of the light source must be in accordance with the simulation type (BLT, DOT, and FMT). In FMT, the luminous type of the light source can be set as 'FMT Excitation' or 'FMT Emission,' where 'FMT Excitation' means the light source is the incident laser and 'FMT Emission' means the light source is the fluorophore which will be excited by the incident laser.

Table 6 Description of the parameters of the light source with an irregular shape

Shape File Path	The path of the triangle mesh file used to describe the surface of the tissue. The file format can be PLY/OFF/SURF/MESH.
Change Path	Change the path of the triangle mesh file.
The rest parameters on the list are the same as that in Table 5.	

Table 7 Description of the optical parameters of the light source

Wavelength	The central wavelength of the spectrum (corresponds to the emission wavelength while the light source is a fluorophore in FMT).
Number of Photons	Number of photons corresponding to the spectrum (no need to set this parameter while the light source is a fluorophore in FMT).
Spectrum Energy	The energy of the light source corresponding to the spectrum (no need to set this parameter while the light source is a fluorophore in FMT).
Excitation Wavelength (nm)	The excitation wavelength of the fluorophore in FMT.
Quantum Yield	The quantum yield of the fluorescence in FMT.
Absorption Factor	The absorption factor of the fluorescence in FMT.
Life Time	The life time of the fluorescence in FMT (Unit: ps).

Click '**Add Light Source**,' and the selection dialog box "Shape Type" will pop up as shown in Figure 26.

Click '**Del Light Source**,' and the optical parameters of the light source selected in the list will be deleted.
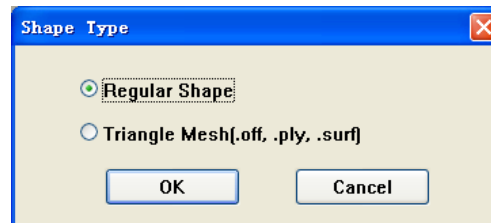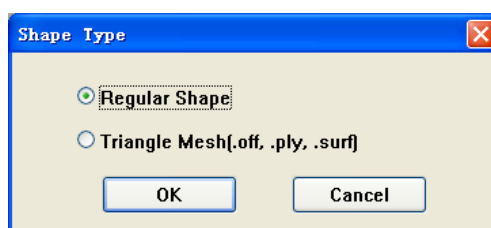

Figure 26 Selection dialog box of the light source shape.

After selecting the shape, users will enter the interface shown in Figure 27 or 28. Figure 27 shows the added interface of the light source with a regular shape, corresponding to Tables 5 and 7. Figure 28 shows the added interface of the light source with an irregular shape, corresponding to Tables 6 and 7.

Figure 27 Dialog box of the added light source with a regular shape.

Figure 28 Dialog box of the added light source with an irregular shape.

4. Detector Interface

As shown in Figure 29, the parameters of the detector and lens can be set on this sub-page. The parameters on the list are described in detail below.
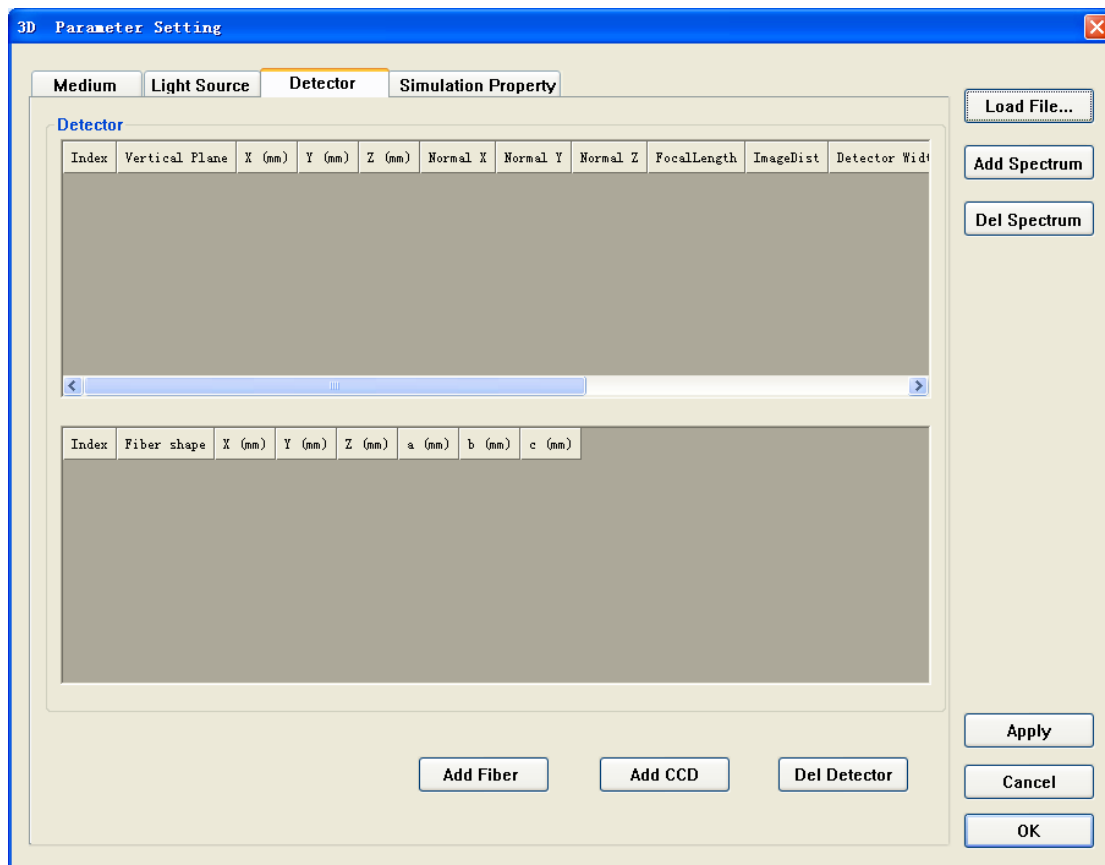
Figure 29 Interface of the setting of the detector parameters.

Table 8 Description of the CCD detector parameters

Vertical Plane	The plane of the detector that its perpendicular to (three options: XY, YZ, and ZX).
X	The central coordinate of the tissue shape along the X-axis.
Y	The central coordinate of the tissue shape along the Y-axis.
Z	The central coordinate of the tissue shape along the Z-axis.
Normal X	The normal vector of the detector plane along the X-axis (**NOTE**: All normal vectors must point to the medium for imaging).
Normal Y	The normal vector of the detector plane along the Y-axis.
Normal Z	The normal vector of the detector plane along the Z-axis.
Image Distance	The image distance of the detector.
Detector Width	The actual width of the detector.
Detector Height	The actual height of the detector.
Width Resolution	The resolution of the detector width.
Height Resolution	The resolution of the detector height.
Focal Length	The focal length of the lens.
Lens Radius	The radius of the lens.

Click 'Add CCD,' and users will enter the 'Add Detector' dialog box as shown in Figure 30.

Figure 30 Dialog box for adding the CCD detector.

Table 9 Description of the fiber detector parameters

Index	内窥探测器编号
fiber shape	内窥探测器的形状
X	The central coordinate of the fiber detector shape along the X-axis.
Y	The central coordinate of the fiber detector shape along the Y-axis.
Z	The central coordinate of the fiber detector shape along the Z-axis.
a	Half length of the fiber detector shape along the X-axis.
b	Half length of the fiber detector shape along the Y-axis.
c	Half length of the fiber detector shape along the Z-axis.

Click '**Add Fiber'**, and users will enter the 'Add Detector' dialog box as shown in Figure 31.
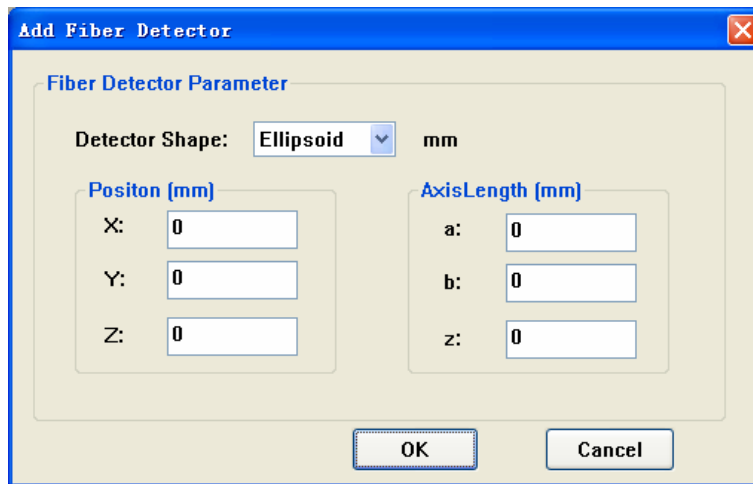
Figure 31 Dialog box for adding the fiber detector.

Click '**Del Detector**,' and the optical parameters of the detector selected from the list will be deleted.

5. Interface of the Simulation Property

On this sub-page, users can set the simulation properties of the light propagation in the medium and free-space as shown in Table 10.
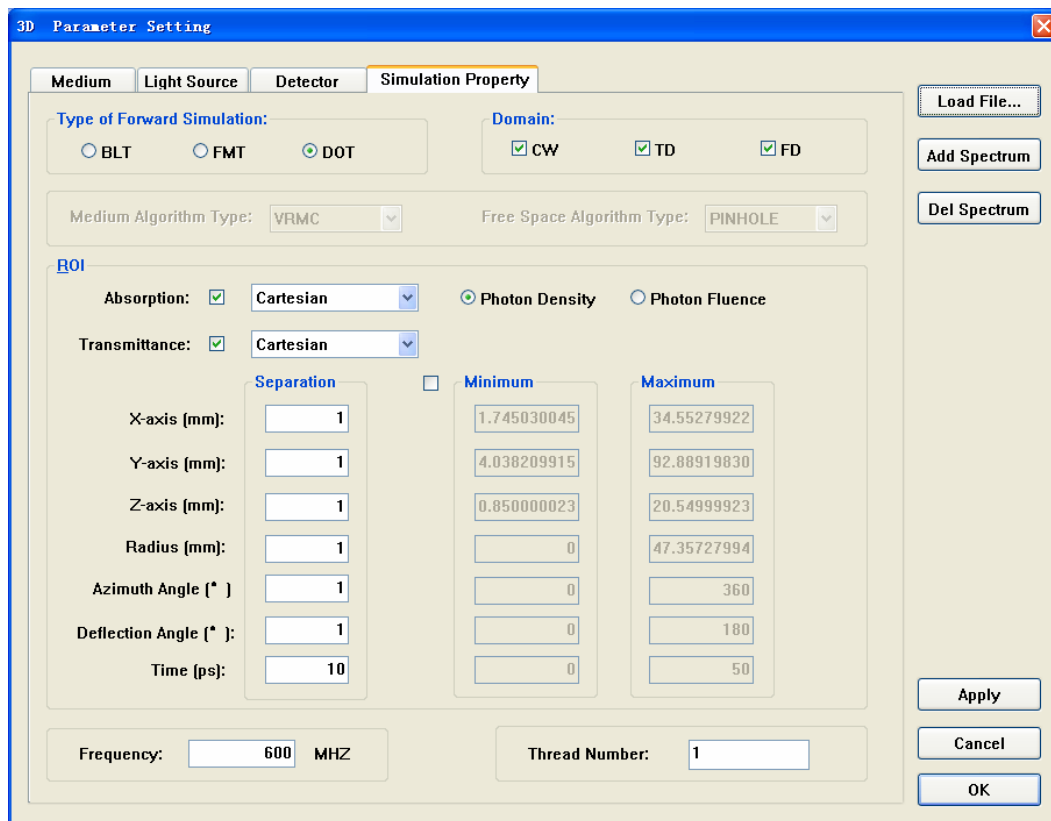
Figure 32 Interface for the setting of the simulation properties.

Table 10 Description of the simulation properties

Type of Forward Simulation	The type of the forward simulation, including BLT, DOT and FMT. Users can choose any one of these for each simulation.
Domain	Simulation domain including CW, TD, and FD. Users can choose all of these for each simulation.

Medium Algorithm Type		The simulation algorithm of light propagation in the medium. Currently, the algorithms only have the variance reduction Monte Carlo (VRMC).
Free-space Algorithm Type		The simulation algorithm of light propagation in free-space. Currently, the algorithm is based on a pinhole projection.
ROI	Absorption	Setting of the coordinate system (2D: Polar, Cartesian; 3D: Cartesian, Cylindrical) used to save the absorption results. The raw absorption results can be saved as the photon density or the photon fluence, and users need to choose one type.
	Transmittance	Setting of the coordinate system. The type of coordinate system is correlated to the shape of the medium. Currently, the type will be modified automatically by the program to avoid using the wrong setting.
	Separation	Setting of the separations in ROI along different directions, including the X-axis, Y-axis, Z-axis, radius, azimuth angle, deflection angle and time. Please refer to Figure 66 in Section 3.2.2.
	Minimum	Setting of the minimum values for the ROI.
	Maximum	Setting of the maximum values for the ROI.
Frequency (MHZ)		The modulating frequency under FD, where the unit is MHZ..
Thread Number		The thread number.

Users will enter the interface of the optical simulation shown in Figure 33 after finishing the parameter setting and clicking "OK" in the main interface of the parameter setting.
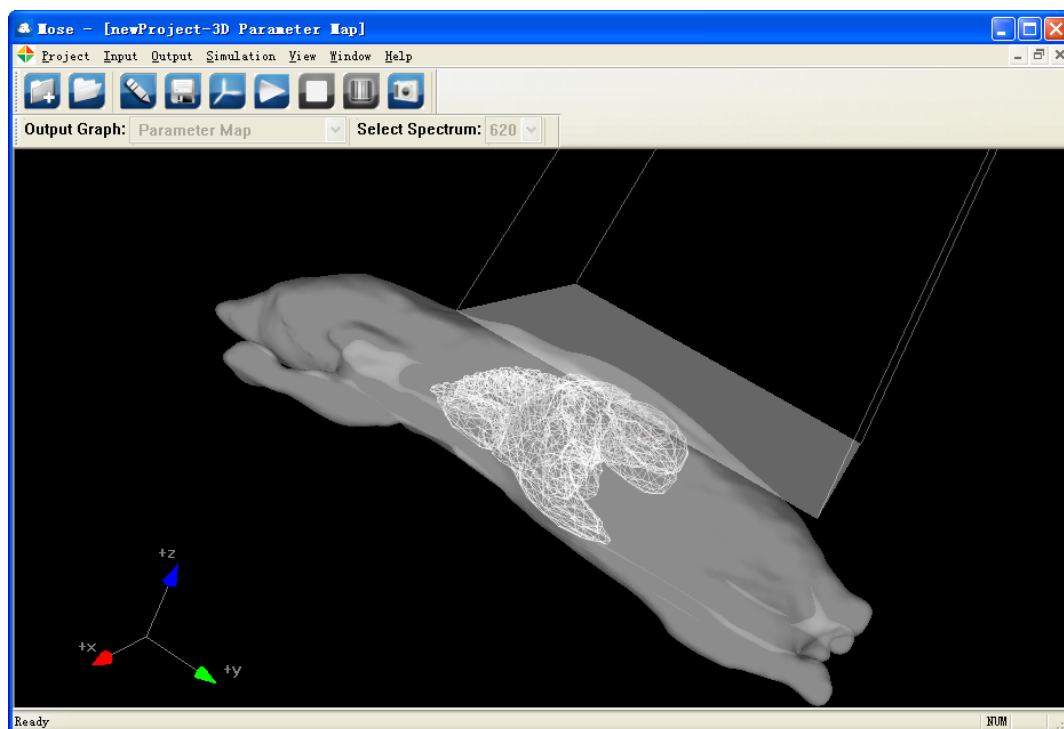
Figure 33 Interface after completing the parameter setting.

