PMOD Geometric Models and Simulation (PGEM)

USER MANUAL
Version 4.1

PMOD is a software
FOR RESEARCH USE ONLY (RUO)
and must not be used for diagnosis or treatment of patients.

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π.pmod

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1 PMOD Geometric Models and Simulation Tool (PGEM)

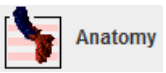
The **PGEM** tool supports various types of analyses and simulations based on anatomical data. Particularly, the following tasks are supported:

- **DTI Tractography**: Diffusion tensors resulting from the analysis of DWI MR data can be imported and three-dimensional tracts generated. They may be visualized in 3D scenes, used for statistics on the diffusion maps, and exported in vtk format for use in external programs.
- **4D Flow Visualization**: MR sequences are able to measure the instantaneous flow vector in vessels over time. In a similar analysis as in tractography, this information can be used for generating streamlines which visualize flow direction and velocity.
- **Generation of Dynamic PET images**: Based on an anatomical atlas and a time-activity curve for each atlas structure, a synthetic dynamic PET image can be generated with a certain noise level. Such data can be used for the evaluation of parametric mapping and segmentation approaches.
- **Construction of Vessel Structures and Computational Fluid Dynamics (CFD) simulation**: In a first step vessel structures can be segmented from anatomical images and converted into a geometric model. In a second step, flow through the vessel is simulated in an external CFD software. The resulting flows can subsequently be retrieved and analyzed.

1.1 User Interface

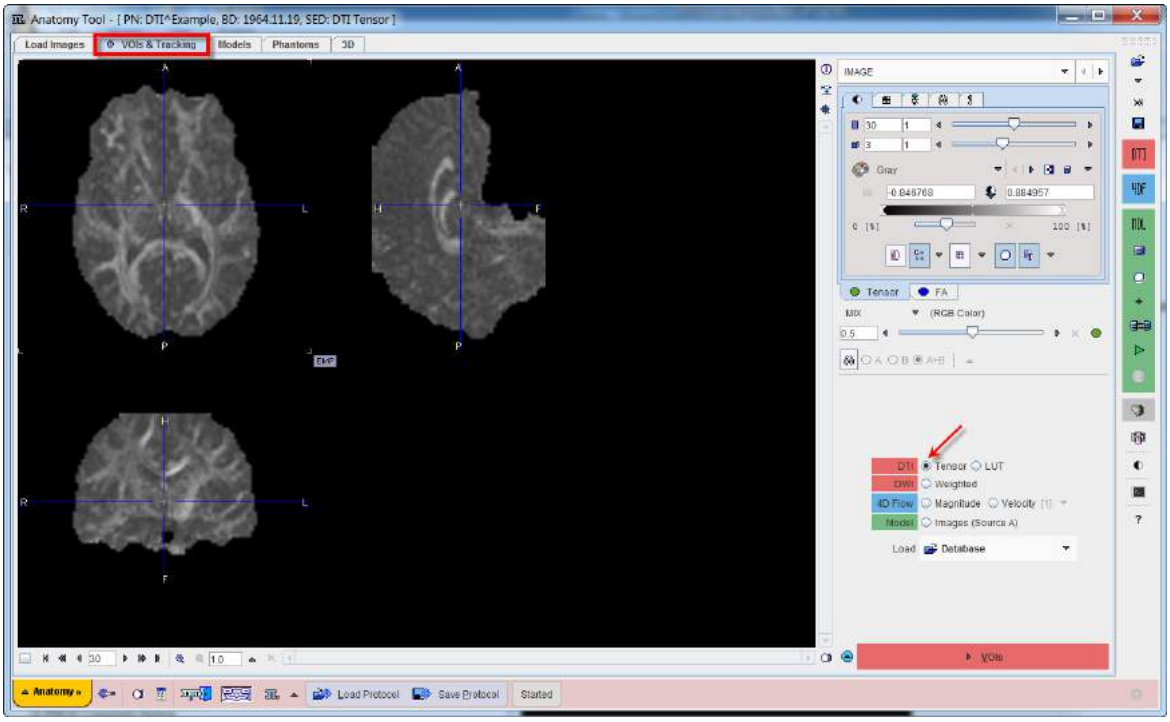
Starting the PGEM Tool

The PGEM tool is started with the **Anatomy** button from the PMOD Toolbox:



The user interface of PGEM consists of five pages which can be selected by tabs:

1. **Load Images** page: This page is only available when using PMOD databases.
2. **VOIs & Tracking** page: Main page for DTI and 4D Flow analysis, as well as the VOI definition for the anatomical models.
3. **Models** page: Page for geometric model definition and calling CFD modeling.
4. **Phantoms** page: Page for using a geometric model for the generation of synthetic images.
5. **3D** page: Page for results are visualized with 3D rendering.

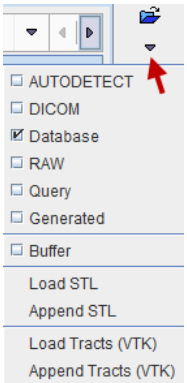


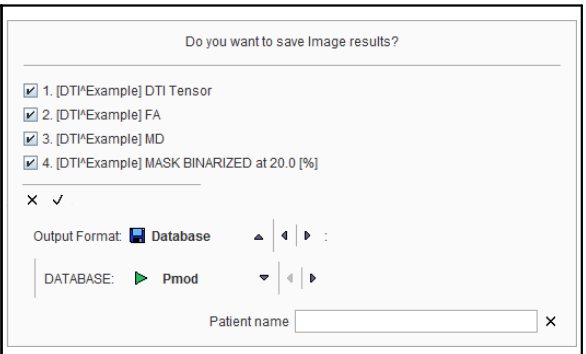
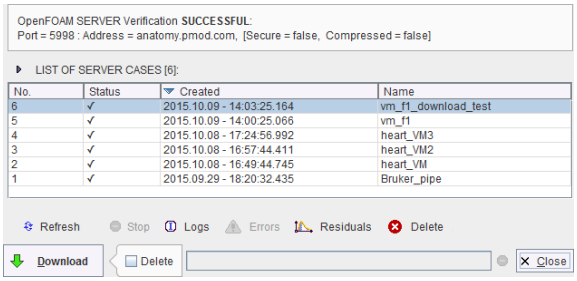
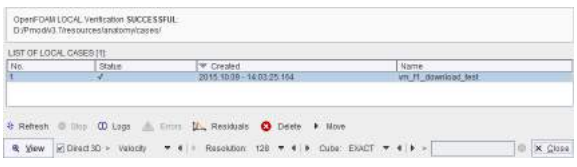
Workflows

The main workflows share the pages. Color coding is therefore applied for highlighting the elements belonging to a certain workflow: red for DTI, blue for 4D Flow, green for anatomical model definition and CFD simulation.

Taskbar

The taskbar to the right of the application window provides shortcut buttons for frequent tasks. Please note the tooltips when hovering over the buttons.

	Load images. The arrow below the loading button allows changing the data format. 
	Clear all data.
	Save results. A dialog window appears for selecting the relevant parts and defining the output format.

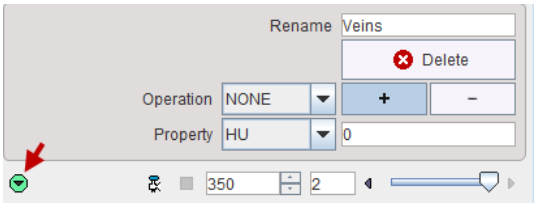
	
	Start DTI workflow by loading tensor images.
	Start 4D Flow workflow by loading MR images with 4D flow information.
	Start model construction workflow by loading anatomical images.
	Create a new anatomic model.
	Open the **VOIs** panel on the **VOIS & Tracking** page.
	Load VOIs from a file and add them to the current model
	Open the manager of the remote OpenFOAM cases. 
	Open the manager of the local OpenFOAM cases. 
	Allows viewing linked CFD case.
	Rendering the selected model structures in 3D.
	Aggregation of VOI statistics results for 4D Flow.

	Hide the control area for more image space. Activate again to show controls again.

Hidden Controls

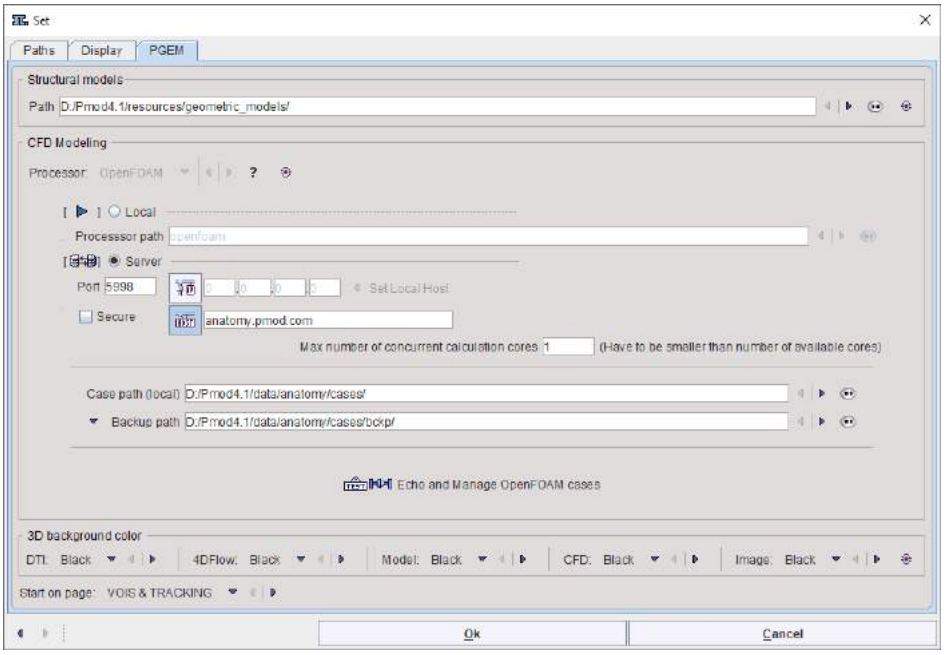
In some places options are hidden to save screen space. This is indicated by a blue up-arrow as in the example below.

When the button is activated, the area expands, showing all the options. It can be collapsed again with the green down-arrow.



1.2 Configuration Settings

The PGEM tool can be configured according to user preference using the icon next to the **Anatomy** menu button.



The **Structural models** path defines, where the created models will be stored.

In the **CFD Modeling** section the OpenFOAM CFD server can be configured. Per default, PMOD comes configured with an **OpenFoam** server hosted on a PMOD machine (anatomy.pmod.com:5998). However, this open foam server should only be used for tests, and not for productive data processing. We recommend users to set up their own server, which is easy to do and free of charge. A description of the OpenFOAM installation on Ubuntu and the PMOD configuration is available in the following section 9.

The **Case path (local)** allows defining the directory where the CFD cases will be downloaded from the OpenFOAM server. Similarly, a **Backup path** can be configured.

The **3D background color** settings serve for predefining the background in the scenes created by the different workflows.

The **Start on page** should be configured such that the most frequently used page is opened when starting PGEM up.

1.3 OpenFoam CFD Server

OpenFoam Installation on Ubuntu

OpenFoam 5.0 installation for Ubuntu is described at: https://openfoam.org/download/5-0-ubuntu/

Installation steps for Ubuntu 16.04 and OpenFoam 5.0:

1. Add OpenFoam repository

   sudo add-apt-repository http://dl.openfoam.org/ubuntu

   sudo sh -c "wget -O - http://dl.openfoam.org/gpg.key | apt-key add -"
2. Update package list

   sudo apt-get update
3. Install OpenFoam and Paraview

   sudo apt-get -y install openfoam5
4. Edit shell configuration, open .bashrc in editor

   gedit ~/.bashrc

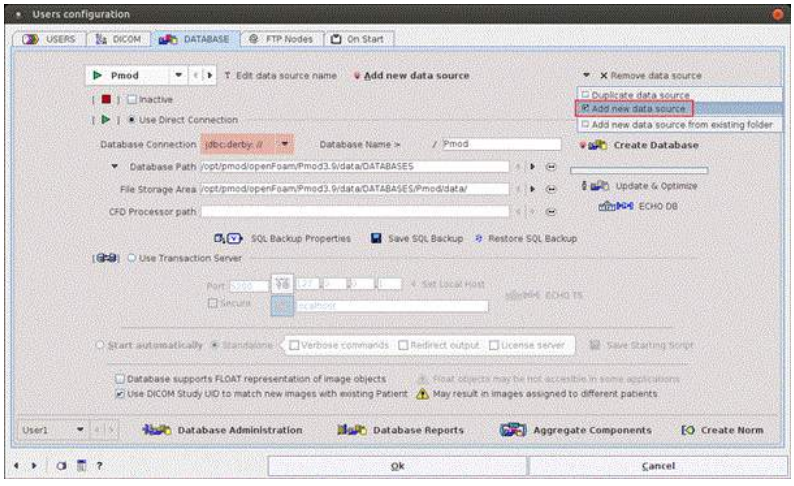
   and add at the end of file:

   source /opt/openfoam5/etc/bashrc

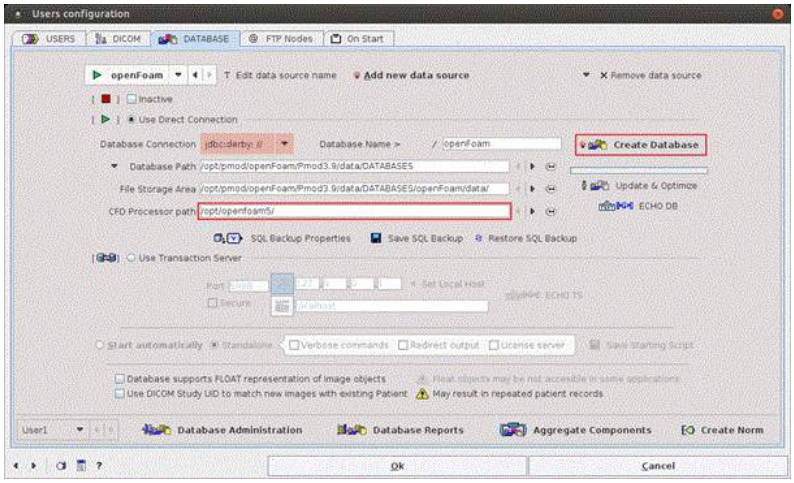
Pmod Configuration for OpenFoam

Once PMOD is properly installed, the OpenFoam CFD server can be easily configured performing the following steps:

1. Open the main configuration interface using the **Config** button available on the **PMOD Toolbox**.
2. Select the **DATABASE** tab and **Add new source** as illustrated below:

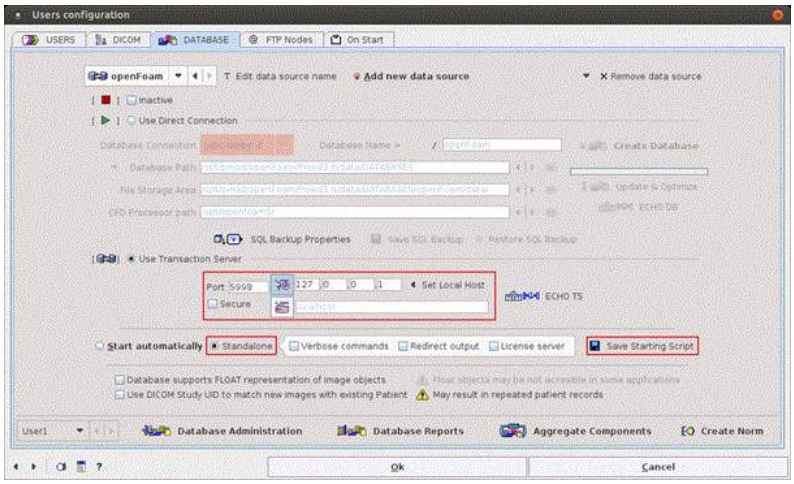


3. Activate the **Create Database** button and configure the **Path** to OpenFoam:



Note that path should point to OpenFoam main folder e.g. */opt/openfoam5/*

4. Switch the radio button from **Use Direct Connection** to **Use Transaction Server:**



5. Configure the properties of the transaction server. The **Secure** box is for enabling secure communication. This mode should be used if the communication is not confined within the institution. Otherwise it will slow down the communication speed unnecessarily.
6. An important property is the IP **Port** for the communication. It must be a unique number not used by any other transaction server or other process. The default port is **5202** if no other transaction server was configured during the PMOD installation.
7. Another important property is the **IP address**. It must contain the address of the host in which the servers are running, so typically the system on which the configuration is performed. For this system the IP address can be obtained by activating the **Set Local Host** button. Note that entering "localhost" in the **HOST** area will NOT work!
8. Check the box **Stand alone** and activate the **Save Starting Script** button. A dialog window appears which shows the contents of the created script. The example below shows the result for Ubuntu system:

9. Select **Yes** to save the starting script with the specified **Name** in the specified subdirectory of the PMOD installation directory:

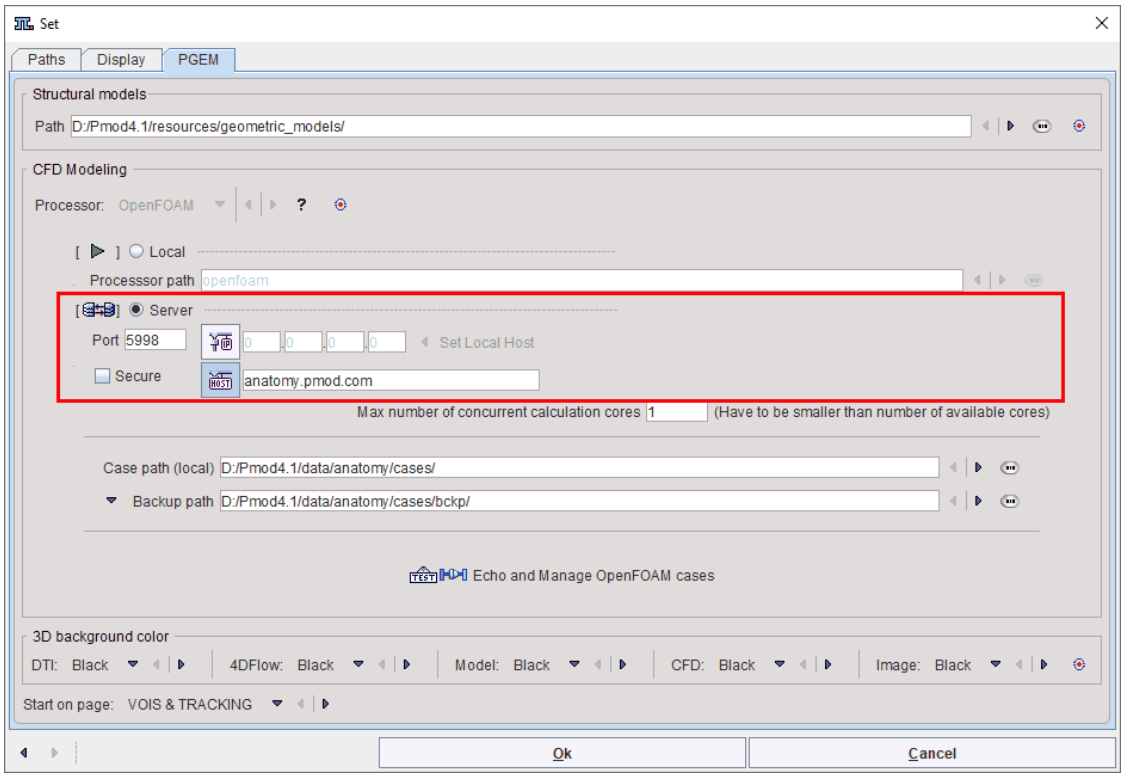
Note: Do NOT switch the radio button back to Use JDBC Connection. The transaction server should run at all times so command window should remain open.

10. Save the PMOD configuration with the **OK** button and exit PMOD.
11. Start the Pmod Transaction Server by double-clicking the script file. Please note that Transaction Server doesn't need a WIBU Key to run, it can be unplugged.

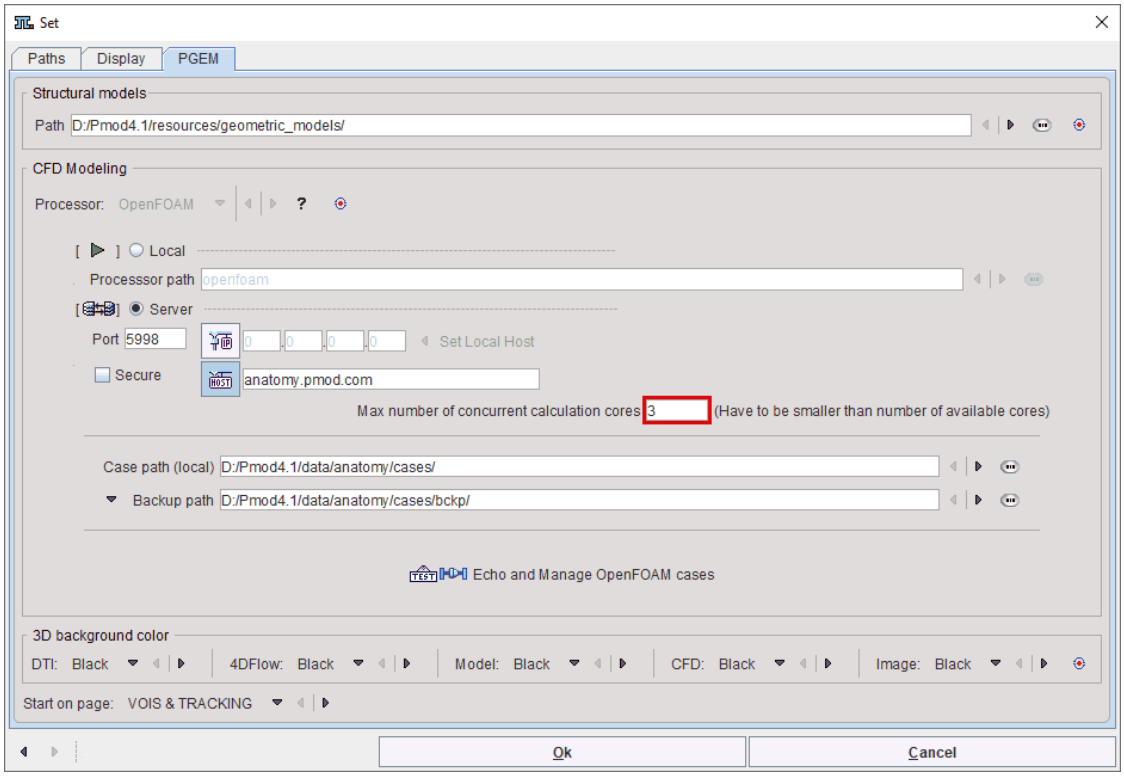
Pmod configuration for OpenFoam (client side)

Start the PGEM local configuration to configure the OpenFoam PMOD client. The steps for an appropriate configuration are as follows:

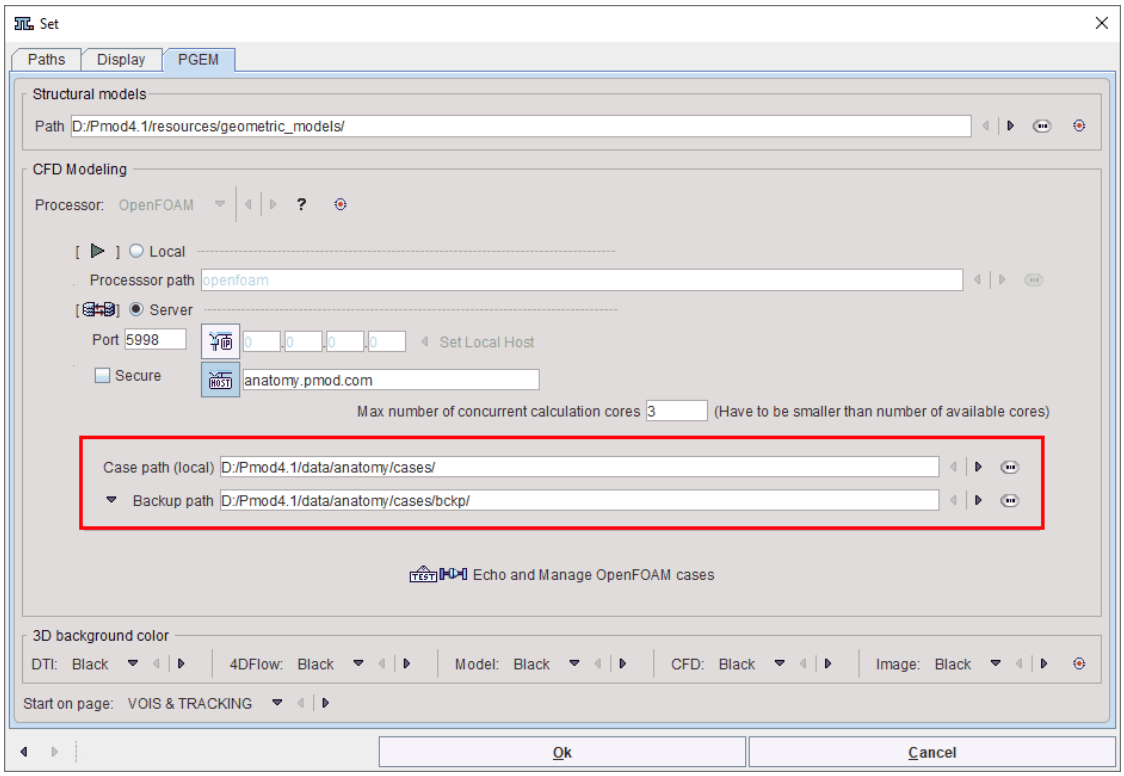
1. In the **CFD Modeling** section enable the **Server** radio button. Define the server by the **host** name or **IP** address and set the **Port** number used in the openFoam transaction server configuration as indicated below:



2. Set the number of cores on the server to be used when solving CFD cases with the OpenFoam:

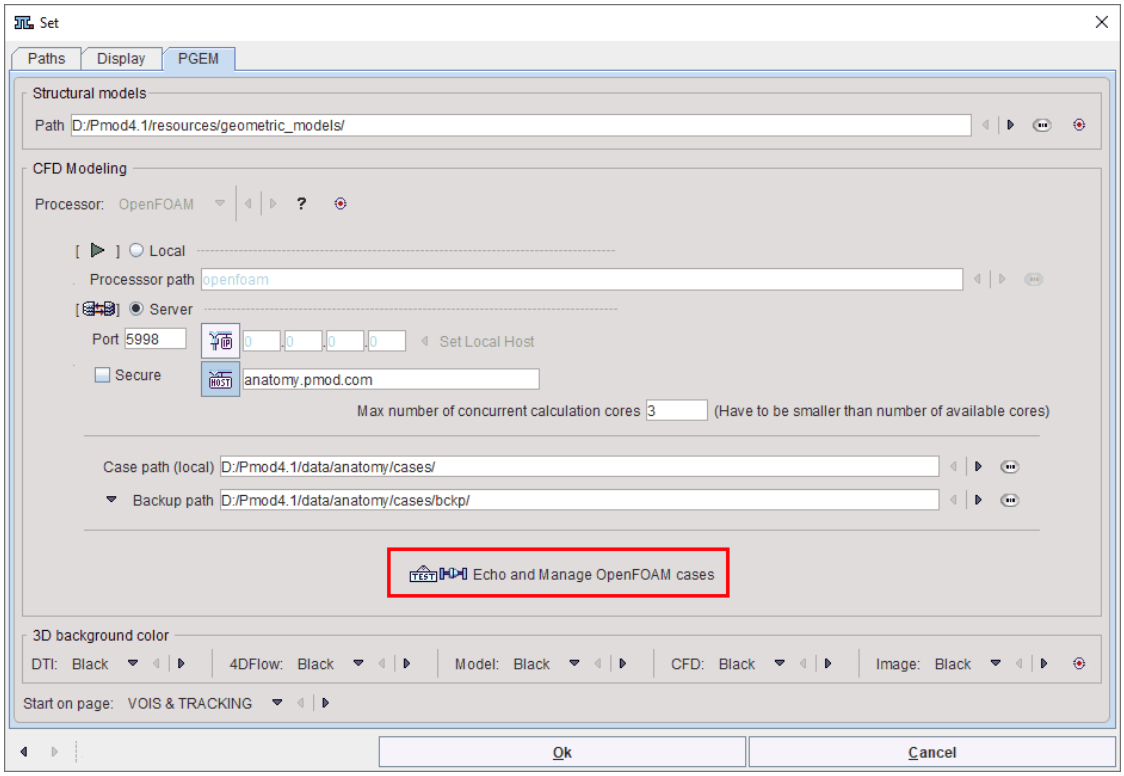


3. Define the local path (client side) to the cases folder:



Note that cases downloaded from the server will be stored on the location specified on the **Case path (local)**.

4. Finally, activate the **Echo and Manage OpenFOAM cases** button to verify the configuration:



1.4 Additional Documentation

The PGEM tool is based on a range of functionalities from the PMOD environment which are not explained in this documentation. Please refer to the

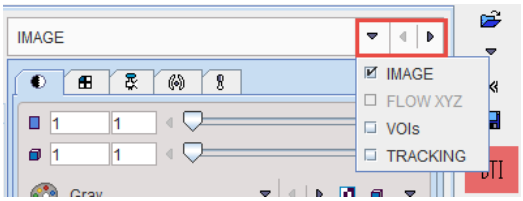
- *PMOD Base Functionality Guide* for information related to data loading, image viewing, volume-of-interest (VOI) definition and the
- *PMOD 3D Rendering Tool Users Guide* for rendering-related information.

2 DTI Tractography

This chapter describes the workflow for loading diffusion tensor data and performing tractography.

2.1 Workflow Organization

The DTI workflow starts on the **VOIs & Tracking** page, which has 4 sub-pages. As illustrated below, the sub-pages can be switched with the selection in the upper right or the adjacent arrows.



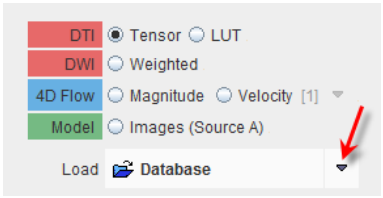
For DTI, only **IMAGE**, **VOIs** and **TRACKING** are relevant. Therefore, FLOW XYZ is disabled as soon as the DTI tensor images have been loaded.

On each page, the user has to perform an operation or configuration, and then activate the red action button in the lower right for proceeding. Correspondingly, an operation is performed and the result shown an the next page. After leaving the **TRACKING** page, the resulting fiber tracks are visualized on the **3D** page.

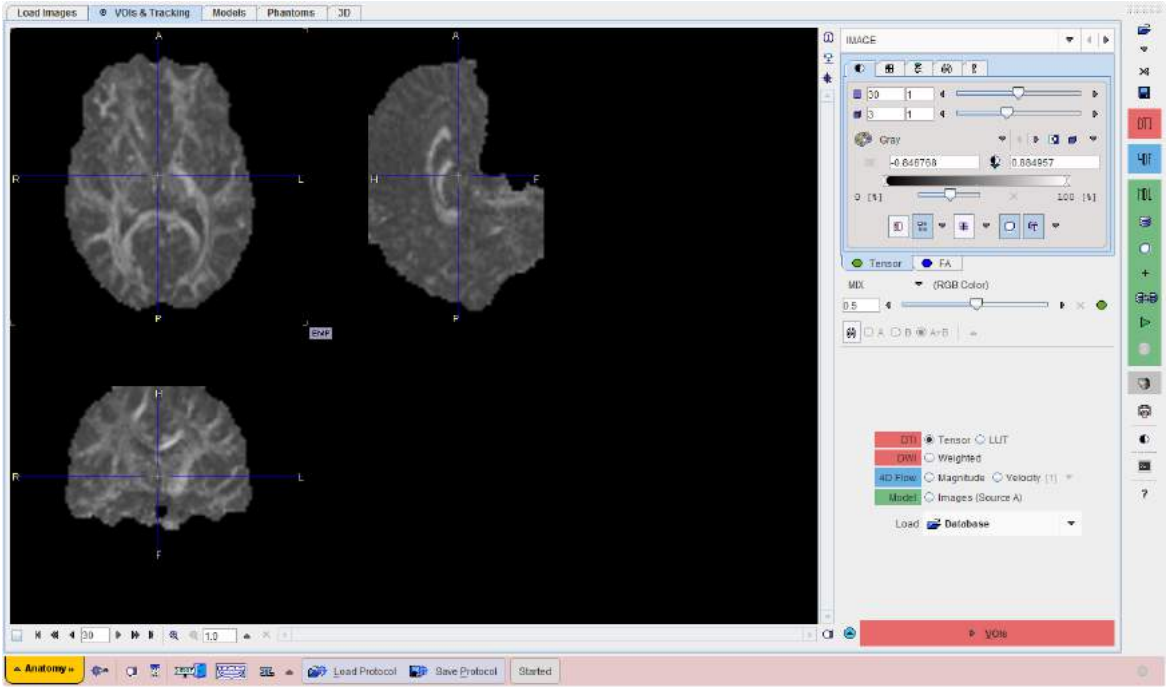
In order to test a different tracking configuration, the user has to return to a prior stage by selecting the **VOIs & Tracking** page again, choosing the appropriate sub-page, and then proceeding from there as with the initial workflow by the red action buttons.

2.2 Loading the Diffusion Tensor Images

Most conveniently, the diffusion tensor images are loaded using the DTI button in the taskbar to the right. As an alternative, the **Tensor** radio button can be set on the **IMAGE** page and the images loaded with the button indicated below.



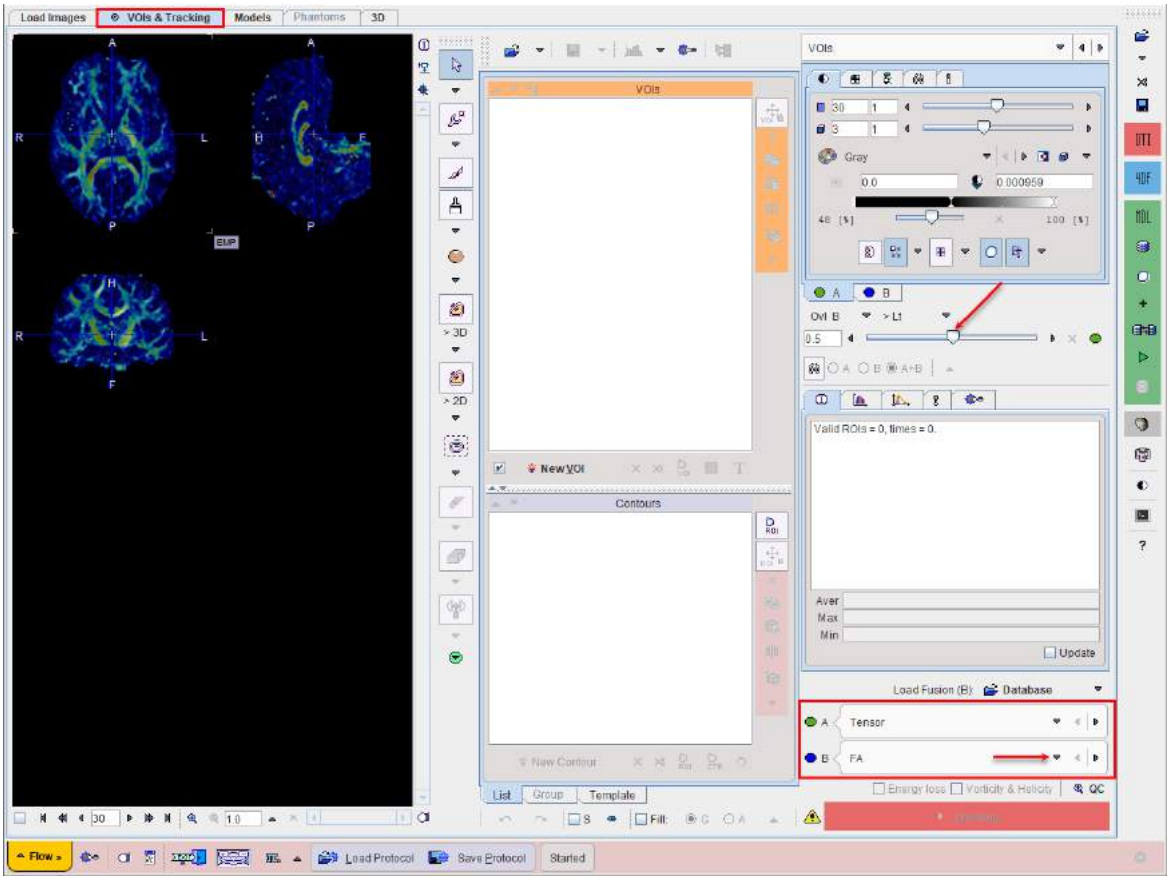
As a result of this loading, the workflow type is defined as "DTI tractography" and the internal program switches are configured accordingly. Particularly, the action button in the lower right is set to red color and indicates that the next step continues on the VOIs sub-page.



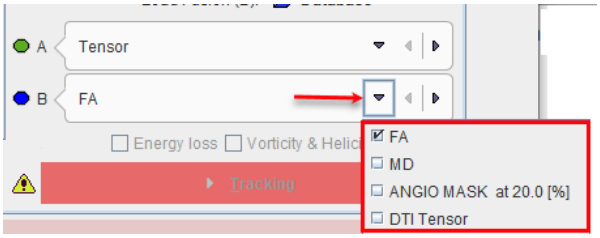
Please activate VOIs to proceed.

2.3 Defining VOIs for Seeding and Imposing Restrictions

When arriving at the **VOIs** sub-page a fusion image is shown to the left which is composed of the **Tensor** image and the **FA** (Fractional Anisotropy) map. Note the two panels **A** and **B** in the upper right which correspond to these images, and the slider for mixing the respective contributions in the fusion image.



In the lower right, the **A** and **B** images can be redefined. The mean diffusivity (**MD**), the **DTI tensor** as well as a masked version of the FA image are available for selection.

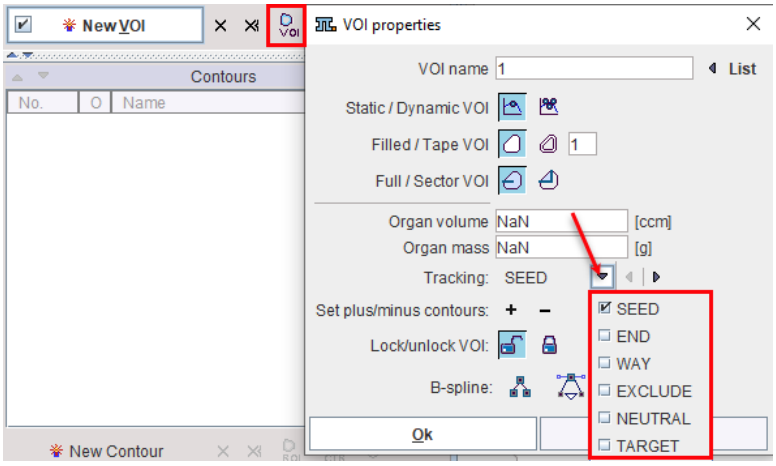


VOI Definition

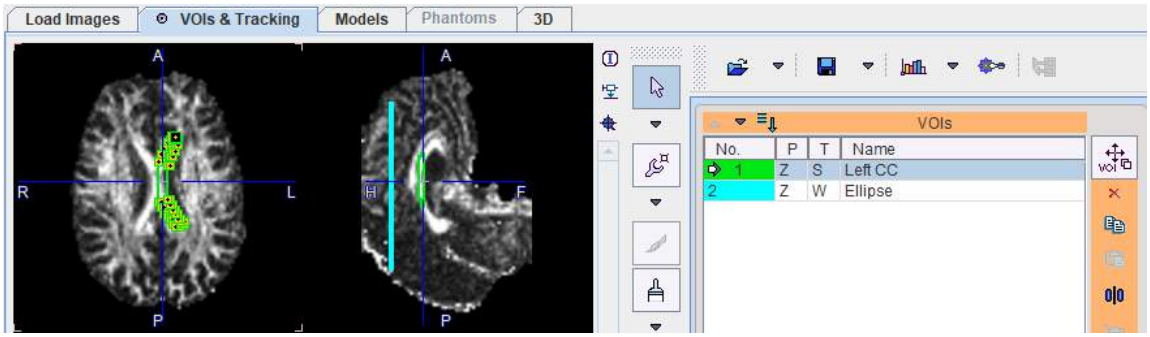
In PGEM, tractography is based on VOIs which can play different roles:

- **SEED** VOIs: Tractography is started from the pixels in seed VOIs, following the local vector directions.
- **END** VOIs: Only tracks ending in this VOI will be used. To avoid excessive pruning of tracks, an **END** VOI should have sufficient volume.
- **WAY** VOIs: Only tracks passing through the **WAY** VOI will be used.
- **EXCLUDE** VOIs: Tracks passing through an **EXCLUDE** VOI will be removed.
- **NEUTRAL** VOIs: Such VOIs have no impact on tractography. Setting VOIs to **NEUTRAL** allows assessing the effect of **END**, **WAY** and **EXCLUDE** VOIs without the need of removing them.
- **TARGET**: Is representing a VOI the track should end with.

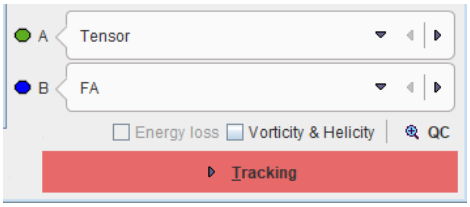
VOIs can be created with the usual PMOD VOI tools. When creating a new VOI, a dialog window pops up which requires defining the appropriate **Tracking** property. Later on, this property can be changed using the **VOI properties** functionality as illustrated below.



In the following sections two VOIs will be used: a **SEED** VOI in the left corpus callosum created using the paint tool, and an elliptic VOI which will be used as a **WAY** VOI. The illustration below shows the VOIs on top of the FA image.



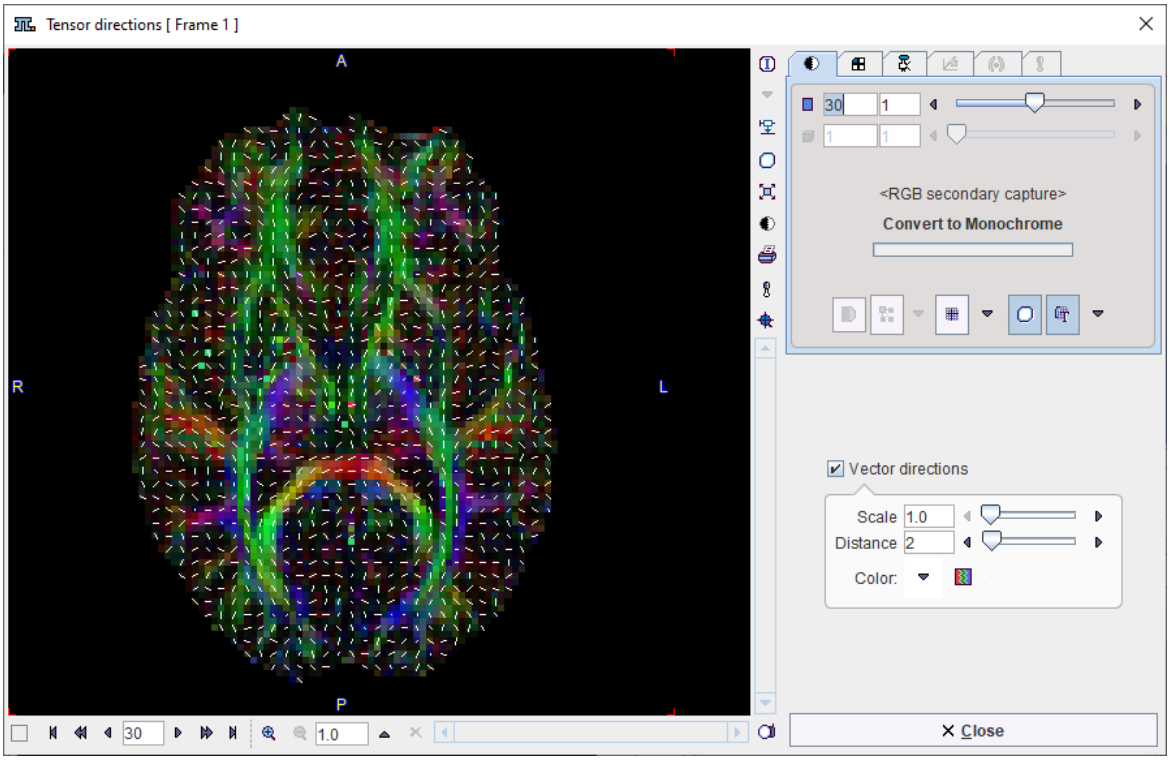
After the VOIs have been defined, please proceed with the **Tracking** button in the lower right.



Note the check box **Vorticity&Helicity**. If it is checked, PGEM calculates parametric maps called **Vorticity Amplitude** and **Absolute Helicity,** respectively. Vorticity is a measure of rotation, whereas helicity relates to the knottedness in fluids.

Tensor Inspection

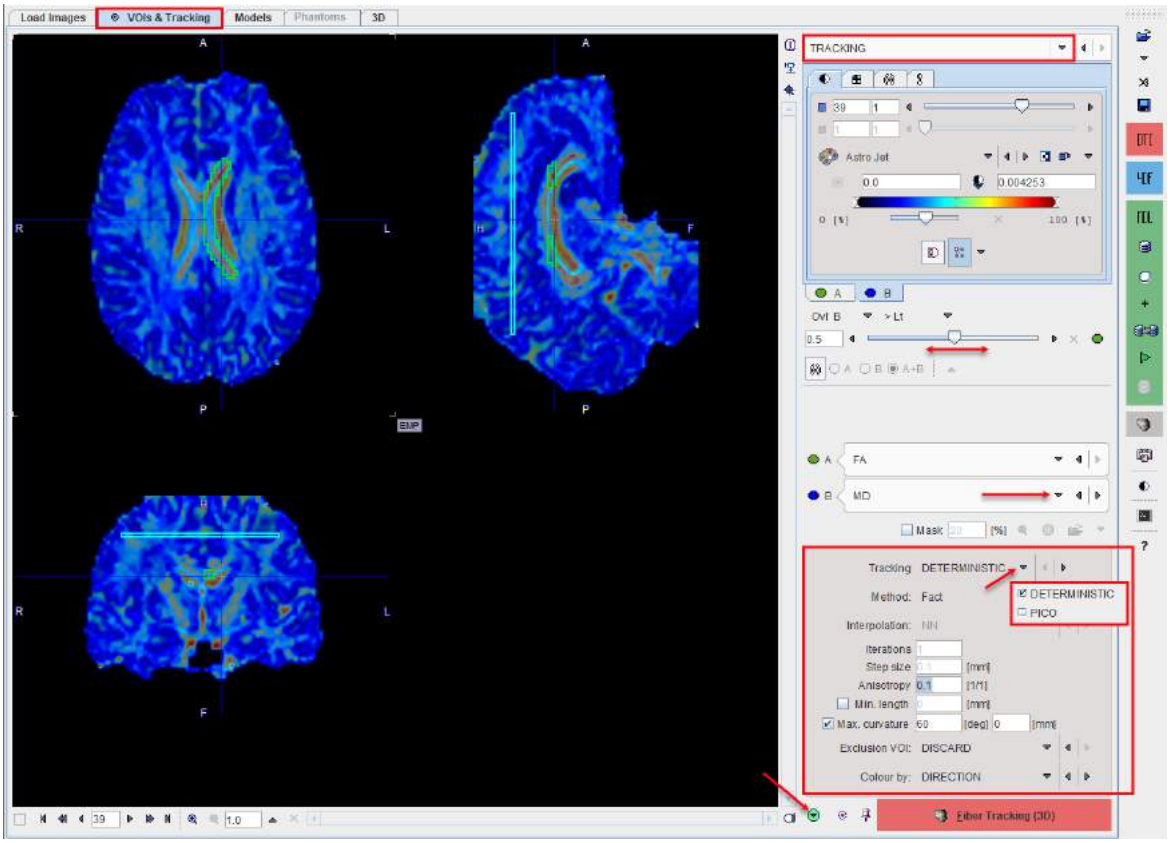
The loaded tensor data can be inspected with the **QC** button. It shows a window with the projection of the principal diffusion direction vectors together with a color-coded direction image. Red indicates diffusion along the x-axis (left-right), green diffusion along the y-axis (posterior-anterior), and blue diffusion along the z-axis (inferior-superior).



2.4 Calculating the Fiber Tracks

When arriving at the **TRACKING** page, the image area shows the **FA** image (**A**), which highlights areas of high diffusion anisotropy. However, a second image (**B**) is available for fusion. To see both images, the fusion slider has to be shifted to the right.

In the example below, the **FA** image is combined with the **MD** image, which highlights the CSF space. Also shown in the overlay are the VOIs.



Tracking Configuration

The area in the lower right serves for defining the tracking algorithm and its parameters. DTI fiber **Tracking** algorithms can be divided into **DETERMINISTIC** and probabilistic methods. PMOD supports the following probabilistic fiber tracking methods: **PICO** for DTI with pregenerated LUT tables (from the PXMOD module) and Bayesian tracking (on simplified tensors, ball and stick model) directly on DWI images.

The **DETERMINISTIC** method initiates fiber trajectories from user-defined voxels. For example, in the fiber assignment by continuous tracking algorithm (FACT) the fiber trajectories, also known as “streamlines”, follow the primary eigenvector from voxel to voxel in 3 dimensions. When the fiber trajectory reaches the edge of the voxel, the direction of the trajectory is changed to match the primary eigenvector of the next voxel. Constraints on the maximum turning angle of the streamline between voxels and on the minimum FA within a voxel for propagation of the streamline can be applied to contain the fiber tracks to regions of the brain where the diffusion tensor model realistically represents the white matter pathways[4].

The deterministic streamline fiber tracking is influenced by the noise, subject movement, and distortion from imaging artifacts which produce uncertainty in the orientation of the diffusion ellipsoid[4].

The probabilistic fiber tracking methods compensate the drawback incorporating the expected uncertainty into the tracking algorithm and can be used to produce a connectivity metric for each voxel. Probabilistic fiber tracking techniques tend to disperse trajectories more than deterministic methods and have the potential to delineate a greater portion of a white matter tract. However, the accuracy of these probabilistic methods is still limited by the information contained in the diffusion tensor and the method of constructing the probability density function[4].

For each tracking algorithm three methods are supported and can be selected in the **Method** list:

1. **FACT:** Similar to the FACT algorithm proposed by Mori et al [1], this method follows the local fiber orientation in each voxel. No interpolation is used.
2. **EULER:** Tracking proceeds using a fixed step size along the local fiber orientation [2]. With nearest-neighbor interpolation, this method may be very similar to FACT, except that the step

size is fixed, whereas FACT steps extend to the boundary of the next voxel (distance variable depending on the entry and exit points to the voxel).

3. **4th order Runge-Kutta** method [2]. The step size is fixed, however the eventual direction of the step is determined by taking and averaging a series of partial steps. Interpolation determines how the fiber direction is determined at a given point in space.

The **Interpolation** setting is not relevant for **FACT**. For **EULER** and **4th Runge-Kutta** the choices are:

1. **NN:** Nearest-neighbor interpolation using the local voxel data directly.
2. **NC:** Probabilistic nearest-neighbor interpolation, similar to the method proposed by Behrens et al [3]. The data is not interpolated, but at each point one of the 8 voxels neighbors is randomly chosen. The probability of choosing a particular voxel is based on how close the point is to the center of that voxel.
3. **TRILINEAR:** Linear interpolation of the vector components using the 8 neighbors.

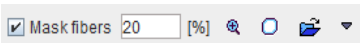
Further parameters and options determine how tracking proceeds and when it ends:

Anisotropy	Track ends if the fractional anisotropy (which is in the range [0,1]) drops below this threshold.
Step size	Distance between points on the track. Not used for FACT as it does not apply interpolation.
Min length	If checked, tracks shorter than the minimal length specified are discarded.
Max curvature	If checked, tracks are terminated in case the curvature exceeds the specified angle within the length specified. If length = 0.0, the curvature is checked at each step.
Exclusion VOI	Defines the behavior, when a track enters an **EXCLUDE** VOI: **DISCARD** the whole track, or **CLIP** it at the entry point.
Colour by	The track lines can be functionally colored as follows: **SEED**: Using the color of the **SEED** VOI. **END VOI**: Using the color of the **END** VOI. **DIRECTION**: Each segment of the track has a color combined from its direction cosines values: Red, Green, and Blue from direction cosines x, y and z respectively. **ANISOTROPY MAP**: Using the FA value along the track for coloring.

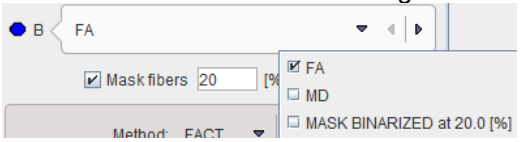
After configuring tracking, please proceed with the **Fiber Tracking (3D)** button. The tracks are calculated and visualized on the **3D** page.

Track Masking

An additional means for restricting the generated tracks is by checking the **Mask fibers** box and defining a mask. The elements in



have the following functionality:

	Generate a mask from the FA image by applying the specified threshold and include it in the image list for viewing. 

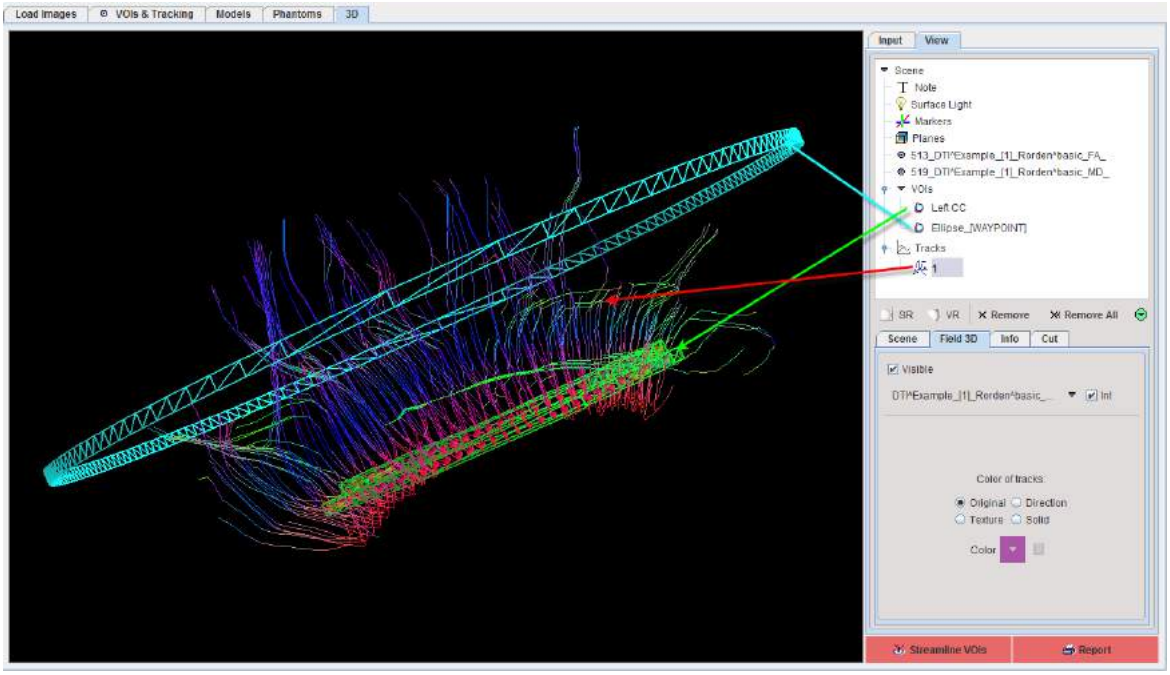
	Open the current mask in the VOI editor and convert it into a VOI. The VOI can be edited, and the mask finally updated from the VOI.
	Select an external mask file.

References

1. Mori S, Crain BJ, Chacko VP, van Zijl PC: Three-dimensional tracking of axonal projections in the brain by magnetic resonance imaging. Ann Neurol 1999, 45(2):265-269.
2. Basser PJ, Pajevic S, Pierpaoli C, Duda J, Aldroubi A: In vivo fiber tractography using DT-MRI data. Magn Reson Med 2000, 44(4):625-632.
3. Behrens TE, Woolrich MW, Jenkinson M, Johansen-Berg H, Nunes RG, Clare S, Matthews PM, Brady JM, Smith SM: Characterization and propagation of uncertainty in diffusion-weighted MR imaging. Magn Reson Med 2003, 50(5):1077-1088. DOI
4. Mukherjeea P , Bermana JI, Chunga SW, Hessa CP, Henrya RG: Diffusion Tensor MR Imaging and Fiber Tractography: Theoretic Underpinnings. AJNR 2008, 29: 632-641. DOI

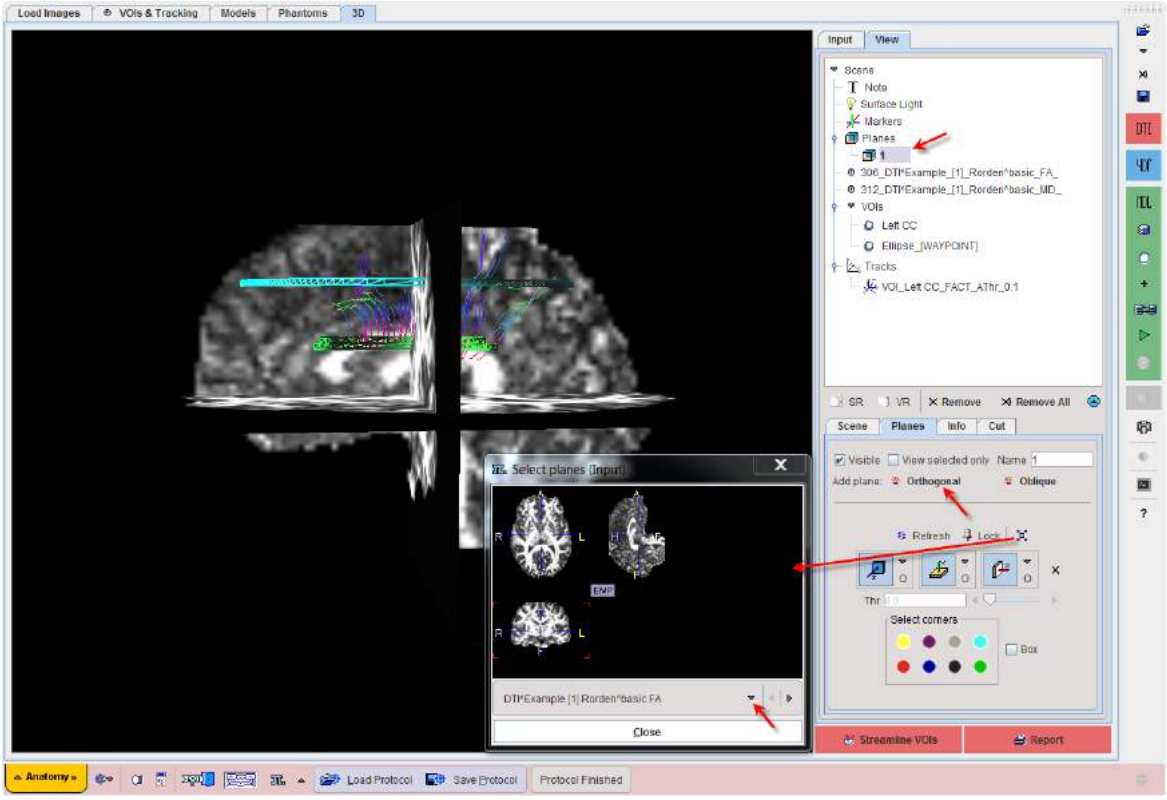
2.5 Visualizing the Fiber Tracks in 3D

The **3D** page initially shows the tracks together with the VOIs.



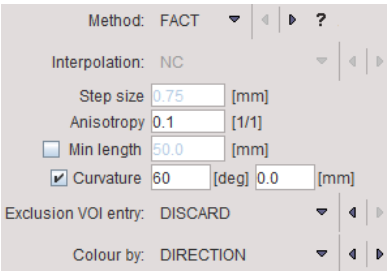
Note the elements in the **Scene** tree in the upper right. An objects can be selected in the tree its appearance changed in the lower part. Please refer to the *PMOD 3D Tool Users Guide* for details about the rendering.

As an example, FA image planes can be added by clicking at **Planes** in the tree, activating the **Orthogonal** button for the **Add planes**, opening the planes locator and finally selecting the **FA** image.

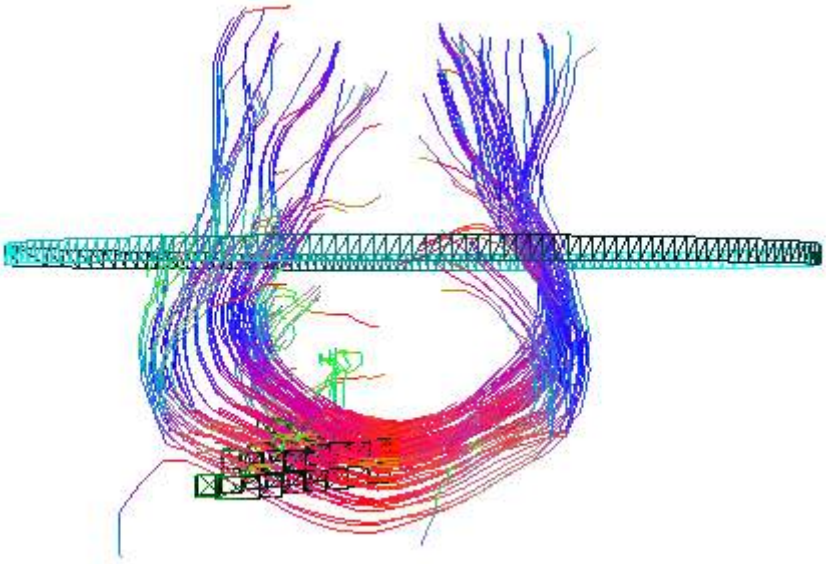
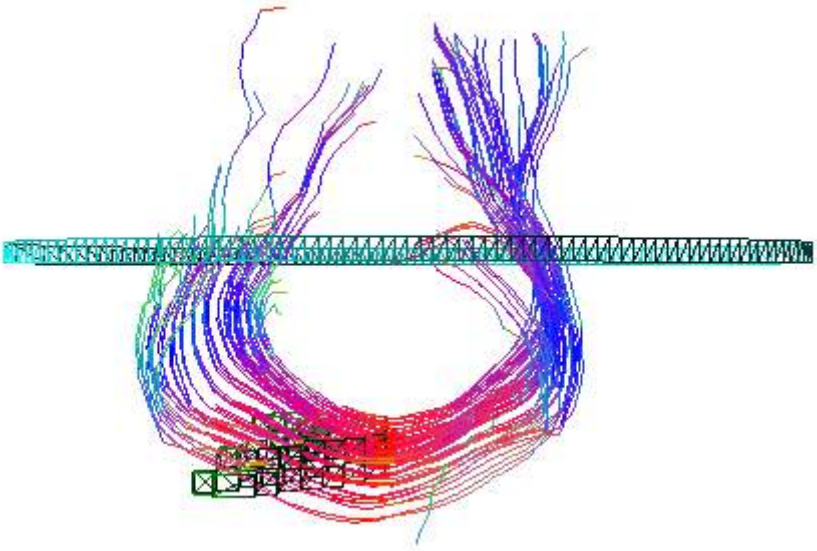
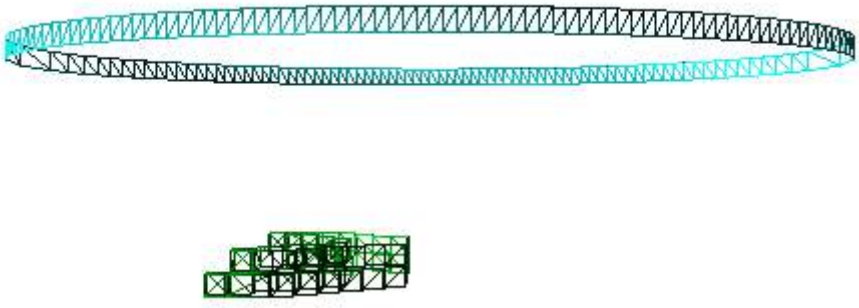


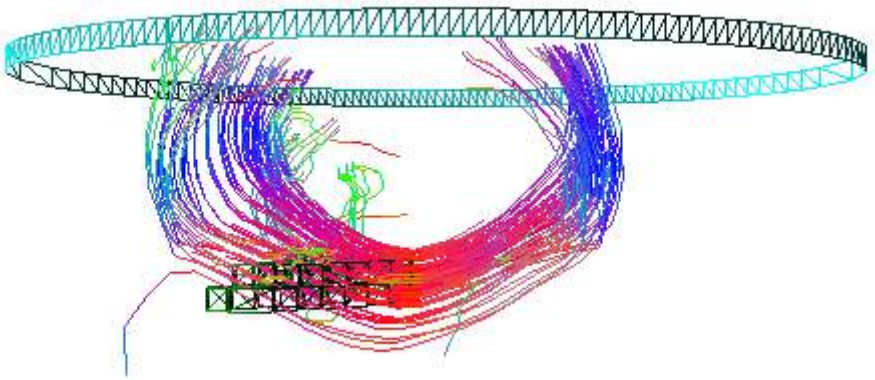
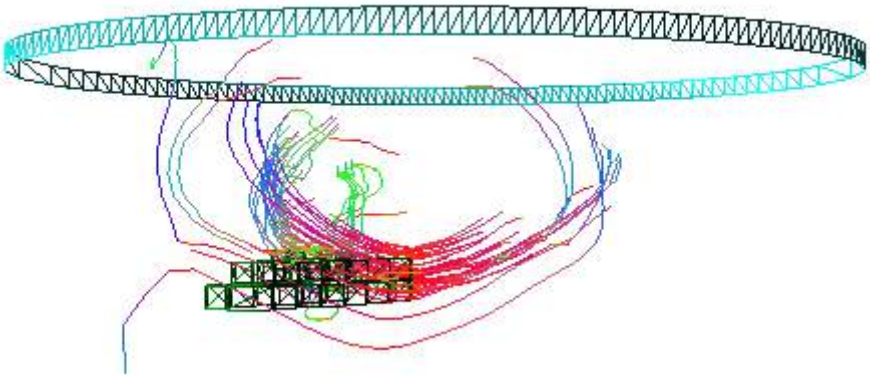
Examples with Different VOI Settings

The two VOIs described above will be used for illustrating the effect of various settings on the resulting tracks. The left corpus callosum VOI used for seeding, and the tracking algorithm is configured by the setting below.

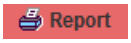


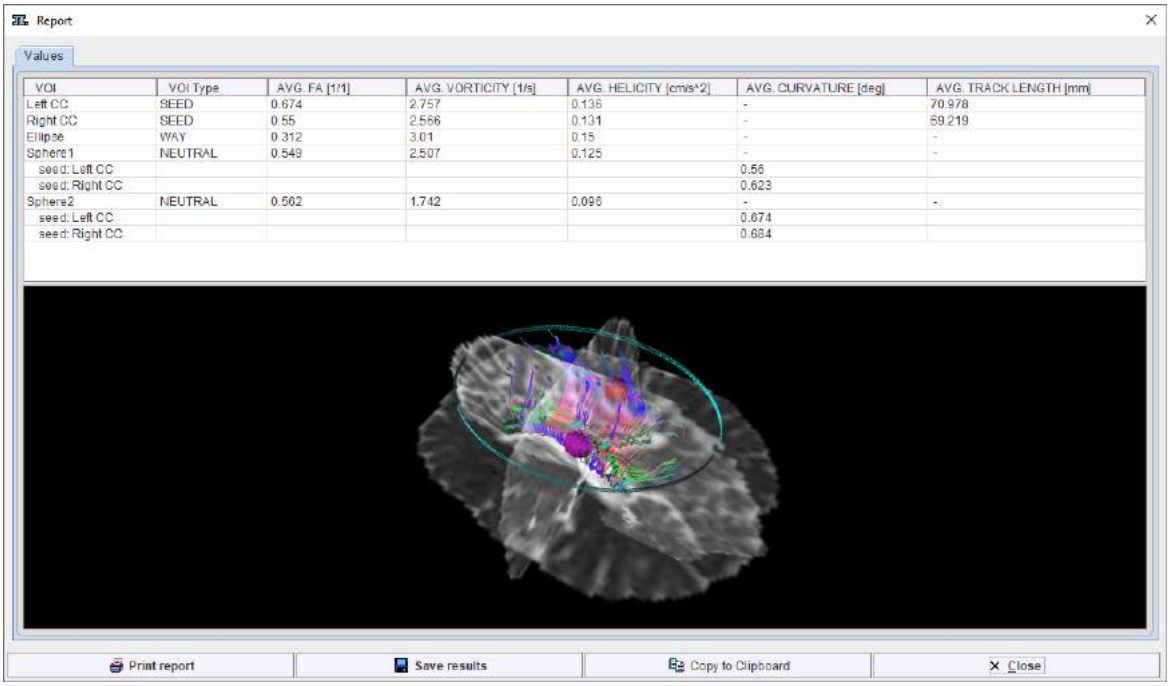
The following results are obtained when changing the role of the ellipse VOI.

Ellipse: **NEUTRAL** VOI	 The scene shows all tracks found with the current algorithm from the seeding VOI.
Ellipse: **WAY** VOI	 By enforcing tracks to pass through the ellipse, the number of resulting tracks is decreased.
Ellipse: **END** VOI	 Enforcing tracks to end within the ellipse VOI results in an empty scene, as none of the tracks fulfills this restriction.

Ellipse: **EXCLUDE** VOI with **CLIP** setting	 Using the ellipse VOI for clipping results in all tracks being shown but clipped at the level of the ellipse.
Ellipse: **EXCLUDE** VOI with **DISCARD** setting	 When discarding all tracks passing the ellipse only few tracks remain in the scene.

2.6 DTI Report

The  button on the 3D page composes a report as illustrated below:



The report is organized on a single page: **Values.**

The report lists on the upper part the statistics of all defined VOIs in table format. For each **VOI** the **Type** is shown. The following statistics measures are displayed:

- **AVG FA[1/1]**: is the fractional anisotropy and is representing a summary measure of microstructural integrity. The **FA** is highly sensitive to microstructural changes, but it is less specific to the type of change [2].

  It is calculated for each VOI type. The table displays the maximum of all the VOI averages.

- **AVG. CURVATURE[deg]**: The DTI tracks allows visualizing the lines along which there is oxygen diffusion. Curvature is a measure of curvilinearity of neural connections.

  It is calculated only for the **NEUTRAL** VOI type in respect to each **SEED** VOI available on the VOIs list.

  The value shown in the table for each neutral VOI is representing the value of the normalized curvature of the set of tracks. The normalized curvature is calculated as the sum of the angles values between consecutive track's parts, divided by the number of angles.

- **AVG. TRACK LENGTH[mm]**: is representing the average length of the tracks which pass through a **SEED** VOI. This parameter is calculated for each **SEED** VOI available in the VOIs list.

Note: Helicity and vorticity parameters are estimated in the DTI workflow when the check box **Vorticity&Helicity** is enabled in the VOI definition step. The **AVG. HELICITY** and **AVG. VORTICITY** shown in the table are representing the average values estimated in each VOI available in the VOIs list.

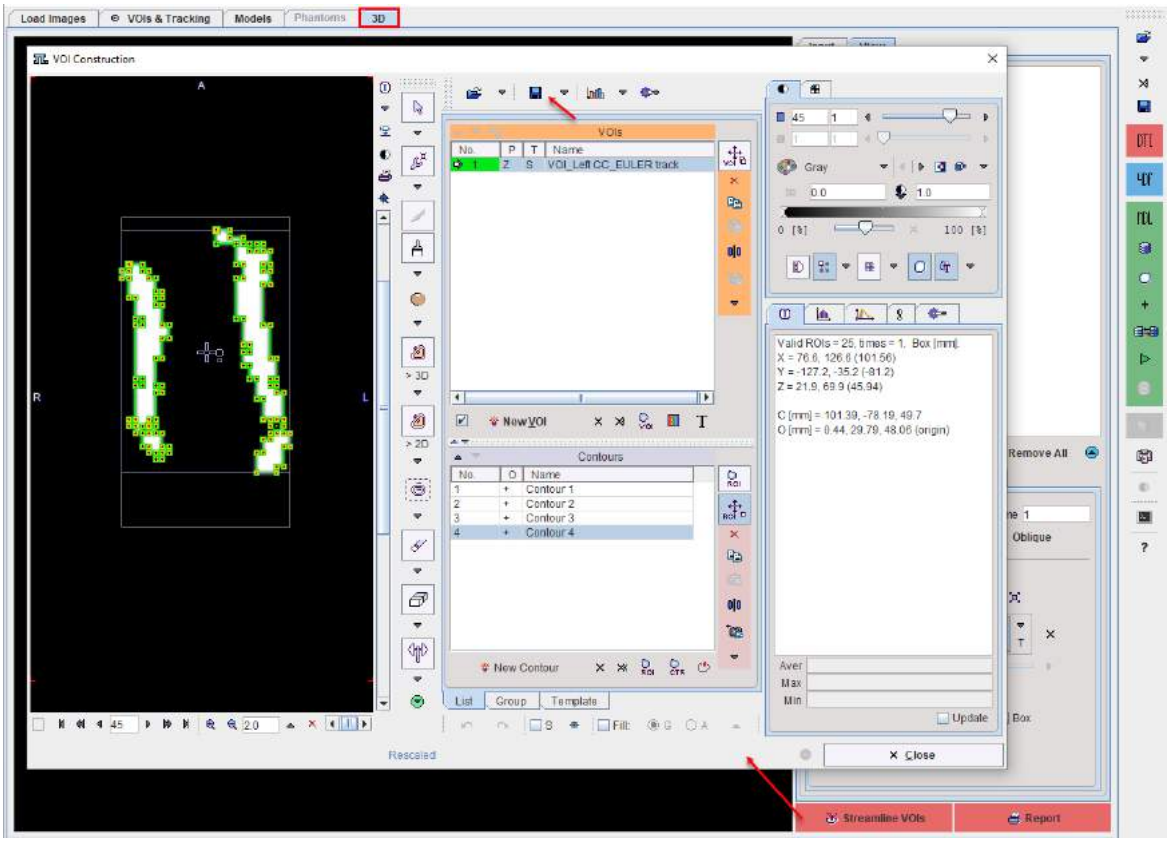
The lower part of the report window shows a capture of the current 3D scene.

As usually, the report can be printed or captured in various formats via **Print report**. **Save results** serves for saving the numeric values, which can also be exported via **Copy to Clipboard**.

2.7 Evaluating Diffusion Images along Tracks

It may be of interest to evaluate diffusion parametric maps such as FA and MD images along the tracks. The solution offered by PGEM is to convert the fibers into VOIs, which can externally be used for statistics.

Please activate the **Streamline VOIs** button on the **3D** page to convert the tracks into VOI outlines and open them in a VOI editor window.

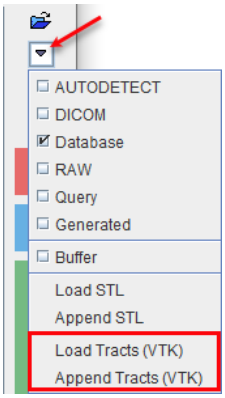


Here they can be modified using the standard PMOD VOI tools, and saved for later usage.

2.8 Saving the Tracks

The generated tracks can be saved in vtk format for use in the standalone 3D tool, or for use with a third-party program. Please make sure that the **3D** page is selected, as the saving functionality is page-specific. Then select the saving button in the taskbar to save the tracks.

Correspondingly, already existing vtk tracks can be loaded or appended as illustrated below.



2.9 Protocol File

The configuration of the DTI analysis can be saved with the **Save Protocol** button in the status line. The adjacent **Load Protocol** button allows retrieving the configuration and repeating the analysis.

3 4D Flow

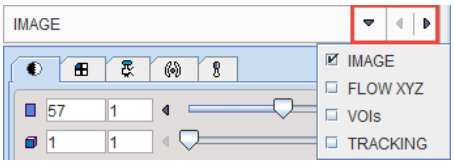
The PGEM allows loading and analyzing data generated by 4D Flow MRI acquisitions. The workflow is very similar to the one described for DTI Tractography 14, and the applied tracking methods are exactly the same.

In 4D Flow analysis, the flow velocity vector takes the role of the principal tensor eigenvector in the DTI analysis. The result of the analysis are "streamlines", comparable to the fiber tracks of DTI tractography. Streamlines connect the velocity vectors at a given acquisition time, and give a general impression of the flow pattern at that time. As 4D Flow measurements acquire the velocity vectors at multiple times, e.g. at different phases of a heartbeat, streamlines can be calculated at every acquisition time. As a result, the change of the flow pattern over time can conveniently be visualized as a movie.

An alternative analysis is the flow tracking along time, connecting the velocity vectors of successive acquisition and thereby mimicking the trajectory a particle might trace during the acquisition. The result of such an analysis are called "pathlines". As of now, PGEM doesn't support the generation of pathlines, only streamlines.

3.1 Workflow Organization

The 4D Flow workflow starts on the **VOIs & Tracking** page, which has 4 sub-pages. As illustrated below, the sub-pages can be switched with the selection in the upper right or the adjacent arrows.



On each page, the user has to perform an operation or configuration, and then activate the blue action button in the lower right for proceeding. Correspondingly, an operation is performed and the result shown an the next page. After leaving the **TRACKING** page, the resulting streamlines are visualized on the **3D** page.

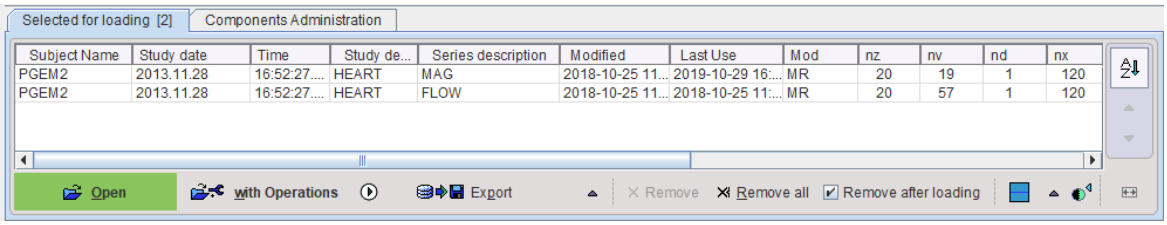
In order to test a different tracking configuration, the user has to return to a prior stage by selecting the **VOIs & Tracking** page again, choosing the appropriate sub-page, and then proceeding from there as with the initial workflow by the blue action buttons.

3.2 Loading the 4D Flow Images

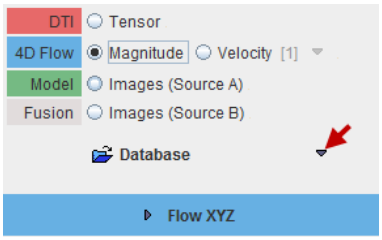
The 4D Flow analysis requires two data sets, "Magnitude" and a "Flow velocity", which are generated by MR reconstruction. The magnitude image shows anatomical detail and has arbitrary scaling, whereas the flow velocity image is a 3D vector field of the flow vector in real-world units.

Most conveniently, the 4D Flow images are loaded using the

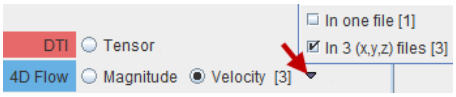
button in the taskbar to the right. Note that the flow magnitude and the flow vectors can be selected and loaded at once. PGEM figures out the roles of the two data sets based on their dimension. In the example below flow has been recorded at 19 different times during the heartbeat. The flow magnitude data set **MAG** therefore has a value of 19 in the **nv** column. The flow velocity in each point is a three-dimensional vector and therefore the **FLOW** data set requires three times as many volumes, namely **57**.



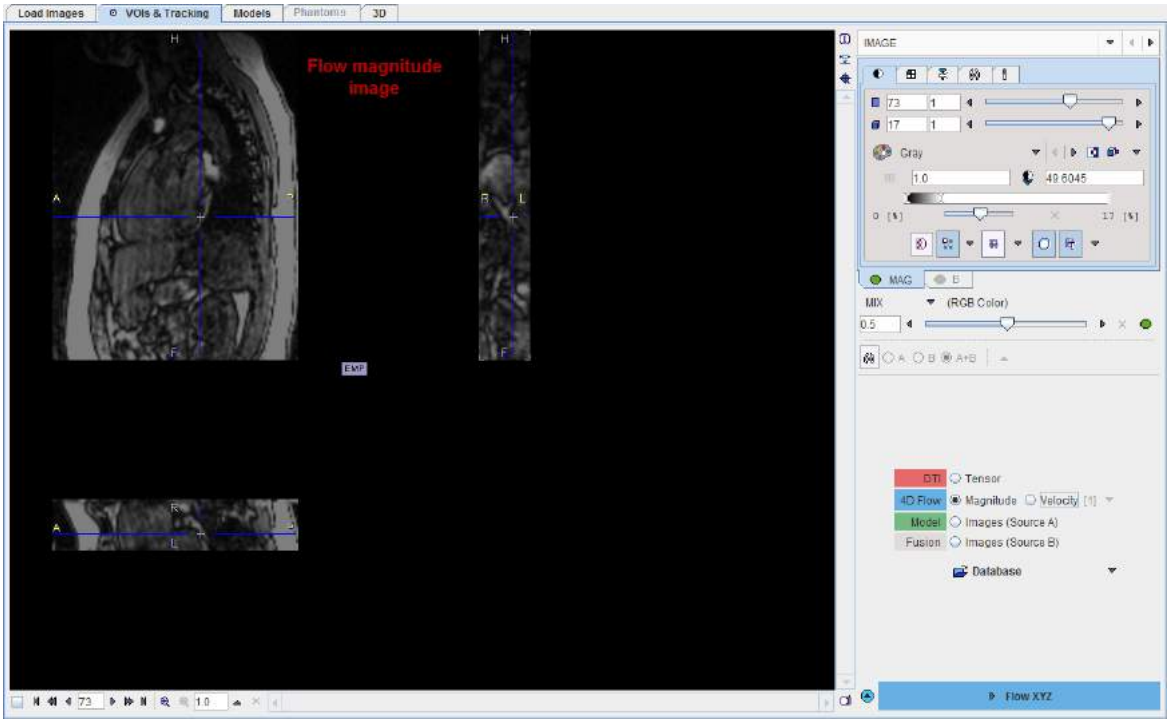
As an alternative, the **4D Flow** radio button can be set to **Magnitude** and the data loaded with the indicated button. Again, both the magnitude and velocity can be loaded at once, if the velocity vector information is in a single file.



In case each flow vector component is stored in a separate file, loading works differently. First load the magnitude image with the radio button **Magnitude**, then the three direction components radio button **Velocity [3]** as illustrated below. Note that the three series have to be selected and brought into the correct order (x, y, z) before loading them.



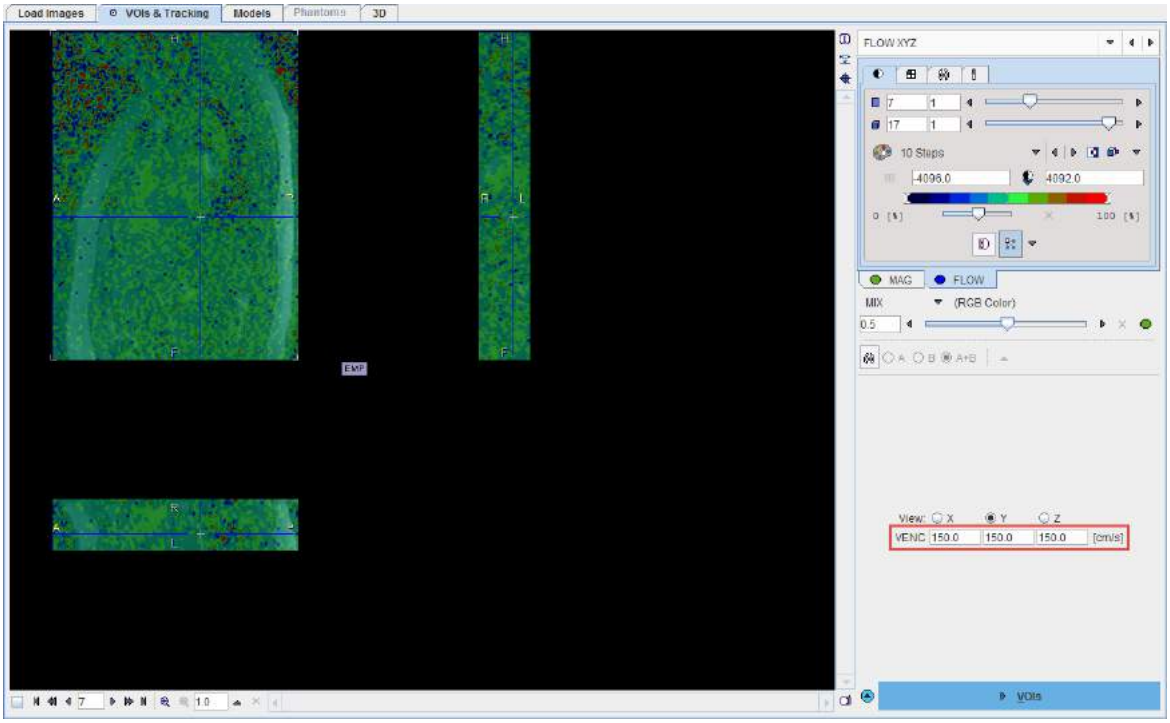
As a result of this loading, the workflow type is defined as "4D Flow" and the internal program switches are configured accordingly. Particularly, the action button in the lower right is set to blue color and indicates that the next step continues on the **FLOW XYZ** sub-page.



Please activate Flow XYZ to proceed.

3.3 Entering the Maximal Flow Value

The loaded images are shown on the FLOW XYZ page in a fusion arrangement. Note the fusion slider for mixing the contributions of the **MAG** and the **FLOW** images. The **X**, **Y** and **Z** radio buttons define, which velocity component of **FLOW** is displayed.