2.2.2.3 Start Simulation

The simulation will start after completing the parameter setting and clicking '**Simulation-Start**' on the menu bar or toolbar as shown in Figure 34. The running time and the percentage are shown on the progress bar which is used as a reference.
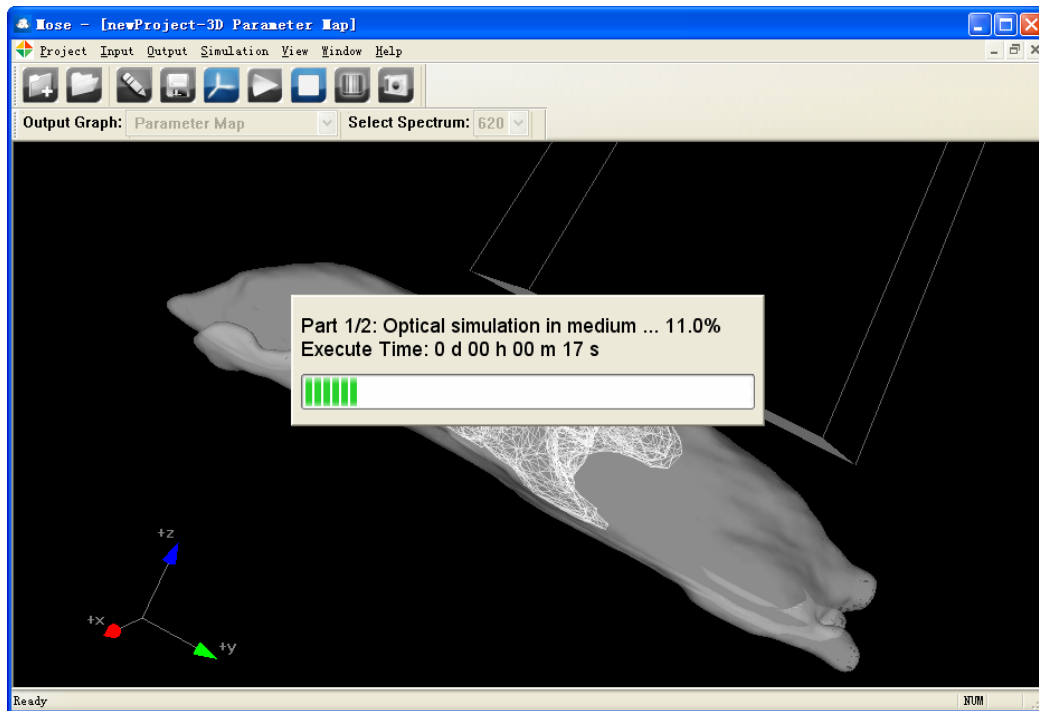
Figure 34 Interface for running the optical simulation.

In the meantime, users can click the shortcuts on the toolbar or select '**Simulation-Stop**' on the menu bar to stop the running operation, thus the simulation will end in failure.
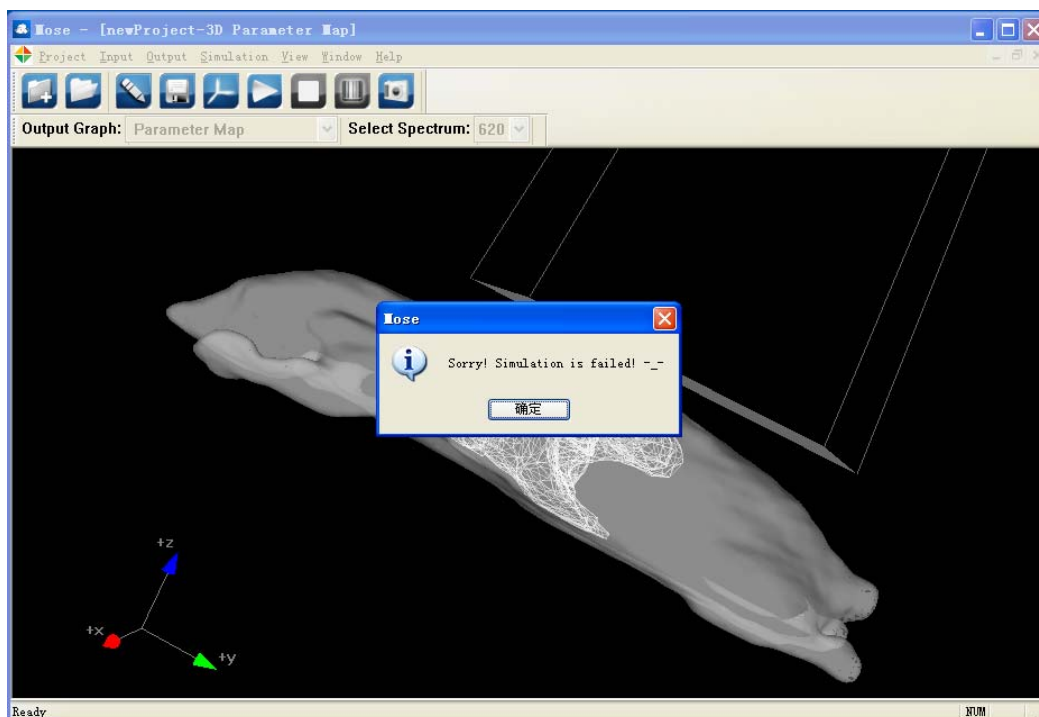
2.2.2.4 Output Simulation Results

Users can choose to output or show the simulation results successfully at the end of the simulation.

Output-Simulation Parameter: Output of the simulation parameters in the project folder.

Output-3D Simulation Result: Output of the simulation results placed in the project folder, including the absorption results, the transmittance results and the detection results.

Output-(CW/TD/FD) Transmit Map: To show the photon transmittance figures under CW, TD and FD respectively. Users can select the spectrum from the drop-down box as shown in Figure 36.
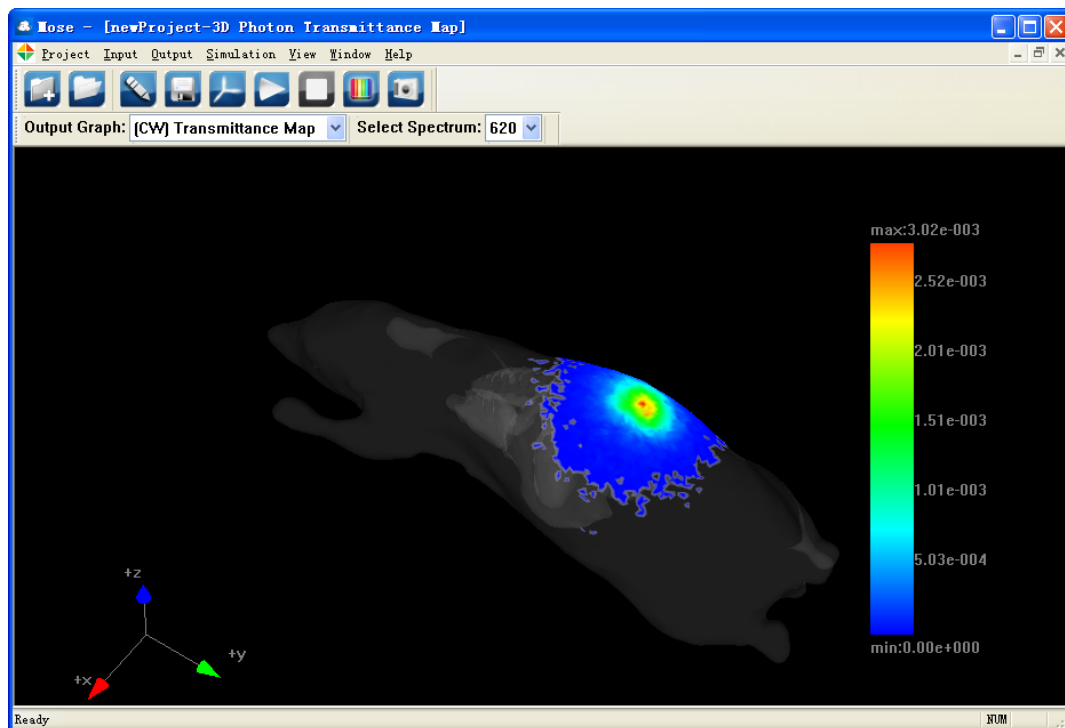
Figure 36 Photon transmittance figure.

Output-(CW) CCD Detector Map: To show the photon detection figure under CW, users can select the spectrum from the drop-down box **Select spectrum: 620** and select the detector number from the drop-down box **Detector Num: 1**, and the order of the numbers will be in accordance with the order of the detectors in the parameter file as shown in Figure 37.
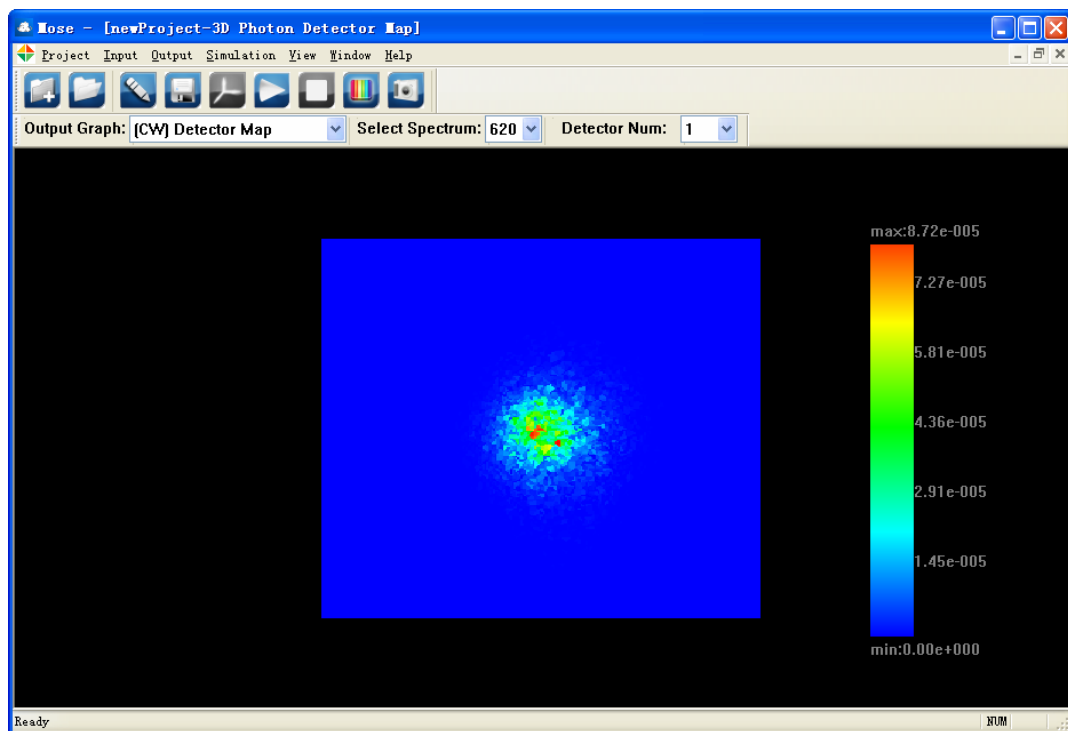
Figure 37 Plane detector figure.

Output-(CW) Fiber Detector Map: To show the photon Fiber detection figure under CW, users can select the spectrum from the drop-down box ![Select spectrum: 620] and select the detector number from the drop-down box ![Detector Num: 2], and the order of the numbers will be in accordance with the order of the detectors in the parameter file as shown in Figure 38.
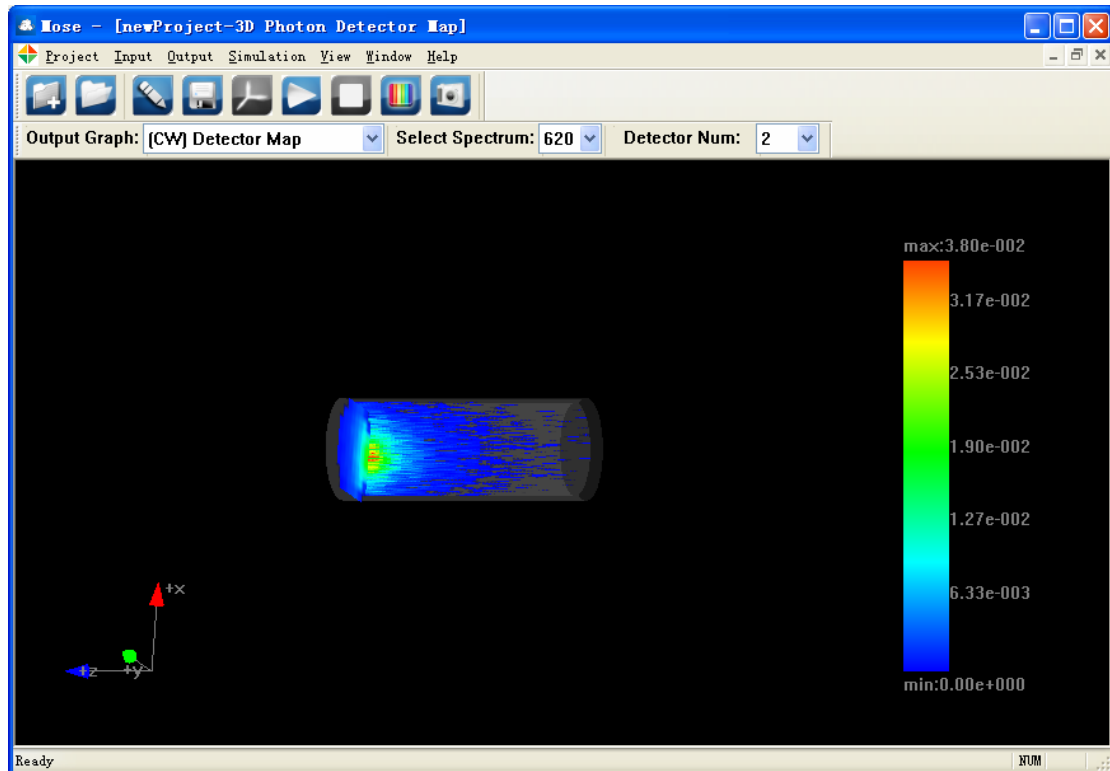
Figure 38 fiber detector figure.

Output-(CW/TD/FD) Absorption Map: Shows the photon absorption figures under CW, TD and FD respectively. There are two ways to show the absorption figure: Single Layer and Multilayer. The slider controls the display of the specific number of the layer when using a single layer display, and the dialog box controls when to use a multilayer display. Figures 39-42 depict the results when using a Cartesian coordinate system. Figures 43-45 show the results when using the Cylindrical coordinate system. The detailed description of these dialog boxes are shown in Table 11.
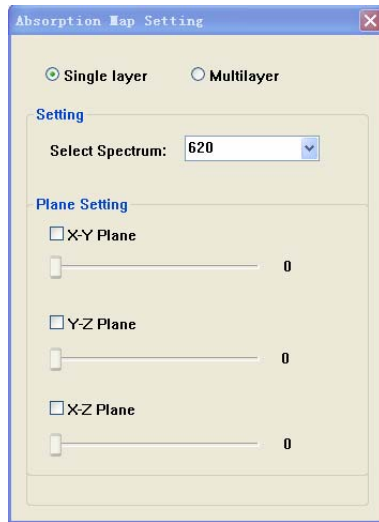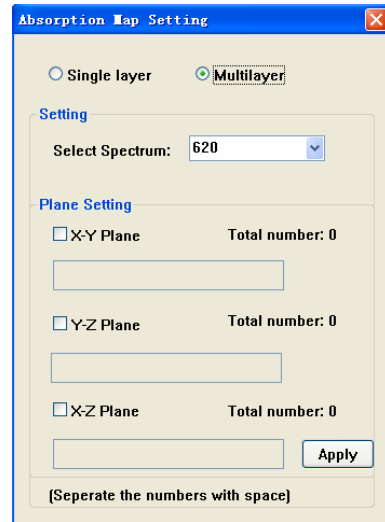
a. Single layer display setting.   b. Multilayer display setting.