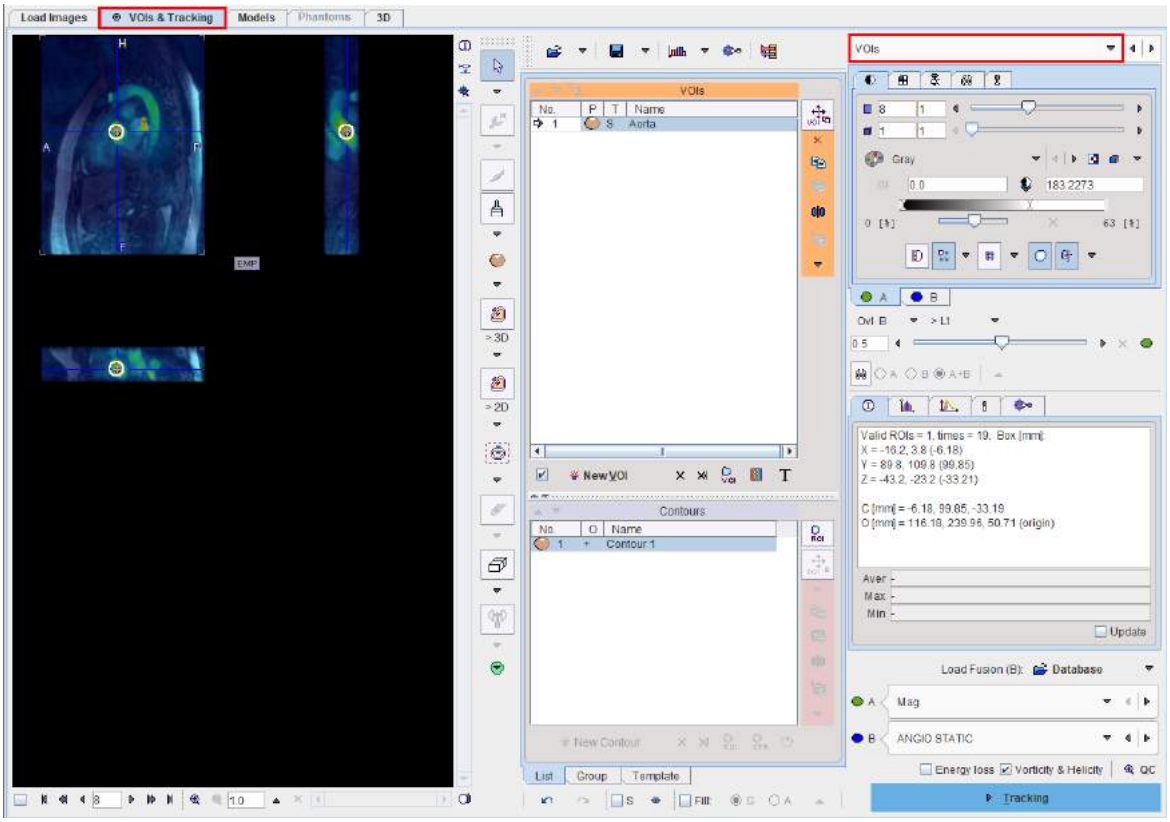


The **VENC** parameter values are required for converting the **FLOW** image values into real-word flow velocities. If they are not encoded in the loaded DICOM file, they have to be edited manually.

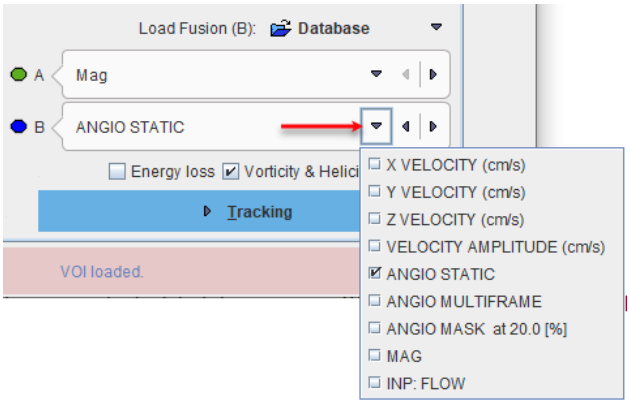
Please proceed with the **VOIs** button to the next page.

3.4 Defining VOIs for Seeding and Imposing Restrictions

When arriving at the **VOIs** sub-page a fusion image is shown to the left which is composed of the **Mag** and the **FLOW MASK (Angio)** images. Note the two panels **A** and **B** in the upper right which correspond to those images, and the slider for mixing the respective contributions in the fusion image.



In the lower right, the **A** and **B** images can be redefined.



The choices are

- the flow **VELOCITY** components in the different directions **X**, **Y**, **Z**,
- the **VELOCITY AMPLITUDE** (length of velocity vector).
- an image **ANGIO STATIC** resembling an angiographic image (calculated by summing SQRT(**VELOCITY*** **MAGNITUDE**) over time),
- an image **ANGIO MULTIFRAME**
- a masked version of **ANGIO STATIC** at the 20% threshold level,
- the **MAG**
- the **INP:FLOW**

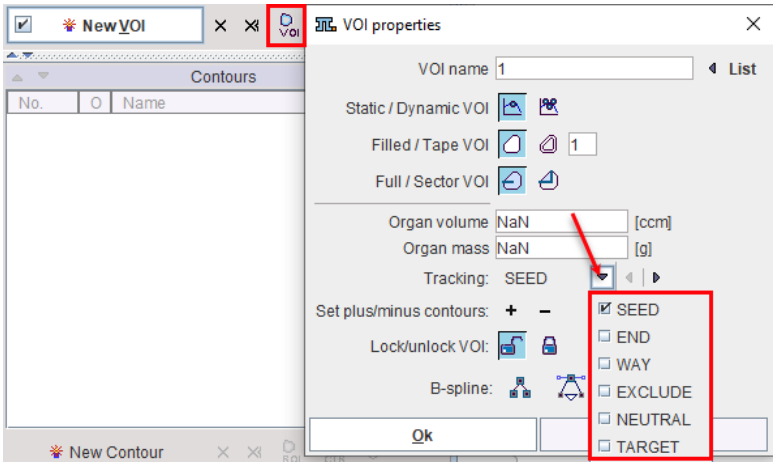
VOI Definition

The calculation of streamlines is based on VOIs which can play different roles:

- **SEED** VOIs: Streamlines tracking is started from the pixels in seed VOIs, following the local velocity vector directions.

- **END** VOIs: Only streamlines ending in this VOI will be used. To avoid excessive pruning of streamlines, an **END** VOI should have sufficient volume.
- **WAY** VOIs: Only streamlines passing through the **WAY** VOI will be used.
- **EXCLUDE** VOIs: streamlines passing through an **EXCLUDE** VOI will be removed.
- **NEUTRAL** VOIs: Such VOIs have no impact on streamlines tracking. Setting VOIs to **NEUTRAL** allows assessing the effect of **END**, **WAY** and **EXCLUDE** VOIs without the need of removing them.
- **TARGET**: Is representing a VOI the track should end with.

VOIs can be created with the usual PMOD VOI tools. When creating a new VOI, a dialog window pops up which requires defining the appropriate **Tracking** property. Later on, this property can be changed using the **VOI properties** functionality as illustrated below.

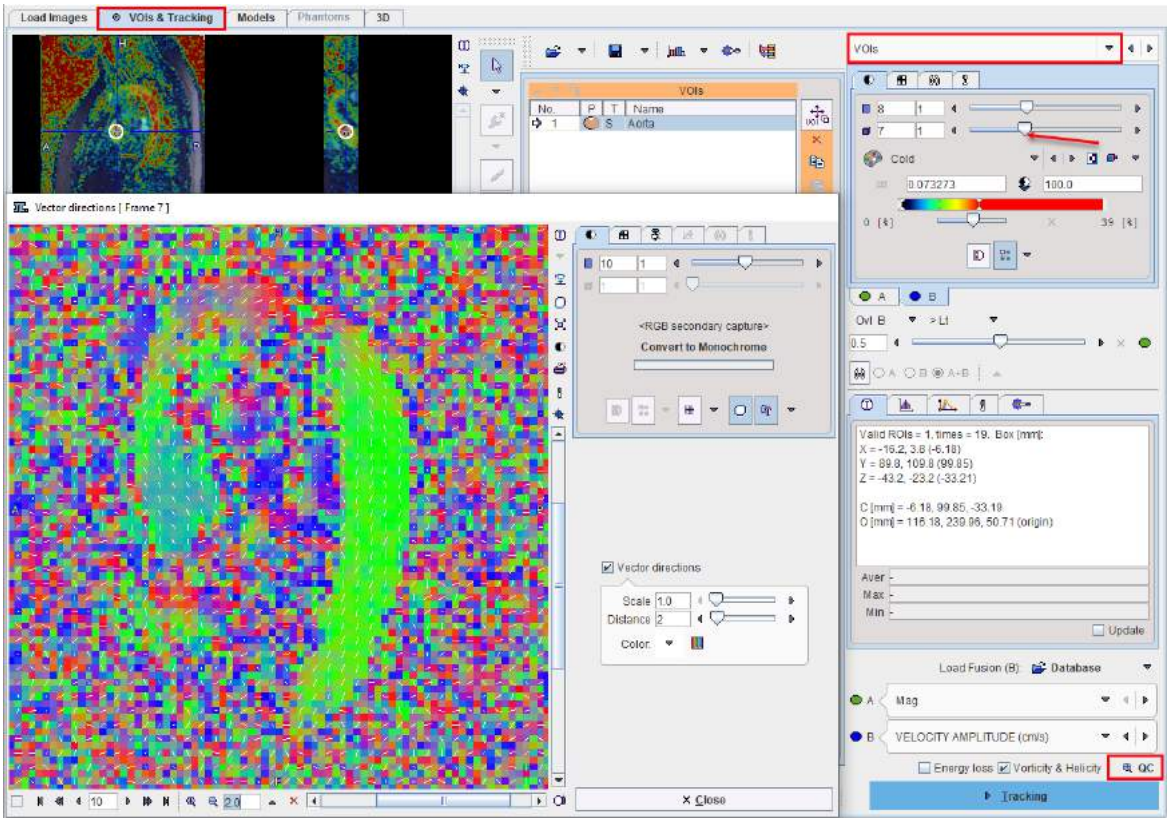


Note the check boxes **Energy loss** and **Vorticity&Helicity**. If they are checked, PGEM calculates energy loss map and **Vorticity Amplitude** and **Absolute Helicity** parametric maps, respectively. Vorticity is a measure of rotation, whereas helicity relates to the knottedness in fluids, and they can be used for assessing the degree of flow non-laminarity.

Vector Inspection

The loaded velocity vectors can be inspected with the **QC** button. It shows a window with the projection of the flow direction vectors together with a color-coded direction image. Red indicates diffusion along the x-axis (left-right), green diffusion along the y-axis (posterior-anterior), and blue diffusion along the z-axis (inferior-superior).

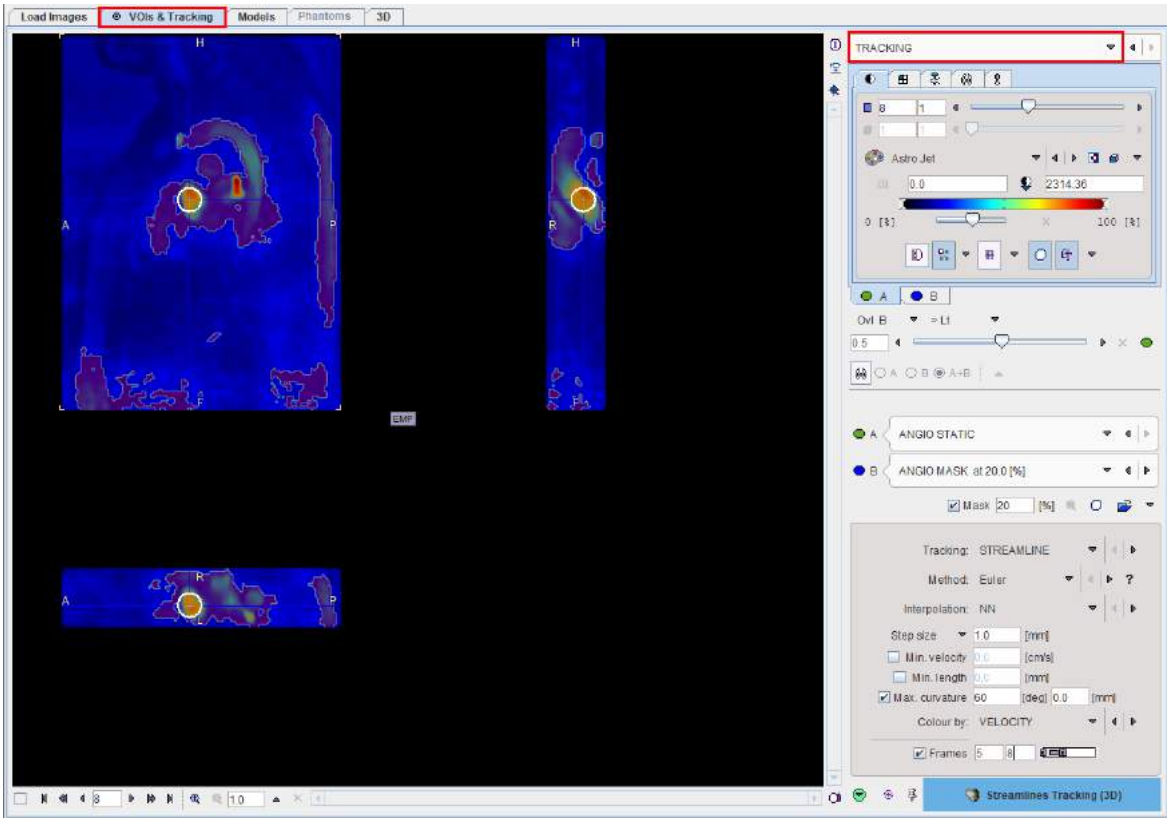
Note that the time frame has to be selected before starting Vector QC, as the velocity vector field is four-dimensional.



Please proceed with the Tracking button in the lower right.

3.5 Calculating the Streamlines/Pathlines

When arriving at the **TRACKING** page, the image area shows a fusion of the Angio image (**A**) and the masked Angio image for highlighting areas with high flow. Also shown in the overlay are the VOIs.



Tracking Configuration

The area in the lower right serves for defining the tracking algorithm and its parameters. Two types of tracking options are available for selection:

1. **STREAMLINE**: is a curve that is instantaneously tangent to the velocity vector of the flow. It shows the direction in which a massless fluid element will travel at any time point.
2. **PATHLINE**: is a trajectory that an individual fluid particle follows. It can be thought of as *recording* the path of a fluid element over a certain period. The direction the path takes will be determine by the streamlines of the fluid at each moment in time.

Two algorithms are supported for any of the tracking option and can be selected in the **Method** list:

1. **EULER:** Tracking proceeds using a fixed step size along the local fiber orientation [2]. With nearest-neighbor interpolation, this method may be very similar to FACT, except that the step size is fixed, whereas FACT steps extend to the boundary of the next voxel (distance variable depending on the entry and exit points to the voxel).
2. **4th order Runge-Kutta** method [2]. The step size is fixed, however the eventual direction of the step is determined by taking and averaging a series of partial steps. Interpolation determines how the fiber direction is determined at a given point in space.

The **Interpolation** setting is not relevant for **FACT**. For **EULER** and **RK4** the choices are

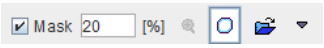
1. **NN:** Nearest-neighbor interpolation using the local voxel data directly.
2. **NC:** Probabilistic nearest-neighbor interpolation, similar to the method proposed by Behrens et al [3]. The data is not interpolated, but at each point one of the 8 voxels neighbors is randomly chosen. The probability of choosing a particular voxel is based on how close the point is to the center of that voxel.
3. **TRILINEAR:** Linear interpolation of the vector components using the 8 neighbors.

Further parameters and options determine how tracking proceeds and when it ends:

Step size	Distance between points on the streamlines. Not used for FACT as it does not apply interpolation.
Min velocity	Track ends if the velocity amplitude drops below this threshold.
Min length	If checked, streamlines/pathlines shorter than the minimal length specified are discarded.
Max curvature	If checked, streamlines/pathlines are terminated in case the curvature exceeds the specified angle within the length specified. If length = 0.0, the curvature is checked at each step.
Colour by	The streamlines can be functionally colored as follows: **SEED**: Using the color of the **SEED** VOI. **END VOI**: Using the color of the **END** VOI. **DIRECTION**: Each segment of the track has a color combined from its direction cosines values: Red, Green, and Blue from direction cosines x, y and z respectively. **VELOCITY**: Using the velocity amplitude value along the track for coloring. **Last VOI:** using the color of the last VOIs in the list.
Frames 	Tracking is relatively time-consuming. With the box enabled it can optionally be restricted to a certain section of the acquisition.

Masking

An additional means for restricting the generated streamlines/pathlines is by checking the **Mask** box and defining a mask. The elements in



have the following functionality:

	Generate a mask from the **ANGIO STATIC** image by applying the specified threshold and include it in the image list **B** for viewing.
	Open the current mask in the VOI editor and convert it into a VOI. The VOI can be edited, and the mask finally updated from the VOI.
	Select an external mask file.

Note: Please first perform tracking without masking, and only afterward gradually increase masking, if necessary.

After configuring all tracking parameters, please proceed with the blue action button. Based on the selected **Tracking** option, the streamlines or the pathlines are calculated and visualized on the **3D** page.

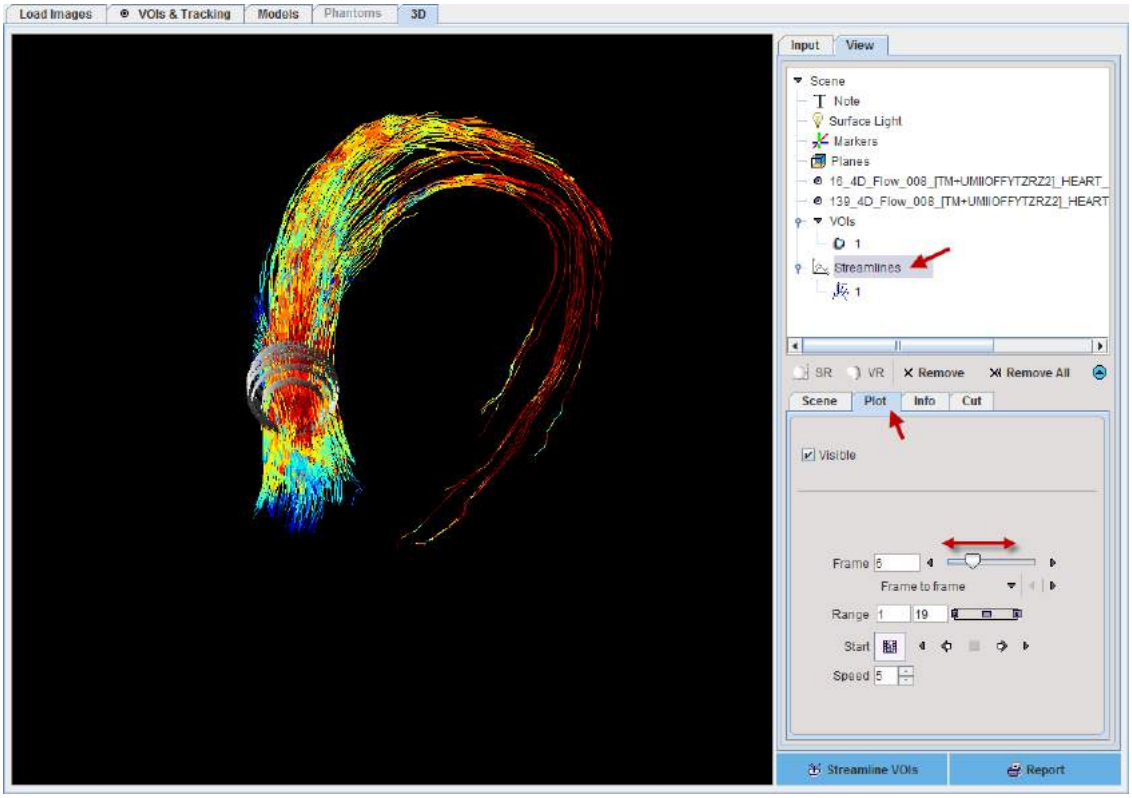
References

1. Mori S, Crain BJ, Chacko VP, van Zijl PC: Three-dimensional tracking of axonal projections in the brain by magnetic resonance imaging. Ann Neurol 1999, 45(2):265-269.
2. Basser PJ, Pajevic S, Pierpaoli C, Duda J, Aldroubi A: In vivo fiber tractography using DT-MRI data. Magn Reson Med 2000, 44(4):625-632.

3. Behrens TE, Woolrich MW, Jenkinson M, Johansen-Berg H, Nunes RG, Clare S, Matthews PM, Brady JM, Smith SM: Characterization and propagation of uncertainty in diffusion-weighted MR imaging. Magn Reson Med 2003, 50(5):1077-1088. DOI

3.6 Visualizing the Streamlines/Pathlines in 3D

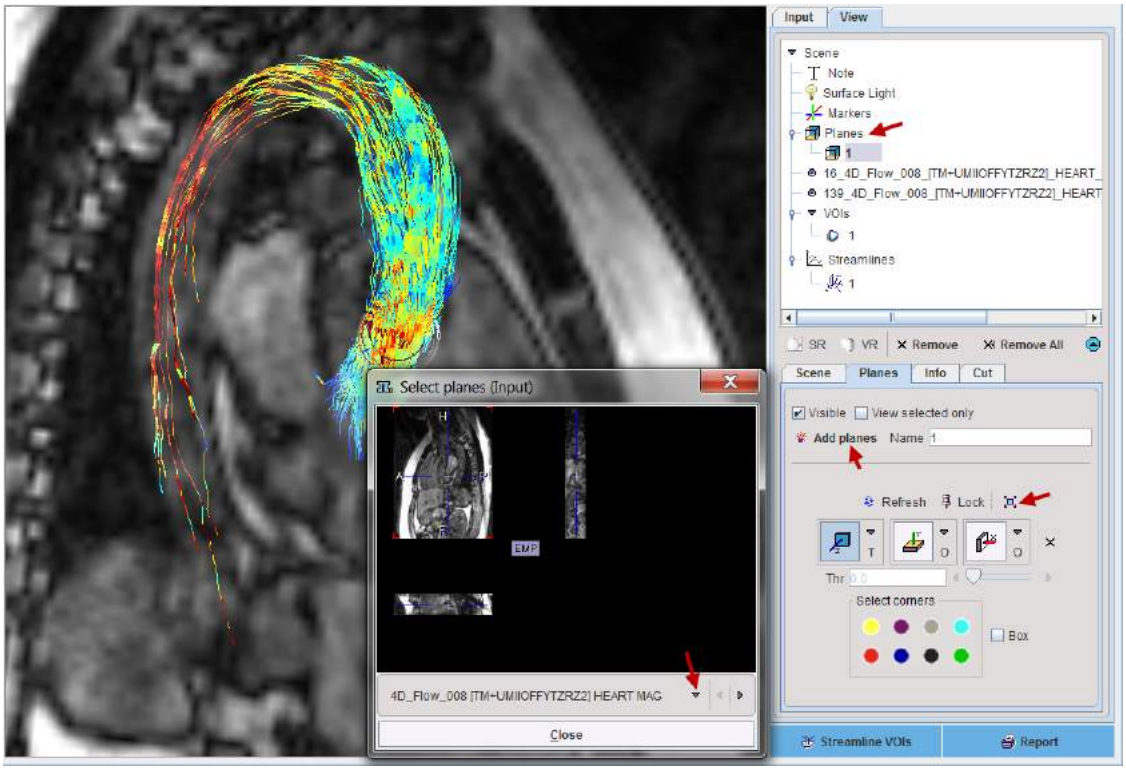
The **3D** page initially shows the streamlines together with the VOIs.



Note the elements in the **Scene** tree in the upper right. An objects can be selected in the tree its appearance changed in the lower part. Please refer to the *PMOD 3D Tool Users Guide* for details about the rendering.

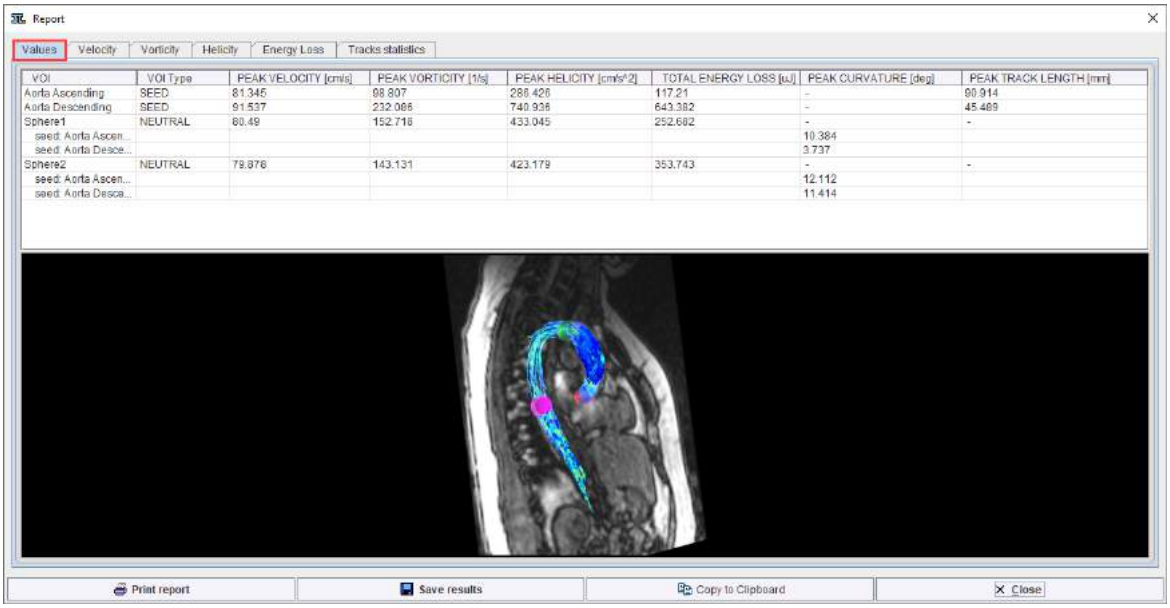
Initially the streamlines/pathlines of the first frame are shown, when typically there is low flow. To visualize the pattern at later times select the **Streamlines/Pathlines** entry in the object tree, activate its **Plot** properties panel, and drag the **Frame** slider or start a cine.

Image planes can be added by clicking at **Planes** in the tree, activating **Add planes**, opening the planes locator and finally selecting the **MAG** image. The plane location can easily be changed by clicking into the **Select planes** window, and the color on the **Input** panel.



3.7 4D Flow Report

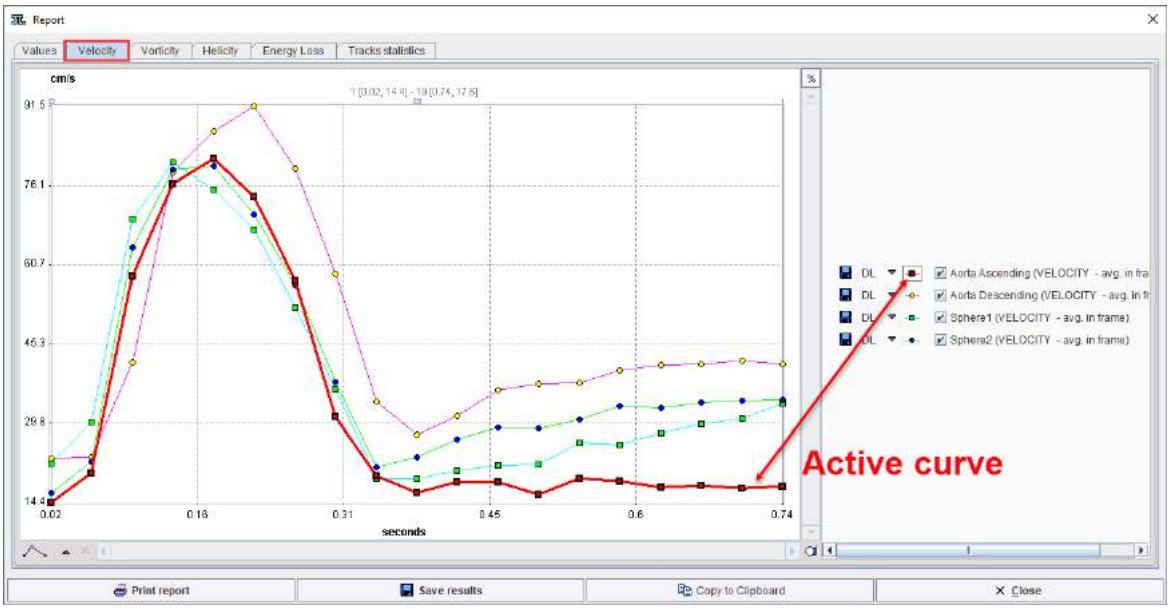
The Report button on the 3D page composes a report as illustrated below:



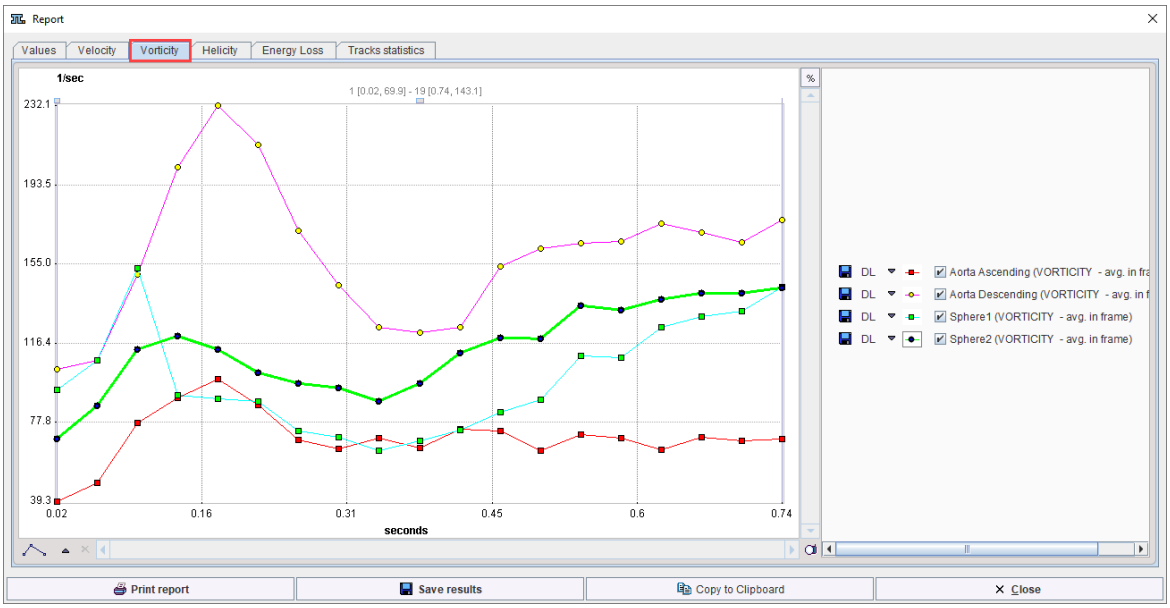
The report is organized on six pages: **Values**, **Velocity**, **Vorticity**, **Helicity**, **Energy loss**, **Tracks statistics**

The **Values** page lists on the upper part the statistics of all defined VOIs. Shown is the maximum of all the VOI averages calculated along the time axis. The lower part shows a capture of the current 3D scene.

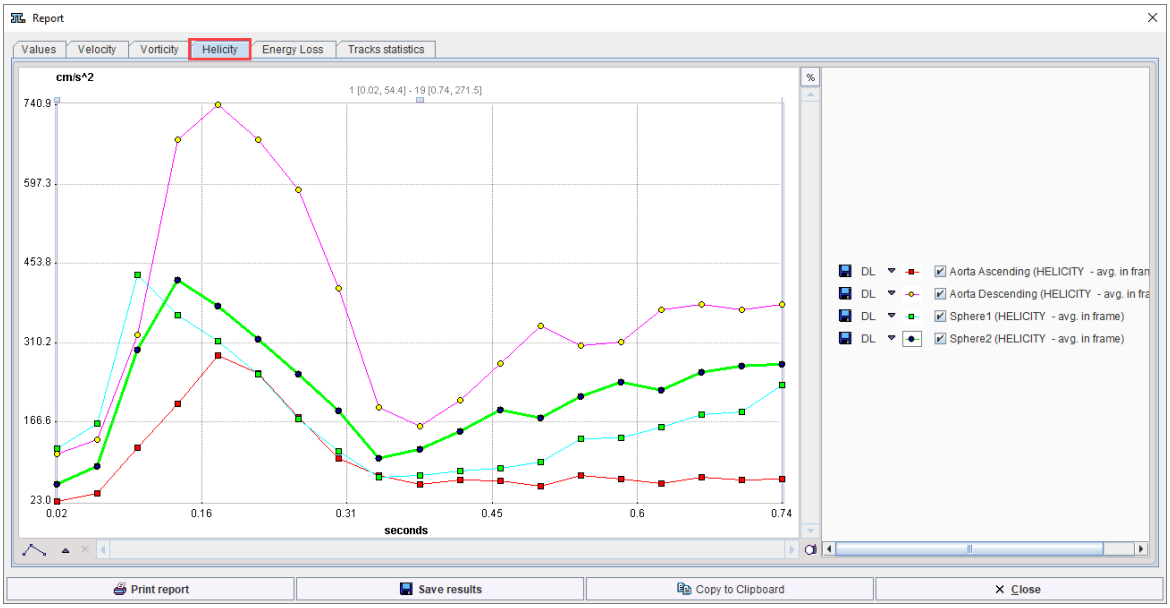
The **Velocity** page shows the plots of the averages **VELOCITY** amplitude for each time point in each VOIs:



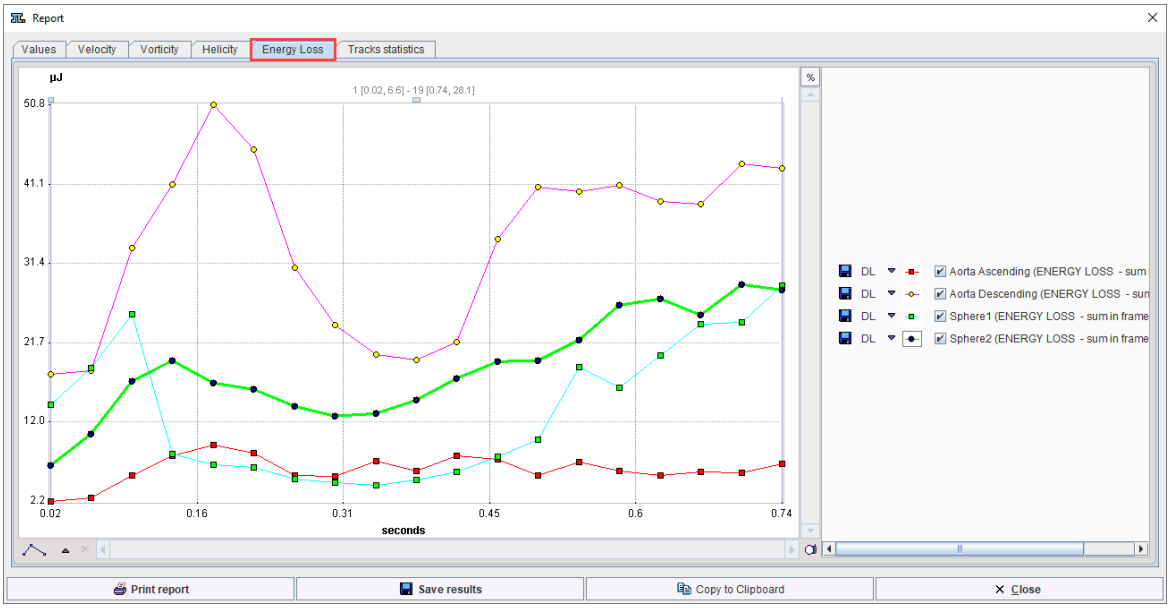
The **Vorticity** page shows the plot of the average **VORTICITY** for each time point in each VOIs:



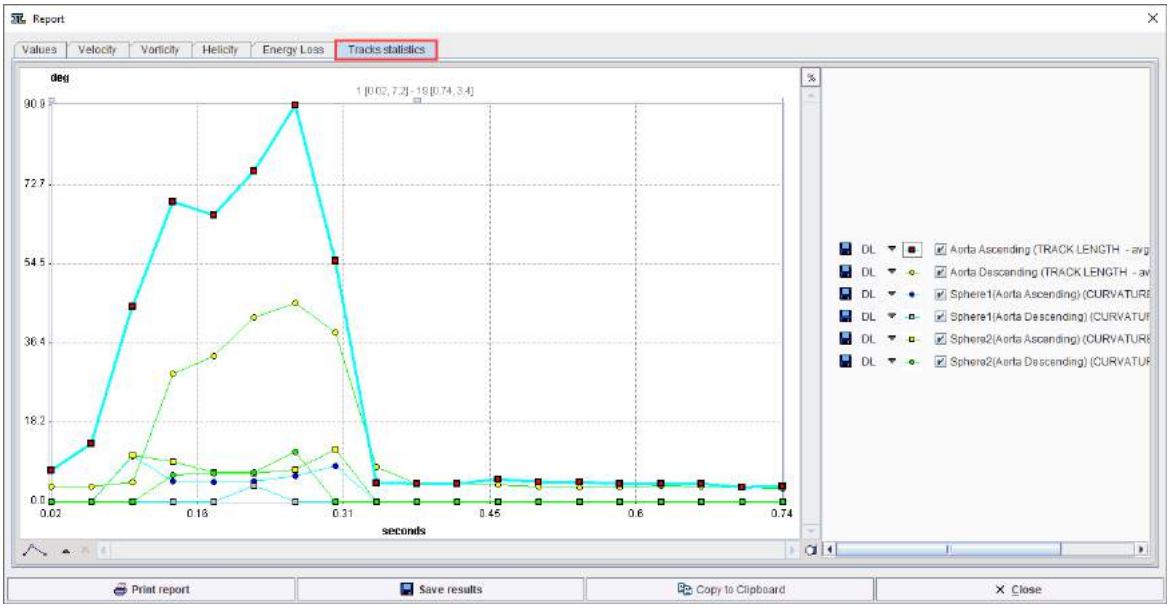
The **Helicity** page shows the plot of the average **HELICITY for each time point** in each VOIs.



The **Energy loss** page shows the total sum of the **ENERGY LOSS** for each time point in each VOIs.



The **Tracks statistics** page shows the average **TRACK LENGTH** in all **SEED** VOIs along time axis. The mean curvature (**CRV[dgr]**) is calculated and displayed for each **Neutral** VOI at each time point:

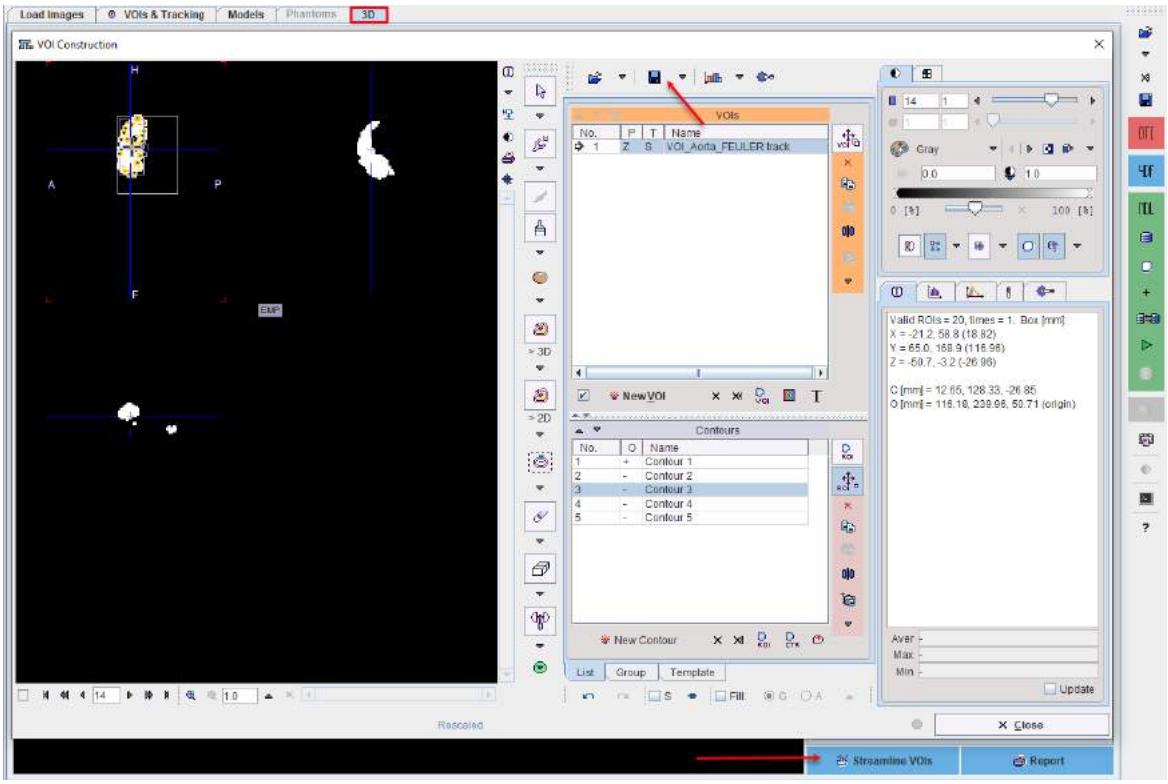


As usually, the report can be printed or captured in various formats via **Print report**. **Save results** serves for saving the numeric values, which can also be exported via **Copy to Clipboard**.

3.8 Creating VOIs along the Streamlines/Pathlines

It may be of interest to evaluate some of the images along the streamlines. The solution offered by PGEM is to convert the streamlines into VOIs, which can externally be used for statistics.

Please activate the **Streamlines VOIs** (or **Pathlines VOI** depending on the context) button on the **3D** page to convert the streamlines into VOI outlines and open them in a VOI editor window.

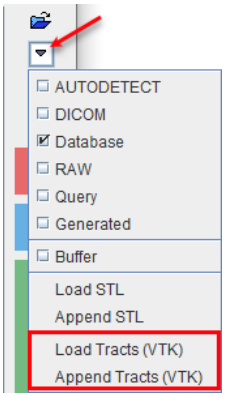


Here they can be modified using the standard PMOD VOI tools, and saved for later usage.

3.9 Saving the Streamlines/Pathlines

The generated streamlines can be saved in vtk format for use in the standalone 3D tool, or for use with a third-party program. Please make sure that the **3D** page is selected, as the saving functionality is page-specific. Then select the saving button in the taskbar to save the streamlines.

Correspondingly, already existing vtk track definitions can be loaded or appended as illustrated below.



3.10 Protocol File

The configuration of the 4D Flow analysis can be saved with the **Save Protocol** button in the status line. The adjacent **Load Protocol** button allows retrieving the configuration and repeating the analysis.

4 Generation of Dynamic PET Phantom Images

There is a particular workflow within PGEM for the generation of dynamic PET images representing defined kinetics in well-defined anatomical structures.

Input to this workflow is a set of VOIs which define the target anatomy. Additionally, the time course of the activity concentration (TAC) in each VOI must be provided. Such data can for instance easily be obtained by applying the PNEURO tool to an experimental dynamic PET study, optionally with an MRI.

Within PGEM, the VOIs are first transformed into an anatomical model. For each pixel within an anatomical structure the corresponding TAC is then used, optionally with some noise added, to generate a synthetic dynamic series with well-defined noise level. Finally, the images can be saved and, for instance, used to study the performance of a parametric mapping method in PXMOD.

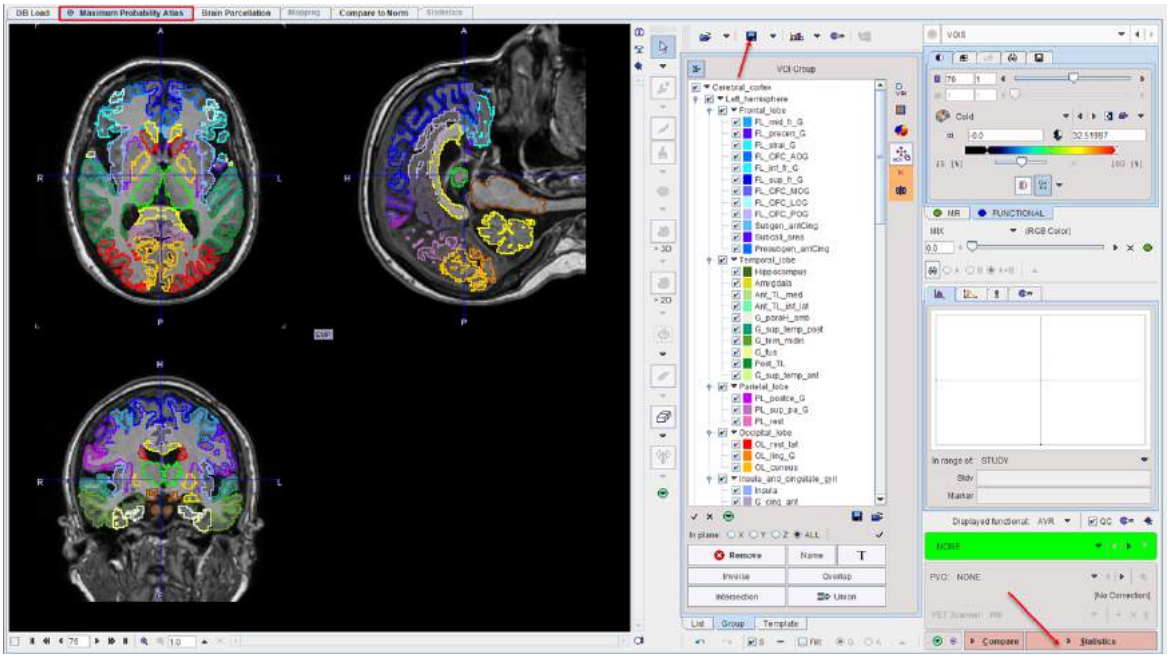
4.1 External Preparations

Before starting the phantom generation process in PGEM two files should be prepared

1. a set of VOIs which define the anatomy,
2. a set of time-activity curves named exactly the same as the VOIs.

4.1.1 Phantom VOIs

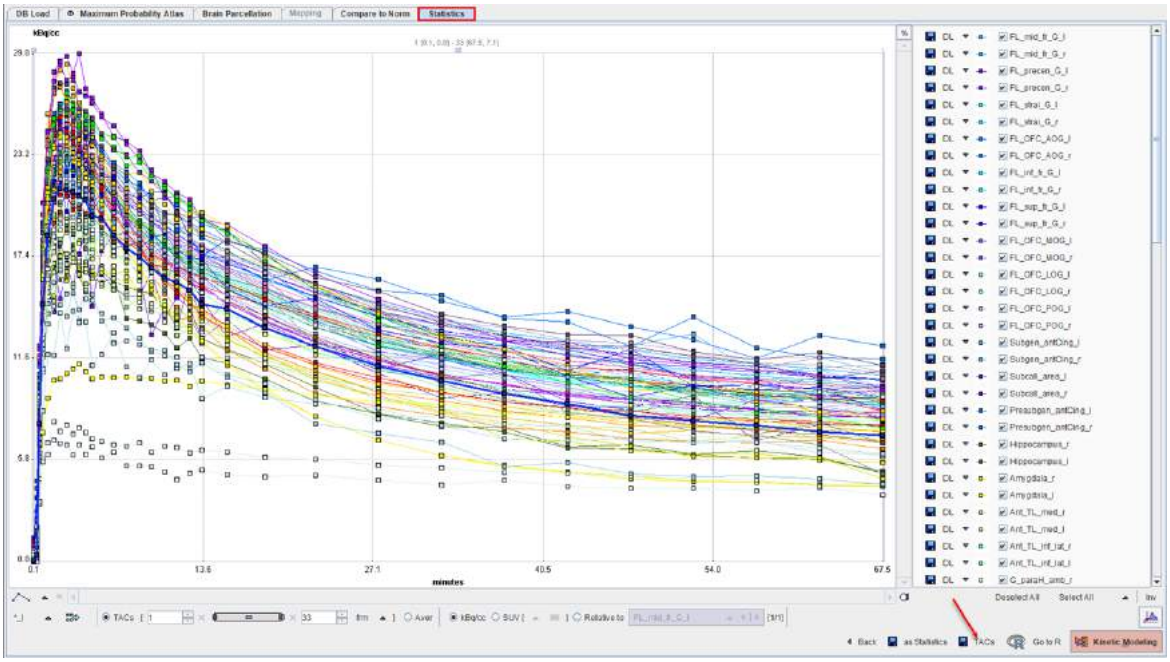
The example below illustrates the results from analyzing a DASB PET/MR data set using the **Brain Parcellation** methodology in the PNEURO tool.



The VOIs can be saved with the button indicated by the upper arrow. The corresponding TACs are calculated with the **Statistics** button in the lower right.

4.1.2 Phantom Dynamic TACs

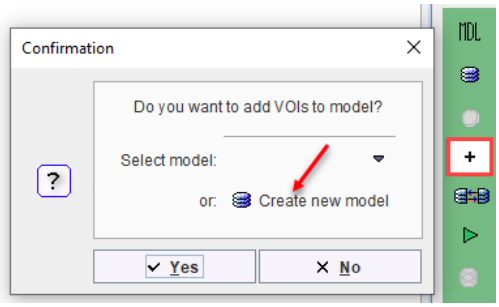
The resulting TACs are shown on the **Statistics** page of PNEURO and can be saved with the button indicated below.



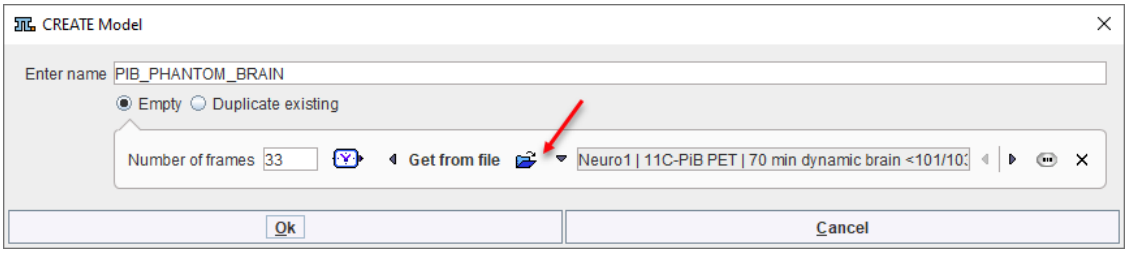
4.2 Dynamic PET Image Creation

4.2.1 Anatomical Model Definition

The first step is to create a new model on the **Models** page. This can be done most easily by activating the **+** button in the taskbar and selecting the VOIs file followed by choosing **Create new model** in the dialog window as illustrated below.

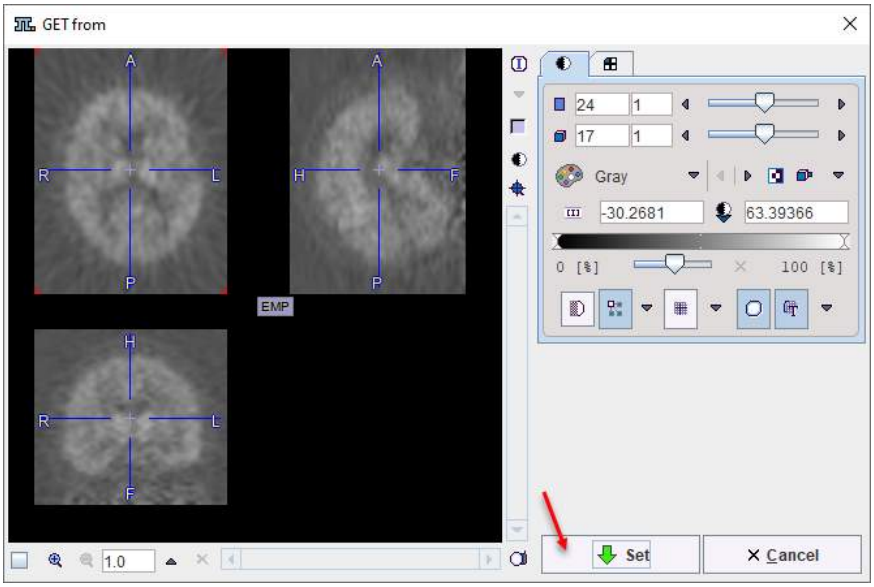


A dialog window opens for defining the name and the timing of the series.

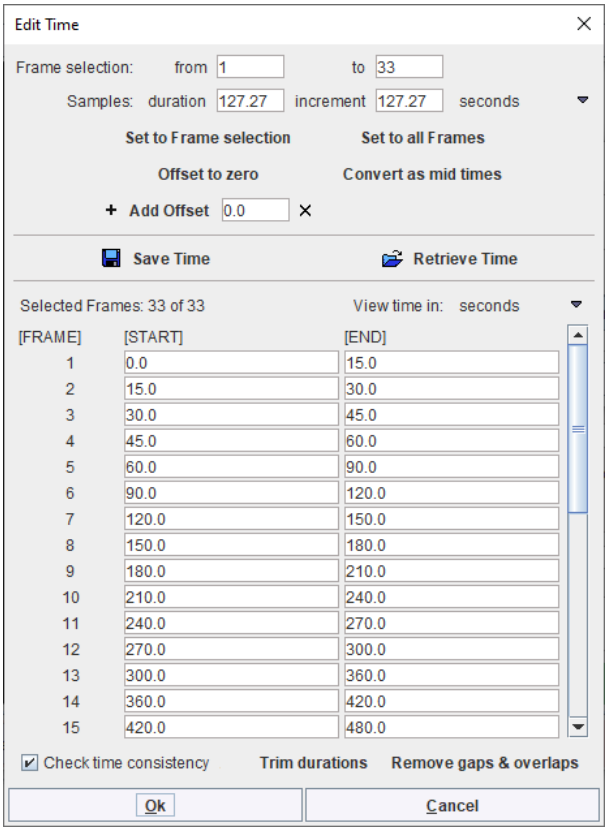


Timing from Existing Dynamic Image

The timing may be extracted from an actual image by selecting it with the open button and then activating **Get from file**. The image is read and displayed in a window.



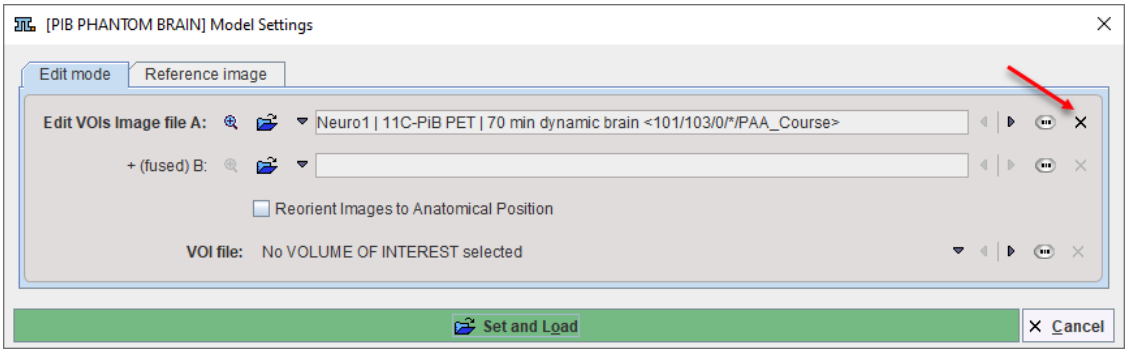
After confirmation with **Set** the timing is opened for editing and confirmation with **Ok**.



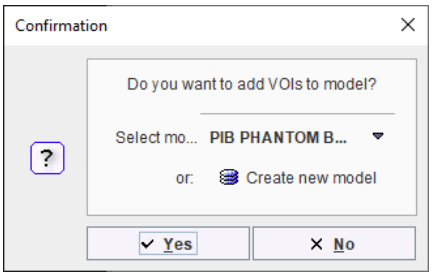
Timing Specified per Dialog Window

The alternative way for timing definition is entering the **Number of frames** and opening the timing window illustrated below with the button:

When closing the model creation window with **Ok**, another window appears, requesting model settings. In this context it is easier to avoid loading the image, so it can be removed from **Edit VOIs Image file A** with the **x** button.



After closing with **Set and Load** the model is ready for the VOIs to be added. To do so, please confirm the dialog window

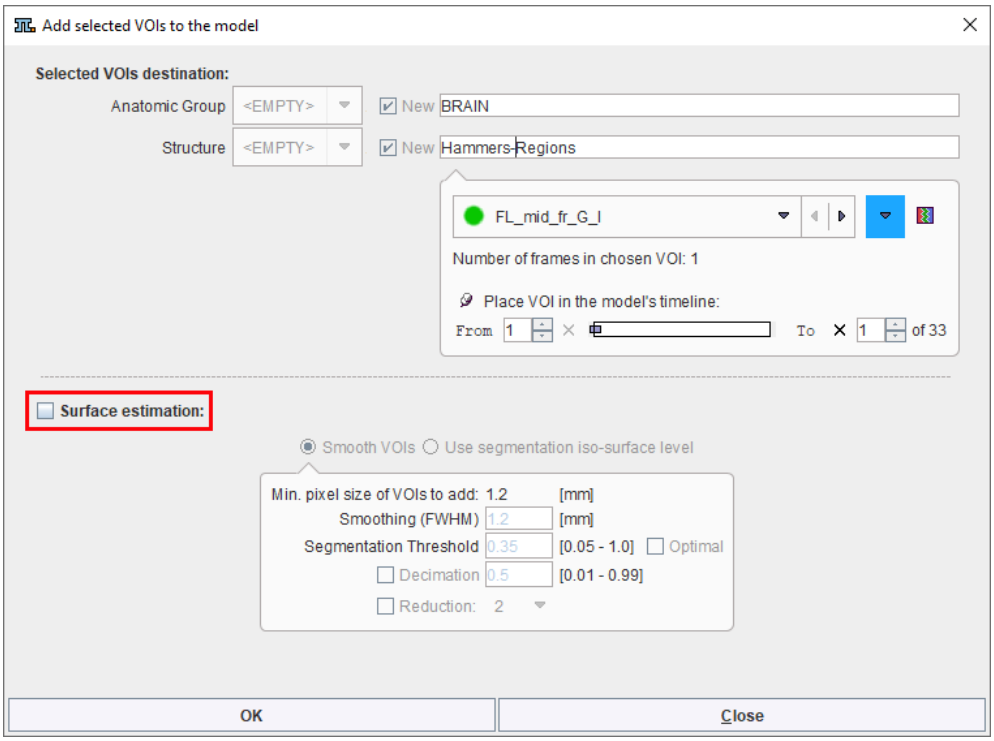


with **Yes**.

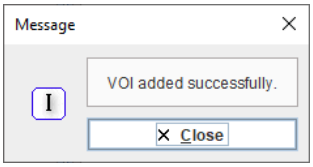
Note: The timing specified should exactly correspond to the timing of the TACs.

4.2.2 VOI Addition

A dialog window comes up for defining VOI properties. This is useful for hierarchical anatomical models. For the generation of the dynamic PET phantom the **Surface estimation** should be switched off, while all other settings can remain as is.

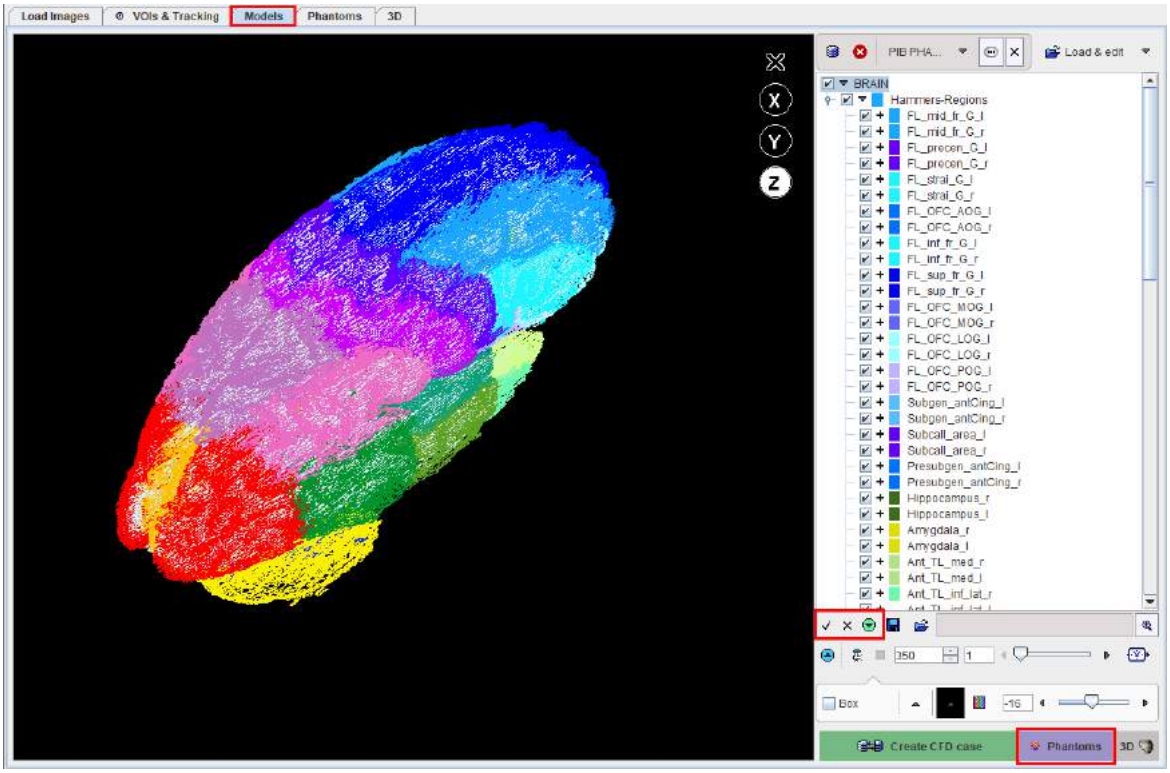


After closing this dialog window with **Ok**, the VOIs are added and a confirmation message appears.



4.2.3 Anatomical Model

At this time the model is prepared and shown on the **Models** page. The left area provides an impression of the VOIs, the right area the incorporated structures in a tree arrangement. Note the indicated arrow button for unfolding/collapsing the tree, and the buttons for checking/unchecking all the structures.

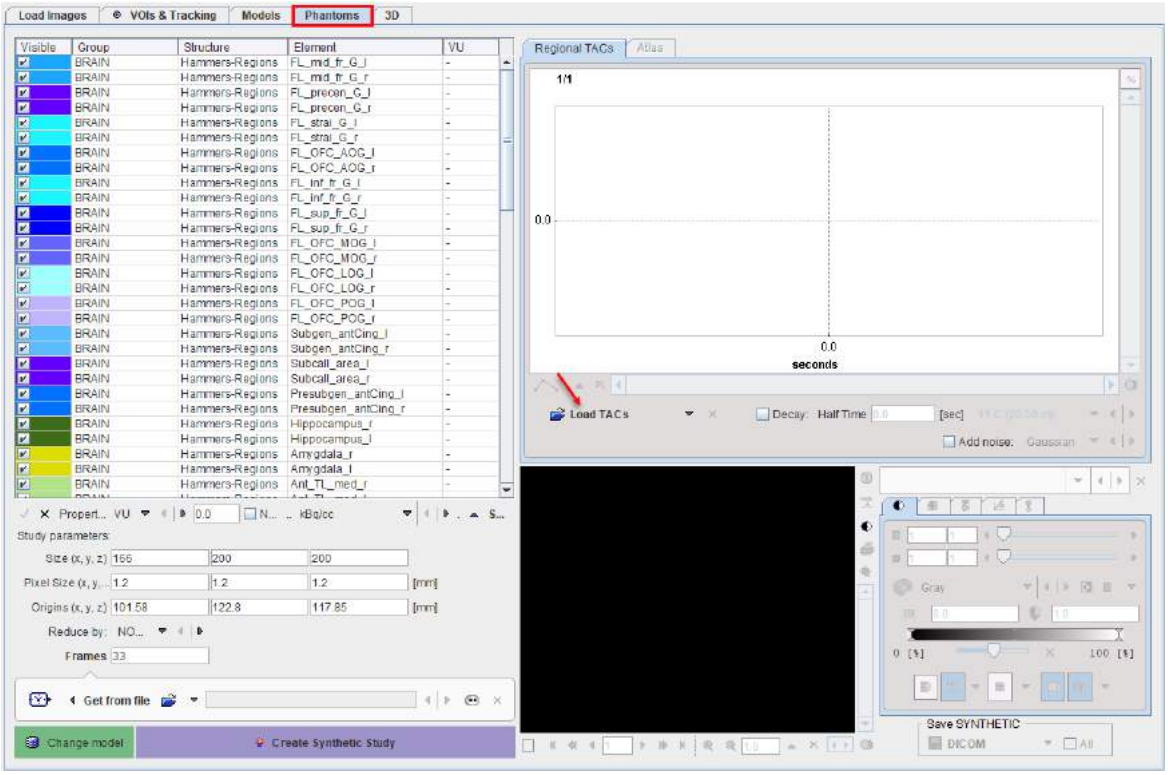


It is important that all structures relevant for the phantom images are checked.

Please continue with the **Phantoms** button.

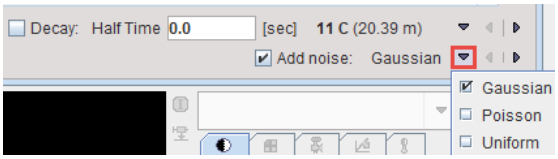
4.2.4 Phantom Creation

The **Phantoms** page lists the structures in the upper right. The timing is already defined, but could be changed in the lower left.



The next steps consists of loading the prepared TACs with the **Load TACs** button, such that they are shown in the **Regional TACs** curve panel.

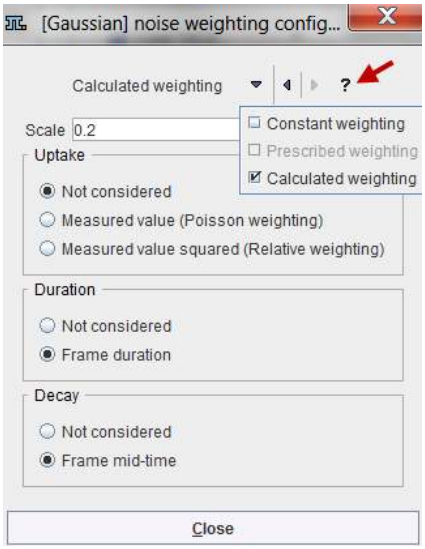
Two options may be configured as illustrated below



before generating the synthetic image: the introduction of radioactive decay, and the the addition of noise.

The choices for configuring the noise properties are the same as the ones available in the PKIN tool for weighted fitting and Monte Carlo simulations. Once **Add noise** is checked, the random number distribution can be selected in the list. Consequently, a dialog window is opened for specifying the noise standard deviation. Please refer to the help entry for details as indicated below.

As the **Calculated weighting** takes the decay into account, the proper isotope has to be selected form the list. otherwise it has no impact. Note that the **Scale** factor scales the standard deviation, not the variance.



If the generated data should represent non-decay corrected data, the **Decay** box needs to be checked, and the appropriate isotope selected.

Create Synthetic Study starts data generation and shows the result in the lower right, where they can be saved using **Save SYNTHETIC**.

5 Geometric Model Construction and CFD Simulation

PGEM module is aimed to provide user with a comprehensive tool for fast and intuitive processing of 3D/4D image datasets from a wide range of scan modalities (MRI, CT, PET, microCT ...). The technical core of PGEM is converting 3D images in models.

This chapter describes the workflow for a geometric model construction, CFD simulation and visualization of the CFD results.

5.1 Geometric Model Construction

The geometric model is representing the functional core of the PGEM tool. It needs for input only images and consists of volumes of interest (VOIs) and auto-generated STereoLithography structures (STLs). Once the model is created and saved, it gives the user the possibility to focus only on applications. Still, the user can redefine the model structures at any time point. This "stop in the middle" of processing data, represented by the model, is a big advantage: the user does not have to repeat the path image data-data segmentation because everything is available within the model.

The model can be used to create:

- Phantom Simulation as explained in the dedicated chapter 42.
- Education-driven application: educational 3D visualization of structures complemented by graphics, pictures and text - knowledge base associated with geometry. It is similar to an atlas of human physiology and is important for education and research as well.
- Surface meshes suitable for CFD modeling. The surface meshes are compatible with CFD solvers like OpenFoam and Fluent. The user can create CFD cases directly through PMOD for OpenFoam. The results can be readily visualized in the interactive PMOD 3D environment in order to obtain new understanding about the blood-flow behavior. The visualization is based on volume rendering and aims to convert nonvisual data into readable and recognizable images.

PGEM is a promising solution which supplements the limited spatial and temporal resolution of imaging data with physically based fluid dynamic.

5.1.1 Workflow Organization

The geometric model construction starts on the **Model** page with the creation of a new empty model and the definition of the time and the input image.

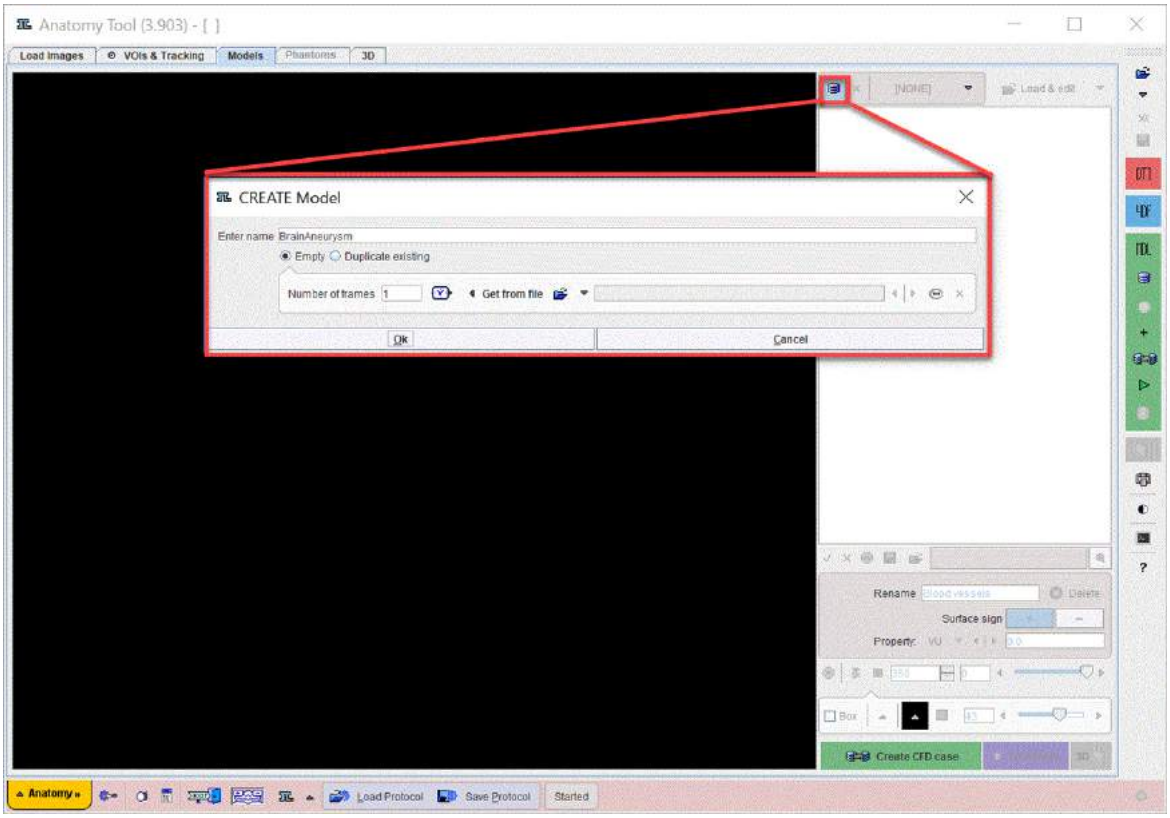
The input image is loaded and displayed on the **VOIs&Tracking/Image** sub-page. If necessary, the image can be cropped before starting the VOI definition.

The work continues on the **VOIs&Tracking/VOIs** sub-page with the VOIs definition.

Finally, the VOIs (geometry) are added to the model in the model builder interface. This will result in the model tree structure. STL structures are auto-generated and saved for each VOI added to the model. Optionally, additional characteristics can be defined for each element present in the model tree structure.

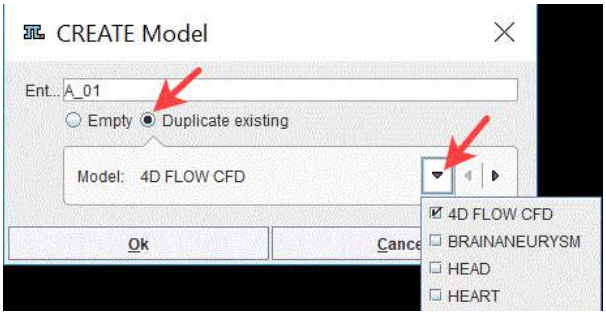
5.1.2 Start of the Model Definition

The first step in the building process consists in creating a new empty model on the **Models** page. This can be easily achieved by activating the **Create new model** icon as illustrated below:



A dialog window opens and allows defining the name and the timing of the series. The name of the model is defined in the **Enter name** filed: e.g.**BrainAneurysm**. Use the **Empty** radio button to create an empty model.

The **Duplicate existing** radio button allows making an exact copy of one of existing models in the list as illustrated below:

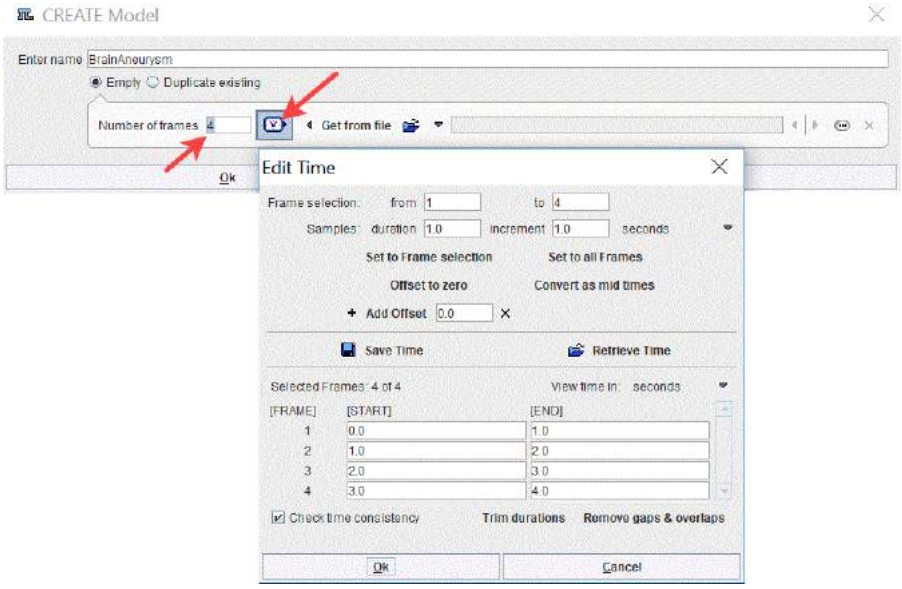


The duplicated model will be stored with the new name provided in the **Enter name** field. The modifications done in the duplicated model will not affect the source model.

Continue with the time definition for the model.

5.1.3 Time Definition

The models can be static or dynamic. The time definition for the **Empty** model is done in the bottom section of the window as illustrated below:



Note: The timing definition cannot be modified when **Duplicate existing** radio button is used to create a new model. In such case the timing defined in the source model will be set for the new model.

Timing Specified per Dialog Window

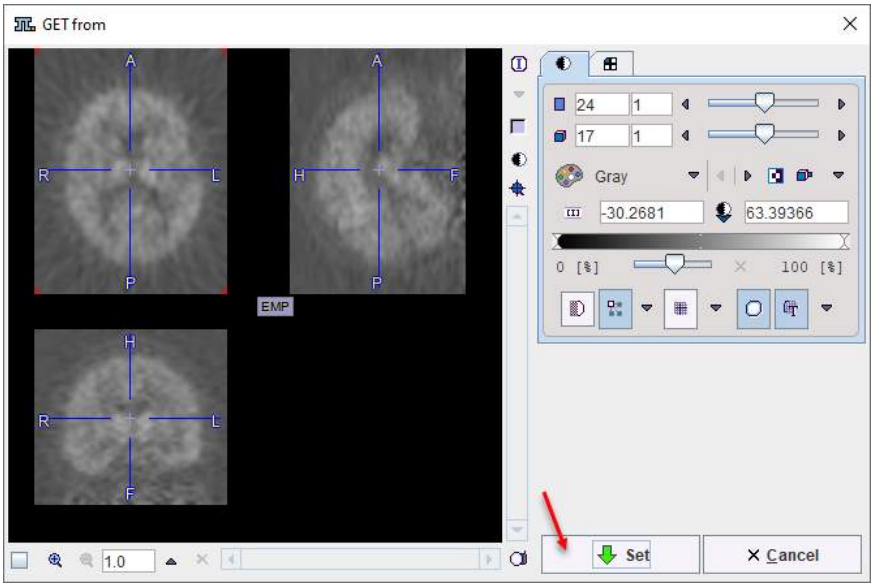
The specification of timing is done entering the **Number of frames** and opening the timing window illustrated above with the button.

The **Save Time**/**Retrieve Time** buttons allow saving/retrieving the timing of the dynamic frames to/from a file. It is possible to select a subset of frames in the **Frame selection** specifying the frames number in the **from** and the **to** text fields. The specified frame **duration** in samples is **Set to Frame selection** or **Set to all Frames.** The **Trim durations button** ensures that the end times are not after the following start times. The **Remove gaps & overlaps** button ensures that there are no empty time intervals between frames and that the start or end times do not extend beyond the previous or following times respectively.

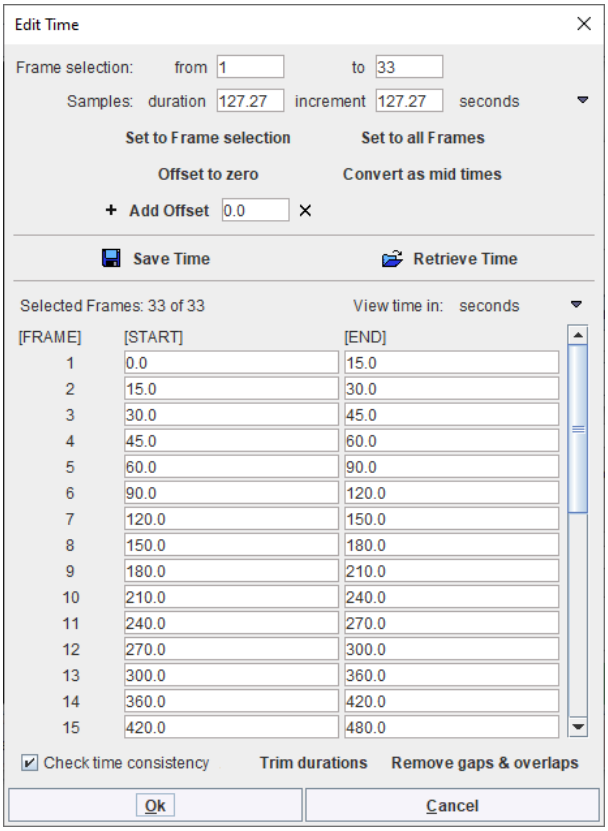
A number of 1 frame is set to the **BrainAneurysm** model. It indicates a static model.

Timing from Existing Dynamic Image

The timing may be extracted from an actual dynamic image by selecting it with the open button and then activating **Get from file**. The image is read and displayed in a window.



After confirmation with **Set** the timing is opened for editing and confirmation with **Ok**.



Note: The timing definition cannot be edited later on.

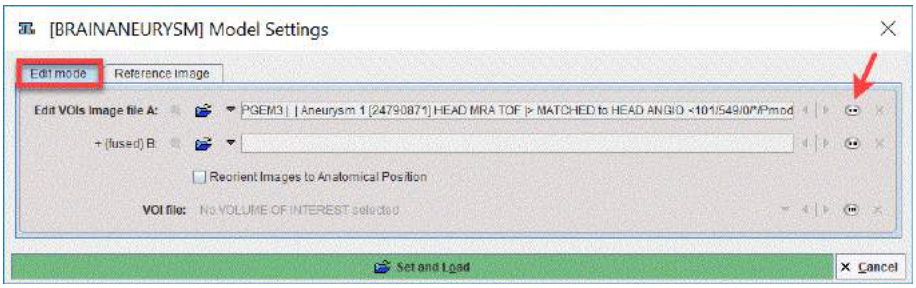
Close the **Create Model** window with **OK** to continue with the image definition.

5.1.4 Image Definition

The following steps are described using the **Aneurysm 1** series of the **PGEM3** subject available in the Pmod database.

Image Definition in Model Settings Window

When closing the **CREATE Model** window with **Ok**, another window appears, requesting image(s) definition:



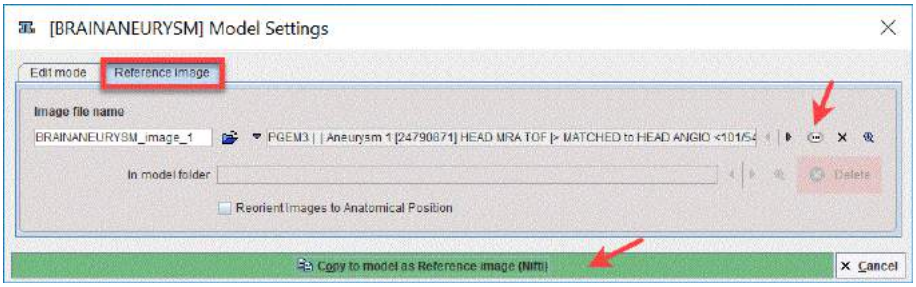
The **Edit mode** tab allows defining two images: image **A** and image **B**.

Image **A** is the image that will be loaded when the **Load & edit** button is activated. It will be considered the basic image for editing VOIs. Image **B**, if defined, has to be matched to the image **A** beforehand, as the two will be shown using the fusion mode on the **Images** page.

With the **Reorient to Anatomical Position** box enabled, the images are brought into the radiological HFS orientation after loading.

Use the button to add a **VOI file** to the model at this stage. Please note that the VOIs have to be previously outline and saved as *.voi* file on image A or B.

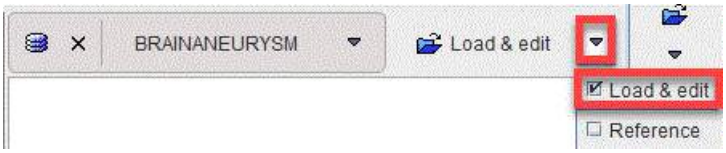
The **Reference Image** tab provides additional settings:



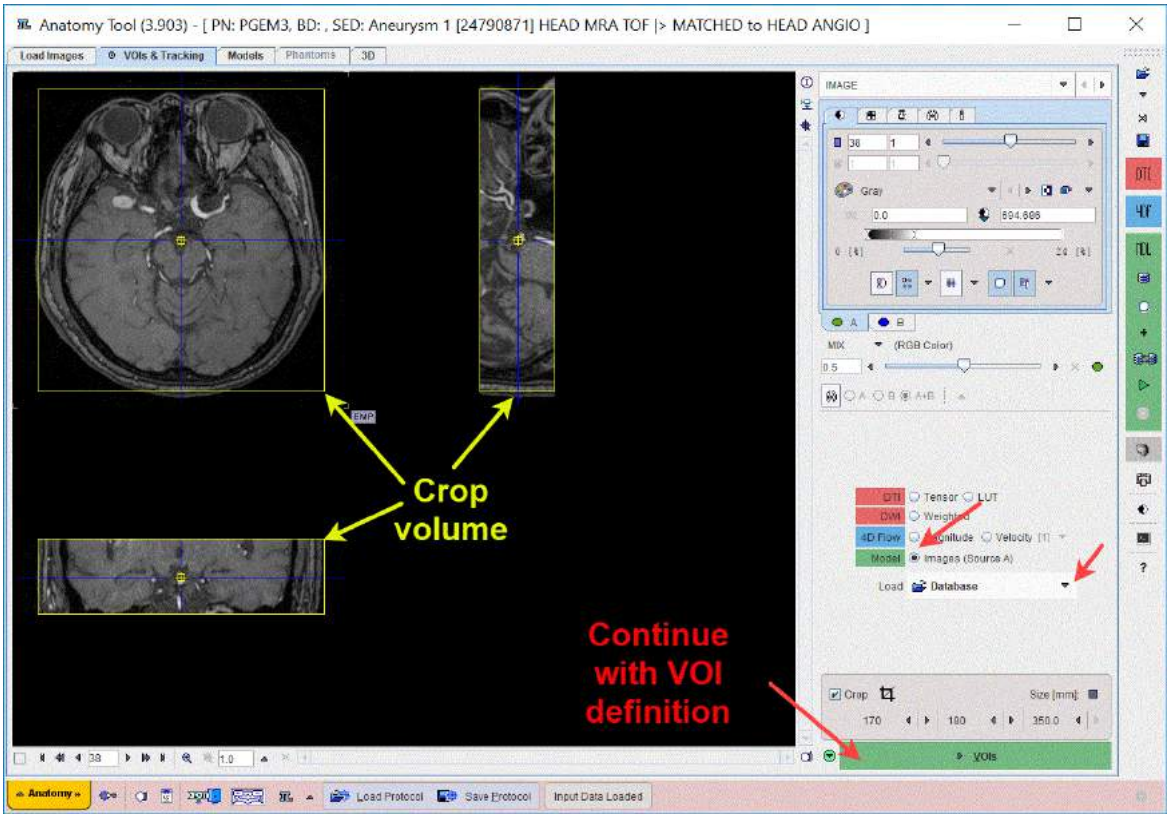
It allows defining a reference image which can be **A** or **B** or any other image in the same space. The **Image file name** field allows assigning a name to the image. The default name is assigned based on the model name followed by the suffix **_image_1** as shown in the example above. The preview button allows visualizing the images set for the model. Enable the **Reorient to Anatomical Position** box to bring the image into the radiological HFS orientation. Activate the **Copy to model as Reference Image (Nifti)** green button to copy the image in the model folder as a Niftii image. A confirmation dialog will appear asking the confirmation of the saving procedure. Close the dialog with **YES** to save the reference image in the model folder.