Figure 39 Settings for the absorption figure under CW using a Cartesian coordinate system.
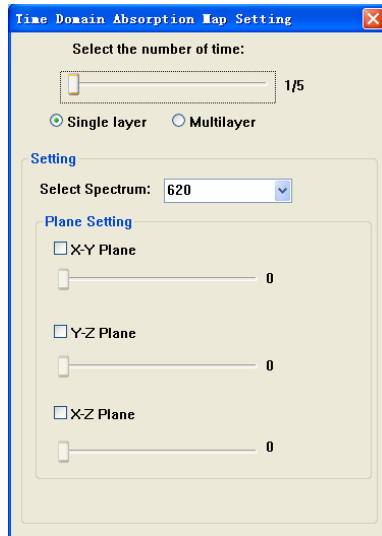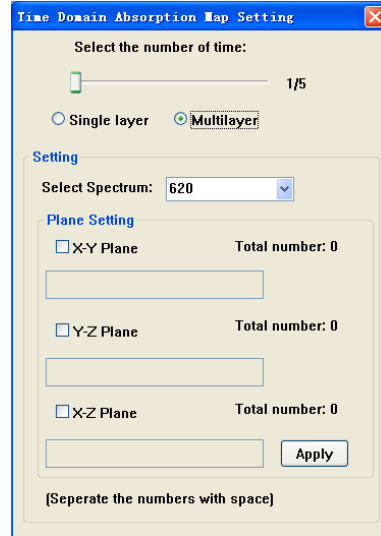
a. Single layer display setting.   b. Multilayer display setting.

Figure 40 Settings for the absorption figure under TD using a Cartesian coordinate system.
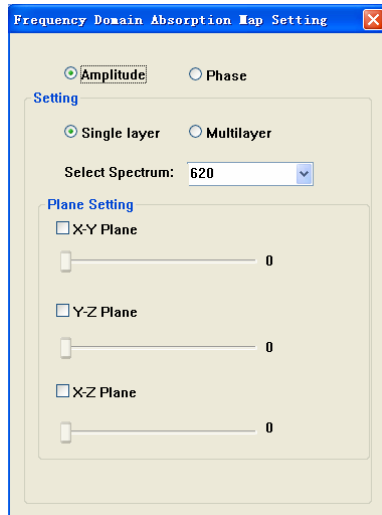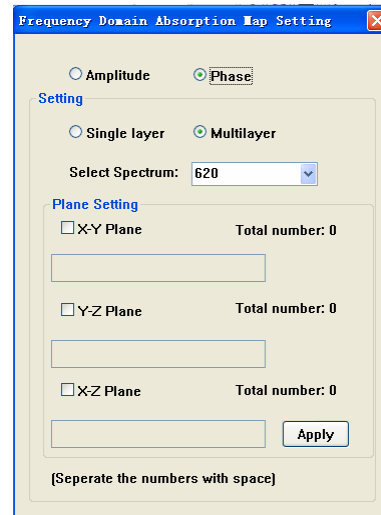
a. Single layer display setting.   b. Multilayer display setting.

Figure 41 Settings for the absorption figure under FD using a Cartesian coordinate system.
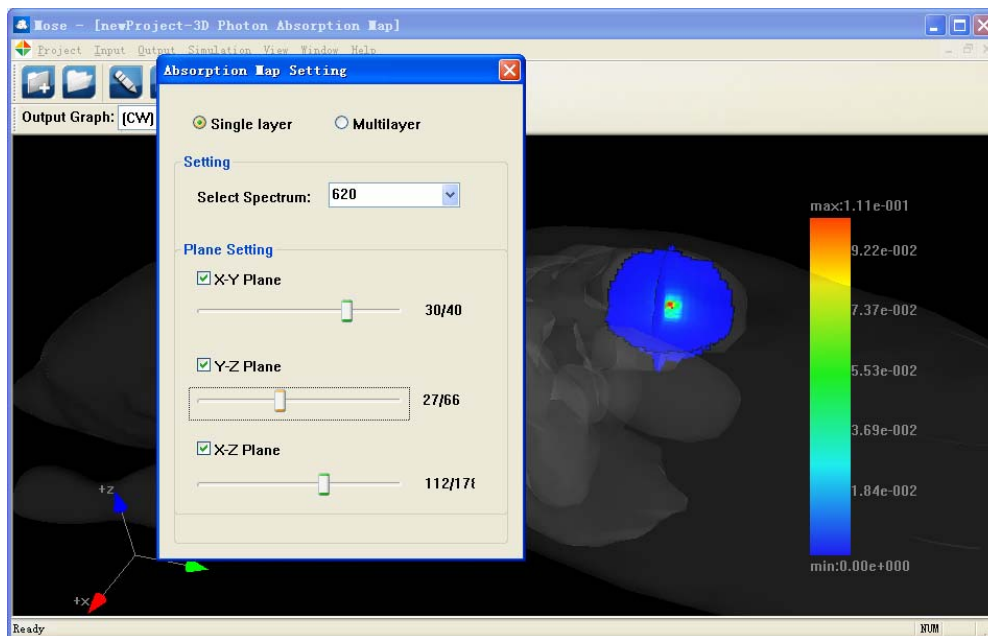
Figure 42 Absorption figure using a single layer display under CW with a Cartesian coordinate system.
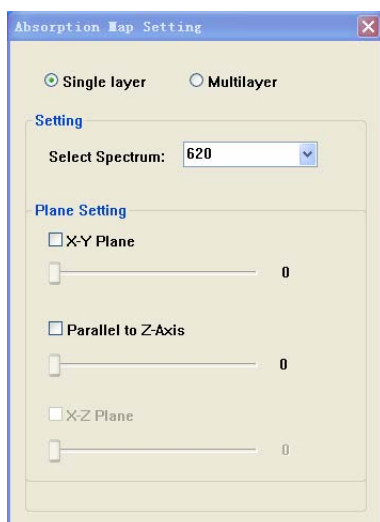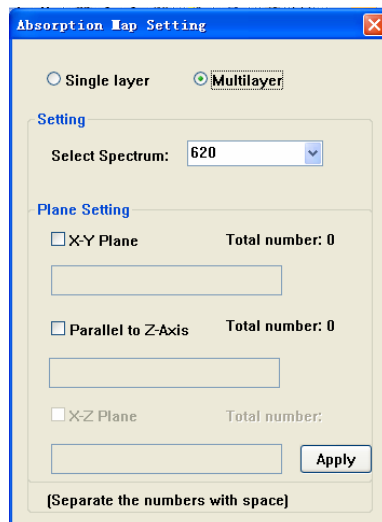
a. Single layer display setting.　　　　b. Multilayer display setting.

Figure 43 Settings for the absorption figure under CW using a Cylindrical coordinate system.
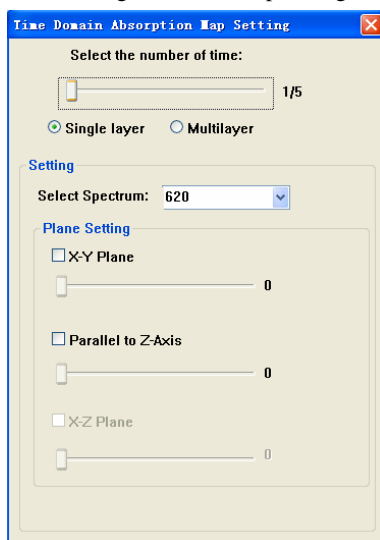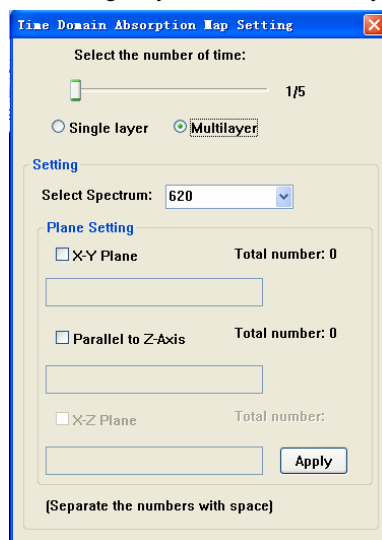
a. Single layer display setting.　　　　b. Multilayer display setting.

Figure 44 Settings for the absorption figure under TD using a Cylindrical coordinate system.
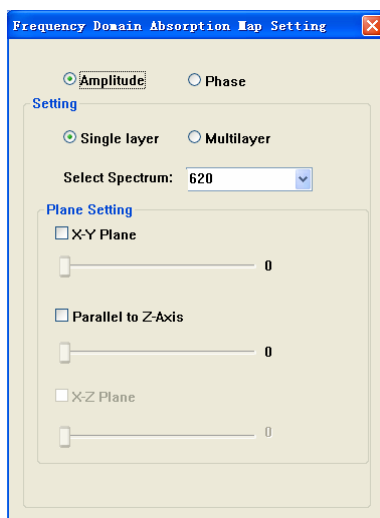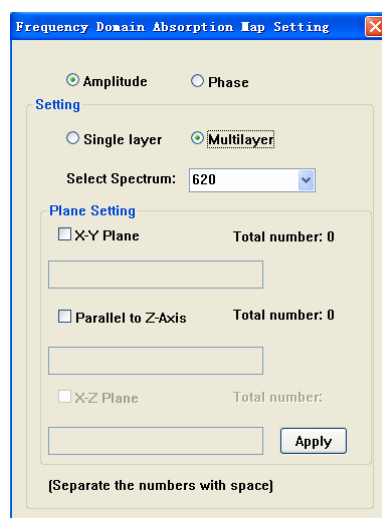
a. Single layer display setting.　　　　b. Multilayer display setting.

Figure 45 Settings for the absorption figure under FD using a Cylindrical coordinate system.

Table 11 Description of the dialog boxes for displaying the absorption figure

Select Spectrum	Select the absorption results based on the spectrum.
Single layer	Single layer display of the absorption results.
Multilayer	Multilayer display of the absorption results. The numbers of the layers are inputted by the dialog and separated with a space.
Select the number of time	Select the number of the time under TD.
Amplitude	Display the amplitude of the absorption results under FD.
Phase	Display the phase of the absorption results under FD.
X-Y Plane	Display of the absorption results on an X-Y plane.
Y-Z Plane	Display of the absorption results on a Y-Z plane.
X-Z Plane	Display of the absorption results on an X-Z plane.
Parallel to Z-Axis	Display of the absorption results parallel to the Z-axis.

2.2.2.5 Open Project

Users can also open the project built previously by selecting '**Project-Open**' from the menu bar or by clicking the shortcut on the toolbar to find the previously saved project file (.MPJ) and open it. MOSE will then load the related data corresponding to the project including the parameter file, the absorption results, the transmittance results, and the detection results.
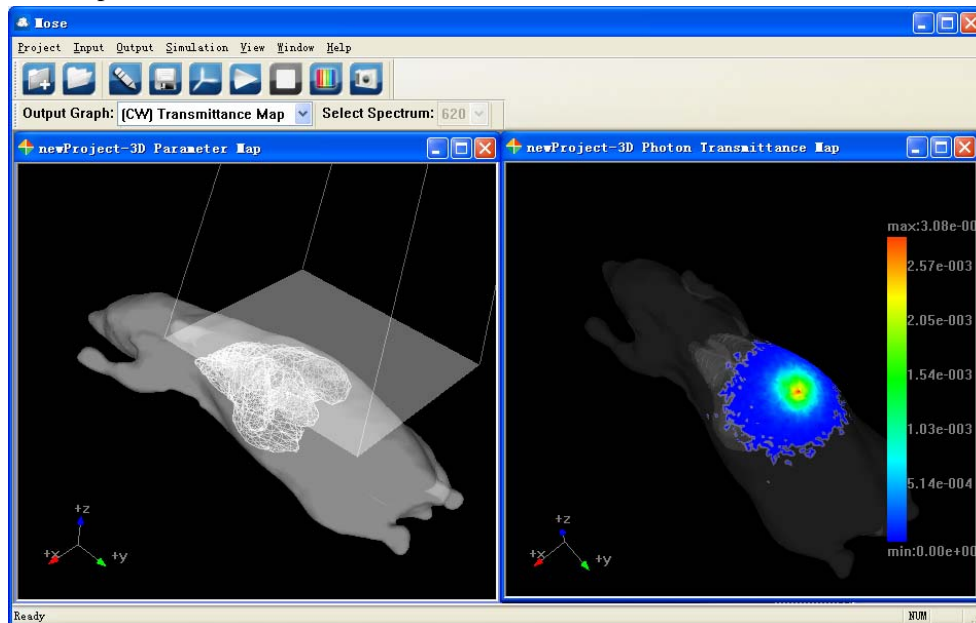
Figure46 Open a project.

NOTE: Reading a larger amount of data may be time consuming. The program state after reading is determined by the recording in the project file. For example, if only the parameters are inputted into the last run of the project, it's required to simulate and output the results. If none of the parameters is inputted, it's also required to set the parameters. If the simulation is done and the results have been outputted, users can observe the results obtained from last run directly after opening the project at this time.

2.3 Energy Mapping From 2D to 3D

It can build a map from 2D photographic images to a 3D spatial distribution on the body surface. In addition, combined with the algorithm for solving the inverse problem based on the photon transport model, we can reconstruct the spatial distribution of the optical properties of the medium or of the bioluminescent source inside of the medium.

Click 'File-new' or 'New Project' on the toolbar and select '2D-3D energy mapping' as shown in Figure 47.
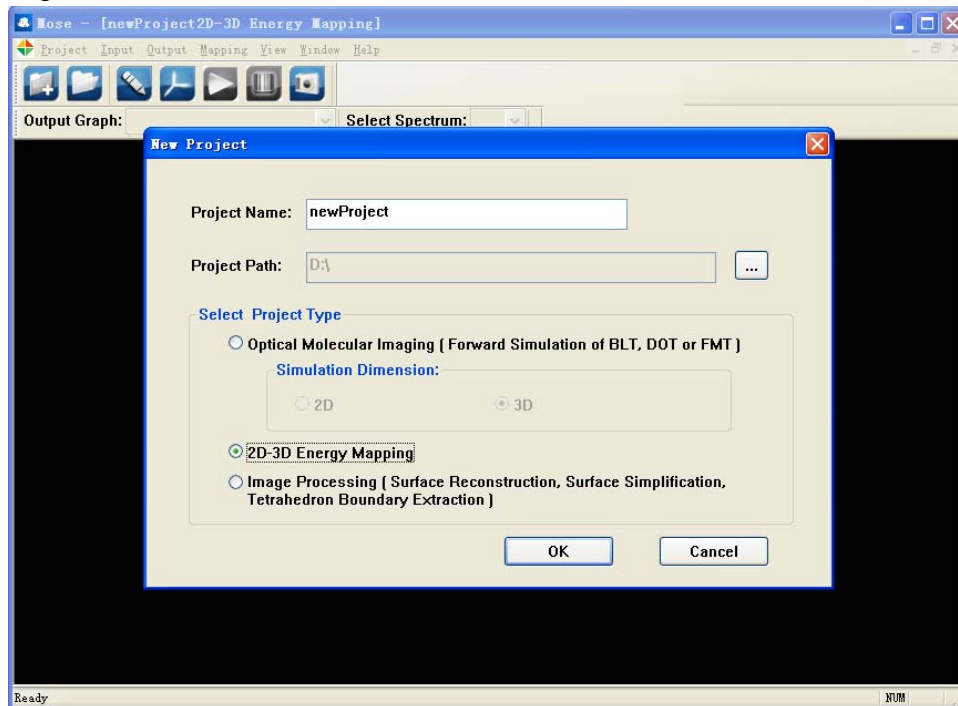
Figure 47 Building a project for 2D-3D energy mapping.