In the example above the same image was defined as image **A** and as **Reference Image**.

Activate the **Load & edit** button to proceed to the VOI definition step:



The program switches to the **VOIs & Tracking** page, **Image** sub-page while loading and displaying the image defined as **A**:



The images data with large field-of-view can be reduced in order to save RAM and optimize processing. This can be achieved enabling the **Crop** box. A yellow crop volume appears on the image. Place the yellow crop volume by clicking in the center of the area of interest such that is fully enclosed. The edge **Size** in [mm] can be adjusted for each direction by selecting the size in the corresponding list. The **Crop** button initiates cropping, whereby the original data are replaced. If cropping is not initiated manually, a request will be shown when proceeding to the **VOIs** step.

Note:

To use the **Reference** image for the VOIs definition select the corresponding entry under the **Load & edit** selection list, as illustrated below:

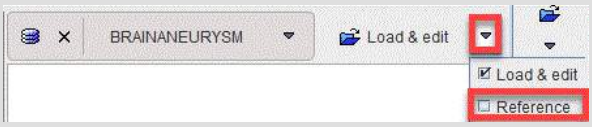


Image Definition by Model Image Loader

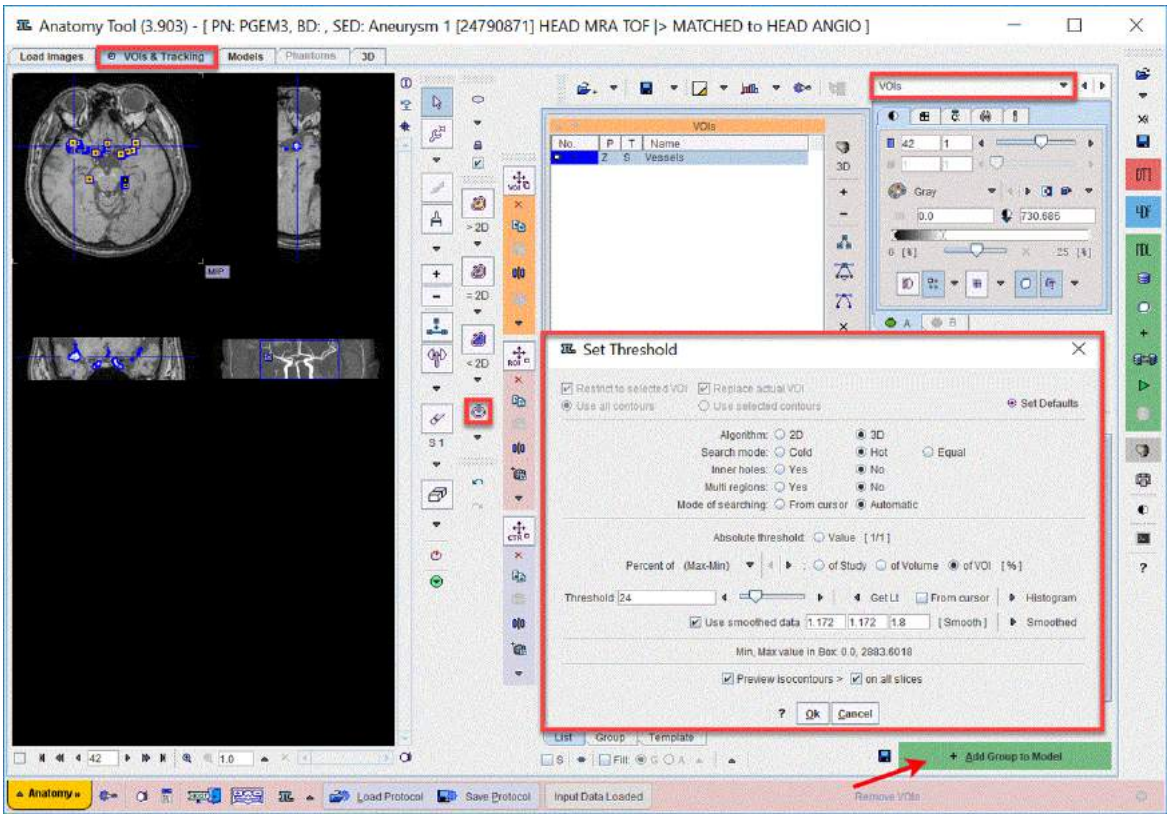
When no image is defined in the **Model Settings** interface, after pressing **Load & edit** button, the user will be asked to provide such configuration. In case there is no intention to provide such configuration, the user has to manually select the **VOIs & Tracking** page **Image** sub-page, enable the **Model** radio button and load an image configuring the available **Load** button. This image will be used for the **VOIs** definition in the next step.

Continue the VOI definition activating the **VOIs** action button.

5.1.5 VOI Definition

When arriving at the **VOIs** sub-page a fusion image is shown to the left which is composed of the image **A** and image **B.** In the current example only image **A** was defined in the Model settings 50 window.

The VOIs are created with the usual PMOD VOI tools. Please refer to the *PMOD Base Functionality Guide* for information related to volume-of-interest (VOI) definition. In the example illustrated below the **Automatic Isocontouring Detection** tool was used for outlining the first VOI:

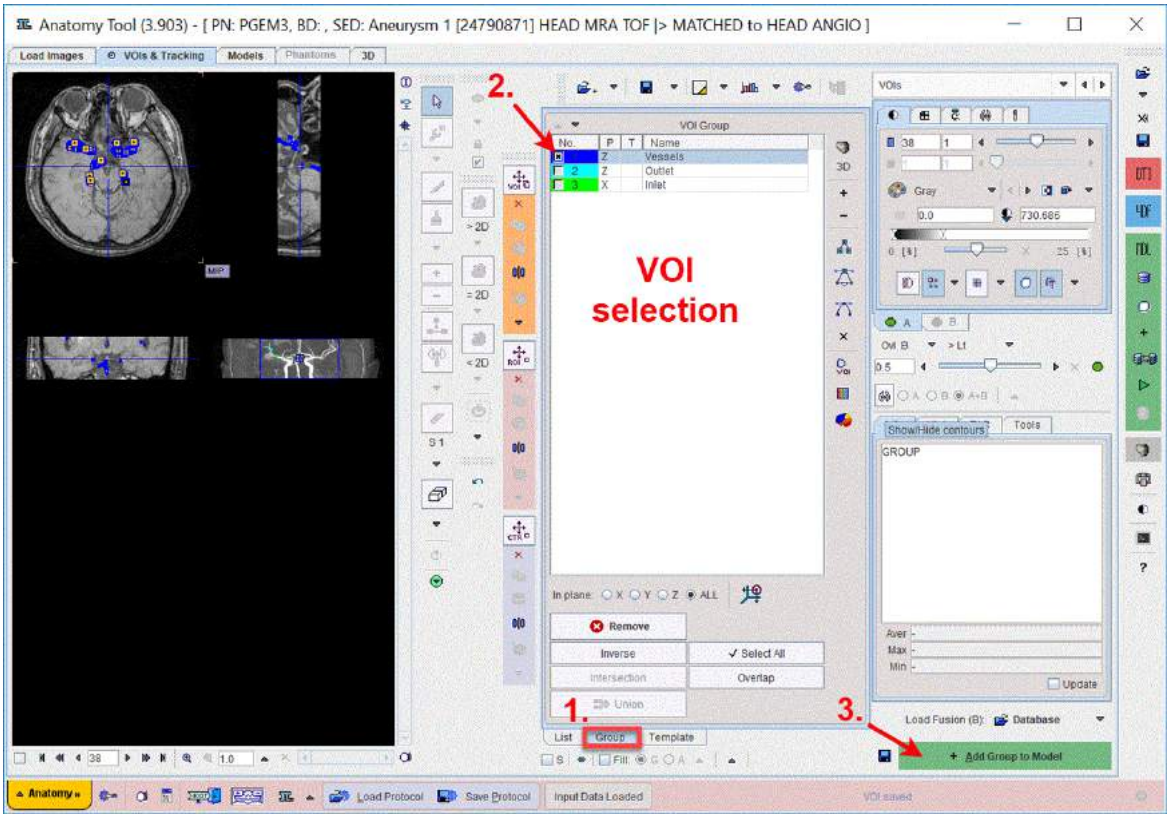


Please note that as soon as a VOI is available in the **VOIs** list the **Add Group to Model** green button becomes active.

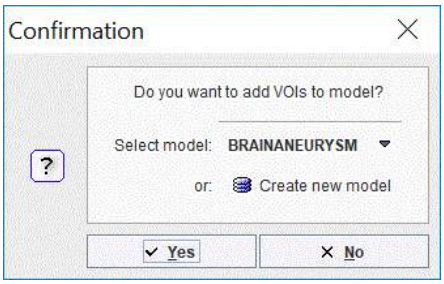
Note:
There is no limitation to the number of VOIs to be defined. It is recommended to define the VOI on the plane which is most perpendicular to the vessel axis.
For CFD simulation it is recommended to create individual contour ROI: e.g. each branch of a bifurcation should be a separate VOI. However, different VOIs can overlap. In case of joining structures (e.g. bifurcation) the VOIs should overlap on a couple of slices.

5.1.6 VOI Addition

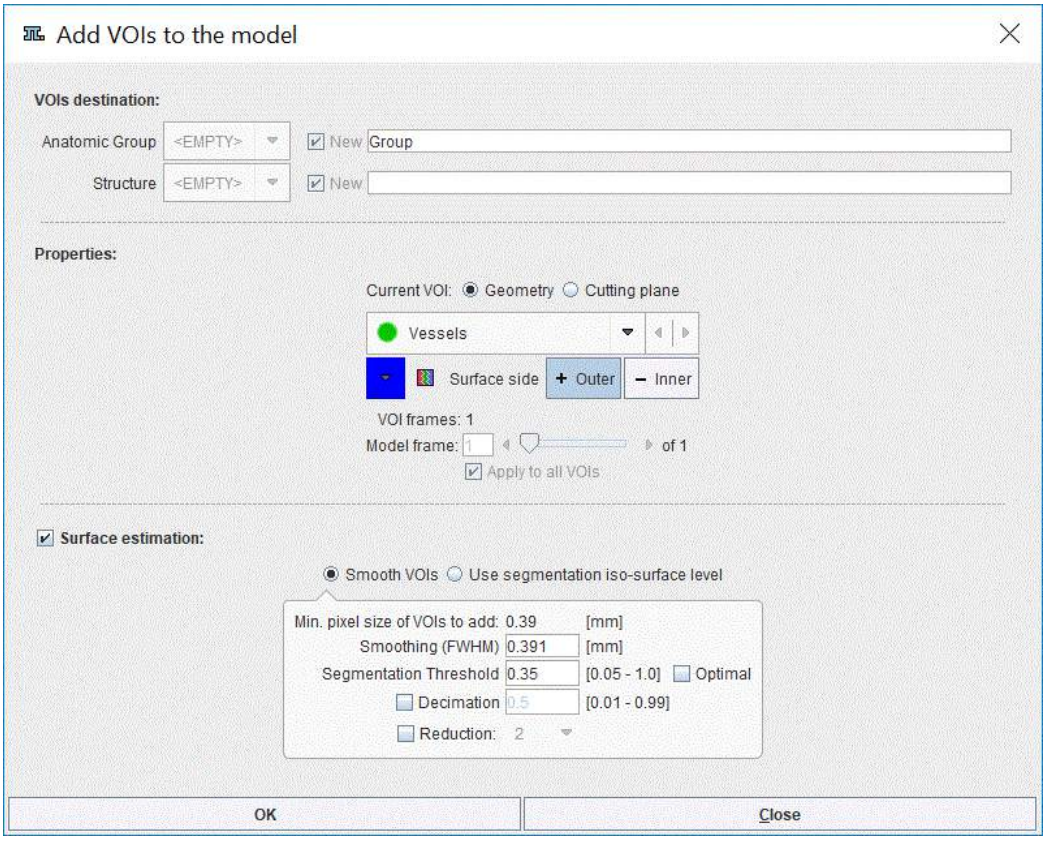
Start adding VOIs to the model selecting the **Group** tab as illustrated below:



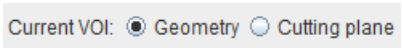
Activating the **Add Group to Model** green button the currently selected VOI is added to the model. Please note that more than one VOI at a time can be added to the model. A confirmation window appears and allows choosing to which model the geometric structures should be added:



Activate the **Yes** button to confirm the default settings which point to the currently selected model on the **Model** page. The model builder interface comes up and allows defining the VOI destination and the properties in the anatomical model:



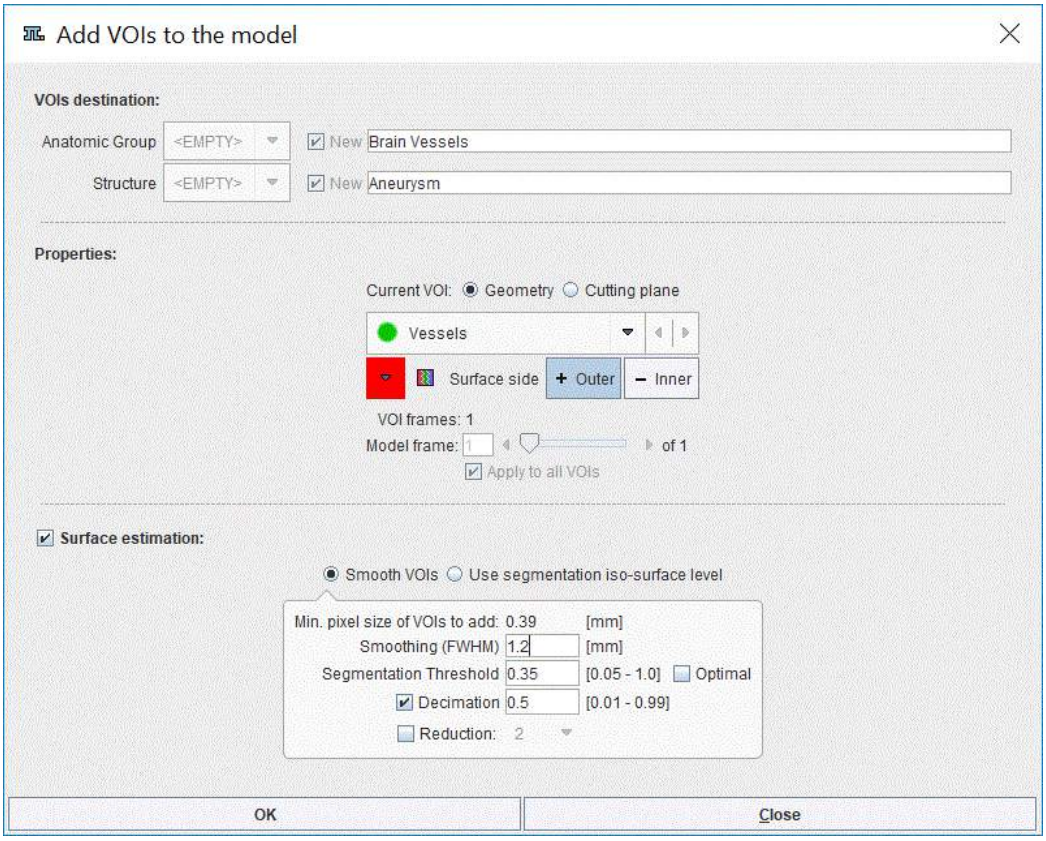
The VOIs can be added to the model as geometry or as cutting planes:



Both options are described in detail in the next sections.

5.1.6.1 Add VOI to the Model as Geometry

In the **Properties** section of the model builder interface, select the **Geometry** radio button for the **Current VOI** .



The appearance of the model builder interface is adjusted according to the **Current VOI** setting. The window is organized in three main sections:

1. **VOIs destination**: allows defining the **Anatomic Group** and the **Structure**.
2. **Properties**: allows defining the VOIs properties for the model.
3. **Surface estimation**: allows defining settings to build the STL structure of the model.

VOIs Destination

The **VOIs destination** section requires definitions for the **Anatomic Group** and **Structure**. When VOIs are added to the model for the first time, these settings are **<Empty>** and **New** names need to be provided in the dedicated field. To this end, the *Brain Vessels* and the *Aneurysm* were set as **Anatomic Group** and **Structure** respectively.

The settings available in this section are summarized in the table below:

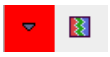
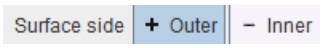
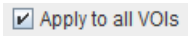
Anatomic Group	Corresponds to the highest hierarchy level in the model tree structure: the *Group* Allows defining the model **Anatomic Group** to which the VOIs will belong. To define a new **Anatomic group** the **New** checkbox has to be enabled and the name specified in the dedicated text field. Confirm and add the entry to the list with the **Enter** button on the keyboard. The drop down arrow becomes active when more than one anatomic structure was defined. It allows selecting among the currently available **Anatomic Group.**
Structure	Corresponds to the second hierarchy level entry in the model tree: the *Structure.*

	Allows defining the model **Structure** to which the VOI will belong. To define a new **Structure** the **New** checkbox has to be enabled and the name specified in the dedicated text field. Confirm and add the entry to the list with the **Enter** button on the keyboard. The drop down arrow becomes active when more than one structure was defined. It allows selecting among the currently available **Structure.** **Note**: Multiple **Structures** can belong to the same **Anatomic Group.** To this end turn off the **New** checkbox for the **Anatomic group**, select one of the **Anatomic Group** available on the list and proceed with the definition of a new **Structure** as described above.

Properties

While adding VOIs to the model as **Geometry**, the various **Properties** are defined in the dedicated section. In the example above the VOI color is set to red while the rest of the properties are the default ones.

The properties settings are summarized below:

	Allows changing or editing the color of the VOI(s) to be added to the model structure.
	Allows setting the VOI(s) as an **Outer** or **Inner** surface. For example the epicardium and endocardium in the heart muscle.
	When enabled applies the same properties to all the VOIs available on the **Current VOI** selection list. Please note that more than one VOI at the time can be added to the model.
VOI frames	Provides information related with the VOI type: • a value of **1** indicates the user is adding static VOIs to the model. • a value >**1** indicates the user is adding a dynamic VOI to the model
Model frame	Allows setting the model frame where the VOIs will be added. In case of dynamic VOIs the number indicates the starting frame of appearance in the model. Please note that the frame number for the model has to be defined previously. 50

Surface Estimation

The **Surface estimation** section allows defining characteristics for the STL model structures. While adding VOIs to the model surfaces (STL files) are generated automatically with the **Surface estimation** box enabled. These STL files will be stored in the model folder and will be used for 3D model presentation. Generating them will allow rendering faster the whole model in 3D.

Note:
Please note that these STL files are not the STL files used as surface meshes while creating CFD case process.

With **Smooth VOIs** radio button active the settings are as follows:

Min pixel size of VOI to add	Displays the pixel size [mm] in the data

Smoothing (FWHM)	It is a Gaussian filter and allows smoothing the data before creating the STL structure. The default value corresponds to the pixel size in the data. It is recommended to use a smoothing value 3 times the minimum pixel size. **Note**: Please note that for complex VOI shape less smoothing should be applied
Segmentation Threshold	All pixels with the value above the threshold are included in the segment. The default value is 0.35. When the **Optimal** checkbox is enabled the threshold will be calculated automatically such that the volume of selected VOIs is preserved.
Reduction	If enabled, allows creating simplified mesh based on data simplification. The defaults value is 2 and is representing the smallest value to be defined. Initially, the program will use this number and multiply the pixel size of the data with this value. Finally, the mesh will be generated on the new data. It is a faster procedure and the results will consist in mesh being less precise. Please note that if only this checkbox is enabled the generated files will be bigger and change in topography of the mesh will occur.
Decimation	Allows simplifying the mesh by removing triangles from the surface mesh without changing the mesh. Please note that in such case the simplification procedure is done after the mesh is created. The defined value should be between 0 and 1. The number represents percentage of the triangles to be thrown out. Usually „0.5" is a good compromise. The smaller the number of triangles, the faster is the 3D visualization. It is a slow procedure which generates smaller files. **Decimation** only changes the number of STL nodes, particularly the vertices of the surface mesh. However, no change in the mesh geometry occurs, preserving thus the mesh topology.

In alternative, the **Use segmentation iso-surface level** radio button can be used. It is recommended to use this option when the VOI was outlined using the isocontouring VOI tool and the image data loaded is the image data on which the VOI was created. With these two conditions fulfilled, the threshold value used for VOI isocontouring has to be set as **Original Segmentation Threshold**.

Note:

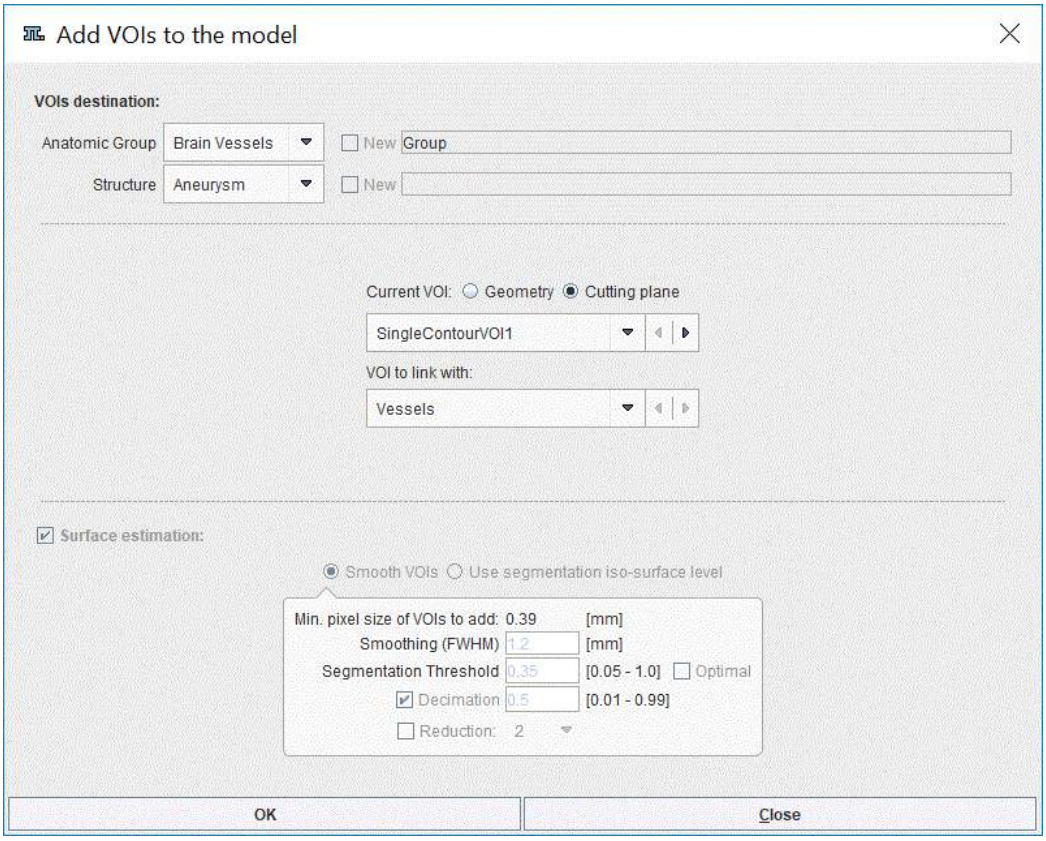
The iso-surface is recommended to be used for big geometries like skull.

In the current example the **Smooth VOIs** radio button is enabled. The **Smoothing (FWHM)** parameter is set to 3 times the pixel size (1.2 mm), **Decimation** is set to 0.5 while **reduction** is avoid.

Activate the **OK** button to start adding the VOI available in the **Current VOI** list to the model. The VOI will correspond to the lowest hierarchy level in the model tree structure: the *Element.* STL structures are auto-generated and saved for each VOI added to the model. This is encoded in the model tree by the letter **s** between round brackets which precede the *Element* and the *Structure* name. The result of the above processing is illustrated below:

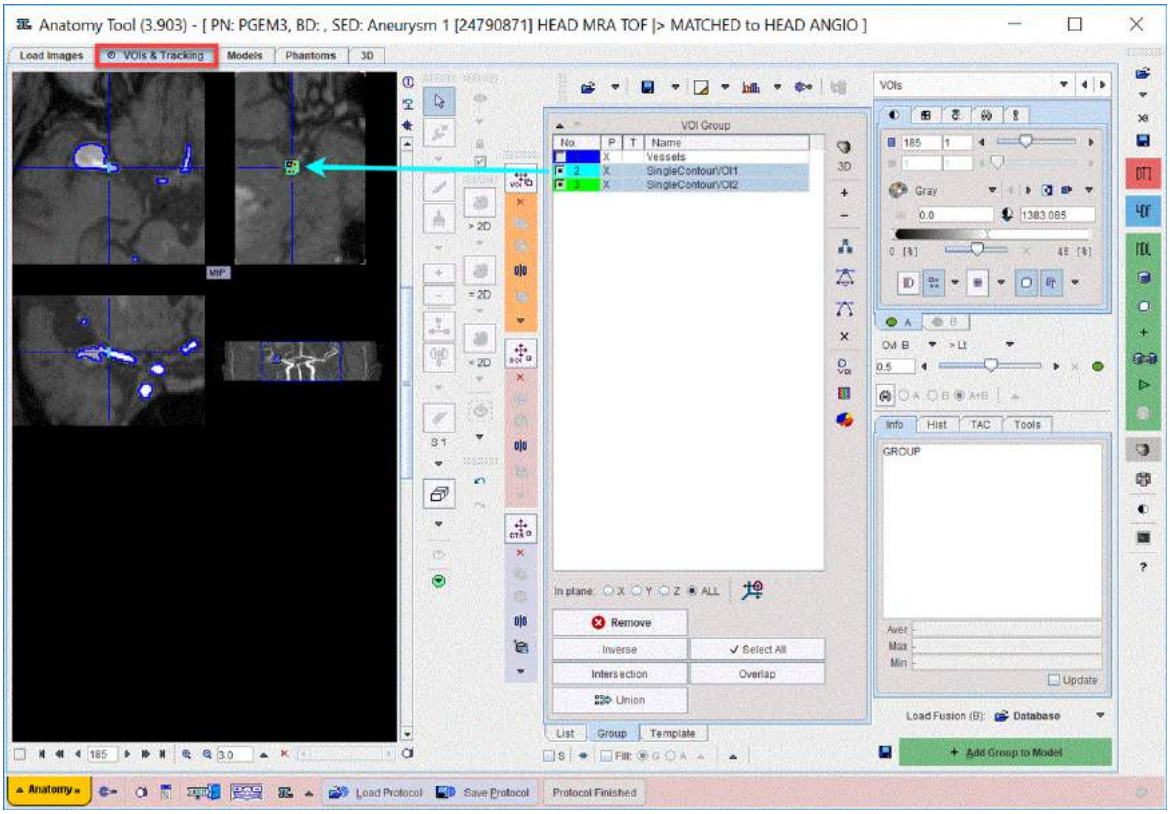
5.1.6.2 Add VOI to the Model as Cutting Plane

In the **Properties** section select the **Cutting plane** radio button for the **Current VOI**.



This setting can be used for single contour based VOIs. Particularly, only single contour VOIs outlined in the VOI definition step can be added to the model as predefined cutting planes. These will be used in the creation of the CFD case. Cutting plane VOIs can only exist when linked with existing structure. Therefore it is recommended to create single contour VOI based on an existing multicontour VOI available on the VOI list. This can be easily achieved creating an empty VOI in the list and pasting a single contour from the VOI of interest. Please note that location of the predefined cutting planes cannot be modified in the creation of the CFD case.

In the example below, two single contour VOIs, **SingleContourVOI1** and **SingleContourVOI2** were created based on two contours belonging to the **Vessels** VOI:



It is mandatory to add the linking VOI to the model as Geometry 57 beforehand. Please note that in the example above all VOIs are outlined in the same direction: **X**.

Note: The direction of the VOI to be added as a cutting plane is required be the same as the VOI to be linked with.

In the model builder interface only the two upper most sections are active:

1. **VOIs destination**: allows setting to which **Structure** in the selected **Anatomic Group** the VOI will be linked to as a cutting plane.
2. **Properties**: allows selecting the **VOI to link** with the selected cutting plane.

The **OK** button is activated to start adding the cutting plane to the model. The cutting plane will be linked to the selected *Element* in the model tree structure.

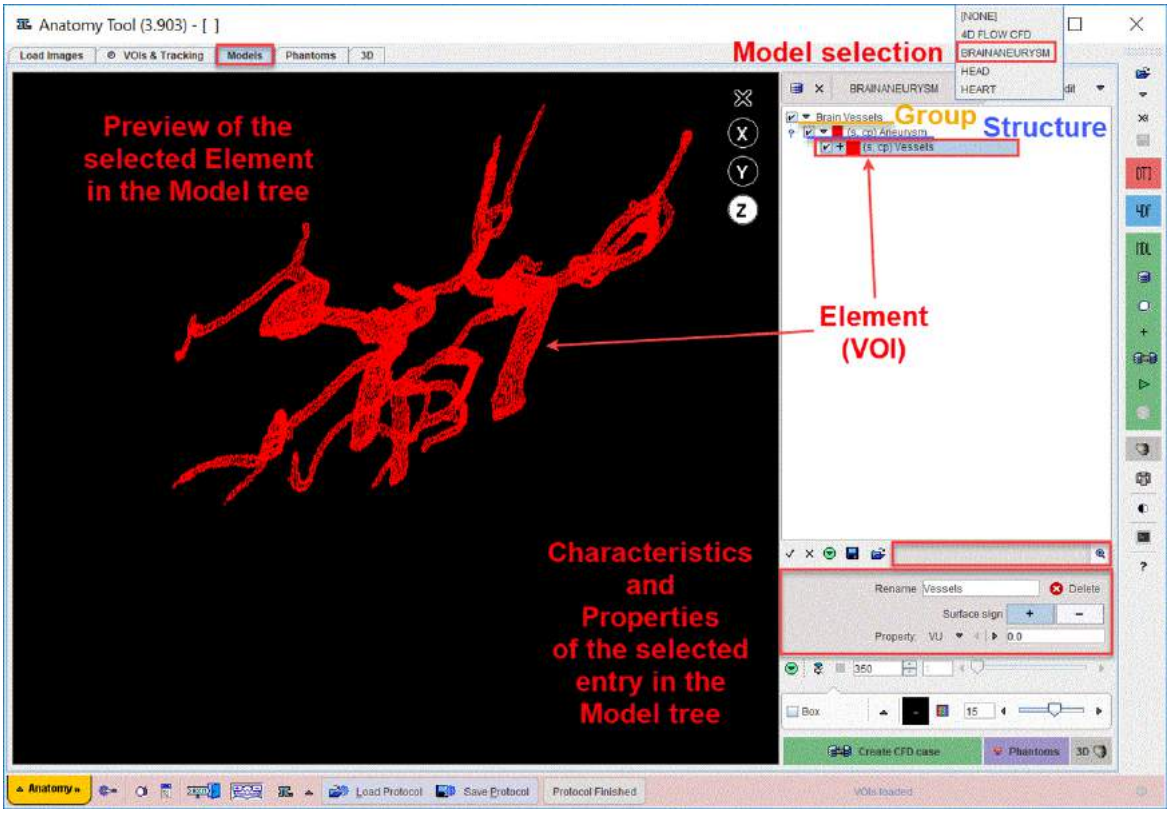
The result of adding a VOI as a cutting plane is illustrated below:

The VOI added as a cutting plane does not appear as an additional *Element* in the model tree. It is linked with the specified *Element* and encoded in the naming procedure by the **cp** entry. The plane will be available in the workflow of the CFD creation.

5.1.7 Anatomical Model

The anatomical model consists of VOIs (*Elements*) and auto-generated STereoLithography structures (STLs). The process of adding VOIs to the model results in the model tree structure. Multiple models may coexist in the same time but only one model is visible at a time

The **Models** page has the layout illustrated below:



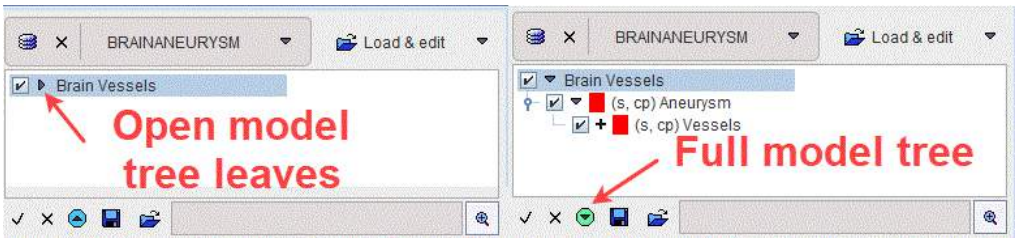
The model is available for selection in the model list, in the upper right. The model tree structure is displayed in the right panel, under the model selection list.

The viewport area to the left shows the selected elements in the model tree, whereas the characteristics and the properties of the visualized objects can be previewed and/or edited using the panel to the right.

5.1.7.1 Tree Organization of the Anatomical Model

The result of adding VOIs to the model is structurally organized in the model tree on the **Models** page.

The selection of a subset of elements in the model is supported by the dedicated panel as illustrated below:



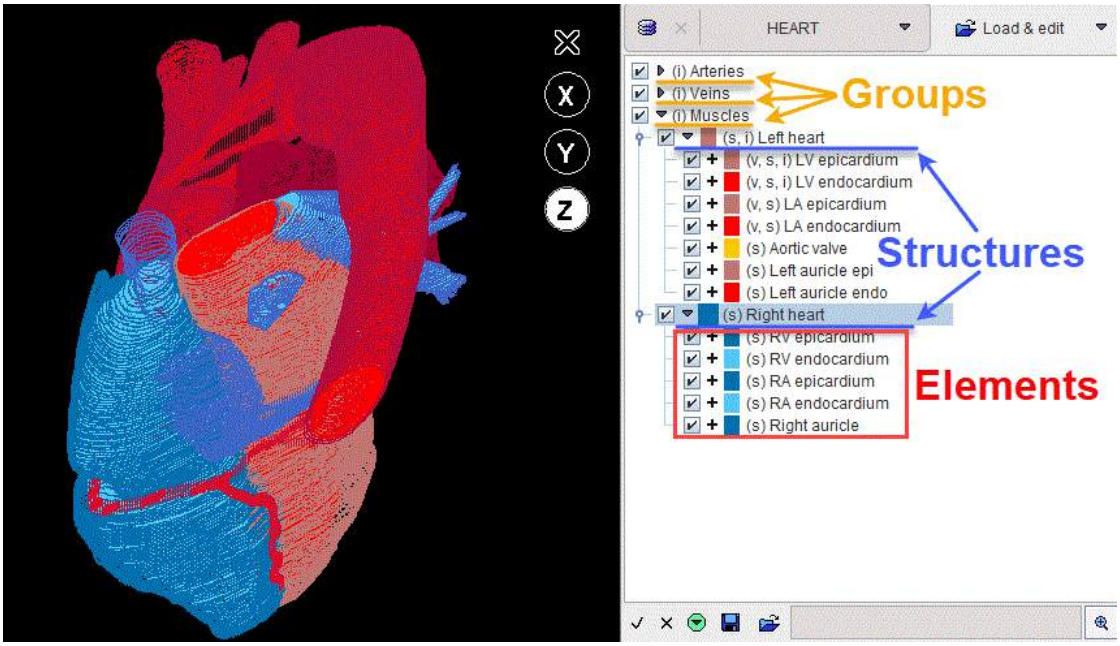
The model structure is organized as a hierarchical tree on three levels: top, middle and low level. The hierarchy corresponds to the **VOIs destination** settings defined in the model builder interface during the VOI addition 56.

The branch on the top level is represented by the *Group,* e.g. the **CFD_Structure**, as indicated in the left panel. It corresponds to the **Anatomic Group** defined in the model builder interface.

The full tree can be opened easily by the button indicated in the right panel. The middle level entry in the model tree is represented by the *Structure* node, e.g. the **ExperimentalPipe**. It corresponds to the **Structure** defined in the model builder interface.

The single entry in the tree is called *Element* and corresponds to a VOI in the VOIs list. It represents the low level entry in the model hierarchy, e.g. **1**.

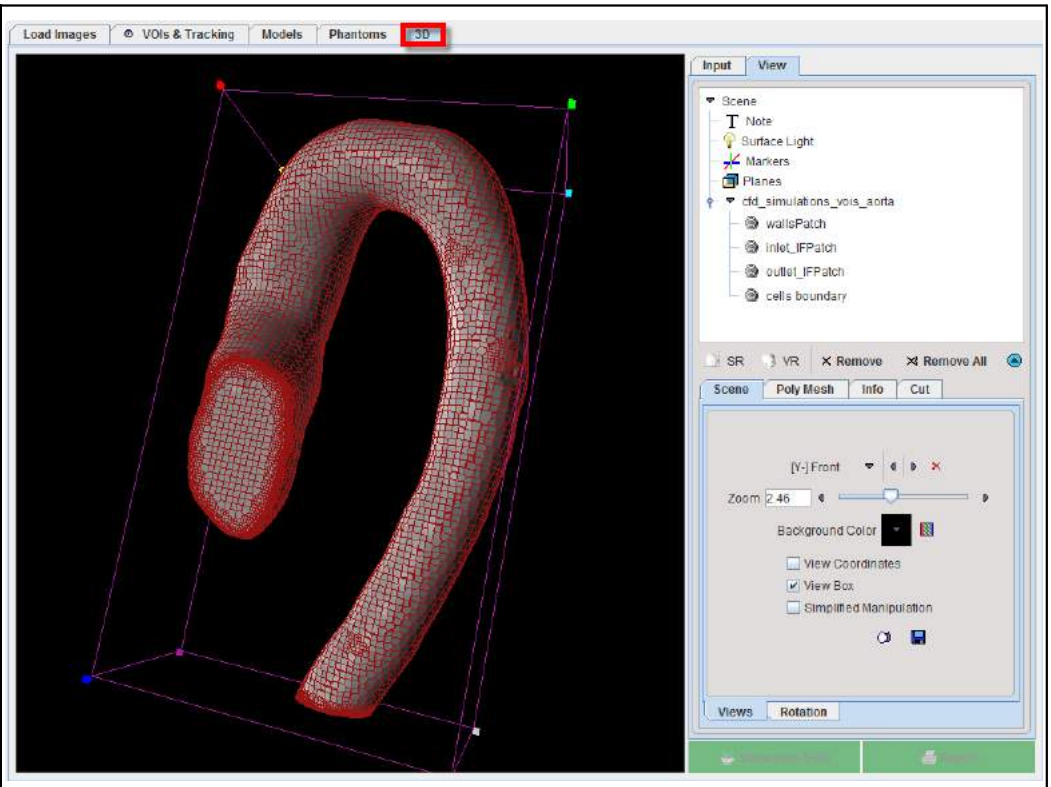
In general, the *Structure* node consists of at least one *Element*. The *Group* consists of at least one structure node. A model may consist of one or several *groups of structures*. An example of such model (**HEART**) is illustrated below:



It consists of three groups: **Arteries**, **Veins** and **Muscles**. Each group contains multiple structure nodes: e.g. the **Left heart** and **Right heart** in the **Muscles** group.

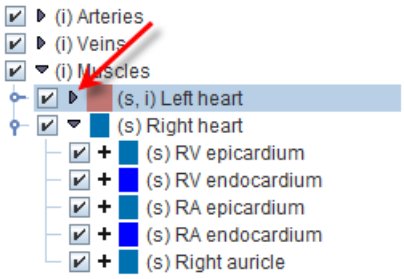
Round brackets are used to add encoded information for each entry in the model tree. Such information precedes the name of the entry and is summarized in the table below:

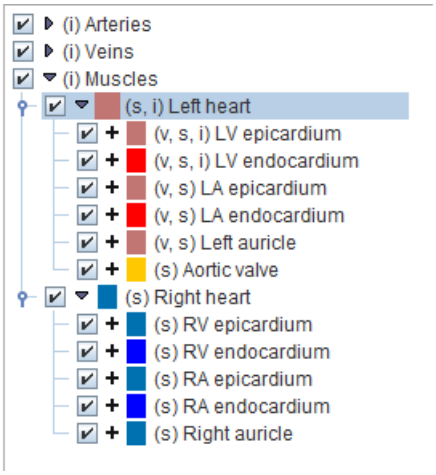
s	Stands for *surface mesh* and indicates that a VOI was added to the model as geometry. STL structure is auto-generated and saved for each such VOI. Note that each middle and low level entry in the model tree has such information available. When an element is selected in the model tree a preview of the simplified mesh structure is shown in the viewport.
cp	Stands for *cutting plane* and indicates that a VOI was added to the model as a cutting plane. This information will appear in the tree for the structure and the element to which the VOI was linked in the model builder interface Note that a cutting plane is not visible in the model tree: it will be available to be used in the CFD workflow.
c	Stands for *case* and indicates that a CFD simulation result was linked to the selected entry in the model through the local cases manager. When such encoding is available for a selected entry in the model tree the button in the taskbar becomes active. It allows viewing the linked CFD case in the 3D interface like a polymesh (volume mesh):

	
i	Stands for *image* and indicates that at least one image was defined as characteristics 70 for that entry.
v	Stands for *volume mesh*. The volume meshes are generated in the process of the CFD case creation and they can be linked with the model element through the local cases manager.

Tree Manipulations

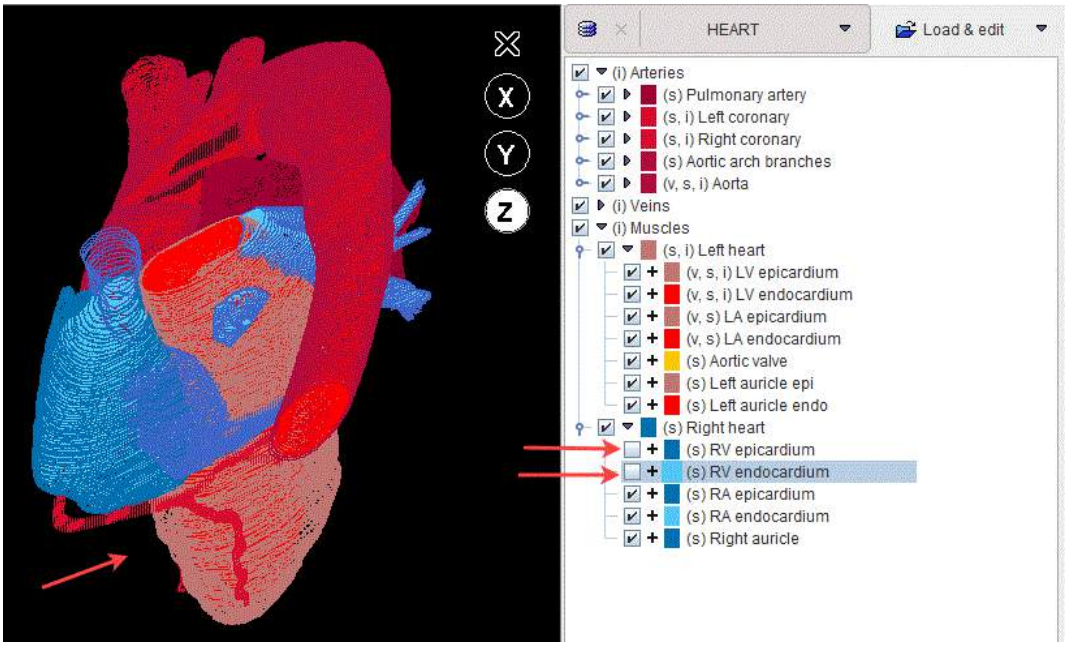
Branches in the tree can be opened/closed with the little arrows left to the branch names.



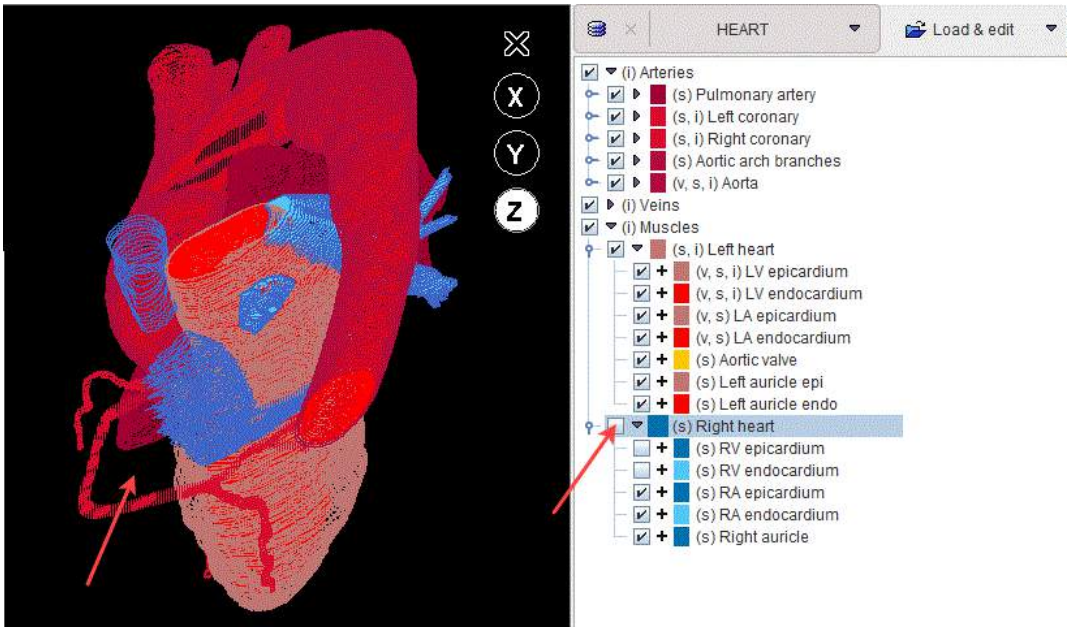


Tree Selections

The structures of interest are the ones with checked boxes to the left of their color code. Simply click into a box for changing the selection. In the example below the **RV epicardium** and **RV endocardium** have been de-selected.

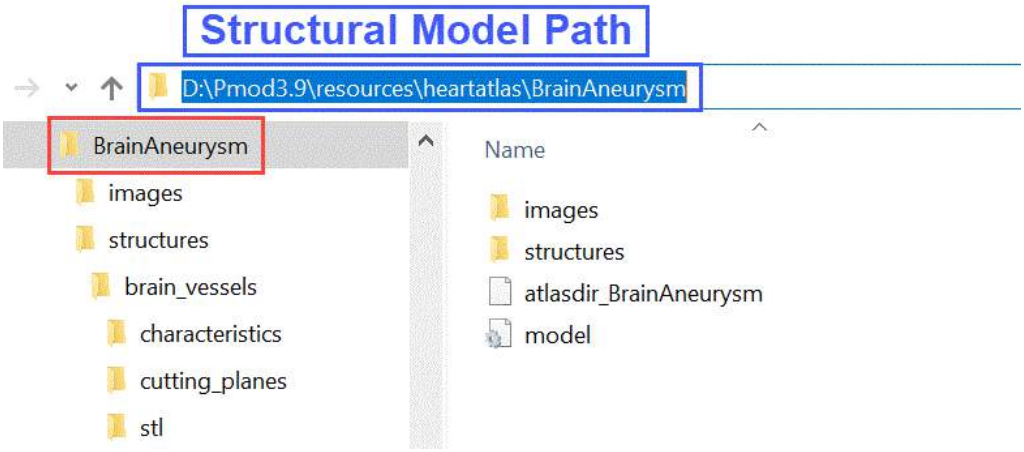


If the selection of a branch is removed, all elements belonging to it will be de-selected.

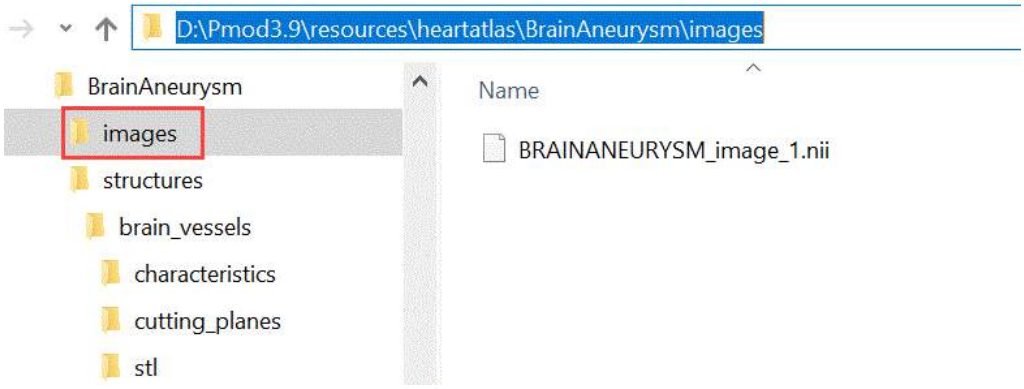


5.1.7.2 Components of the Model Folder in PMOD

The model is stored in the **Structural model Path** defined in the PGEM configuration settings. The model directory contains two folders and two files as illustrated below. :



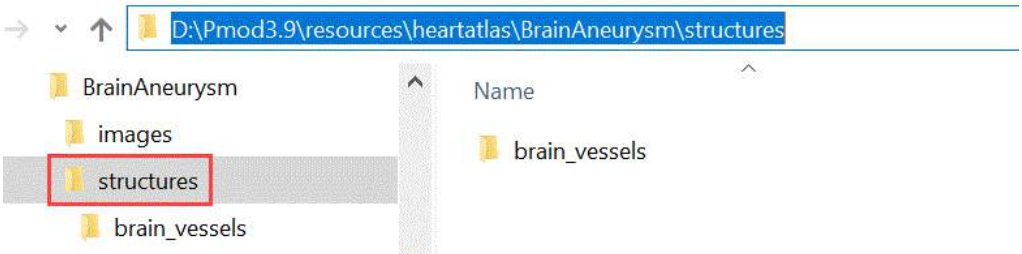
1. The **image** folder contains the image copied to the model folder as the reference image in niftii format.



2. The **structures** folder contains all the information related to the entries in the model tree.
3. The **atlasdir_*** file stores the frame time definition, reference image file information, settings used in the model builder interface.
4. The **model** file stores the information related to the PMOD version used to create the model and the definition of the model images .

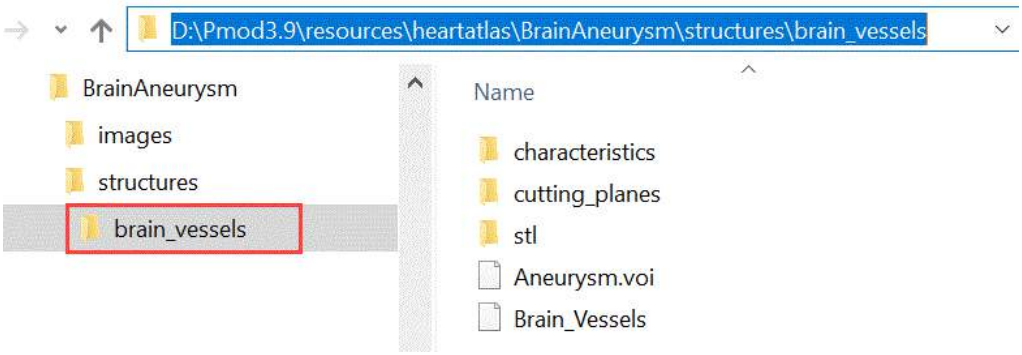
The Structures Folder

The information related to each top level entry in the model hierarchy is organized in subdirectories with the same name. Their location is in the **structures** folder of the model directory as illustrated below:



The number of the subdirectories present in the **structures** folder equals the number of top level entries in the model tree. In the example above a single subdirectory is present: the **cfd_structure**. It indicates the model has a single top level entry.

The content of such subdirectory is shown below:

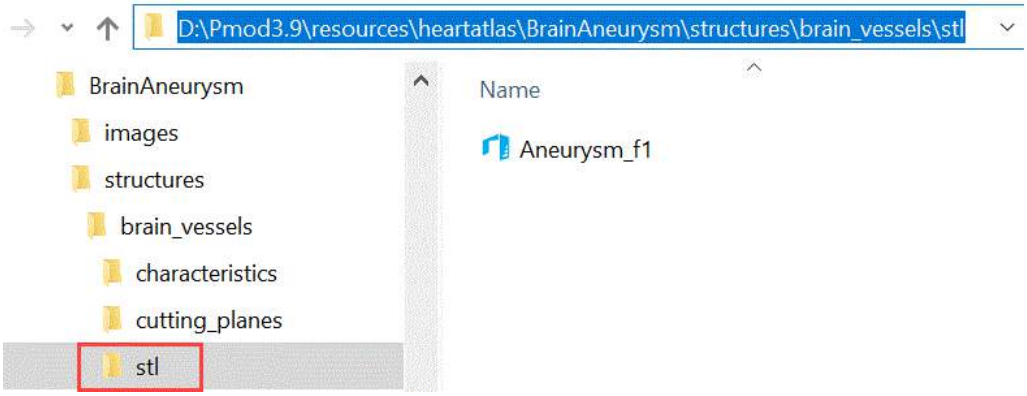


It contains:

1. The **.voi** file(s): the number of these files equals the number of middle level entries belonging to the same top level entry in the model tree. The name of the middle level entry in the model tree is used as the name of the *.voi* file: e.g. **Aneurysm.voi**.
2. The **.XML** file: the name of the top level entry in the model tree is used as the name of the *.xml* file: e.g. **Brain_Vessels**. It stores information of the edition dates and the name of the top level entry in the model hierarchy as illustrated below:

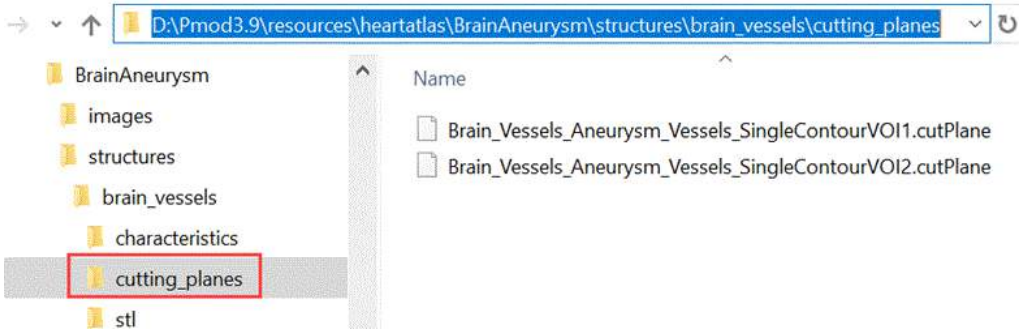
```
<?xml version="1.0"?>
<!--Put all new tags under <entry> level.-->
<!--Order of the groups under the <entry> level, such as f.ex. <Name>,
<Description> does not matter.-->
<!--Do not remove or rename defualt groups, which are: Name, Geometrical,
Physical, Description and Images.-->
<!--Xml preserves the formatting of text between tags (it does not ignore
spaces and empty lines).-->
<!--Information between <descrpition> tags must be put in between in such
way that the text is not in the same line as opening and closing tags-->
- <entry>
  - <Edition_dates>
      <First_addition_date>2017.12.05</First_addition_date>
    </Edition_dates>
  - <Name>
      <model>Brain Vessels</model>
    </Name>
</entry>
```

3. The **stl** folder: contains the STL file of each middle level entry belonging to the same top level entry in the model tree. Particularly, for each **.voi** file the corresponding STL file is saved.



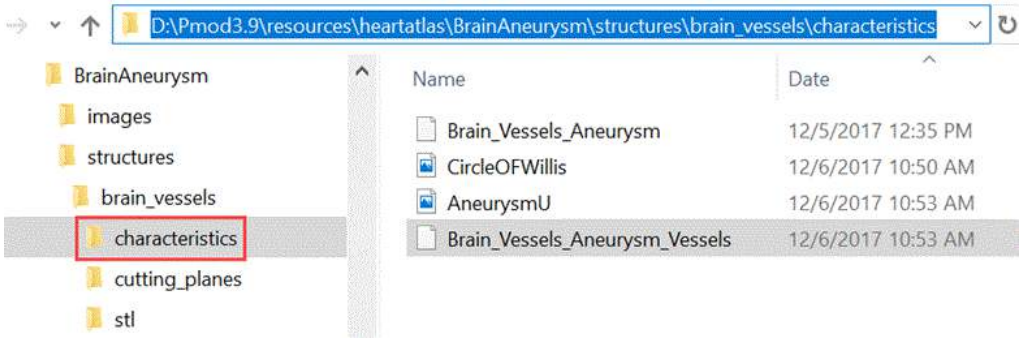
Please note that a suffix, e.g. *_f1* is appended to the name: it corresponds to the **Model frame** definition in the **Properties** section in the model builder interface. This indicates that in the VOI adding procedure the **Model frame** field was set to 1. The static models (1 frame model) will always have **Model frame** set to 1. The STL files are used for 3D simplified preview of the model.

4. The **cutting_planes** folder: if VOI was added to the model as a cutting plane, such information is stored in a *cutPlane* file. The number of the files in the folder indicates the number of VOIs added as cutting planes. In the example illustrated below two VOIs were added as cutting planes:



The cutting plane is always linked with a low level entry in the model tree as described in the model builder interface. The name of the top level entry (**Brain_Vessels**) in the model followed by the middle (**Aneurysm**) and low level entry (**Vessels**) ones is used as the root name for the *cutPlane* file. The name of the VOI added as cutting plane is appended as suffix to the root name: e.g. **_SingleContourVOI1.**

5. The **characteristics** folder: stores the definitions provided as characteristics 70 for each entry belonging to the respective top level entry in the model tree.



Such definitions are stored separately for each entry level in *.xml* files. The number of *.xml* files equals the number of middle and low level entries belonging to that specific top level branch.

The name of the top level entry in the model followed by the middle level entry one is used as the corresponding name for the *Struture .xml* file: e.g. **Brain_Vessels_Aneurysm.**

The name of the top level entry in the model followed by the middle and low level entry ones is used as the corresponding name for the *Element .xml* file: e.g. **Brain_Vessels_Aneurysm_Vessels.**

In the example below is illustrated the content of the **Brain_Vessels_Aneurysm_Vessels**:

```
<?xml version="1.0"?>
<!--Put all new tags under <entry> level.-->
<!--Order of the groups under the <entry> level, such as f.ex. <Name>, <Description> does not matter.-->
<!--Do not remove or rename defualt groups, which are: Name, Geometrical, Physical, Description and Images.-->
<!--Xml preserves the formatting of text between tags (it does not ignore spaces and empty lines).-->
<!--Information between <descrpition> tags must be put in between in such way that the text is not in the same line
as opening and closing tags-->
- <entry>
  - <Edition_dates>
      <First_addition_date>2017.12.05</First_addition_date>
    </Edition_dates>
  - <Name>
      <model>Vessels</model>
    </Name>
  - <Description>
    - <description>
      - <![CDATA[
          <html>  <b>Circle of Willis</b><br><br>The blood supply 
        ]]>
      </description>
    </Description>
  - <Images>
      <image>CircleOFWillis.png</image>
      <image>AneurysmU.png</image>
    </Images>
</entry>
```

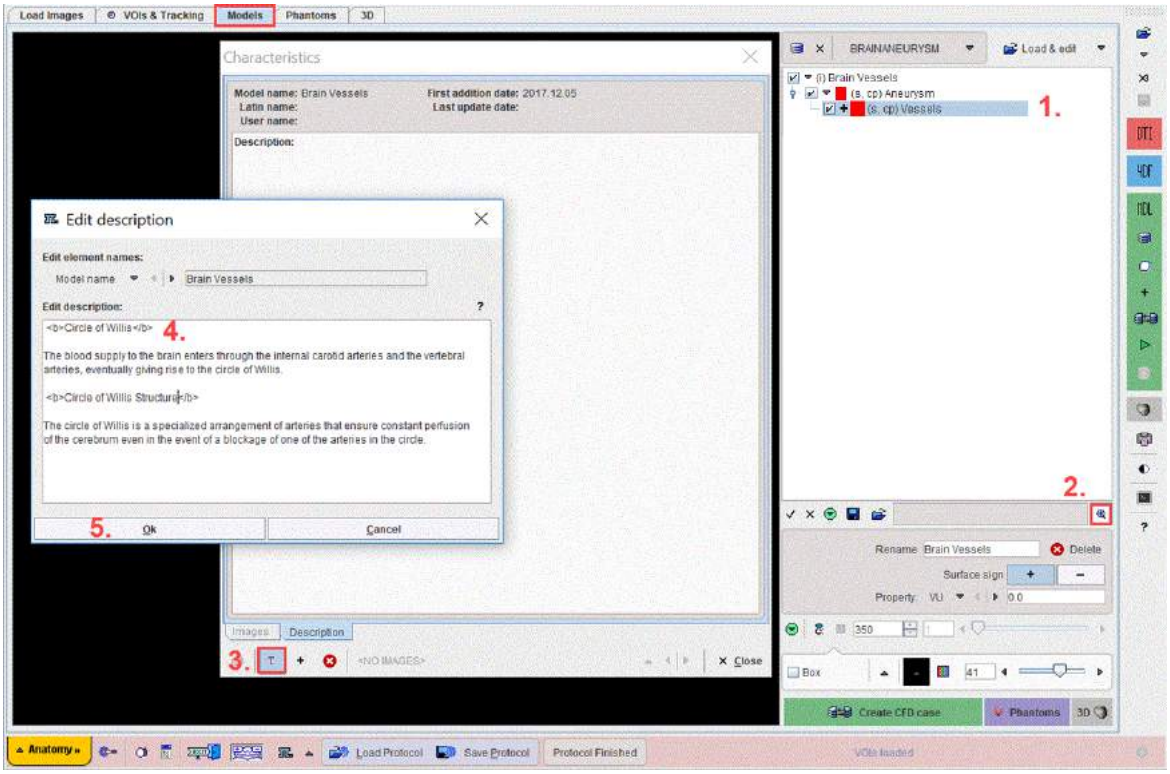
Each *.xml* file stores information about the edition dates, the level entry name encoded as described above, the text description and the images file names. The images, if defined, are stored as .jpg files with the specified name: e.g. *CircleOFWillis* and *AneurysmU* in the example above.

Note: To share a model with another PMOD user simply copy the model folder (e.g **BrainAneurysm**) to another PMOD installation in the **Structural model Path** defined in the PGEM configuration settings.

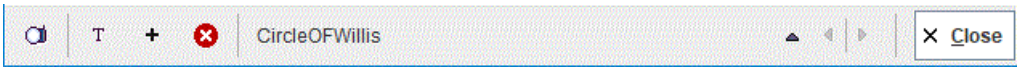
5.1.7.3 Definition of the Characteristics for the Model's Elements

Use the characteristics section on the **Models** page to provide images and text description for the entries in the model tree. The characteristics of the models and the 3D visualization are representing the education-driven application of the models.

Select an entry in the model tree (**1**) and activate the **View Characteristics** button (**2**) to start the characteristics definition. A dialog window opens and allows allowing editing and adding captured images:



The window is organized in two main tabs, **Images** and **Description.** The characteristics can be easily edited using the buttons available in the bottom section of the window.



Please note the tooltips which provide short explanation of the buttons functionality.

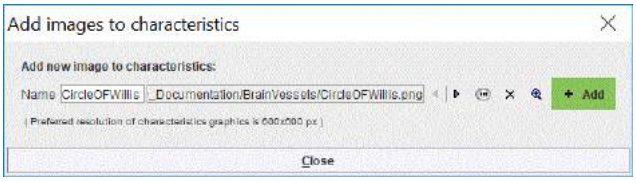
Initially, only the description tab is active as no image is defined in the characteristics. Activate the **T** icon (**3**) to start **Edit description**. Please note that text sections entered in this area should be formatted using HTML tags (**4**): and . In the example above two sections are formatted using the HTML tags:

Circle of Willis

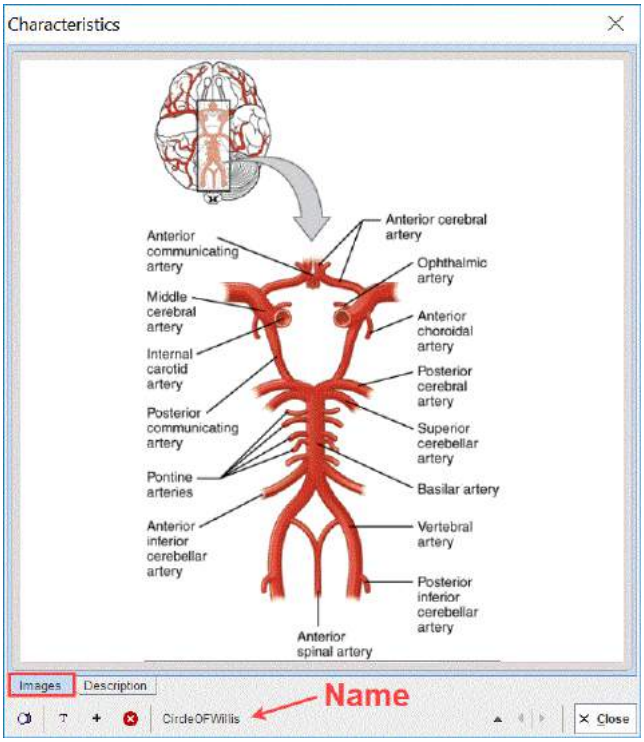
Circle of Willis Structure

Close the dialog window with the **OK** button (**5**) to transfer the content of the edit dialog to the **Characteristics.** Use **Cancel** button if no text should be transfer to the **Description** tab.

Activate the + button to start adding an image. Its activation opens a dialog window as illustrated below:



It allows defining the **Name** for the image. Once the image is selected the activation of the **Add** green button stores the image as a characteristic. Select the button to preview the image added as characteristics. Finally **Close** the window. The image is available on the **Images** tab and the assigned name is displayed on the status line of the window as shown below:



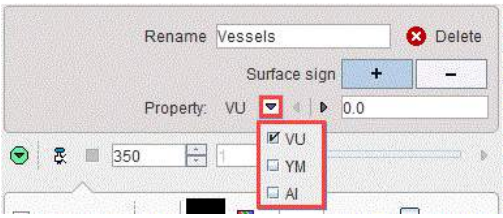
The arrow button becomes active when multiple images are added as characteristic to the selected element. It allows selecting the image to be displayed on the **Images** tab. Activate the **Delete image** button to discard an image.

Use the **Close** button to exit the **Characteristics** window.

Note: The recommended graphic size for images is 600x600 pixels.

5.1.7.4 Definition of the Properties for the Model's Elements

The properties section on the **Models** page allows modifying the properties of the element selected in the model tree:



The **Rename** text field allows changing the name of the entry in the tree by simply typing a new name. To set the new name it is mandatory to press the **Enter** key on the keyboard. A dialog window opens: activate the **OK** button to confirm the change.

To eliminate an entry in the model tree, select the element or the node and activate the **Delete** button. A dialog window appears allowing to **Completely remove from the model** the selected entry or to **Delete the definition from the specified frame**.

The **Property** available for selection is as follows:

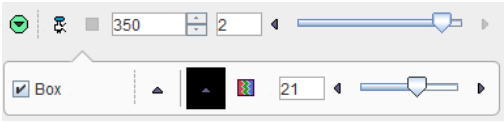
1. VU is representing the user defined units.
2. YM stands for Young's module.
3. AI stands for acoustic impedance.

To assign a certain e.g. **VU** value to one or more entry in the model tree please proceed as follows:

1. Select the element in the model tree. For multiple selection use *Shift+click* or *CTRL+click*.
2. In the text field aside the **Property** selection (e.g. VU) type the value (e.g. 100).
3. Confirm the action with the *Enter* button from the keyboard.

Note:
In case property value is entered for a top level entry it will affect all the nodes beneath it.
The property will be applied to all selected nodes: the selection is referring to the node, not to the checkbox aside the node.
To define different properties to the elements in a node start the definition with the highest hierarchical node and then continue with the lower level nodes beneath it.
If no value is entered for the current selection the property field displays "0".

Below the properties panel additional functionality buttons are available:



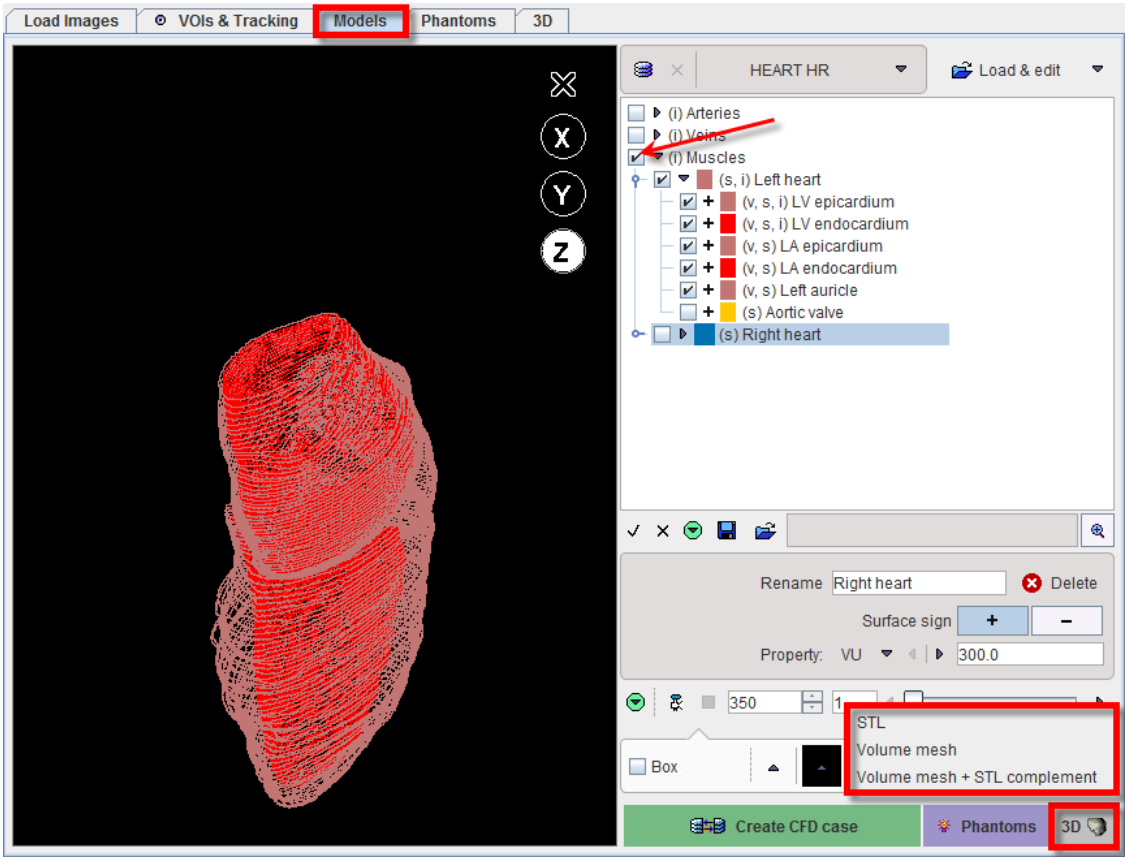
offering the following functions:

/	Hide/show the properties panel to free some space in the user interface. With the panel hidden, the icon changes to . When this button is activated, the panel is shown again.
	Allows starting the movie when dynamic models are defined. The text box aside allows defining the movie delay 500. The slider allows selecting for preview a specific frame in a dynamic model.
	Allows stopping the movie
Box	If enabled shows 3D Cartesian coordinate system.
	Allows selecting the number of the 3D vertices to be displayed in the view port. The higher the number the less vertices will be shown.
	List selection for changing the background color.
18	Allows rotating 360 degrees the 3D simplified model preview in the view port.

5.1.7.5 Interactive Exploration of the Model

Start on the **Model** page by selecting a model and then the elements in the model tree to be visualized in 3D.

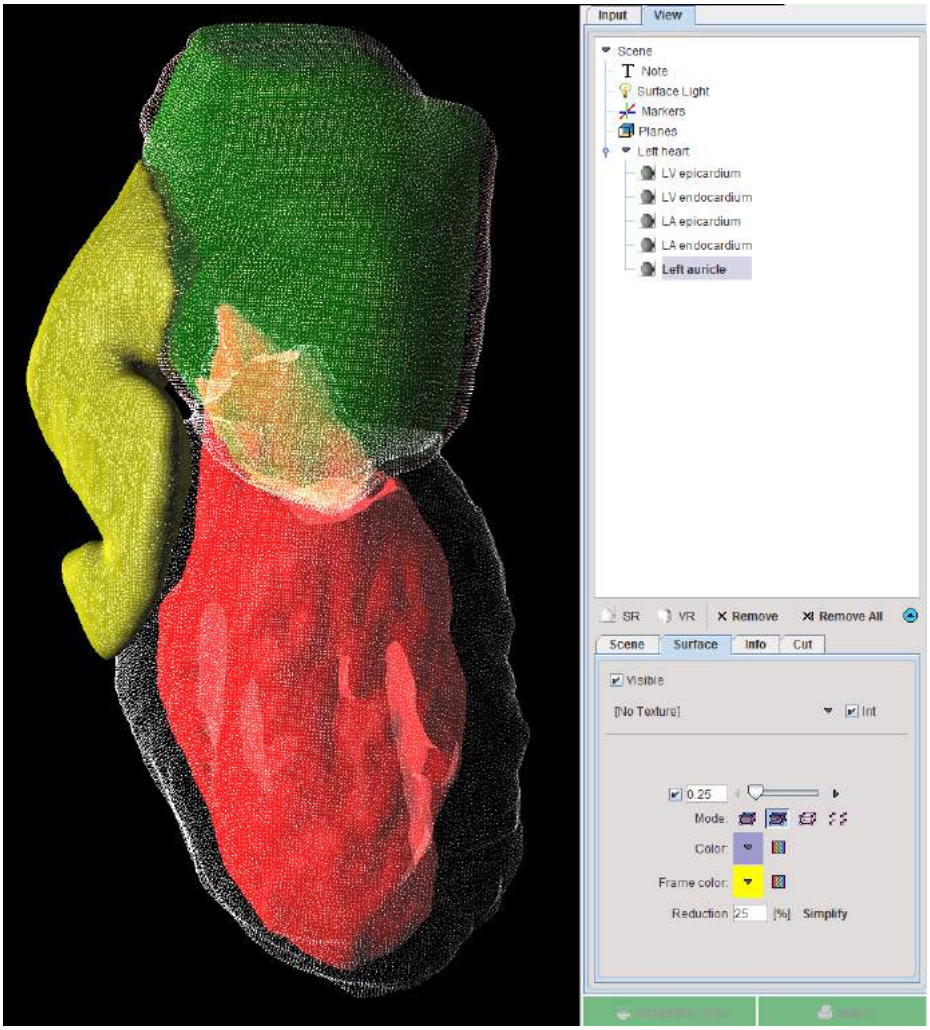
In the example illustrated below the **Muscles/Left heart** branch in the **HEART** model tree is selected for exploration:



Activate the 3D button to start the interactive exploration of the model.

The program will render the selected elements of the model and show them in the **3D** page as: **STL**, **Volume Mesh** or **Volume Mesh +STL complement**.

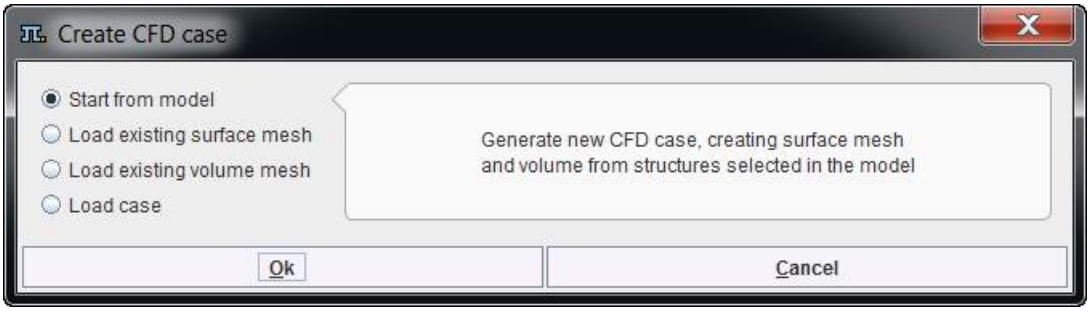
The **STL** rendering result is illustrated below:



Note that default properties of the elements in the 3D **View** tree were changed for exploration purposes. Please refer to the *PMOD 3D Rendering Tool Users Guide* for rendering-related information.

5.2 CFD Simulation and Implementation in PGEM

The CFD simulation is started activating the **Create CFD case** green button.



A dialog window opens and allows selecting the starting point to create the CFD case: a geometric **model**, an **existing surface mesh** (SM), an **existing volume mesh** (VM) or loading a previously saved **case.**

Start CFD case from the Model

This is the most detailed workflow and is based on the selected geometry in the model. The other workflows are essentially simplified variants of it but require the availability of the starting point files usually created in a detailed workflow.

The creation of the CFD case requires performing the following steps in order:

1. select the geometric element in the model
2. create surface meshes based on the selected model geometry
3. create volume meshes based on the surface meshes
4. set boundary conditions for the simulation problem
5. set parameters for the solver (e. g. OpenFoam)

It is advised saving all the steps definitions in a case file once the CFD case creation is completed. This allows retrieving the case configuration at any later time point. The case definitions can be modified to try variations of the processing parameters.

Start CFD case from existing Surface Mesh (SM)

If a SM is available with properly define solids the following steps are required:

1. load the SM file.
2. create volume meshes based on the surface meshes
3. set boundary conditions for the simulation problem
4. set parameters for the solver (e. g. OpenFoam)

Start CFD case from existing Volume Mesh (VM)

If a VM is available on the file system or in the local case manager, the following analysis steps are required:

1. load the VM file.
2. set boundary conditions for the simulation problem
3. set parameters for the solver (e. g. OpenFoam)

Start CFD case from Existing Case

To start the CFD simulation from an existing case the * **.cfdCase** file has to be loaded and send to the solver. Such file includes surface meshes definition, the volume mesh settings as well as the definitions of the boundary condition and the parameters for the solver.

4D Flow CFD case

The creation of a CFD case based on 4D Flow data requires performing initially the 4D Flow analysis 28 up to the VOI definition step. Next, the user has to switch to the **Model** page and select the anatomical model built using the same 4D Flow images data. The CFD case creation may start using any of the above scenarios: from the model, from an existing SM, from an existing VM or from an existing case.

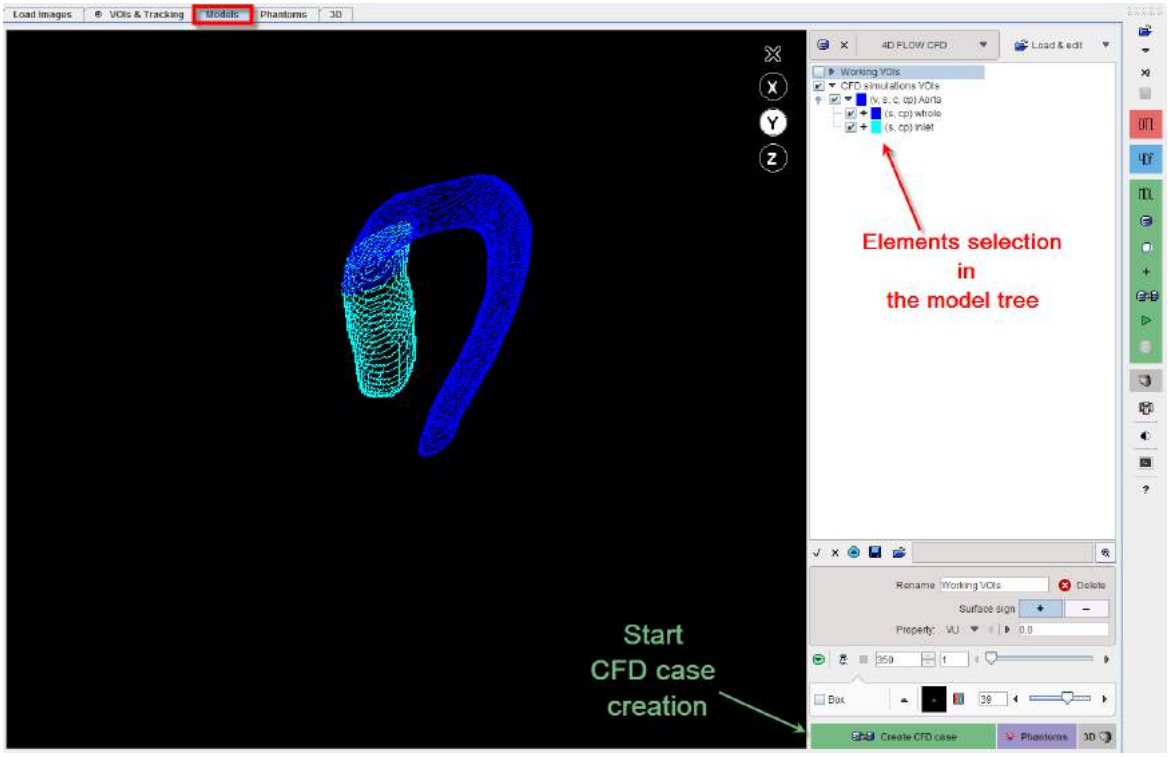
In the 4D Flow CFD case study the velocity profile can be calculated and visualized for the defined cutting planes.

The **4D FLOW CFD** model will be used for the description of all CFD case creation.

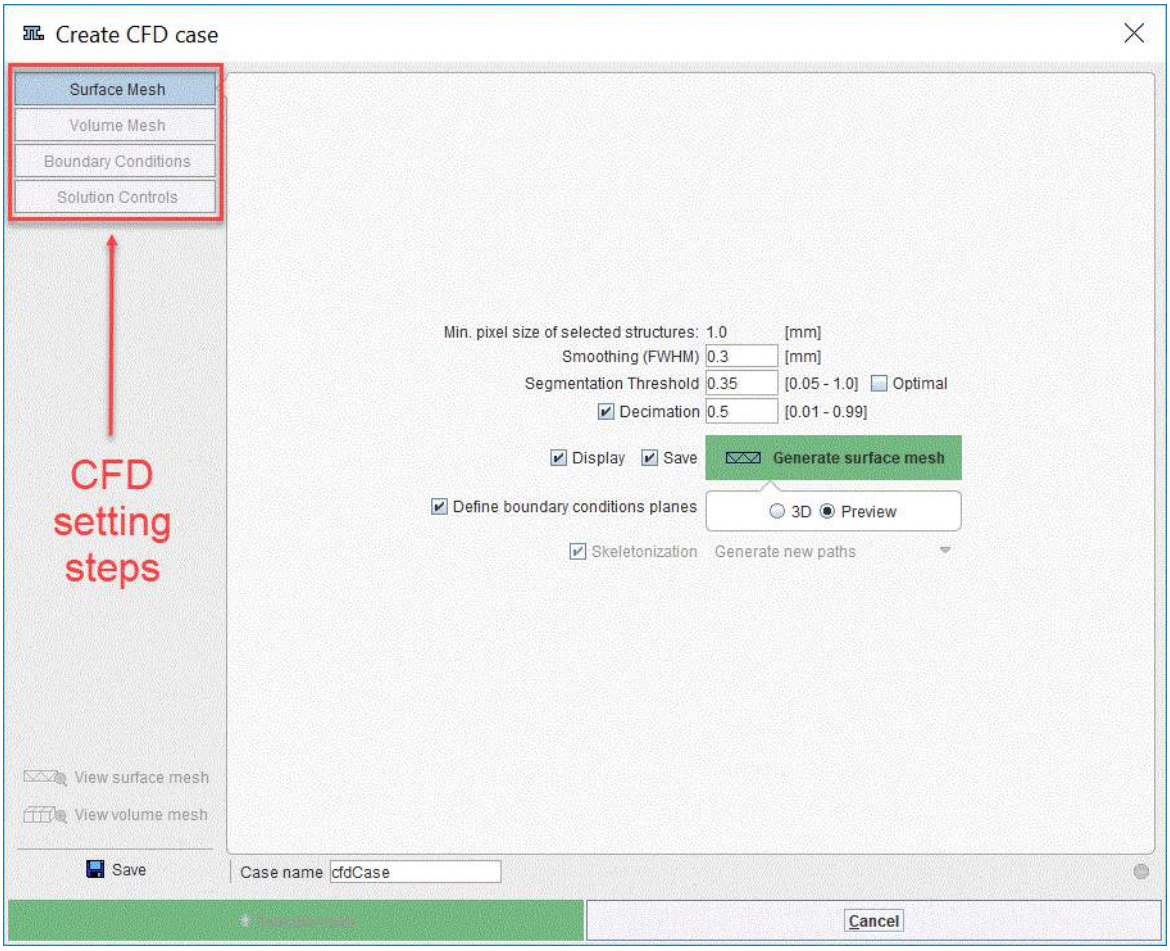
5.2.1 Create CFD Case from the Geometric Model

5.2.1.1 Geometry Selection in the Model

Start the workflow selecting the elements in the model tree. In the example illustrated below all the elements in the **CFD simulation VOIs** branch are selected in the **4D Flow CFD** model tree:



The creation of the CFD case is started with the **Create CFD case** green action button. A dialog window opens allowing to select the starting point for the case: enable the **Start from the model** radio button. The appropriate **Create CFD case** interface appears. It provides a step-by-step guidance through the CFD setting process:



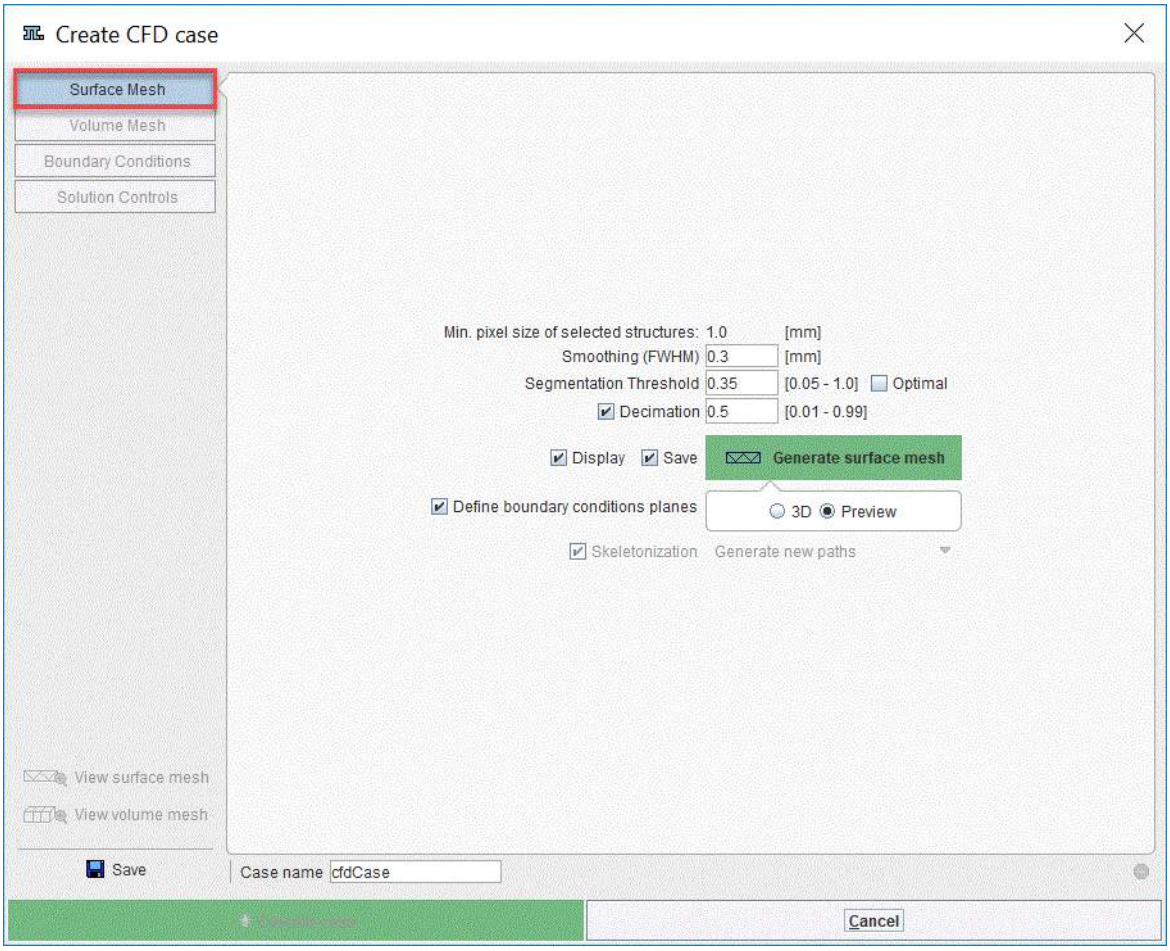
The definition steps are mandatory and have to be completed for the CFD process.