The interface is shown in Figure 48 after clicking 'OK.'
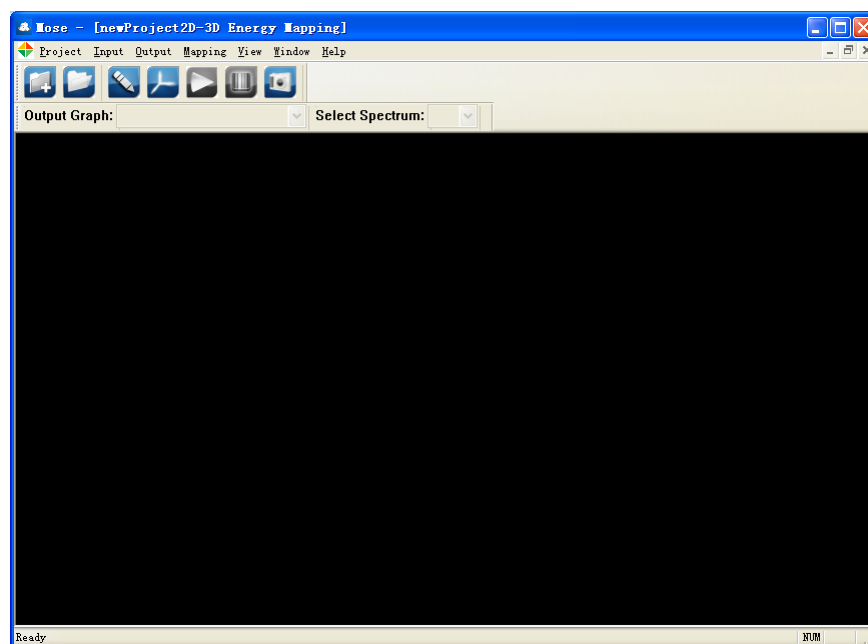
Figure 48 Interface after building the project for 2D-3D energy mapping.

Click '**Input-3D Parameter**' or '**Input Parameter**' on the toolbar, and the interface for the parameter setting is shown in Figure 49.
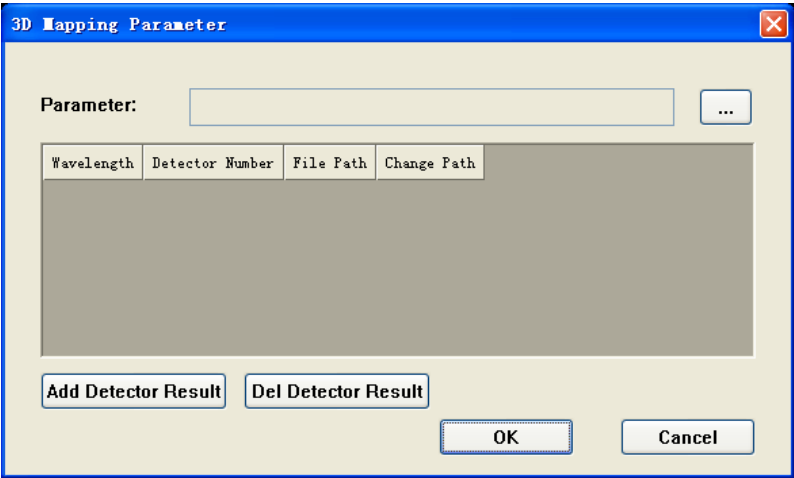
Figure 49 Interface for the parameter setting.

Table 12 Description of the parameters of the interface for the parameter setting

Parameter	The path of the parameter file.
Add Detector Result	Add a detection result.
Del Detector Result	Delete a detection result.
Wavelength	The central wavelength of the spectrum.
Detector Index	The number of the detector.
File Path	The file path of the detection result.
Change Path	Change the file path of the detection result.

The interface after inputting the parameters is shown in Figure 50.
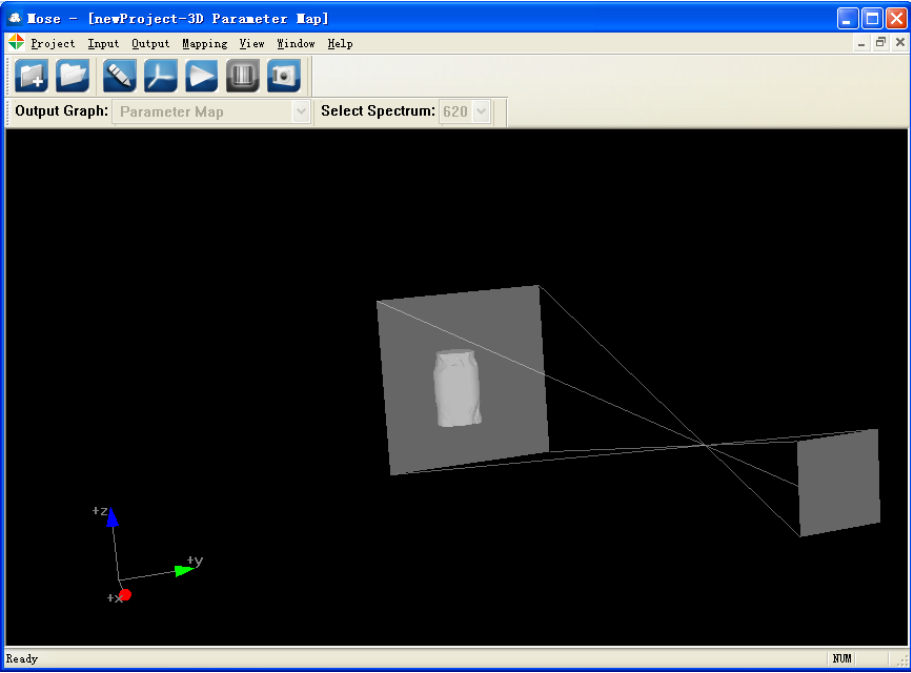
Figure 50 Display after setting the parameters for 2D-3D energy mapping.

Click '**Simulation-Start'** to start the mapping process as shown in Figure 51.
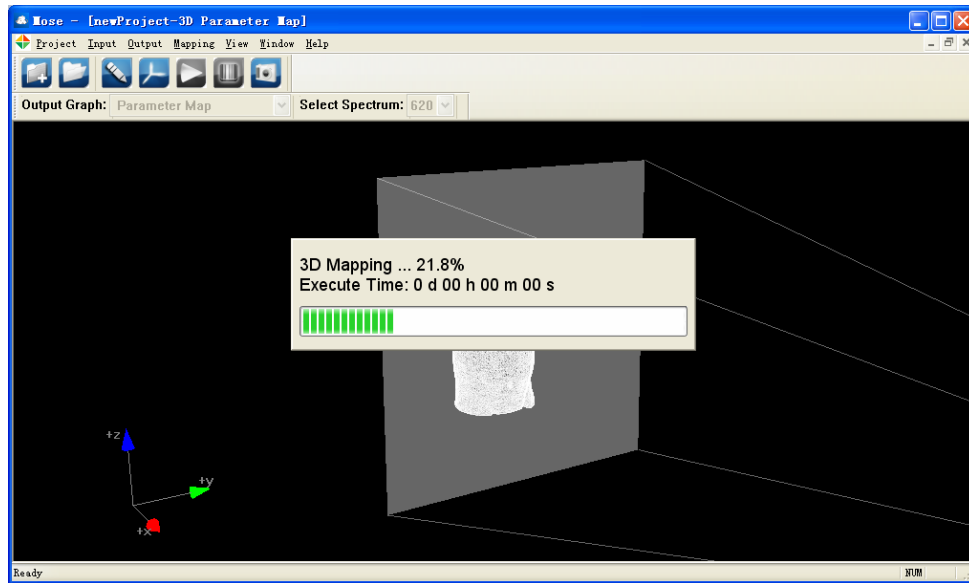
Figure 51 Interface for 2D-3D energy mapping.

The mapping result after the run is shown in Figure 52.
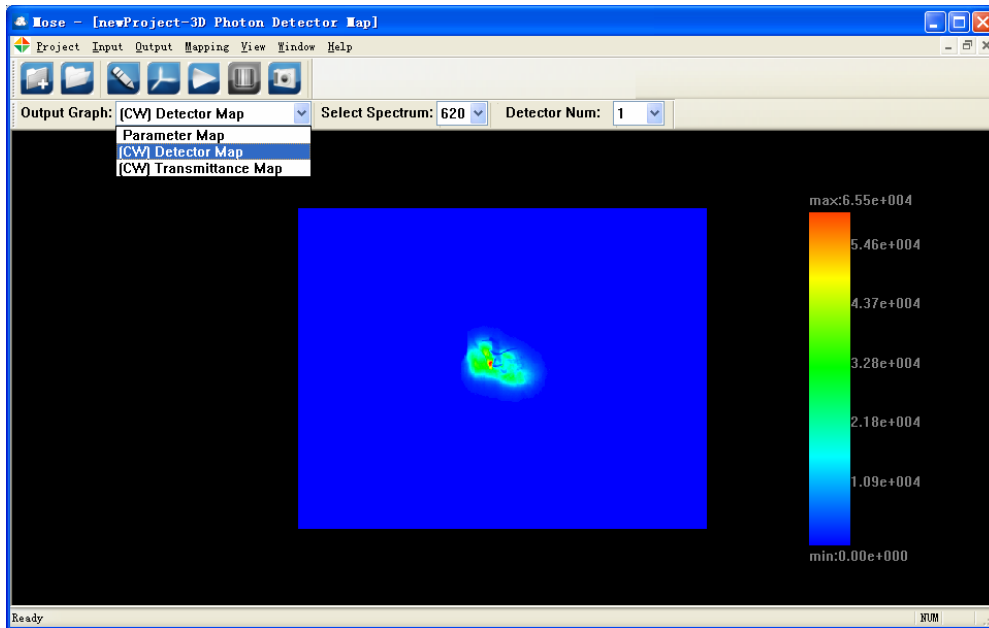
Figure 52 Display of the detection result.
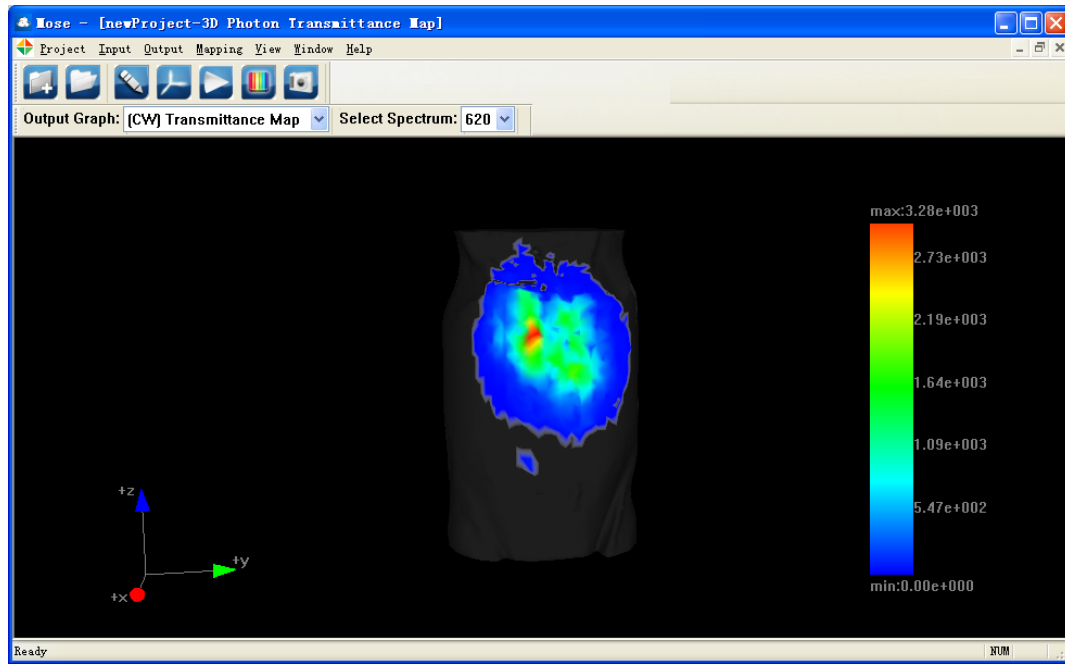
Figure 53 Display of the mapping result on the surface of the medium.

2.4 Image Processing

Select the type of image processing project and enter its interface. This project has two functions: threshold extraction and mesh simplification.

2.4.1 Threshold Extraction

The function of the threshold extraction is to extract the surface within a certain threshold from the RAW date captured by CT/MRI, and the surface is constructed by a triangle mesh.

For example, select 'File-Load Volume-RAW/IMG file' and enter the parameter setting dialog box as shown in Figure 54. A detailed description of the dialog is in Table 13.

Figure 54 Dialog box for reading the RAW format file.

Table 13 Description of the parameter setting while reading the RAW format file

Filename	The path of the RAW/IMG file.
Data type	The data type of the RAW/IMG file.
Requested	Calculated size of the file according to the input parameters. Check the accuracy of the input parameters by comparing the calculated size to the actual size of the file.
Filesize	The actual size of the RAW/IMG format file.
Width	The width of each slice and the size of each pixel.
Height	The height of each slice and the size of each pixel.
Number of slice	The number of slices and the interval distance of the slices.
Number of channels	Channel number: 1. Gray image; 2. RGB image; 3. RGBA image.
Head length	The head length of the data.
Little Endian	Selection of the endian format.
Interleaved Storing	Whether or not each channel data is cross stored.

Click 'OK' after finishing the parameter setting. The interface should look like that in Figure 55 if the input data are correct.
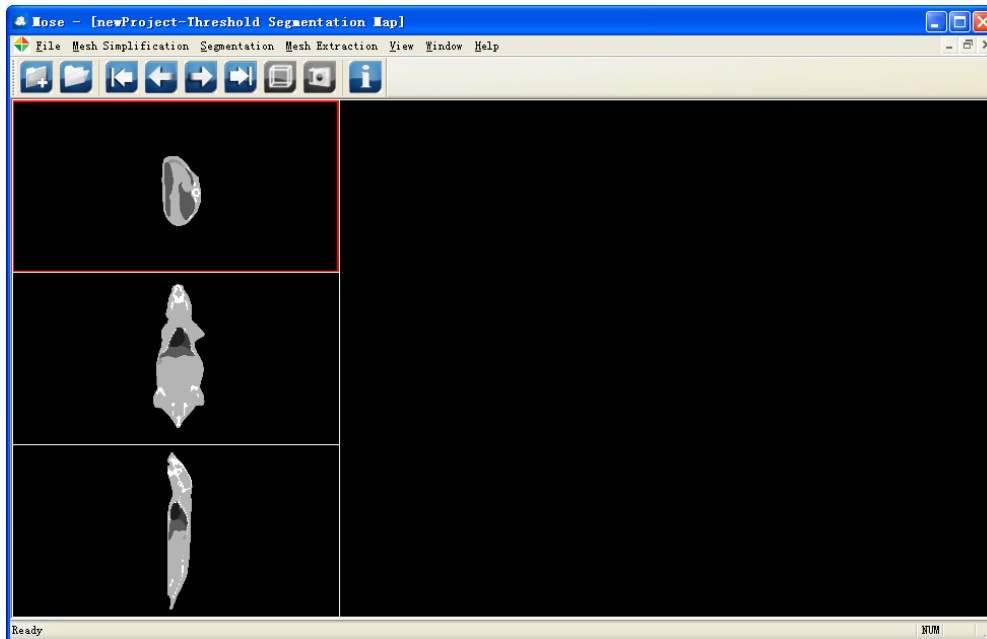
Figure 55 Display after reading the .RAW format file.