Note:

The geometric model can be used to repeat simulation as VOIs editing step is a fast process. Starting from the base geometry a series of different geometries can be built: narrow, widen, with extra branches. The new geometries (VOIs) can be easily added to the model, as explain previously 56, and use to run CFD experiments.

5.2.1.2 Surface Mesh Creation

The first step in the CFD case preparation is the creation of the surface meshes. Initially, only the **Surface Mesh** tab is active as illustrated below:



The SM settings are described in the table below:

Min pixel size of selected structure	Displays the pixel size [mm] in the data.
Smoothing (FWHM)	It is representing a Gaussian filter and allows smoothing the data before creating the STL structure. The default value corresponds to the pixel size in the data. It is recommended to use a smoothing value 3 times the minimum pixel size.
Segmentation Threshold	All pixels with the value above the threshold are included in the segment. The default value is 0.35. When the **Optimal** checkbox is enabled the threshold will be calculated automatically such that the volume of selected elements is preserved.
Decimation	Allows simplifying mesh by removing tringles from the surface mesh without changing the mesh. Please note that in this case the simplification procedure is done after the mesh is created. The value ranges between 0 and 1. The number represents the percentage of triangles to be thrown out. Usually a value of **0.5** is a good compromise. The smaller the number of triangles, the faster will be the 3D visualization. It is a slow procedure which generates smaller files. **Decimation** only changes the number of STL nodes, particularly the vertices of the surface mesh. However, no

	change in the mesh geometry occurs, preserving thus the mesh topology.
☑ Save	When enabled allows saving the generated STL file in the *surface-meshes* folder. This folder is located in the directory set as **Case path (local)** in the PGEM configuration settings. The SM STL files stores information related with the Bounding Box and Point in mesh location. This information is used for the calculation of the VM.
☑ Display	When enabled shows the SM generated based on the definition of the cutting planes
Define boundary condition plane	When enabled allows starting the definition of the cutting planes. The cutting planes definition is mandatory for the CFD simulation. When disabled allows creating SM for visualization purposes. Such SM are used to create VM of selected geometries for visual presentations and cannot be used for CFD simulation

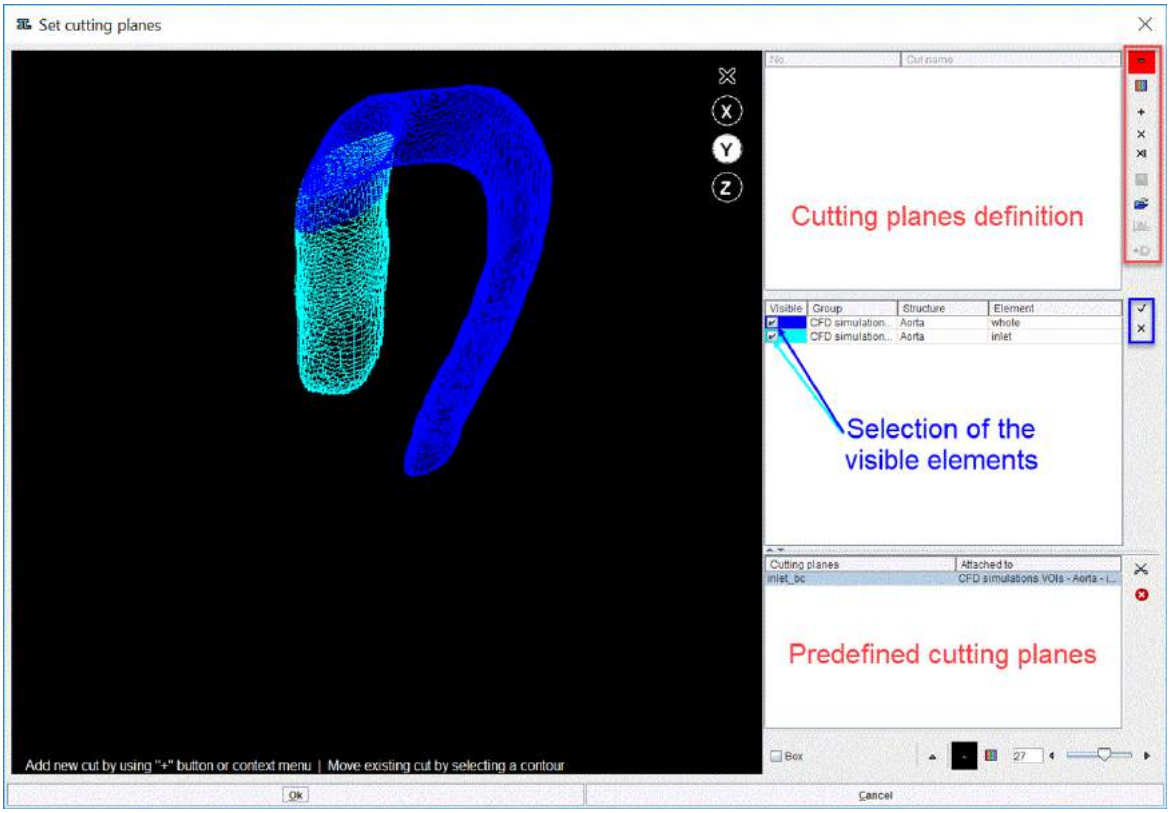
In the example above the **Smoothing** was set to 3 mm while the default settings were used for **decimation** 0.5 and **segmentation threshold** 0.35. Toggle the **Save** and the **Display** checkboxes in order to save and preview respectively the result of the definition of the cutting planes.

Enable the **Define boundary condition plane** checkbox to start the definition of the cutting planes.

Two methods are available for the definition of the cuttings planes: **Preview** and **3D**. Enable one method radio button followed by the activation of the **Generate surface mesh** green button.

5.2.1.2.1 Cutting Planes Definition with Preview

The **Preview** interface for the definition of the cutting planes is illustrated below:



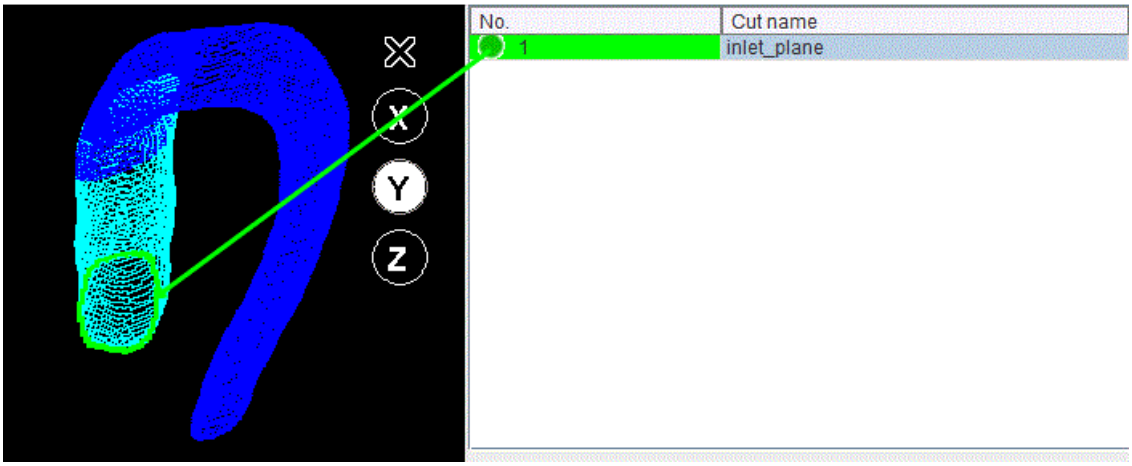
The window consists in an image area on the left and control and definition panels on the right. Note the divider buttons which can be used for enlarging/reducing the relative areas.

Elements List

The entries selected in the model tree are listed in the central panel on the right hand side of the window. Initially all the elements are displayed in the viewport area. Select/deselect the **Visible** check boxes for the structure of interest to change the appearance in the viewport. In the example above all elements are set to **Visible**.

Definition of cutting planes based on predefined cutting planes

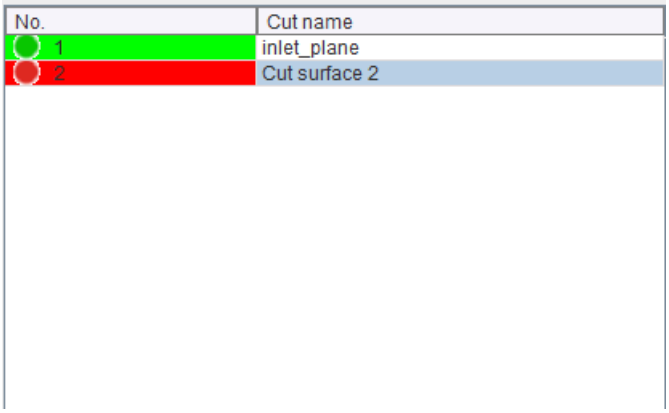
When VOIs were added to the model as cutting planes, they were linked with the specified element in the model builder interface and consequently with the element entry in the model tree. The predefined cutting planes listed in the **Cutting planes** panel, bottom right, are linked to the entries in central elements panel. Select the entry in the list (e.g. *inlet_bc*) and activate the icon from the lateral task bar to cut the geometry with the selected cutting plane. The cutting plane is shown on the image on the linked geometry. The cutting plane definition panel, top right, list the copy of the predefined cutting plane as the first defined cutting plane.



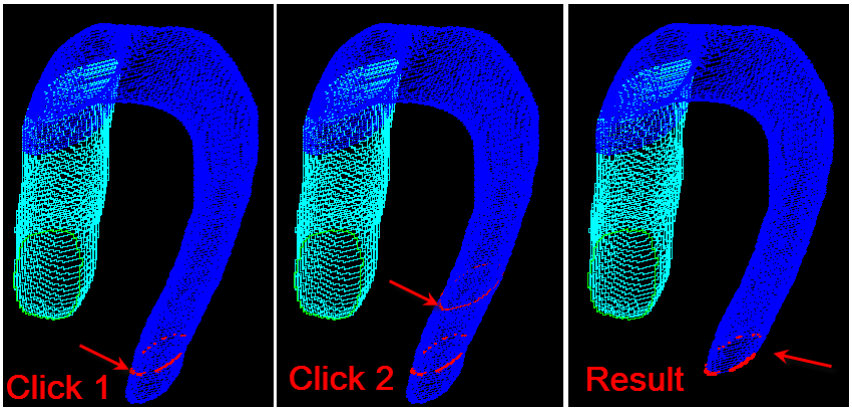
Double click in the **Cut name** field to assign a different name to the first cutting plane in the list: e.g. *inlet_plane*.

Definition of new cutting planes

Activate the **+** icon in the taskbar to create a new cutting plane. A new entry appears in the top right panel with the default name **Cut_Surface_2**:



Successively click twice on the structure displayed in the viewport: the first click defines the cutting contour while the second click selects the part of the geometry to be used in the simulation. The opposite part of the geometry is discarded. The process is illustrated below:

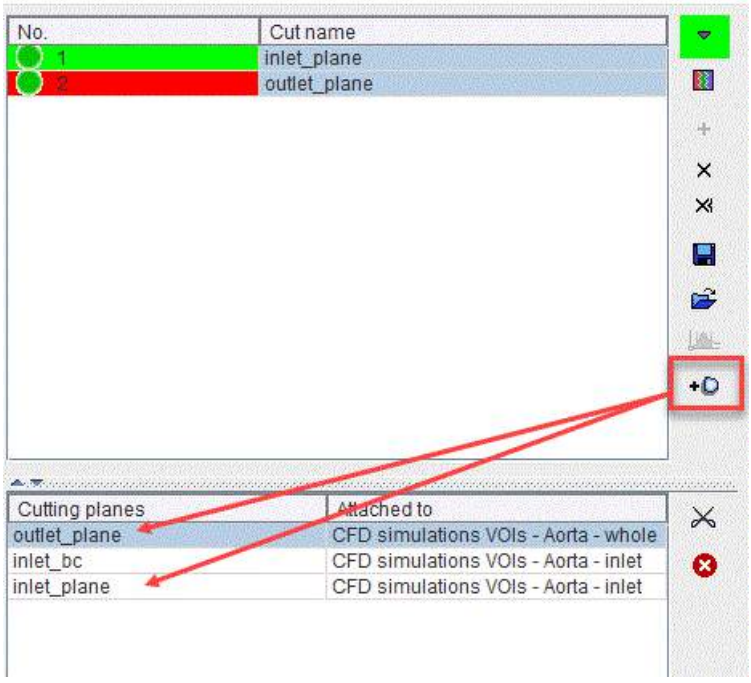


Rename the new cutting plane to *outlet_plane*.

Saving the cutting planes

Saving of the cutting planes definition is started with the button in the lateral taskbar. It allows saving the entries in the list as **.cutPlane* files. By simply retrieving those with the button de definitions are recovered.

Alternatively, add the cut definitions to the model as cutting planes with the button. The cutting planes will be linked in the model with the element being cut and they will be appended to the existing predefined **Cutting planes** list as illustrated below:



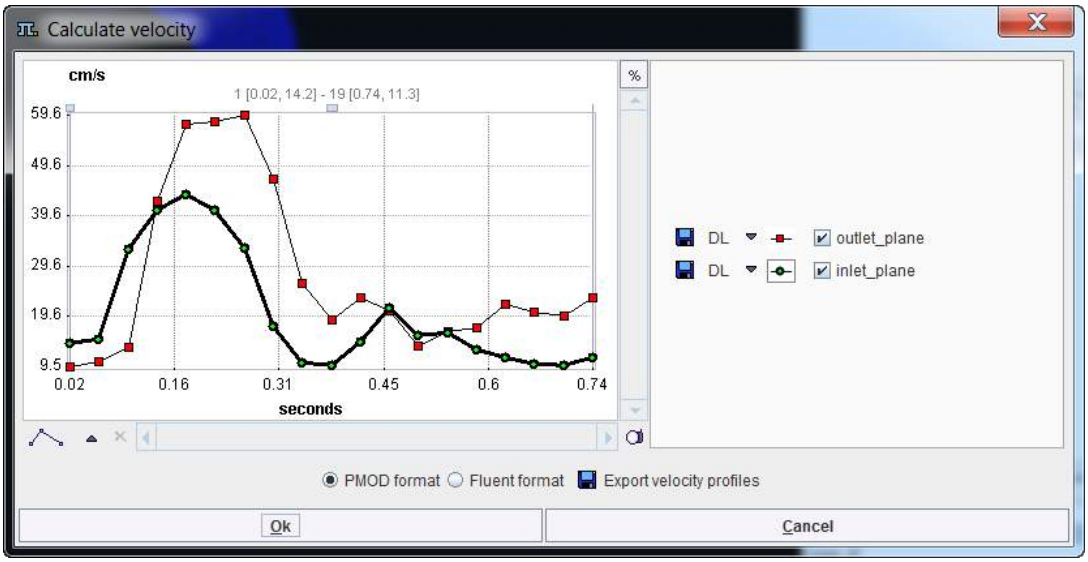
Modify a cutting plane

The process to modify a cutting plane is very similar to the definition of a new plane. First, the plane is selected in the list. Successively are requested two clicks on the image: the first click defines the new cutting contour while the second click selects the part of the geometry to be used in the simulation. The opposite part of the geometry is discarded.

Alternatively, discard the selected cutting plane from the definition list with the button. The button removes all the cutting plane definitions available in the list. Start the definition of a new cutting plane as described above.

Velocity profiles for the cutting plane definitions

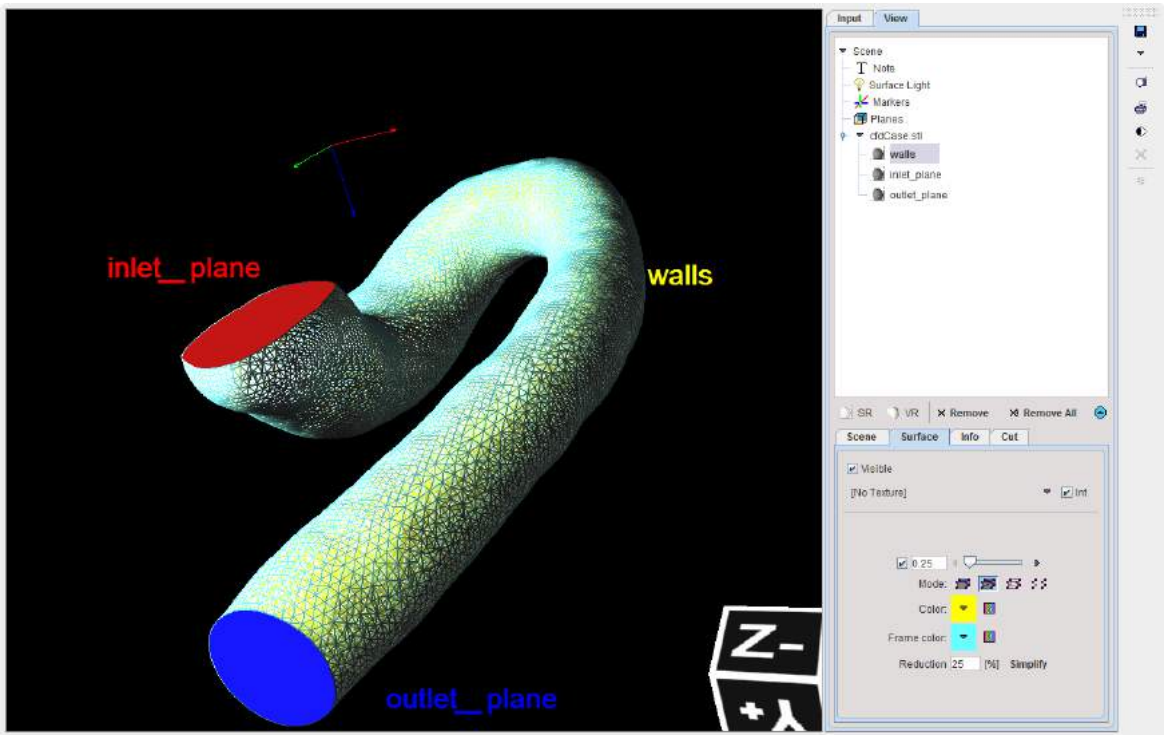
When the creation of a CFD case is based on 4D Flow data the icon on the lateral taskbar becomes active. It allows calculating and visualizing the velocity profiles of the 4D flow data on the defined cutting planes. The result of such a calculation is shown below:



Save the velocity profiles with the **Export velocity profiles** button in one of the available formats: **PMOD format**, **Fluent format**. To close the window activate the **OK** button.

Note: It is mandatory that the 4D Flow data used in the creation of the CFD case are the same data used to build the currently selected anatomical model on the **Model** page.

Close the **Preview** interface with the **OK** button to generate the surface mesh. The calculation process may take a couple of minutes. The results are shown in a 3D window as illustrated below:



It allows exploring interactively the generated surface mesh. **Close** the window and continue with the VM creation.

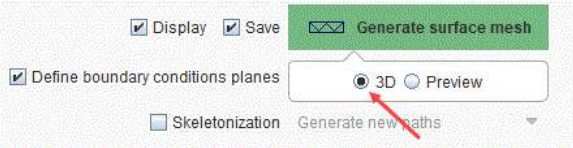
The cutting planes will be used to define the boundary conditions for the CFD simulation.

5.2.1.2.2 Cutting Planes Definition with 3D

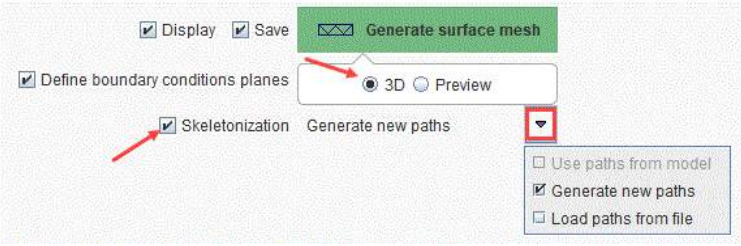
It is recommended to use the oblique planes to create cutting planes for the CFD simulation. The oblique planes allow creating cutting surfaces which are perpendicular to the vessel axis.

PMOD supports two ways of cutting planes definitions with 3D:

1. Without Skeletonization: the oblique plane needs to be interactively placed perpendicular to the vessel axis. In this case the 3D radio button is active as illustrated below:



2. With Skeletonization: the oblique plane is automatically place orthogonal to the vessel skeleton when bound to the selected path. In this case the 3D radio button is active and the Skeletonization box is enabled:



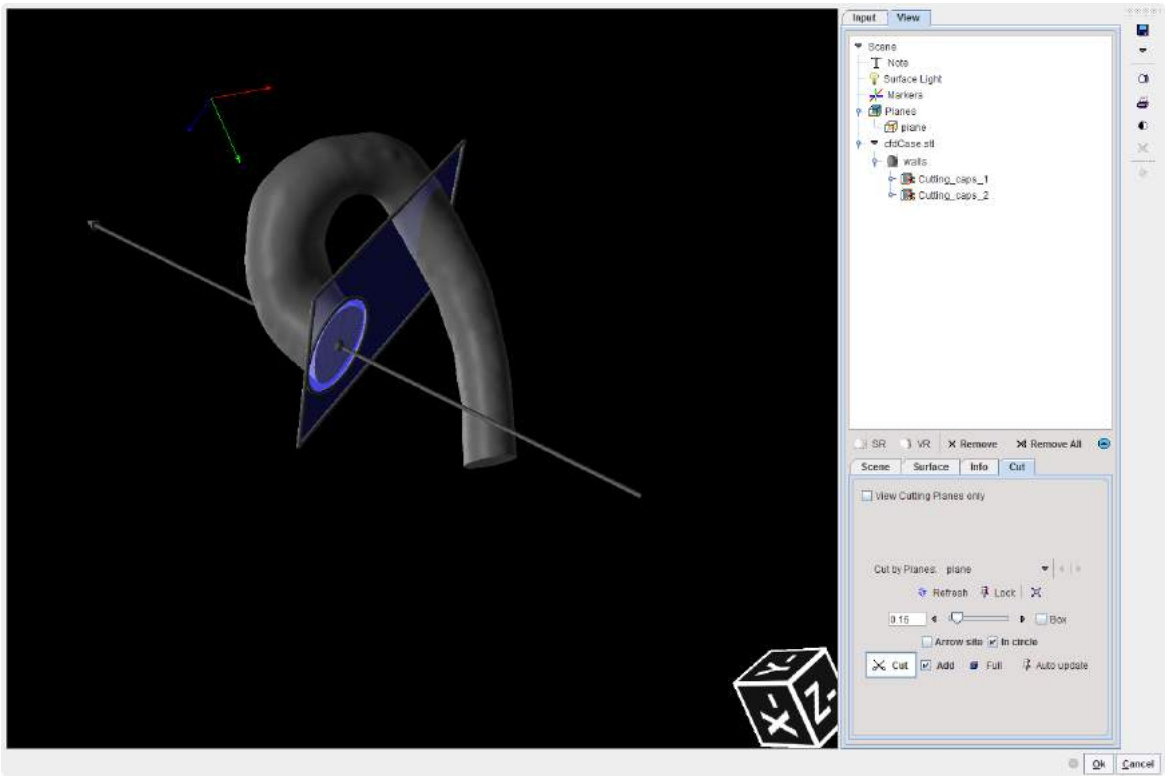
With Skeletonization enabled a selection list becomes active allowing to **Use paths from model** if available, to **Generate new paths** or to **Load path from file** previously saved in the P3D module.

Both approaches will be briefely described.

Please refer to the *PMOD 3D Rendering Tool Users Guide* for any further details about the skeletonization, oblique planes and cutting-related information.

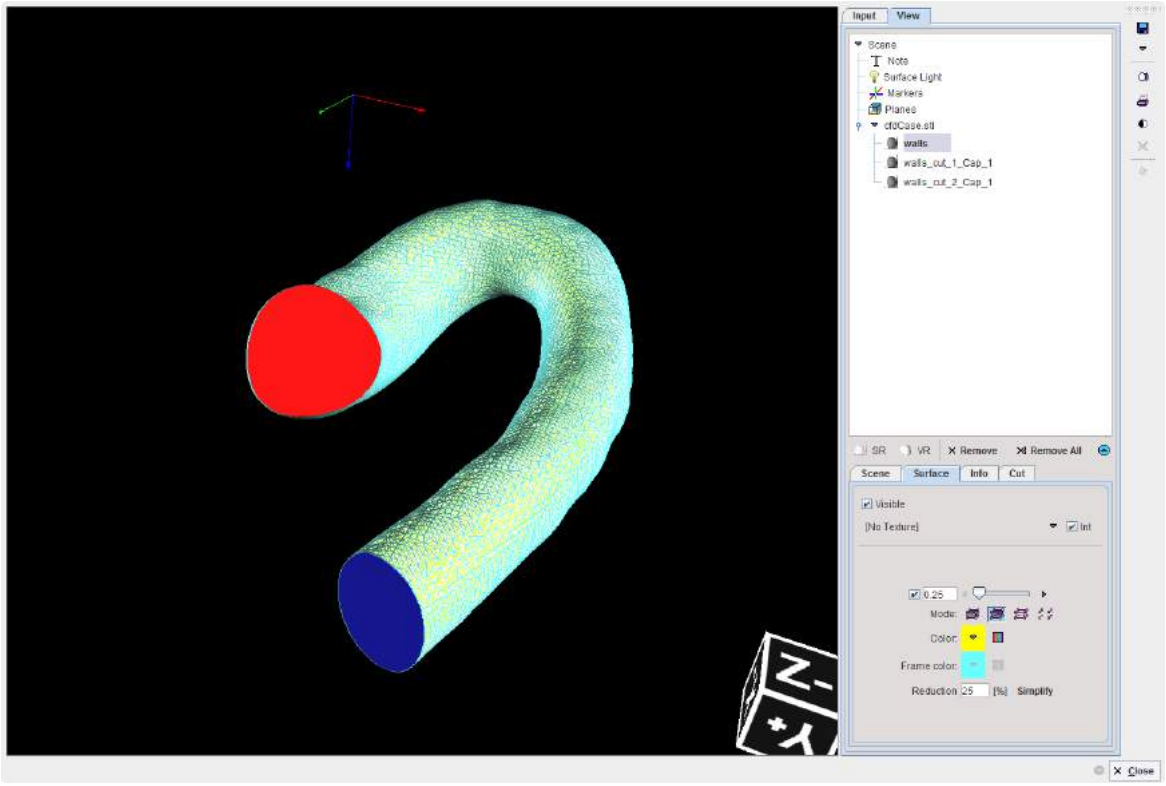
5.2.1.2.2.1 Without Skeletonization

The **3D** interface for the definition of the cutting planes is illustrated below:



In the example above one oblique **plane** was used to create the cutting planes on the selected surface render object: the walls. The results are two entries in the **View** tree, in the **walls** branch: the **Cutting_caps_1** and **Cutting_caps_2.**

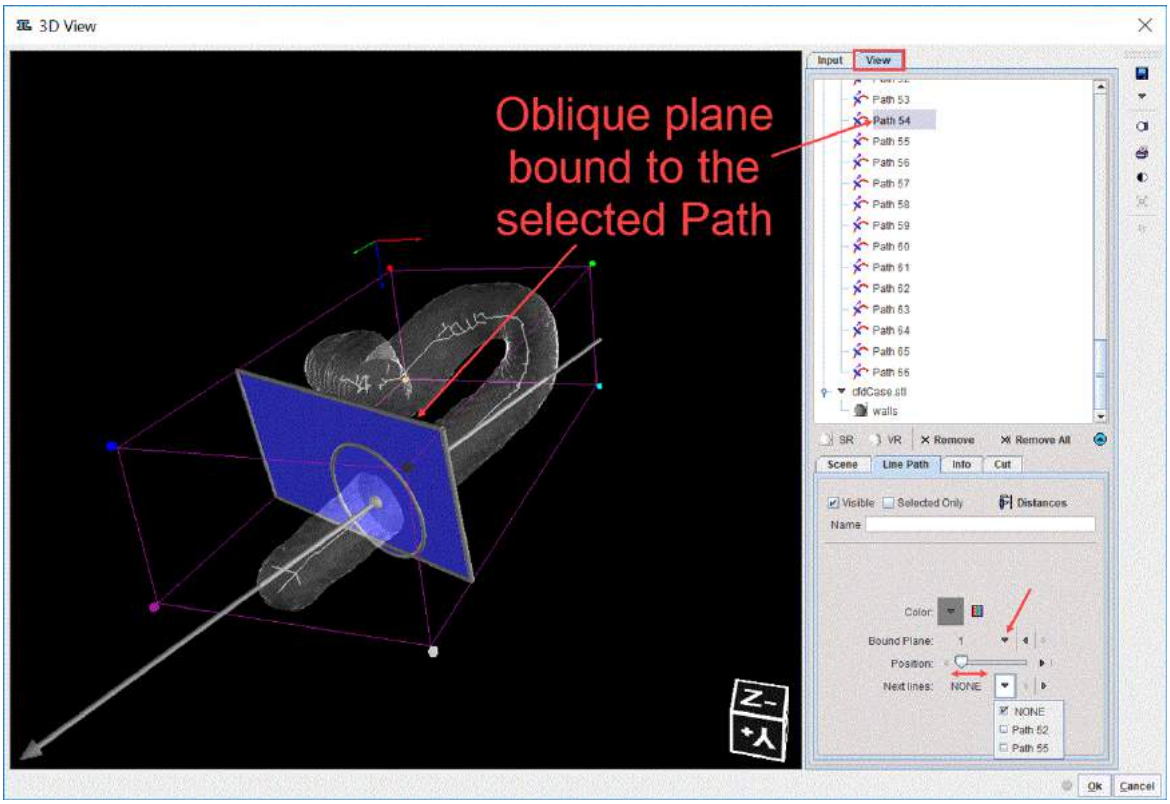
Close the **3D** interface with the **OK** button to generate the surface mesh. The calculation process may take a couple of minutes. The results are shown in a **3D** window as illustrated below:



The 3D interface allows exploring interactively the generated surface mesh. **Close** the window and continue with the VM creation. The cutting planes will be used to define the boundary conditions for the CFD simulation.

5.2.1.2.2.2 With Skeletonization

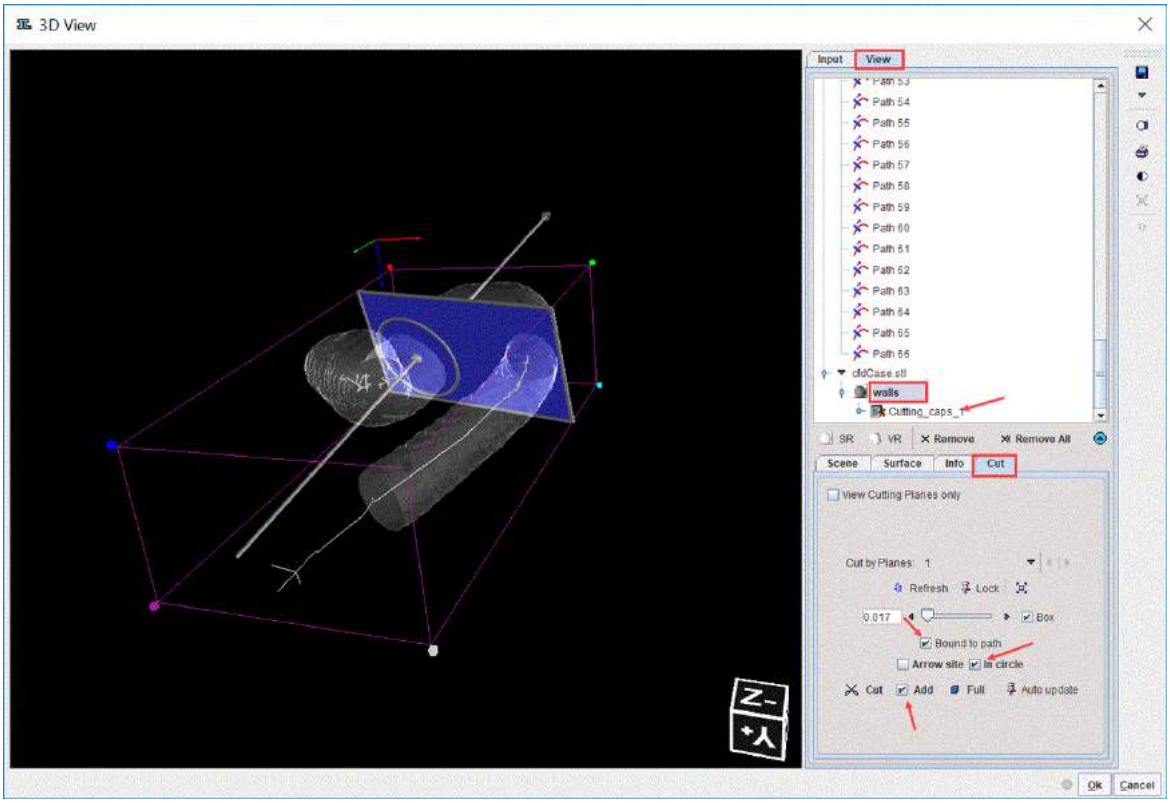
The **3D** interface for the definition of the cutting planes using generated paths is illustrated below:



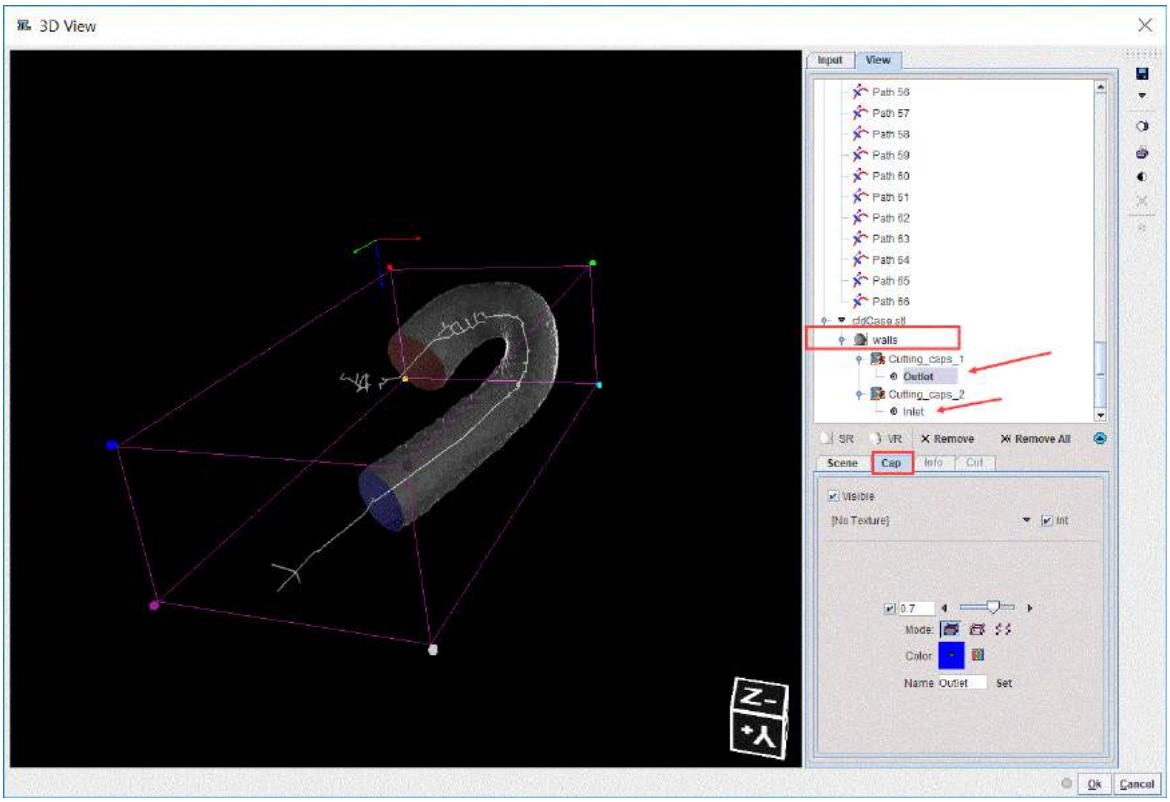
The paths are representing the skeletons components and are immediately available in the **View** tree when the 3D interface appears.

In the example above one oblique plane **1,** was used to create the cutting planes on the selected surface render object: the walls. The blended transparency was enabled for the walls in order to allow the visibility of the skeleton paths. The **Path 54** is selected in the **View** tree and the **Bound Plane** selection is set to the oblique plane **1**. The oblique plane is placed orthogonally to the vessel skeleton as soon as it is bound to a selected path. The **Position** slider allows moving the plane along the active path while preserving the orthogonality.

To cut a part from the SR object used for the skeletonization select the SR object (**walls**) in the **View** tree and subsequently the **Cut** tab belonging to this object (NOT the Cut tab of the Planes object). With the **Bound to path**, **Arrow site** and **In circle** boxes enabled the **Cut** button is activated. The **Cut** button starts a process which clears all information of the selected object on the defined side and area and refreshes the rendering scene. The part of the SR object on the same side as the arrow head is cut from the scene. There is now an indication in the object tree which objects have been cut:

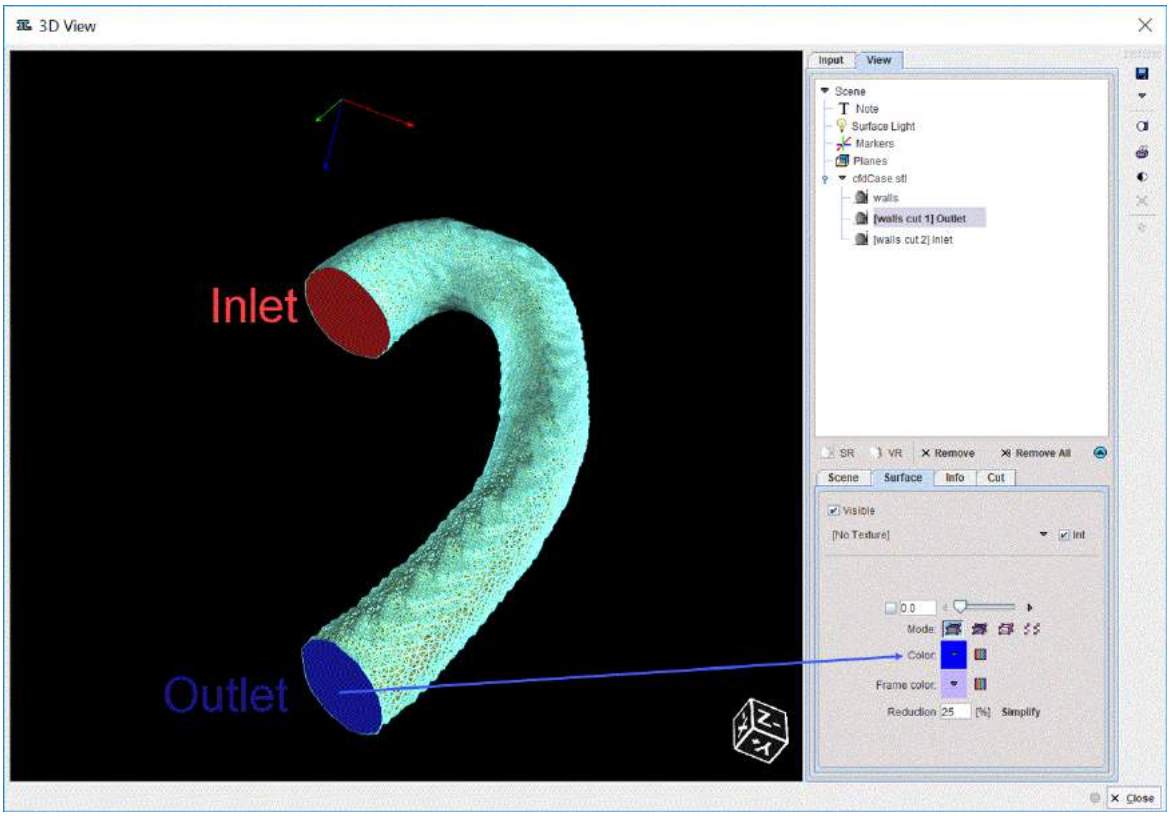


The same oblique plane is used to define another cutting plane for the **walls**. The plane is bound to the Path 33. With the **Bound to path**, **In circle** and **Add** boxes enabled the **Cut** button is activated. With the **Arrow site** box disabled the part of the object on the opposite side of the arrow head will be cut. The final scene is illustrated below:



The resulting cutting planes are renamed to *Outlet* and *Inlet* editing the **Name** field followed by the activation of the **Set** button.