Select 'Segmentation–Threshold Segmentation,' which provides a threshold setting dialog box. Set the upper and lower threshold, and obtain the results as shown in Figures 56 and 57.
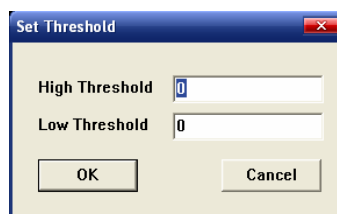
Figure 56 Upper and lower threshold settings in the dialog box.
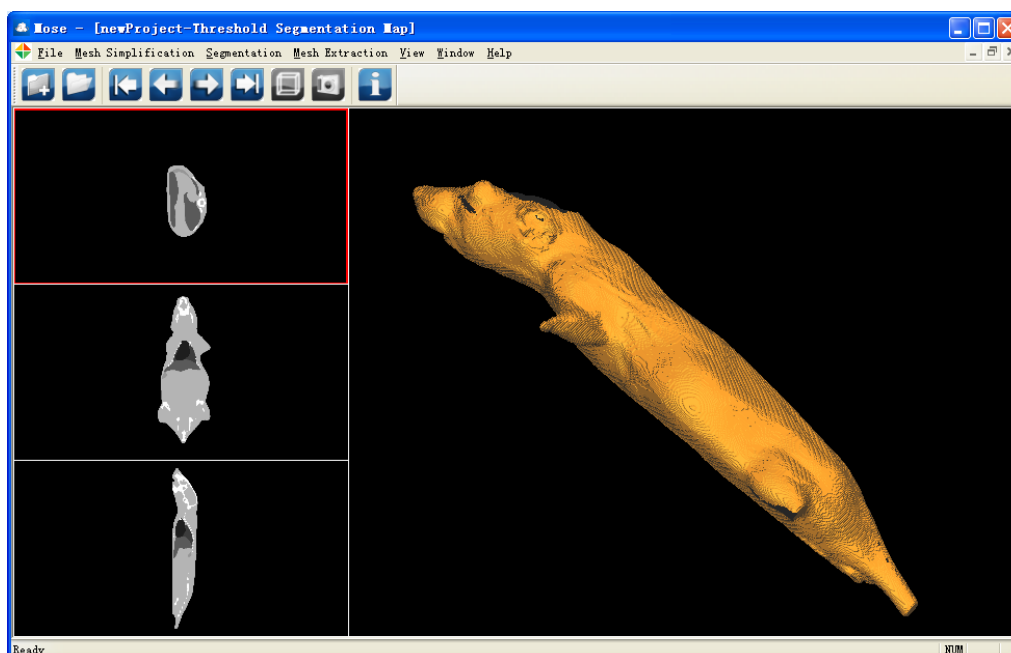
Figure 57 Display of the threshold extraction result.

Select 'Output- Segmentation Result,' the extraction result would be saved in PLY/OFF

format in the project folder.

2.4.2 Mesh Simplification

The function is to simplify the object surface constructed by the triangle meshes, and thus reduce the data size. However, it also reduces the detailed description of the object surface.

Select 'File-Load Data-PLY/OFF file' and input the PLY/OFF format file. The result is shown in Figure 56.
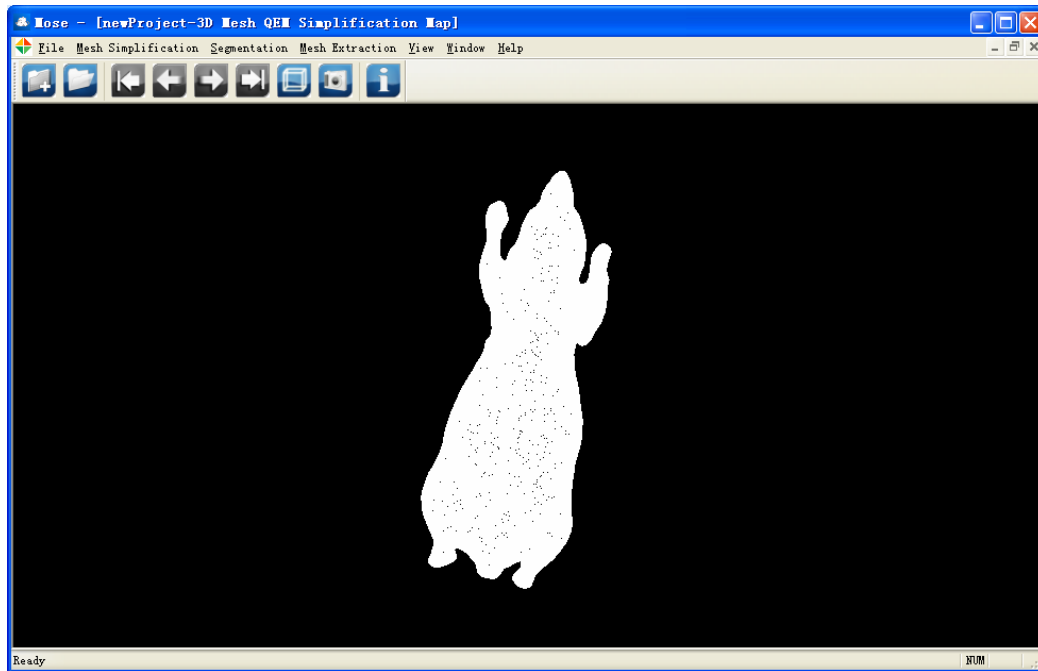
Figure 58 Display of a mesh format file.

Select 'Mesh Simplification-QEM Arithmetic' and enter the dialog box (Figure 59) of the mesh simplification. Set the target number of the mesh simplification; the result is shown in Figure 60.
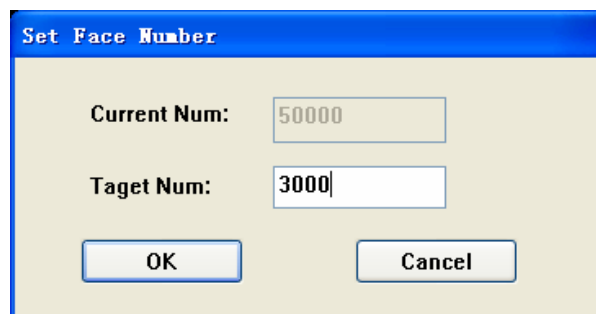
Figure 59 Dialog box for setting the simplification.
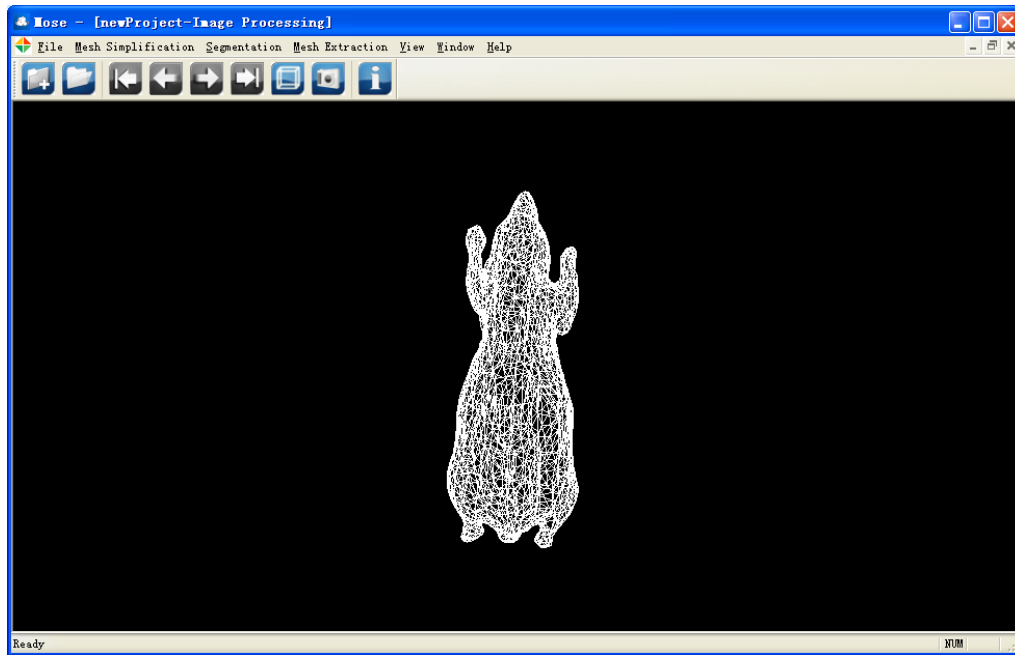
Figure 60 Result of the mesh simplification.

Select '**File-Save Data-Mesh Simplification Result**' and save the simplified result to the project folder.

2.4.3 Tetrahedral Boundary Extraction

The function of boundary extraction from the tetrahedral mesh can be used to obtain the boundary data of the tetrahedral mesh. For example, the tetrahedral mesh can be formed after tetrahedralization of the complex region and can be used in the finite element method. The boundary extraction can be used to obtain the triangle mesh boundary of each region from the tetrahedral mesh.

Select **File-Load Surface-MESH/AM File** after reading the tetrahedral data files in a .mesh or .am format. All of the internal and external boundaries of the tetrahedral mesh are shown in Figure 61.
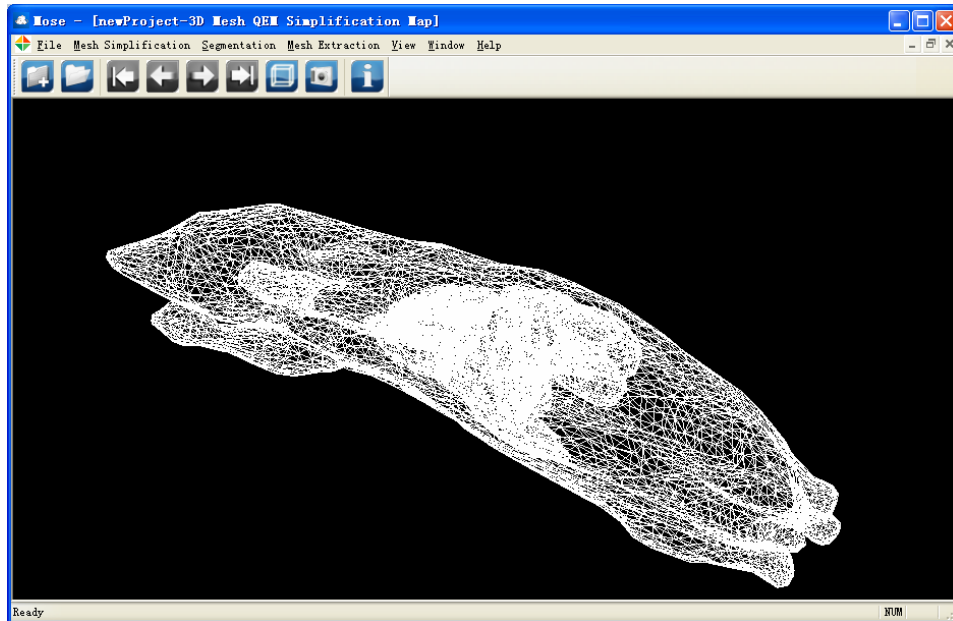
Figure 61 Reading the tetrahedral data.

After reading the tetrahedral data, select **Mesh Extraction-Tetrahedron Boundary Extraction**, and the dialog box shown in Figure 62 will pop up.
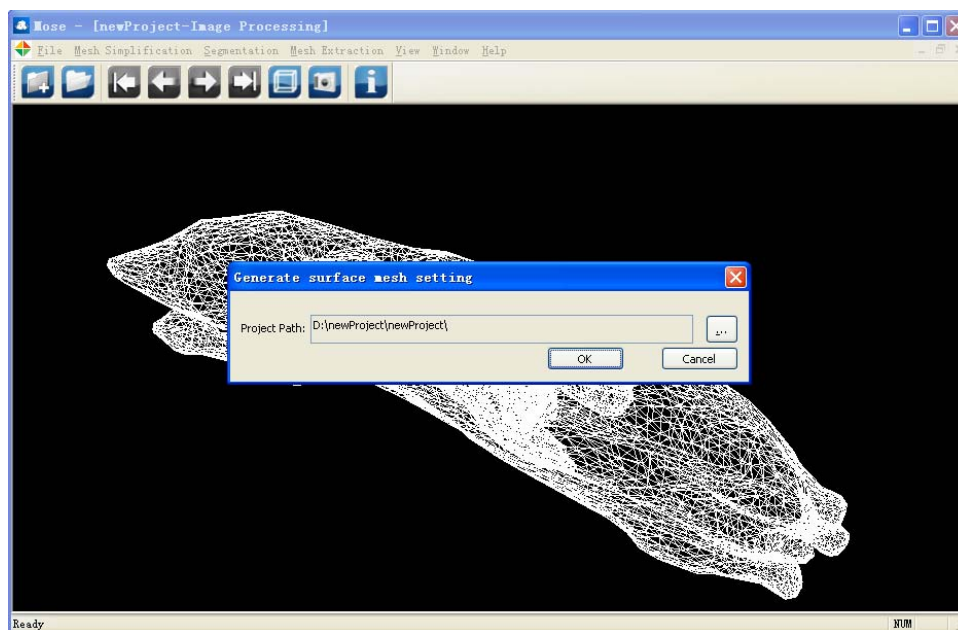
Figure 62 Tetrahedral boundary extraction.

After selecting the file storage path from the dialog and clicking the "OK" button, it starts extracting the tetrahedral regional boundaries from the tetrahedral data and saves it as a grid file in the .off format.

The surface and liver of the digimouse are extracted and shown in Figure 63.
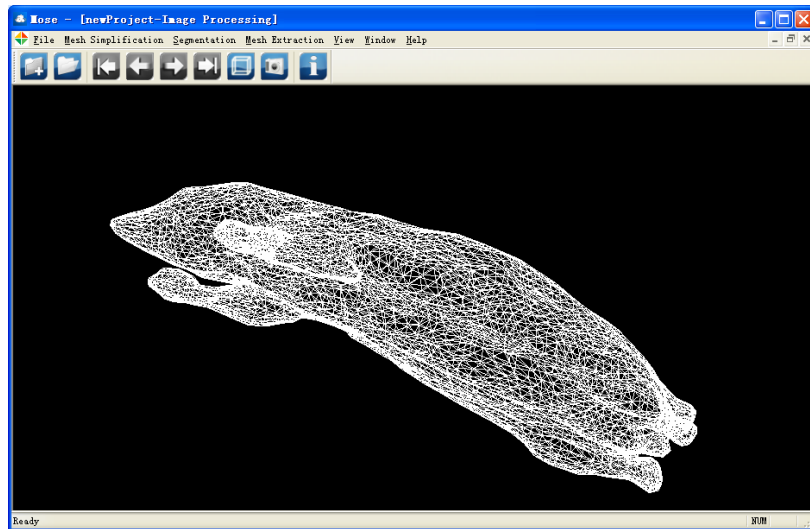
(a) The boundary of the mouse surface.
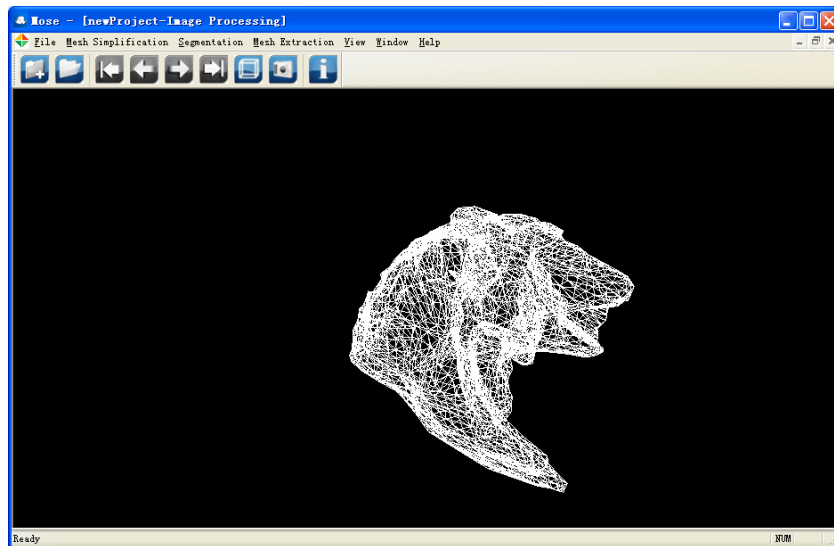
(b) The boundary of the liver.

Figure 63 Extraction results of the digimouse.

3 Description of the File Format in MOSE

This chapter will focus on the format of various documents used in MOSE and the meaning of the parameters. For more details, see below.

3.1 File Type

The file types in MOSE are listed in Table 14.

Table 14 Description of the file type in MOSE

File extensions	File description	File content
.mpj	Project file for MOSE.	Save the information in a MOSE

		operation.
.mse	The file of the simulation parameters.	Save the optical simulation parameters in an MC simulation.
.A.CW	The file of the absorption results under CW.	Save the absorption results under CW in an MC simulation.
.T.CW	The file of the transmission results under CW.	Save the transmittance results under CW in an MC simulation.
.D.CW	The file of the fiber detector results under CW	Save the detector results under CW in an MC simulation.
.A.TD	The file of the absorption results under TD.	Save the absorption results under TD in an MC simulation.
.T.TD	The file of the transmittance results under TD.	Save the transmittance results under TD in an MC simulation.
.A.FD	The file of the absorption results under FD.	Save the absorption results under FD in an MC simulation.
.T.FD	The file of the transmittance results under FD.	Save the transmittance results under FD in an MC simulation.
.D	The file of the detection results under CW.	Save the detection results under CW in an MC simulation.
.raw	The file of raw data.	The input data in threshold segmentation.
.off	The file of triangular data.	Triangle mesh data, which can be used to describe the tissue shape in an MC simulation.
.ply	The file of triangular data.	Triangle mesh data, which can be used to describe the tissue shape in an MC simulation.
.surf	The file of triangular data generated from Netgen.	Triangle mesh data, which can be used to describe the tissue shape in an MC simulation.
.am	The file of tetrahedral data generated from Amira.	Tetrahedral mesh data, which can be used to describe the integral structure of the medium in an MC simulation.
.mesh	The file of tetrahedral data generated from Netgen.	Tetrahedral mesh data, which can be used to describe the integral structure of the medium in an MC simulation.

3.2 Parameter File

This section will specify the format of the parameter file in detail.

3.2.1 Format of the Parameter File

Table 15 Format specification of the parameter file

No.	Keywords	Default	Explanation
1	mse		File type.
	Format ASCII 2.0		ASCII encoding, version 2.0, corresponding to MOSE v2.1.2.
	Comment: This file is generated by MOSE		Comment.
2	SimulationProperty		The keywords to start the setting of the simulation property.
	SimulationType *	BLT	The forward simulation type: 'BLT', 'DOT', or 'FMT.'
	Dimension *	3D	The simulation dimension: '2D' or '3D.'
	SpectrumNum *	0	The total number of spectra.
	LightSourceNum *	0	The total number of light sources.
	TissueNum *	0	The total number of the tissues in the medium.
	DetectorLensNum *	0	The total number of detectors (**NOTE**: Need to set it in 3D CW).
	MediumAlgorithm *	VRMC	The algorithm of light propagation in the medium.
	FreeSpaceAlgorithm *	PINHOLE	The algorithm of light propagation in free-space (**NOTE**: Need to set it in 3D CW).
	ROI * * * * * * * * * * * *		Region of Interest (ROI) (Unit: mm); please refer to Figure 65. 1. 3D: The order is Xmin, Xmax, Ymin, Ymax, Zmin, Zmax, Rmin, Rmax, Amin, Amax, Dmin, and Dmax, which corresponds to the minimum and maximum values along the directions of the X-axis, Y-axis, Z-axis, radial, azimuth angle, and deflection angle respectively. 2. 2D: The order is Xmin, Xmax, Ymin, Ymax, Rmin, Rmax, Amin, and Amax, which correspond to the minimum and the maximum values along the directions of the X-axis, Y-axis, radial, and azimuth angle respectively.
	ROISeparation * * * * * *		The separations of the ROI (Unit: mm); please refer to Figure 65. 1. 3D: The order is Dx, Dy, Dz, Dr, Da, and Dd, which correspond to the format of the ROI in 3D. 2. 2D: The order is Dx, Dy, Dr, and Da, which correspond to the format of the ROI in 2D.
	AbsorptionMatrix *	Cartesian	The coordinate system for saving the absorption results. 1. 3D: 'Cartesian,' 'Cylindrical' 2. 2D: 'Cartesian,' 'Polar'
	TransmittanceMatrix *	Cartesian	The coordinate system for saving the transmittance results. It's related to the shape of the outermost tissue. The program will automatically modify the wrong setting of the coordinate system (**NOTE**: For the 'Cylinder' shape, there are two choices for the coordinate system, including the 'Cartesian' and 'Cylindrical' ones). However, there is only one choice for other shapes, such as an ellipse (Polar), rectangle (Cartesian), ellipsoid (Spherical), cube (Cartesian), and triangle mesh

			(Cartesian).
	FluenceRate *	0	The flag whether or not to calculate the internal fluence rate based on the photon density (Raw absorption). There is only one type of data that can be saved in each simulation.
	PhotonFlyTime *	0	The flag whether or not to record the fly time of the transmitted photons under TD.
	OutermostTissueIndex *	1	The number of the outermost tissue on the tissue list for the medium. The outermost tissue has the largest bounding-box. Index starts from 1.
	AmbientMediumR *	1	The refractive index of the ambient medium.
	Domain *	CW	The simulation domain: 1. 'CW': There are no more parameters that need to be set. 2. 'TD': In addition to the above parameters that need to be set, the parameters related to time also need to be set. The order is Tmin, Tmax, and Dt, which correspond to the minimum time, the maximum time, and the time interval respectively (Unit: ps). 3. 'FD': Under FD, users still need to set the modulating frequency (Unit: MHZ).
	MediumShapeTetraType	0	The flag of the medium shape is 1 for a tetrahedral mesh structure and 0 for others.
	endSimulationProperty		The keywords to end the setting of the simulation property.
3	Spectrum * *		Spectrum list, where the order is the spectrum number and the central wavelength of the spectrum (Unit: nanometer). For example: Spectrum 1 650 Spectrum 2 690
4	LightSource *		The light source parameters and their numbers.
	LightSourceShape *		The shape of the light source. 1. 3D: 'Ellipsoid,' 'Cylinder,' 'Cube,' and 'TriangleMesh' (Irregular shape). 2. 2D: 'Ellipse,' 'Rectangle.'
	LightSourceProperty * * * *	Internal Solid NoSpecular	The optical properties of the light source, including four of its aspects. More information is listed in Table 14. 1. 'Internal, External': Set the position of the light source position, where 'Internal' means inside of the medium and 'External' means outside of it. 2. 'Solid, Face': Set the position of the photon. 'Solid' means the photon is generated inside the shape or on the boundary of the shape of light source. 'Face' means the photon is generated just on the boundary of the shape. 3. 'Specular, NoSpecular': 'Specular' means the specular reflectance will occur while the light source is outside of

			the medium. 'NoSpecular' means no specular reflectance. 4. 'Excitation, Emission': 'Excitation' means the light source is the incident laser. 'Emission' means it is the fluorophore (**NOTE**: Need to set it in FMT).
	LightSourceCenter * * *	0 0 0	The center of the shape (**NOTE**: Do not need to set it while the shape is a triangle mesh).
	LightSourceAxis * * *	0 0 0	Half of the axis length of the shape (**NOTE**: Do not need to set it while the shape is a triangle mesh; see Figures 63 and 64 for more information).
	LightSourcePath *		The path of the triangle mesh file used to describe the irregular shape (**NOTE**: Need to set it while the shape is a triangle mesh).
	LightSourceSpectrumIndex * * * * *		The optical properties of the light source. 1. Non-Fluorophore: the order is a spectrum number, spectrum energy, and photon number. 2. Fluorophore: the order is a spectrum number, excitation wavelength, quantum yield, absorption factor, and fluorescence lifetime (Unit: ps).
	LightSourceAzimuthAngle	0 360	The range of the azimuth angle of the emitted photon. The maximum range is [0, 360].
	LightSourceDeflectionAngle	0 180	The range of the deflection angle of the emitted photon. The maximum range is [0, 180].
5	MediumTetraPath		File path of the tetrahedral mesh while the medium is a tetrahedral mesh structure.
	Tissue *		The tissue parameters and their numbers.
	TissueShape *		Set the shape of the tissue.
	TissueCenter * * *	0 0 0	The center of the shape.
	TissueAxis * * *	0 0 0	Half of the axis length of the shape; see Figures 63 and 64 for more information.
	TissuePath *		The path of the triangle mesh file used to describe the irregular shape.
	TissueSpectrumIndex * * * * *		The optical parameters of the tissue. The order is the spectrum number, absorption coefficient, scattering coefficient, anisotropy factor, and refractive index.
6	DetectorLens *		The detector parameters and their numbers.
	VerticalPlane *	XY	The plane that the detector is perpendicular to, including XY, YZ, and ZX (**NOTE**: The structural design of the detector in MOSE is shown in Figures 66-68).
	DetectorCenter * * *	0 0 0	The center of the detector.
	DetectorNormal * * *	0 0 0	The normal vector of the detector.
	DetectorSize * *	0 0 0	The actual size of the detector; the order is height and width.
	DetectorResolution * *	0 0	The resolution of the detector; the order is height resolution and

			width resolution.
	ImageDist *	0	The image distance of the detector.
	FocalLength *	0	The focus of the lens.
	LensRadius *	0	The radius of the lens.
7	fiberdetector		The detector type and their numbers.
	Fiberdetectorshape	cylinder Ellips- oid	The shape of the fiber detector. The current vision of MOSE only supports cylinder and ellipsoid. The default shape is ellipsoid.
	FiberdetectorCenter	0 0 0	The center of the fiber detector.
	FiberdetectorAxis	0 0 0	The half of the axis length of the fiber detertor.
	endmse		The keywords to end the parameter file.

NOTE: 1. File header; 2. Simulation properties; 3. Spectrum list; 4. Light source parameters; 5. Medium parameters; 6. Detector parameters; 7. Detector parameters

3.2.2 Description of the Light Source, Medium Model, Detector and Region of Interest

3.2.2.1 Light Source

In the latest version of MOSE, the types of light sources include three kinds shown in Table16. Table 16 can be a reference when user set the properties of the light source.

Table 16 Differences in the light source properties from different simulation types

Properties	Forward simulation type		
	BLT	DOT	FMT
Luminescence type	Bioluminescence	Incident laser	Incident laser (Excitation), fluorophore (Emission)
Shape	Not limited	Not limited	Not limited
Position	Inside the medium	Inside or outside the medium	The incident laser can be inside or outside of the medium. The fluorophore must be inside the medium.
Specular reflectance	No	'Yes' can be set while the incident laser is outside of the medium	'Yes' can be set while the incident laser is outside of the medium
Solid/Face	Not limited	Not limited	Not limited
Spectrum parameters	Including central wavelength, spectrum energy, and photon	Including central wavelength, spectrum energy, and photon number	1. The spectrum parameters of the incident laser include central wavelength, spectrum energy, and photon number. 2. The spectrum parameters of the fluorophore

	number		include emission wavelength, excitation wavelength, quantum yield, absorption factor, and fluorescence lifetime (Unit: ps).

3.2.2.2 Medium Model

In the latest version of MOSE, the medium is divided into two types: homogeneous medium (contains one tissue) and inhomogeneous medium (contains more than 2 tissues). In the previous versions, all of the tissues in the medium are "independent," where the boundary of the tissue can be described by regular shape or irregular triangle mesh (the shapes are shown in Figure 64(a), (b), (c) respectively); this kind of medium model is called the "Independent medium model." After version 2.2, MOSE introduces a new structure of the irregular tetrahedral mesh to describe the whole medium. In this structure, the shapes of all of the tissues are constructed with the tetrahedral mesh structure and are joined together as shown in Figure 65; this kind of media model is called the "Integral medium model." The differences between the medium models arise from the differences between the realizations of the MC simulation method, but users only need to know how to set the correct structure for the medium without fully knowing the details of the program, as described in the following.
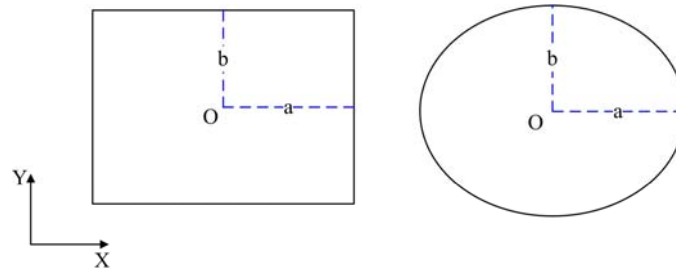
(a) Illustration of the parameters of the 2D shapes. Point O is the center, while a and b are the halves of the axis length along the X-axis and Y-axis respectively.
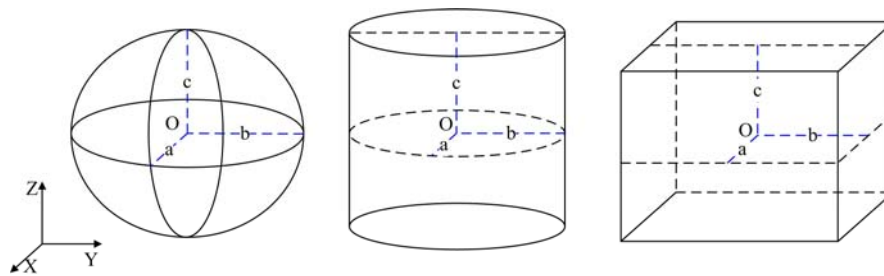
(b) Illustration of the parameters of the 3D shapes. Point O is the center, while a, b, and c are the halves of the axis length along the X-axis, Y-axis, and Z-axis respectively.
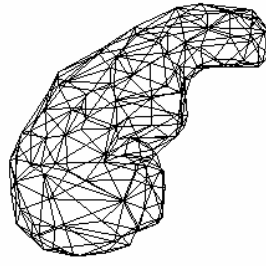
(c) Irregular triangle mesh structure, with an empty interior (this is the shape of a stomach).

Figure 64 Illustration of different shapes in an independent medium model.
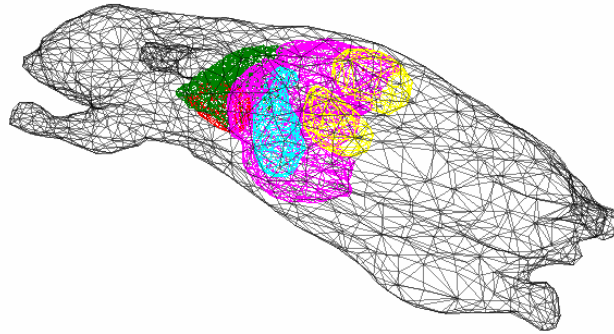
Figure 63 Integral media model (irregular tetrahedral mesh structure). Only the boundaries of the regions are shown here. The interior is constructed by tetrahedrons (it is a whole structure of a mouse which consists of the heart, lungs, stomach, liver and kidneys).
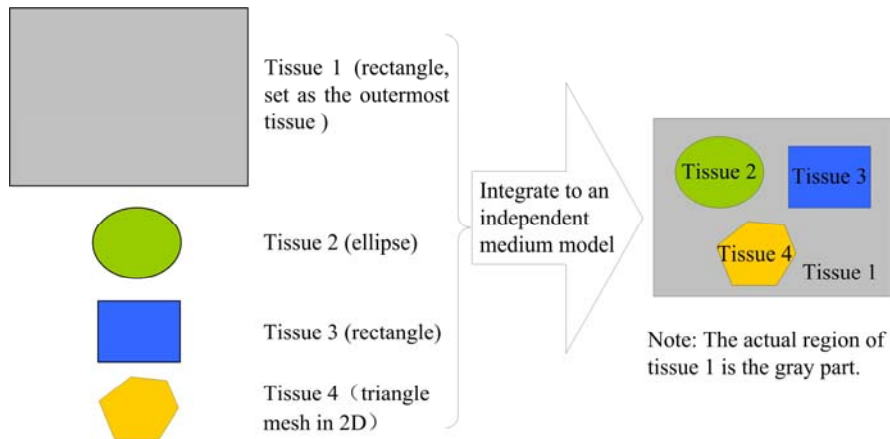
Figure 65 Schematic diagram of the construction of the independent medium model in 2D.

Independent Media Model: In this model, the shapes of all of the tissues need to be described independently and all of the shapes will be integrated into a whole medium. The following parameters need to be set while the user sets the medium to be this model:

1. MediumShapeTetraType: Set the flag of the type of the medium model as "0."
2. TissueShape: Set the shape of the tissue, including the regular shape and triangle mesh structure.
3. TissueCenter and TissueAxis: Set the center of the regular shape and its half axis length.
4. TissuePath: Set the file path when using the triangle mesh structure.
5. OutermostTissueIndex: Set the number of the outermost tissue. User needs to

appoint which tissue shape is the outermost layer on the tissue list, and the number starts from 1. Other shapes of tissues are required to be surrounded by this shape of tissue, otherwise there would be some mistakes in the simulation. It should be noted that the "actual region" of the outermost tissue is the part which equals to the shape of the tissue minus the shapes of the other tissues.

Figure 65 is the schematic diagram for the construction of the independent medium model in 2D.

Integral Medium Model: In this model, the shapes of all of the tissues are constructed with tetrahedral meshes that are then joined together. The following parameters need to be set while the user sets the medium to be this model:

1. MediumShapeTetraType：Set the flag of the type of the medium model as "1."
2. MediumTetraPath: Set the file path of the tetrahedral mesh describing the whole medium; the file format of the tetrahedral mesh structure refers to Section 3.4.

TissueCenter, TissueAxis, TissuePath and OutermostTissueIndex don't need to be set, otherwise this may result in some mistakes.

3.2.2.3 Plane Detector

The structural design of the plane detector in MOSE is shown in Figure 66; there are three designs. Users can set the detector needed in the simulation with the following parameters:

1. VerticalPlane: Vertical plane of the detector. In the current version, the detector cannot be placed randomly. Its detection plane must be perpendicular to the XY plane, XZ plane or YZ plane shown in Figure 66.
2. DetectorCenter: Center of the detector plane; it determines the location of the detector.
3. DetectorNormal: Normal vector of the detector plane; the values are (*, *, 0), (*, 0, *), and (0, *, *) which correspond to the XY plane, XZ plane, and YZ plane respectively. Here * can be any value. The value determines the detection direction of the detector; the correct direction points to the media from the detector plane. Otherwise, the detection result would be zero.

NOTE: When setting the location of the detector, the user needs to ensure that the "virtual detection plane" corresponding to the detection plane is located outside of the medium. Otherwise, this will result in certain mistakes. The location of the "virtual detection plane" is determined by the focal length, the image distance and the center of the detector plane.
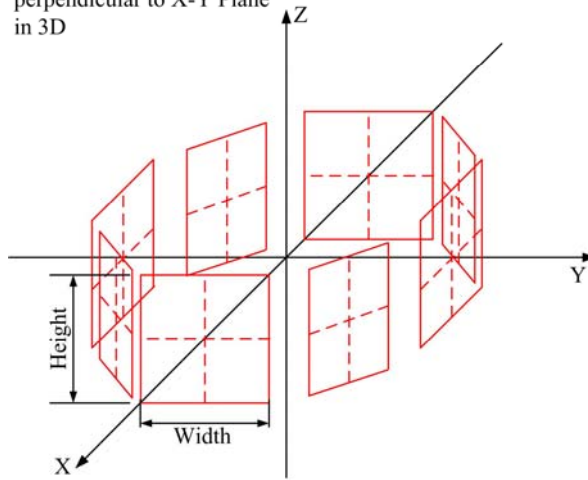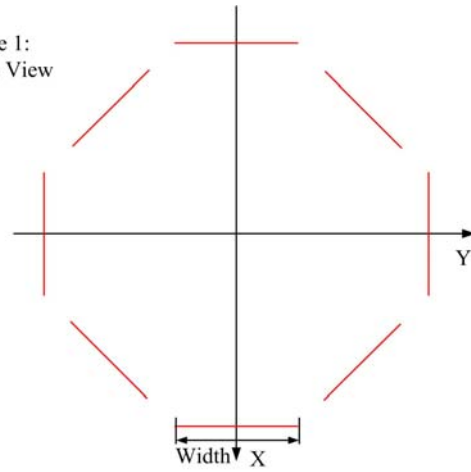
(a) View of the detector perpendicular to the X-Y plane; the normal vector of the detector is (*, *, 0).

(b) View of the detector perpendicular to the X-Z plane; the normal vector of the detector is (*, 0, *).
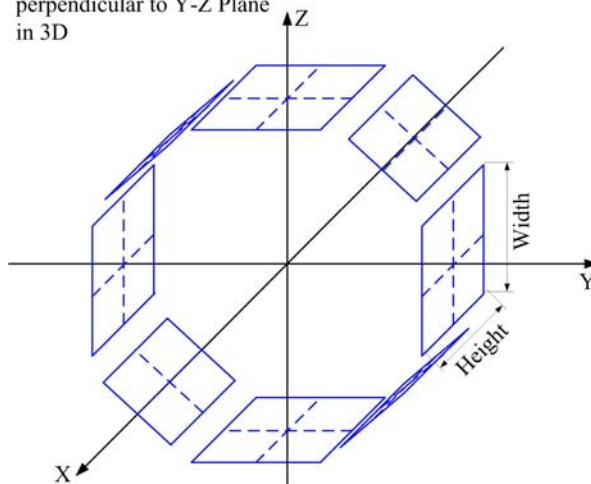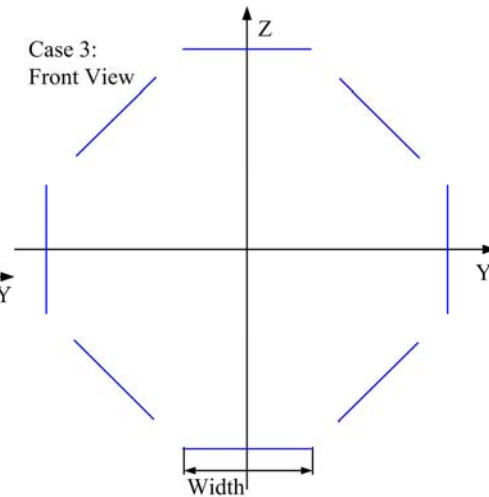
(c) View of the detector perpendicular to the Y-Z plane; the normal vector of the detector is (0, *, *).

Figure 66 Structural design of the detector.

3.2.2.4 Fiber Detector

The structural design of the fiber detector in MOSE is shown in Figure 67; the fiber detector has two kinds of shape. Users can set the detector needed in the simulation with the following parameters:

1. Fiberdetectorshape: The shape of the fiber detector. In the current version, the shape of the detector can be only set as cylinder or ellipsoid.
2. FiberdetectorCenter: Center of the fiber detector; it determines the location of the detector.
3. FiberdetectorAxis: The half of axis length of the fiber detector. (a, b, c) values which correspond to the X-axis, Y-axis and Z-axis respectively determine the size of the fiber detector.

NOTE: The resolution of the fiber detector is the same as that of the tissue. The fiber detector can be only set at the inside of the outermost tissue. The fiber can not intersect the light source. To make the simulation more accurate compared with the real experiment, a cavity tissue which has the same shape and center as the fiber detector is usually set to the boundary of the fiber detector.
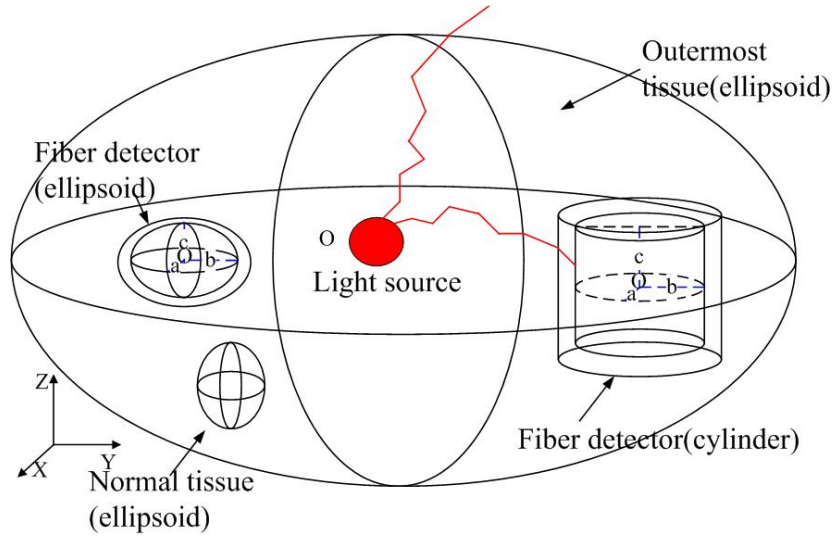
Figure 67 Structural design of the detector.

3.2.2.5 Region of Interest

There are three types of simulation results in MOSE: absorption results, transmittance results and detection results. The format of the first two results is in connection with the region of interest (ROI) and the coordinate system set. The results have different formats with different settings. The detection result is in connection with the detector size and resolution.
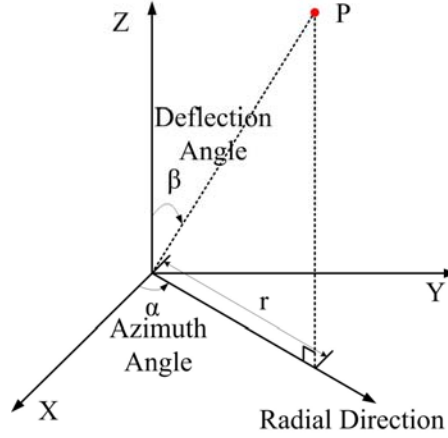
Figure 68 Illustration of the ROI.

The setting of the ROI contains two of the following:

1. ROI: The range of the ROI. There are 4 directions in 2D, such as the direction of the X axis, the direction of the Y axis, the radial direction and the azimuth direction respectively; and there are 6 directions in 3D, such as the direction of the X axis, the direction of the Y axis, the direction of the Z axis, the radial direction, the azimuth direction and the direction of deflection angle respectively. The ROI is determined by the starting and end points and it also has some connection with the coordinate system selected by the user. P is a point in 3D, of which the X, Y, Z, the radial value, the azimuth angle and the deflection angle are all shown in Figure 68.

2. ROISeparation: The unit intervals of all of the directions in the ROI.

NOTE: While setting the "ROI" and "ROISeparation" in the parameter file, the user must obey the order mentioned above and no value can be skipped.

The setting of the coordinate system for saving the absorption result and the transmittance result contains two of the following:

1. AbsorptionMatrix: Coordinate system for saving the absorption matrix; there is the Cartesian coordinate system and Polar coordinate system in 2D; and there is the Cartesian coordinate system and cylindrical coordinate system in 3D.

2. TransmittanceMatrix: Coordinate system for saving the transmittance matrix. The set of the coordinate system is also restricted by the shape of the outermost boundary of the medium. Rectangle (Cartesian coordinate system), ellipse (Polar coordinate system), cube (Cartesian coordinate system), ellipsoidal (Spherical coordinate system), and Cylinder (Cartesian or Cylindrical coordinate systems, which only affect the manner of saving the results on upside and bottom of the cylinder, hence the results on the side of the cylinder are always saved following the Cylindrical coordinate system). For the triangle mesh or the tetrahedral mesh, the value does not need to be set for either one of them. The output order of the transmittance is in accordance with the order of the mesh vertices and the mesh faces.

3.3 Format of the Simulation Results

There are three simulation domains in MOSE, including CW, TD, and FD. The description of the simulation results are also divided into three parts correspondingly. The simulation results include the transmittance results, the absorption results and the detection results.

3.3.1 CW

3.3.1.1 Transmittance Results

The format of the transmittance results is recorded according to the shape of the outermost tissue. The format is shown in Table 17 while the shape is a triangle mesh, and the formats corresponding to the other shapes are listed in Tables 17-24.

Table 17 Format of the transmittance results for the shape of the **triangle mesh** under CW

Content	Explanation
Spectrum *	The central wavelength of the spectrum.
TotalPhotonNum *	The total number of photons at the current spectrum.
Runtime * (second)	The runtime of the simulation (Unit: second).
Domain CW	The simulation domain.
SpecularReflectance *	The specular reflectance of the light sources at the current spectrum.
3DCWTransmittance *	The total transmittance at the current spectrum in 3D.
3DCWTransmittanceMesh *	The total transmittance of the triangle meshes.
CountMeshVertex *	The number of data, which is equal to the number of mesh vertices.
3DCWTransmittanceMeshVertex	The transmittance result on each mesh vertex.
0.00000e+000 …	One-dimensional matrix data; the order is the same as that of the mesh vertices in the shape file of a triangle mesh.
CountMeshFace *	The number of data, which is equal to the number of mesh faces.
3DCWTransmittanceMeshFace	The transmittance result on each mesh face.
0.00000e+000 …	One-dimensional matrix data; the order is the same as that of the mesh faces in the shape file of the triangle mesh.

NOTE：The formats of the contents in the green part of the table above are the same for all of the shapes, and those in the blue part are different for different shapes. The asterisk indicates the value.

Table 18 Format of the transmittance results for the shape of the **tetrahedral mesh** under CW

3DCWTransmittance *	The total transmittance at the current spectrum in 3D.
3DCWTransmittanceTetraMesh *	The total transmittance at the boundaries of the triangle meshes of the medium.
CountMeshTetraVertex *	The number of data, which is equal to the vertex number of the tetrahedral mesh.

3DCWTransmittanceTetraMeshVertex	The transmittance result on each mesh vertex. **NOTE**: The transmittance on the inner vertex would be zero.
0.00000e+000 …	One-dimensional matrix data; the order is the same as that for the tetrahedral mesh vertices.
CountMeshTetraFace *	The data size of the triangle meshes.
3DCWTransmittanceTetraMeshFace	The transmittance result on each boundary face of the tetrahedral mesh. **NOTE**: The transmittance on the inner boundary face would be zero.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data. The first three lines are the vertex number of the triangle mesh on the boundaries of the medium (including the inner boundary and outer boundary); the last line is the transmittance result of each triangle mesh.

Table 19 Format of the transmittance results for the shape of the **rectangle** under CW

2DCWTransmittance *	The total transmittance at the current spectrum in 2D.
2DCWTransmittanceUp *	The total transmittance on the upside of the rectangle.
CountX *	The number of data along the X-axis.
2DCWTransmittanceUpX	The transmittance results on the upside.
0.00000e+000 …	One-dimensional matrix data.
2DCWTransmittanceDown *	Total transmittance on the downside of the rectangle.
CountX *	The number of data along the X-axis.
2DCWTransmittanceDownX	The transmittance results on the downside.
0.00000e+000 …	One-dimensional matrix data.
2DCWTransmittanceLeft *	The total transmittance on the left side of the rectangle.
CountY *	The number of data along the Y-axis.
2DCWTransmittanceLeftY	The transmittance results on the left side.
0.00000e+000 …	One-dimensional matrix data.
2DCWTransmittanceRight *	The total transmittance on the right side of the rectangle.
CountY *	The number of data along the Y-axis.
2DCWTransmittanceRightY	The transmittance results on the right side.
0.00000e+000 …	One-dimensional matrix data.

Table 20 Format of the transmittance results for the shape of an **ellipse** under CW

2DCWTransmittance *	The total transmittance at the current spectrum in 2D.
2DCWTransmittanceSide *	The total transmittance on the side of the ellipse.
CountA *	The number of data along the direction of the azimuth angle.
2DCWTransmittanceSideA	The transmittance results on the side.
0.00000e+000 ……	One-dimensional matrix data.

Table 21 Format of the transmittance results for the shape of an **ellipsoid** under CW

3DCWTransmittanceSide *	The total transmittance on the side of the ellipsoid.

CountD CountA * *	The numbers of data along the directions of the deflection angle and azimuth angle respectively.
3DCWTransmittanceSideDA	The transmittance results on the side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data where the order is: [0 0] [0 1] … [0 CountA] [1 0] [1 1] … [1 CountA] … [CountD 0] … [CountD CountA]

Table 22 Format of the transmittance results for the shape of a **cylinder** in the **Cylindrical coordinate system** under CW

3DCWTransmittanceSideAZ *	The total transmittance on the side of the cylinder.
CountA CountZ * *	The numbers of data along the azimuth angle direction and Z-axis respectively.
3DCWTransmittanceSideAZ	The transmittance results on the side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceTop *	The total transmittance on the top of the cylinder.
CountR CountA * *	The numbers of data along the radial direction and azimuth angle direction respectively.
3DCWTransmittanceTopRA	The transmittance results on the top.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceBottom *	The total transmittance on the bottom of the cylinder.
CountR CountA * *	The numbers of data along the radial direction and azimuth angle direction respectively.
3DCWTransmittanceBottomRA	The transmittance results on the bottom.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

Table 23 Format of the transmittance results for the shape of a **cylinder** in the **Cartesian coordinate system** under CW

3DCWTransmittanceSide *	The total transmittance on the side of the cylinder.
CountA CountZ * *	The numbers of data along the azimuth angle direction and Z-axis respectively.
3DCWTransmittanceSideAZ	The transmittance results on the side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceTop *	The total transmittance on the top of the cylinder.
CountX CountY * *	The numbers of data along the X-axis and Y-axis respectively.
3DCWTransmittanceTopXY	The transmittance results on the top.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceBottom *	The total transmittance on the bottom of the cylinder.
CountX CountY * *	The numbers of data along the X-axis and Z-axis respectively.

3DCWTransmittanceBottomXY	The transmittance results on the bottom.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

<div align="center">Table 24 Format of the transmittance results for the shape of a cube under CW</div>

3DCWTransmittanceTop *	The total transmittance on the top of the cube.
CountX CountY * *	The numbers of data along the X-axis and Y-axis respectively.
3DCWTransmittanceTopXY	The transmittance results on the top.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceBottom *	The total transmittance on the bottom of the cube.
CountX CountY * *	The numbers of data along the X-axis and Y-axis respectively.
3DCWTransmittanceBottomXY	The transmittance results on the bottom.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceLeft *	The total transmittance on the left side of the cube.
CountX CountZ * *	The numbers of data along the X-axis and Z-axis respectively.
3DCWTransmittanceLeftXZ	The transmittance results on the left side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceRight *	The total transmittance on the right side of the cube.
CountX CountZ * *	The numbers of data along the X-axis and Z-axis respectively.
3DCWTransmittanceRightXZ	The transmittance results on the right side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceFront *	The total transmittance on the front side of the cube.
CountY CountZ * *	The numbers of data along the Y-axis and Z-axis respectively.
3DCWTransmittanceFrontYZ	The transmittance results on the front side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWTransmittanceBack *	The total transmittance on the top side of the cube.
CountY CountZ * *	The numbers of data along the Y-axis and Z-axis respectively.
3DCWTransmittanceBackYZ	The transmittance results on the back side.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

3.3.1.2 Absorption results

The format of the absorption results is recorded based on the coordinate system. The format in the Cartesian coordinate system is shown in Table 25, and the formats in the other coordinate systems are listed in Tables 25-28.

<div align="center">Table 25 Format of the absorption results in a 3D Cartesian coordinate system under CW</div>

Content	Explanation

Spectrum *	The central wavelength of the spectrum.
Domain CW	The simulation domain.
3DCWAbsorption *	The total absorption in 3D at the current spectrum.
CountX CountY CountZ * * *	The numbers of data along the X-axis Y-axis and Z-axis respectively.
3DCWAbsorptionXYZ	The absorption results.
0.00000e+000 0.00000e+000 … …	Three-dimensional matrix data where the order is: [0 0 0] [0 0 1] … [0 0 CountZ] [0 1 0] [0 1 1] … [0 1 CountZ] … [0 CountY 0] [0 CountY 1] … [0 CountY CountZ] … [CountX CountY 0] [CountX CountY 1]… [CountX CountY CountZ]

Table 26 Format of the absorption results in a 3D **Cylindrical coordinate system** under CW

3DCWAbsorption *	The total absorption in 3D at the current spectrum.
CountR CountA CountZ * * *	The numbers of data along the radial direction, azimuth angle direction and Z-axis respectively.
3DCWAbsorptionRAZ	The absorption results.
0.00000e+000 0.00000e+000 … …	Three-dimensional matrix data; the order is the same as that in Table 24.

Table 27 Format of the absorption results in a 2D **Cartesian coordinate system** under CW

2DCWAbsorption *	The total absorption in 2D at the current spectrum.
CountX CountY * *	The numbers of data along the X-axis and Y-axis respectively.
2DCWAbsorptionXY	The absorption results.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

Table 28 Format of the absorption results in a 2D **Polar coordinate system** under CW

2DCWAbsorption *	The total absorption in 2D at the current spectrum.
CountR CountA * *	The numbers of data along the radial direction and azimuth angle direction respectively.
2DCWAbsorptionRA	The absorption results.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

3.3.1.3 Plane Detector Results

The format of the plane detector result is shown in Table 29.

Table 29 Format of the detection results under CW

Content	Explanation
Spectrum *	The central wavelength of the spectrum.
3DTotalDetection * *	The number of the detector and total detection at the current spectrum.
HeightResolution WidthResolution * *	The numbers of data along the directions of the height and width respectively.

3DDetectionMatrix	The detection results.
0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.

3.3.1.3 Fiber Detector Results

The format of the fiber detector results is shown in Table 30.

Table 30 Format of the fiber detection results under CW

Content	Explanation
Spectrum *	The central wavelength of the spectrum.
TotalDetection *	The number of the detector
3DFiberDetector *	The total detection at the current spectrum
3DCWFiberDetectorSide *	The detection of the detector on the side when the shape of the detector is cylinder.
CountA CountZ * *	The numbers of data along the azimuth angle direction and Z-axis respectively on the side.
3DCWFiberDetectorSideAZ 0.00000e+000 0.00000e+000 … …	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWFiberDetectorTop *	The detection of the detector on the top when the shape of the detector is cylinder.
CountX CountY * *	The numbers of data along the X-axis and Y-axis respectively on the top.
3DCWFiberDetectorTopXY 0.00000e+000 0.00000e+000 ...	Two-dimensional matrix data; the order is the same as that in Table 20.
3DCWFiberDetectorBottom *	The detection of the detector on the bottom when the shape of the detector is cylinder.
3DCWFiberDetectorBottomXY 0.00000e+000 0.00000e+000 ...	Two-dimensional matrix data; the order is the same as that in Table 20.
CountD CountA * *	The numbers of data along the directions of the deflection angle and azimuth angle respectively.
3DCWTransmittanceSideDA 0.00000e+000 0.00000e+000 ...	Two-dimensional matrix data; the order is the same as that in Table 20.

3.3.2 TD

3.3.2.1 Transmittance Results

Compared to the transmittance results under CW, the transmittance results under TD only increase the time as shown in Table 31.

Table 31 Format of the transmittance results for the shape of a **triangle mesh** under TD

Content	Explanation
Domain TD	The simulation domain.
3DTDTransmittance 2.85103e-002	The total transmittance in all of the time segments.
TDTransmittanceNum 5	The number of time segments.
TD 0 *	The total transmittance in the first time segment.
3DTDTransmittanceMesh	The total transmittance of the triangle meshes in the first time segment.
CountMeshFace *	Same as that in Table 17.
3DTDTransmittanceMeshFace	The transmittance results on each mesh face in the first time segment.
0.00000e+000 …	Same as that in Table 17.
CountMeshVertex *	Same as that in Table 17.
3DTDTransmittanceMeshVertex	The transmittance results on each mesh vertex in the first time segment.
0.00000e+000 …	Same as that in Table 17.
TD 1 *	The total transmittance in the second time segment.
CountMeshFace *	Ibid
3DTDTransmittanceMeshFace	Ibid
0.00000e+000 …	Ibid
CountMeshVertex *	Ibid
3DTDTransmittanceMeshVertex	Ibid
0.00000e+000 …	Ibid

NOTE: The contents in red font are the differences from those in Table 17.

3.3.2.2 Absorption Results

Compared to the absorption results under CW, the absorption results under TD merely increase the time as shown in Table 32.

Table 32 Format of the absorption results in a 3D **Cartesian coordinate system** under TD

Content	Explanation
Domain TD	The simulation domain.
3DTDAbsorption *	The total absorption in all of the time segments.
CountX CountY CountZ * * *	Same as that in Table 24.
TDAbsorptionNum *	The number of the time segments.
TD 0 *	The total absorption in the first time segment.
3DTDAbsorptionXYZ	Same as that in Table 24.
0.00000e+000 0.00000e+000 …	Same as that in Table 24.

…	
TD 1 *	The total absorption in the second time segment.
3DTDAbsorptionXYZ	Same as that in Table 24.
0.00000e+000 0.00000e+000 … …	Same as that in Table 24.

3.3.3 FD

3.3.3.1 Transmittance Results

Compared to the transmittance results under CW, the transmittance results under FD include amplitude and phase as shown in Table 33.

Table 33 Format of the transmittance results for the shape of a **triangle mesh** under TD

Content	Explanation
Domain FD	The simulation domain.
CountMeshFace *	Same as that in Table 17.
3DFDAmpTransmittanceMeshFace	The amplitude of the transmittance on each mesh face.
0.00000e+000 …	Same as that in Table 17.
3DFDPhaTransmittanceMeshFace	The phase of the transmittance on each mesh face.
0.00000e+000 …	Same as that in Table 17.
CountMeshVertex *	Same as that in Table 17.
3DFDAmpTransmittanceMeshVertex	The amplitude of the transmittance on each mesh vertex.
0.00000e+000 …	Same as that in Table 17.
3DFDPhaTransmittanceMeshVertex	The phase of the transmittance on each mesh vertex.
0.00000e+000 …	Same as that in Table 17.

3.3.3.2 Absorption Results

Compared to the absorption results under CW, the absorption results under FD include amplitude and phase as shown in Table 34.

Table 34 Format of the absorption results in a 3D **Cartesian coordinate system** under FD

Content	Explanation
Domain FD	The simulation domain.
CountX CountY CountZ * * *	Same as that in Table 24.
3DFDAmpAbsorptionXYZ	The amplitude of the absorption in a 3D Cartesian coordinate system.
0.00000e+000 0.00000e+000 …	Same as that in Table 24.

…	
3DFDPhaAbsorptionXYZ	The phase of the absorption in a 3D Cartesian coordinate system.
0.00000e+000 0.00000e+000 … …	Same as that in Table 24.

3.4 Other files

In MOSE, there are other types of files except for the optical simulation parameters and simulation results file:

RAW/IMG/IM0/DICOM
Instruction: Image data used in the image processing.

OFF
Instruction:
Only the triangle mesh file in the OFF format is supported by MOSE.
1. The numbers of vertices and triangle meshes.
2. Vertex data: The order of each line is x, y and z coordinates for each vertex.
3. Triangle mesh data: The order of each line is the vertex number of each mesh (triangle mesh is 3) and the vertex indices of each triangle mesh. The index begins from 0.

PLY
Instruction:
Only the triangle mesh file in a PLY format is supported by MOSE; for more information please refer to: http://paulbourke.net/dataformats/ply/

SURF
Instruction:
1. Vertex data: The first part is the number of vertices. In the second part, the order of each line is x, y and z coordinates of each vertex.
2. Triangle mesh data: The first part is the number of triangle meshes. In the second part, the order of each line is the vertex indices of each triangle mesh. The index starts from 1.

AM
Instruction:
The tetrahedral mesh file is generated from Amira, so for more information please refer to: http://www.amira.com/

MESH
Instruction:
The tetrahedral mesh file is generated from Netgen (http://www.hpfem.jku.at/netgen/), which consists of three parts:
1. Vertex data: The first part is the number of vertices. In the second part, the order of each line is x, y and z coordinates of each vertex.

2. Tetrahedral data: The first part is the number of tetrahedrons. In the second part, the order of each line is the region index of each tetrahedron it belongs to as well as the vertex indices of each tetrahedron. Both indices of the region and the vertex begin at 1.

3. Boundary triangle mesh from different regions (Note: This part is not used by MOSE, thus it should be omitted). The first part is the number of triangle meshes. In the second part, the order of each line is the region index of each triangle mesh it belongs to as well as the vertex indices of each triangle mesh. Both indices of the region and the vertex start from 1.

STL

Instruction:

Only the triangle mesh file in a PLY format is supported by MOSE, for example:

```
solid name
  facet normal ni nj nk
    outer loop
       vertex v1x v1y v1z
       vertex v2x v2y v2z
       vertex v3x v3y v3z
    endloop
  endfacet
  ...
  ...
endsolid name
```

4 Frequently Asked Questions (FAQ)

1.   Can I use MOSE in a commercial organization?

Yes, MOSE is free software. You can use it on any computer. You just need to register without purchasing MOSE.

2.   Why does the process of MOSE still reside in the task manager after closing the program?

This is because some amount of memory has not been released after closing MOSE, and it may still reside in the task manager. The process needs to be closed by the user manually in the task manager. MOSE is developed for use at a research institute, thus it is not perfect and we will work continuously to improve it.