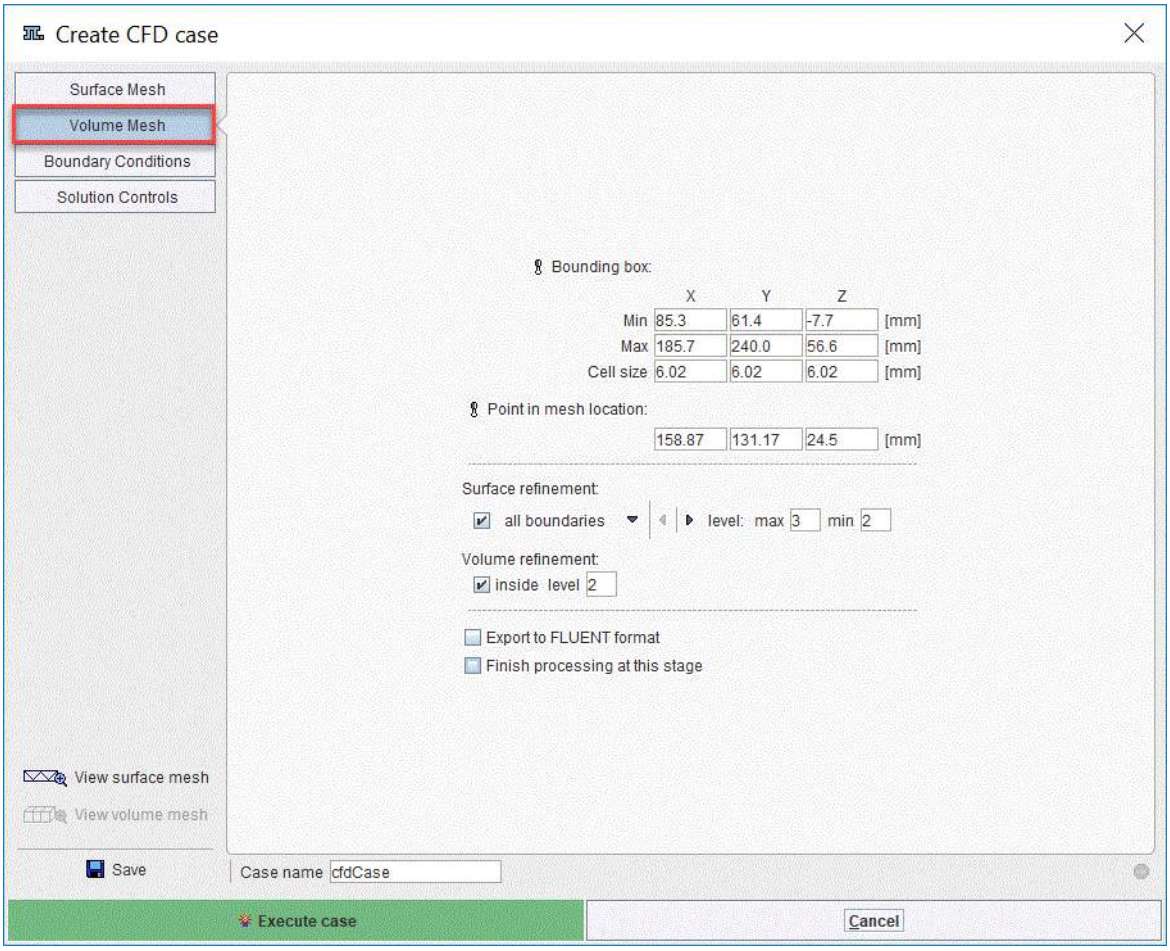
Close the **3D** interface with the **OK** button to generate the surface mesh. The results are shown in a **3D** window. It allows exploring interactively the generated surface mesh as illustrated below:



Close the window and continue with the VM creation. The cutting planes will be used to define the boundary conditions for the CFD simulation.

5.2.1.3 Volume Mesh Creation

The **Volume mesh** tab becomes active once the SM is generated. In the process of SM creation the **Bounding box** and **Point in mesh location** parameters are calculated automatically and displayed as illustrated below:



It is mandatory that the **Bounding box** encloses the whole surface. The **Point in mesh location** represents coordinates of any point inside the SM. It is recommended to preserve the automatically calculated values for the **Bounding box** and **Point in mesh location** and optionally change the **Cell size** parameter. This parameter determines the size of the initial cube cells. In the example above the values calculated automatically are used for the simulation purposes.

Note:

The bounding box and location in mesh can be edited via image data - using the screwdrivers buttons.

The **Surface refinement** is representing the parameter that will steer division of cells of a volume mesh in the surface's neighbourhood. Particularly, the **max**imum number of divisions (**level**) will be applied to the curved parts of the surface while the **min**imum number of division anywhere else in the neighbourhood. It can be defined for each surface (**walls**, **inlet** or **outlet**) separately or on all surfaces selecting **all boundaries**. Please note that the parameters for a particular surface (e.g. **walls**, **inlet**, **outlet**) will overwrite the **all regions** settings. In this particular case the surface refinement was set for all boundaries to a **max** level of 3 and a **min** level of 2.

The **Volume refinement** is representing the number of cell divisions inside the whole volume of the geometry (each cell of the volume mesh). A **level** of 2 is set in the example above.

Note:

The default settings always build rather simple volume mesh and are recommended to be to use for the first estimation of a solution. The cells number of a volume mesh and its quality is always a compromise between accuracy of the solution and the time of calculation. Using a bigger number of cells does not change the quality of the solution.

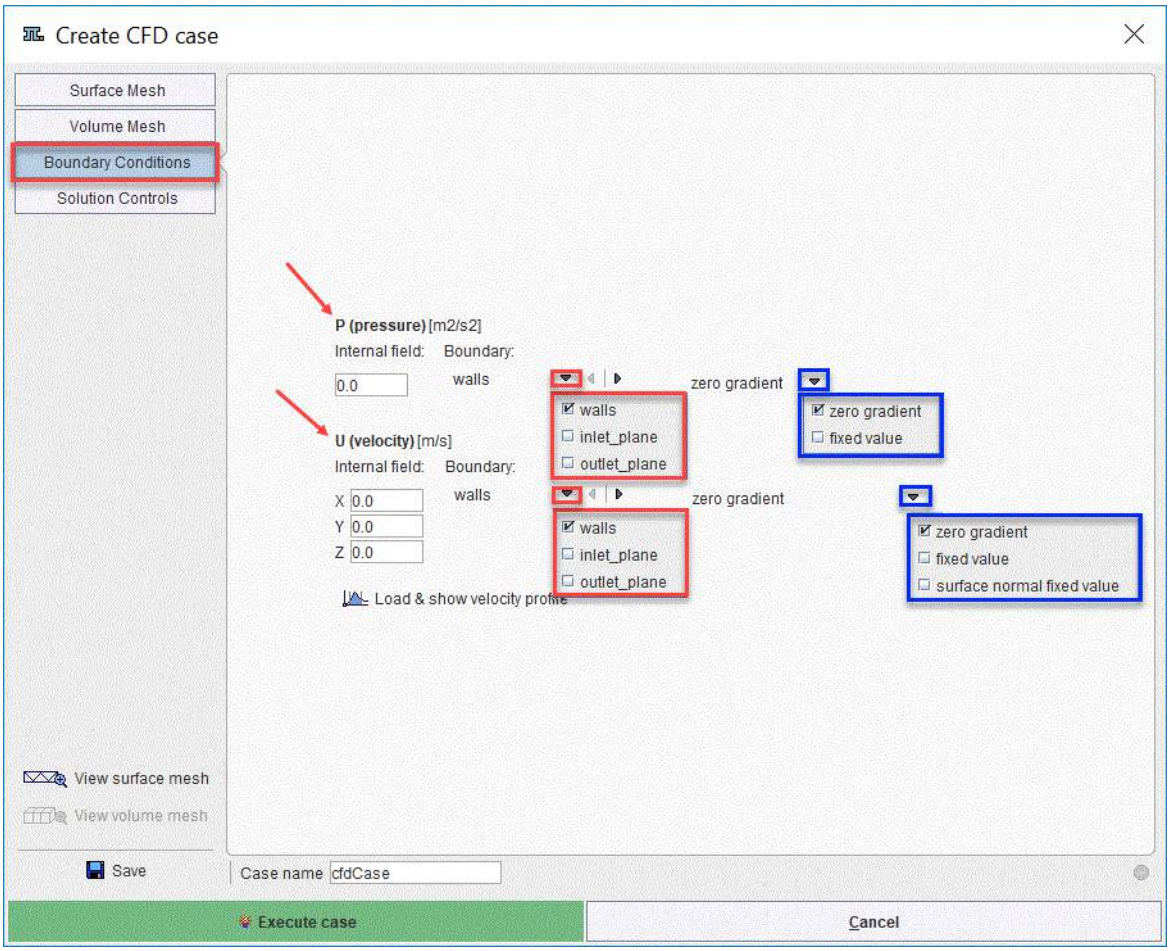
With the **Finish processing at this stage** box enabled the **Generate volume mesh** green button becomes available. It allows calculating the volume mesh but exits the **Create CFD case** dialog. The result is an OpenFoam case storing only the volume mesh. To create a volume mesh compatible with Fluent solver activate the **Export to Fluent format** check box.

To continue with the CFD case creation select the boundary condition tab.

5.2.1.4 Boundary Condition Settings

In this step the boundary conditions are defined for the cutting planes and for the wall. There are two physical variables which characterize the fluid flow: the pressure and the velocity.

The **Boundary Conditions** interface is illustrated below:



The **Internal field** allows setting initial values for both physical variables. These values will be assigned to every cell in the volume mesh. It allows starting the simulation from field with non-zero values. In the example above the zero value is used both for the pressure and velocity in the CFD simulation.

The **P (pressure)** is a scalar and is defined as a kinematic pressure (pressure/fluid density) and measured in [m2/s2]. There are two types of pressure boundary conditions: **fixed value** and **zero gradient**. With the **fixed value** selection the value of the variable will stay as defined throughout the simulation. With the **zero gradient** selection it is assumed that there is no value gradient along the flow direction. Particularly, it is assumed that the flow is fully developed at this boundary, and the value will be calculated by the solver.

In the CFD simulation example above the **zero gradient** is set for the *walls* and the *inlet_plane* surfaces and a **fixed value** of *0* for the *outlet_plane* surface.

The **U(velocity)** is a vector and is measured in [m/s]. There are three types of velocity boundary conditions: **fixed value**, **surface normal fixed value** and **zero gradient**.

When the **fixed value** is set the value of the variable will stay as defined throughout the simulation. A similar situation is obtained with the **surface normal fixed value** selection but in this case the vector alignment is always normal to the surface for which the boundary condition is applied. The inflow is defined by a negative value. The outflow is defined as a positive value. The **zero gradient** significance is the same as for the pressure variable: assumes the flow is fully developed at this boundary, and the value will be calculated by the solver.

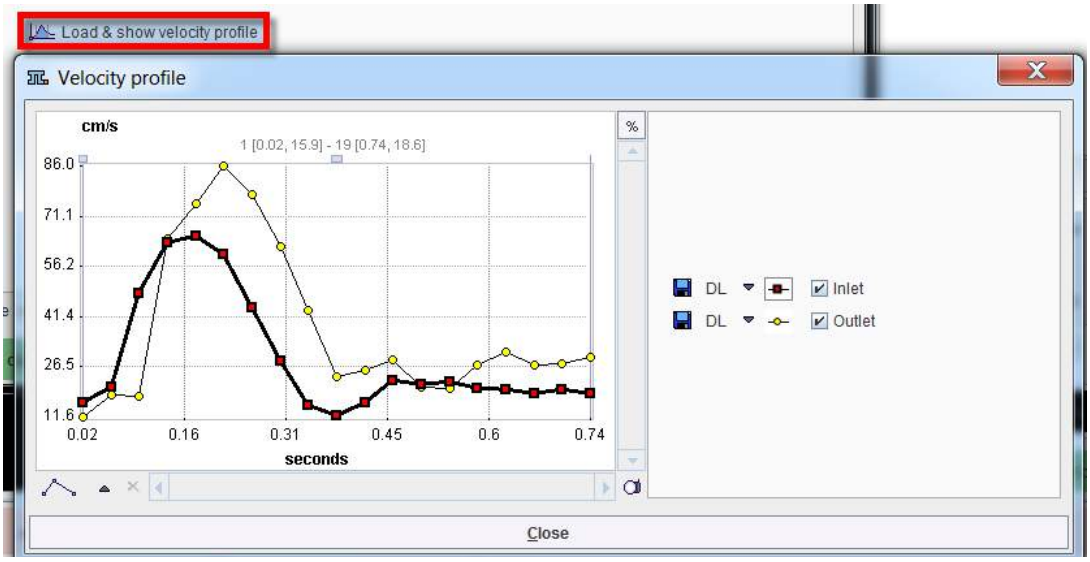
In the example above, the following settings are done for the **U** variable:

- *walls* surface: **fixed value***0 0 0* (the so called *no slip boundary condition*)
- *inlet* surface: **surface normal fixed value** with a value of **-0.26**
- *outlet* surface: **zero gradient**

Note:

It is recommended NOT to set fixed constraints on the flow at one surface for both variables, e.g. pressure and velocity set as fixed values at the inlet.

Activate the **Load and show velocity profile** button to visualize previously saved 4D flow velocity profiles.

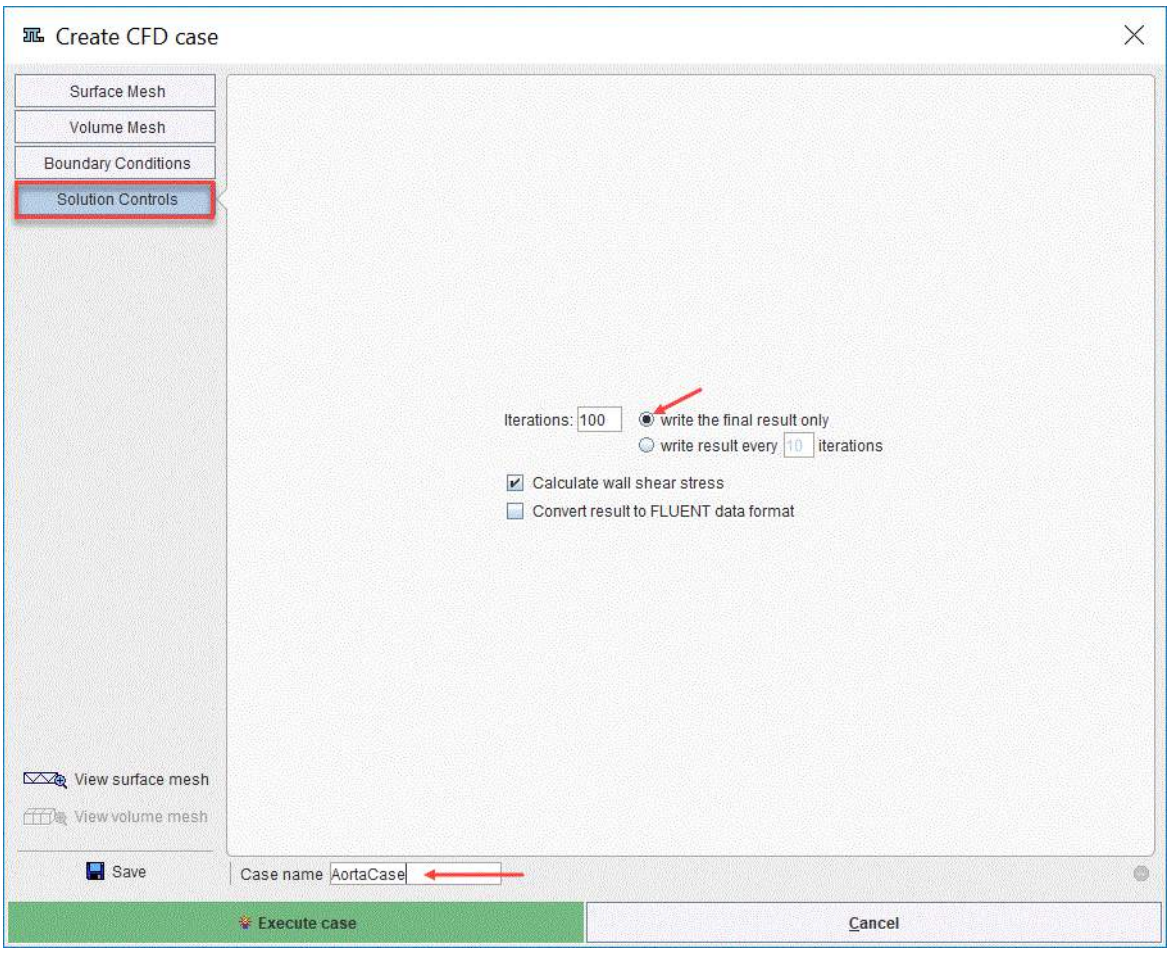


Such profiles are saved in the cutting plane definition step of a 4D Flow CFD case creation.

Note: In the current implementation the velocity profiles for the cutting planes are not used in the simulation process.

5.2.1.5 Solution Control

The last step consists in setting the parameters for the solver as illustrated in the capture below:



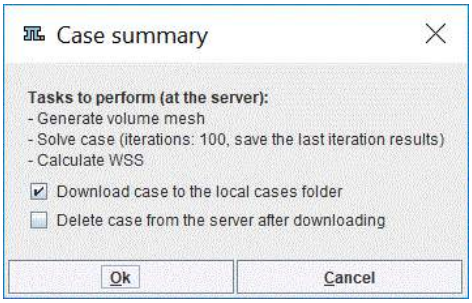
The number of **Iterations** is recommended to always be rounded to full tens. Toggle the **write final result only** radio button to save only the final solution for the simulation. Consequently, the wall share stress (*WSS*) will only be calculated for the last point when the dedicated box is enabled.

The best way for reproducing a simulation is to save the entire case configuration with the **Save** button in the lower left. All the information will be saved in a **.cfdCase** file.

The **Case name** field allows assigning a meaningful name to the CFD case. This facilitates the management of the OpenFoam remote and local cases. In the example above the *AortaCase* was assigned as the name for the CFD experiment.

With the **Convert result to FLUENT data format** box enabled the case will become compatible with the FLUENT software.

Activate the **Execute case** button. A confirmation panel appears listing the **Case summary**:

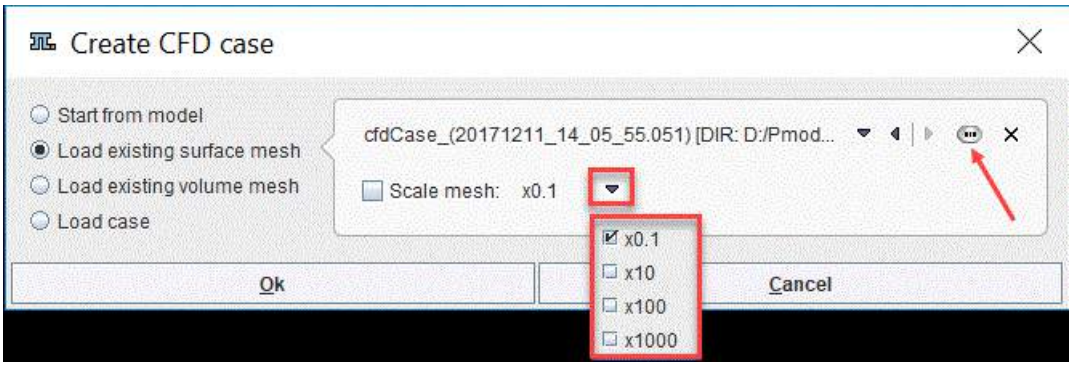


With the **Download case to the local cases folder** box enabled the CFD simulation results are automatically downloaded when calculations are completed. The **Delete case..** box enabled allows deleting the case from the remote location.

Close the confirmation window with **OK** to send the CFD case to the OpenFoam interface and exit the CFD settings interface. A message will confirm the success of sending the case to the server or not.

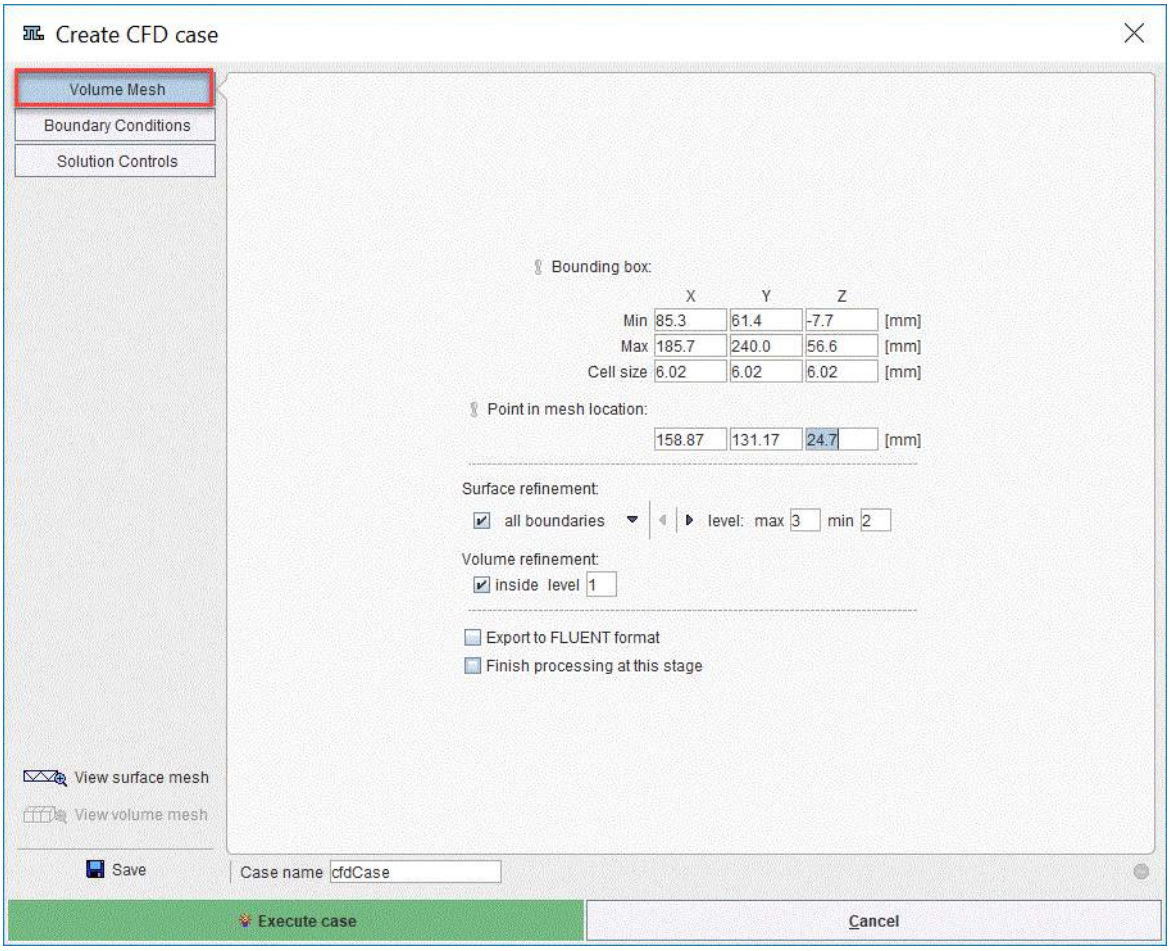
5.2.2 Create CFD Case from a Surface Mesh

Start the CFD simulation activating the **Create CFD case** green button. A dialog window appears as illustrated below:



Toggle the **Load existing surface mesh** radio button to start the creation of the CFD case from a SM. Use the open button to load a SM file. To scale the SM enable the **Scale mesh** box and select one of the scaling size available on the list.

Close the dialog window with the **OK** button to continue the creation of the CFD case. The CFD interface appears displaying the **Volume Mesh** as the first step of the analysis.



The **View surface mesh** button allows exploring interactively the loaded surface mesh in the 3D interface.

The **Bounding box** and the **Point in mesh location** parameters are initially set to 0 and 1 respectively. It is mandatory for the user to know these parameters and interactively type them in the dedicated text boxes.

The **Surface refinement** parameters are set to **all boundaries** to a **max** level of 3 and a **min** level of 2. This indicates that a **max**imum number of 3 divisions will be applied to the curved parts of the surface while a **min**imum number of 2 divisions anywhere else in the neighbourhood.

The V**olume refinement** is set to a **level** of **2**. This indicates that each cell in the volume mesh will be divided in two.

Continue with the definition of the **Boundary Conditions** as explained previously 91.

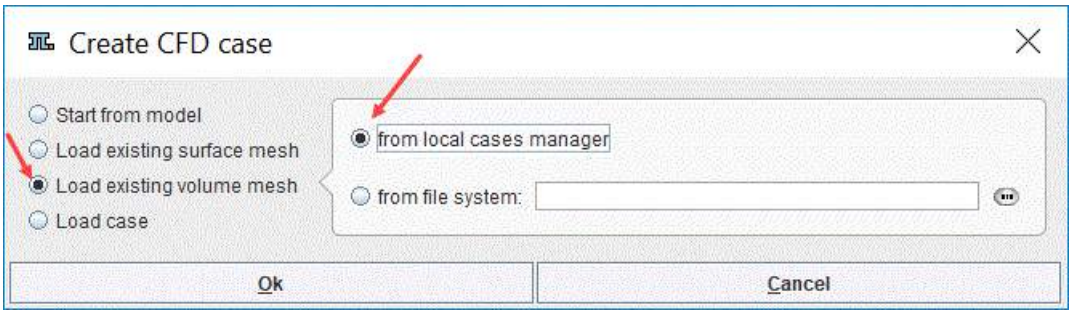
Finally, define the parameters for the solver. Set the number of **iterations** to a full tens number, e.g. 100 and enable the **write the final result only** radio button to save only the final solution for the simulation. Enable **Calculate wall shear stress** box for WSS calculation.

Note: Assign a meaningful name to the CFD case in the **Case name** field. This facilitates the management of the OpenFoam remote and local cases.

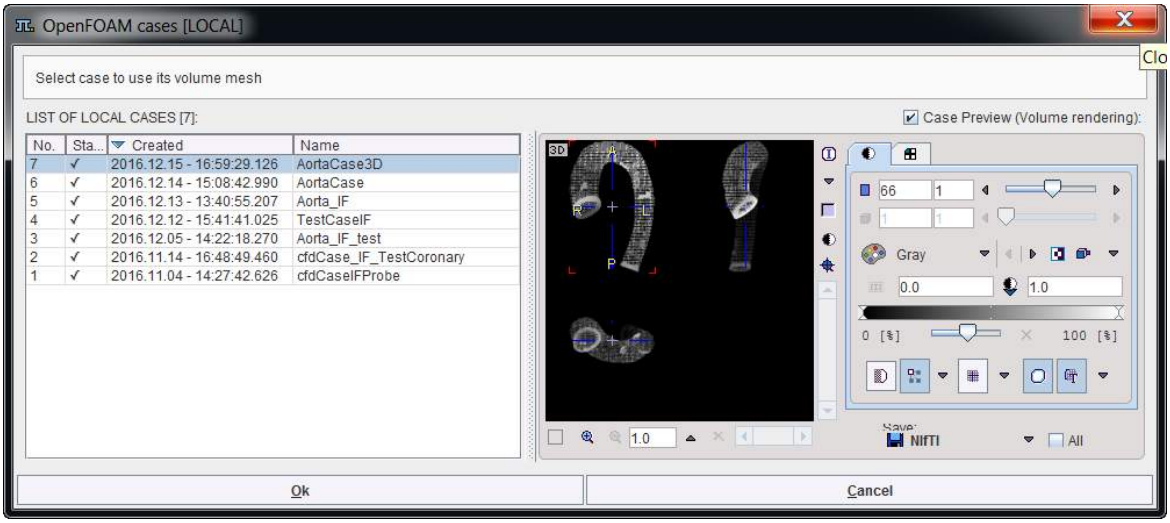
Activate the **Execute case** button to send the CFD case to the OpenFoam interface

5.2.3 Create CFD Case from a Volume Mesh

Start the CFD simulation activating the **Create CFD case** green button. A dialog window appears as illustrated below:

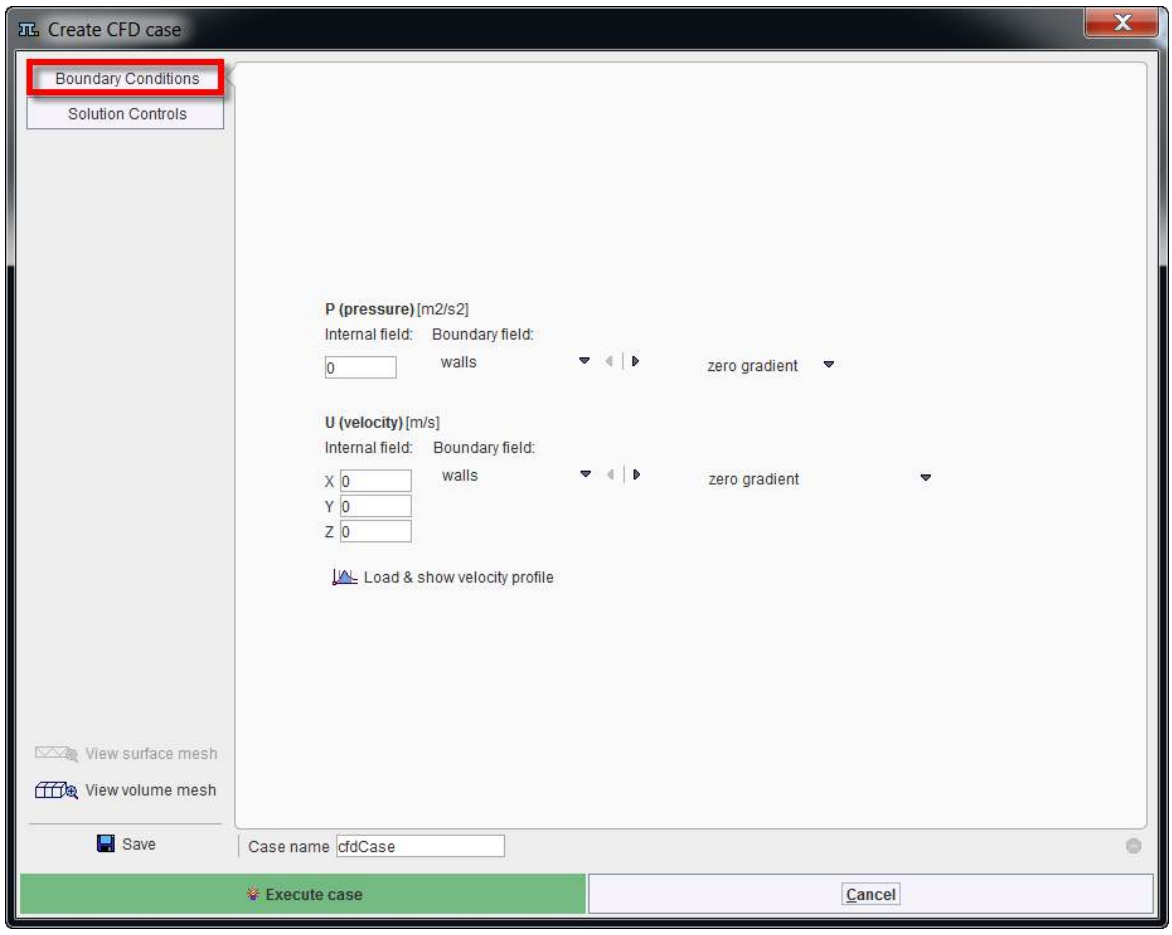


Toggle the **Load existing volume mesh** radio button to start the creation of the CFD case from a VM. Enable the **from local cases manager** radio button. The local cases are listed in a dialog window as illustrated below:



The left side shows the list of the available local cases. The list allows selecting one of the volume meshes for simulation. With the **Case Preview** box enabled, the selected VM is shown in the image port. The general image manipulation panel is available on the right hand side. It allows changing the appearance of the image in the viewport. The volume rendering displayed in the viewport can be saved as an image with the **Save** button.

Activate the **OK** button to exit the window and continue with the creation of the CFD case. The interface is simplified as shown below:



It consists of the **Boundary Conditions** and the **Solution Controls** panels. Define the **Boundary Conditions** as explained previously. Finally, define the parameters for the solver. Set the number of **iterations** to a full tens number, e.g. 80 and enable the **Get final results only** box to save only the final solution for the simulation.

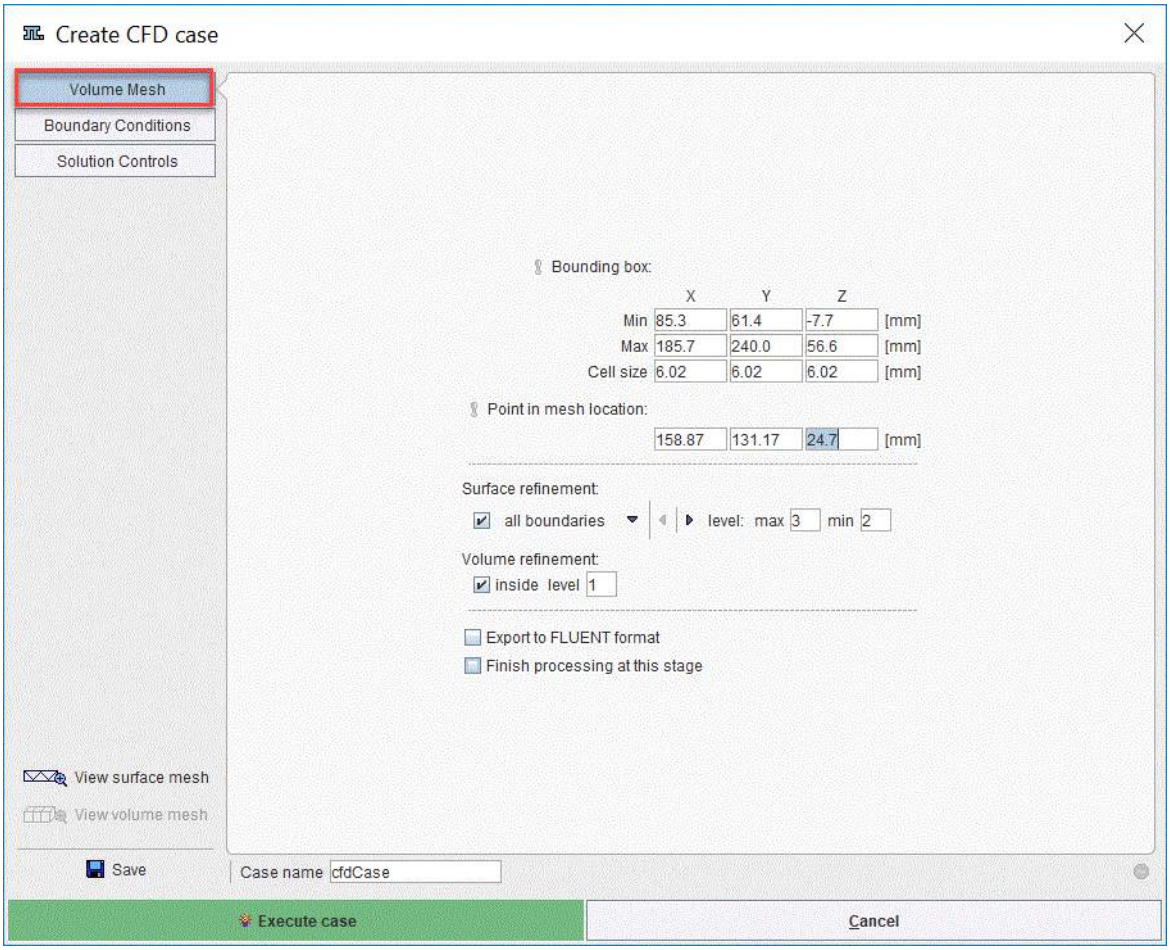
Note:
Assign a meaningful name to the CFD case in the **Case name** field. This facilitates the management of the OpenFoam remote and local cases.
The **View volume mesh** button allows viewing the VM in the 3D interface and interactively explore it.

Send the CFD case to the OpenFoam interface by activating the **Execute case** button.

5.2.4 Create CFD case from an Existing Case

Start the CFD simulation activating the **Create CFD case** green button. A dialog window appears as illustrated below:

Enable the **Load case** button to start the CFD simulation from a previously saved case. Close the window with the **OK** and select a **.cfdCase** file. The CFD interface appears displaying the **Volume Mesh** as the first step of the analysis.

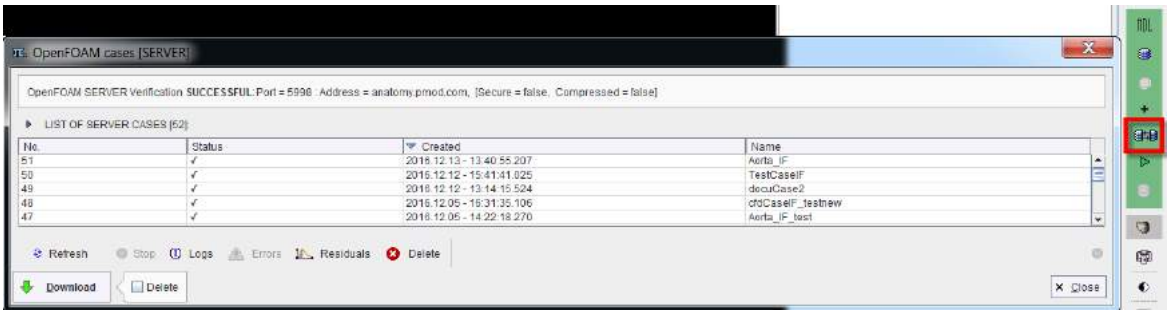


The **.cfdCase** file contains all the settings necessary for the CFD simulation: **Volume Mesh**, **Boundary Conditions** and **Solution Controls**. Modify the case definitions (e.g. **Boundary Conditions**) in order to try variations of the processing parameters. Save the new case settings with the **Save** button and finally send the new CFD case to the server with the **Execute case** button.

Note:
Assign a meaningful name to the CFD case in the **Case name** field. This facilitates the management of the OpenFoam remote and local cases.
The **View surface mesh** button allows viewing the SM in the 3D interface and interactively explore it.

5.2.5 Management of the OpenFoam Remote Cases

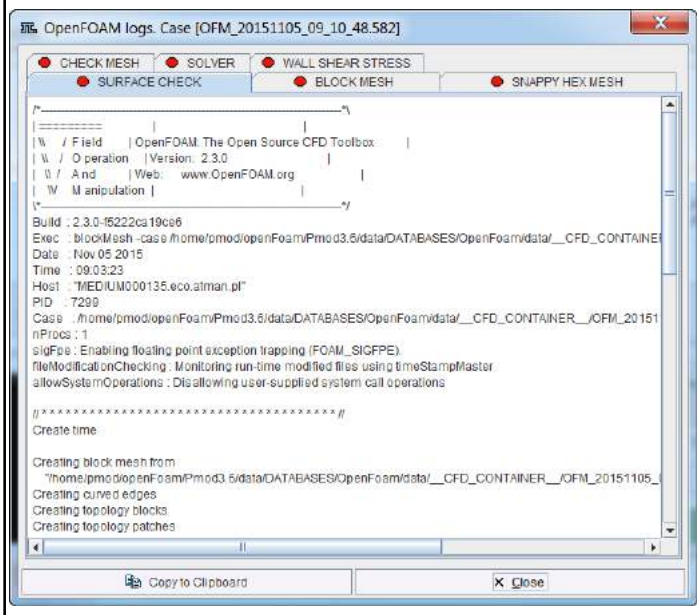
The Open Foam remote cases are easily accessible via the dedicated button available in the lateral task bar. A dialog window opens as illustrated below:

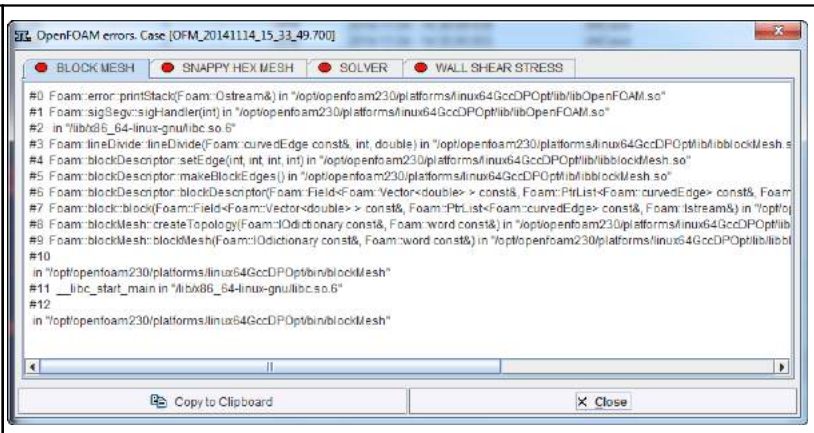
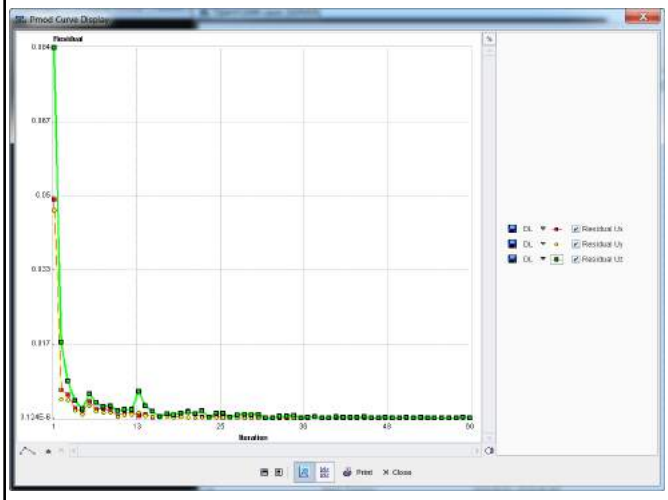
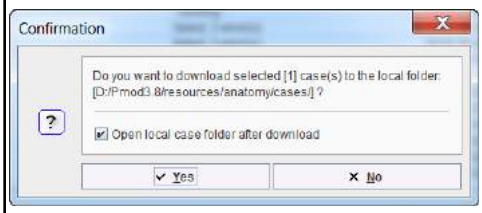


The information related with the OpenFoam server is displayed in the upper section.

The cases available on the server are centrally listed in table format. The status of each case is displayed on the **Status** column: it can be either **running**, **failed** (giving number of errors), or just ticked √ if successfully finished as in the capture above.

The functionality of the action buttons available at the bottom of the page are summarized in the table below:

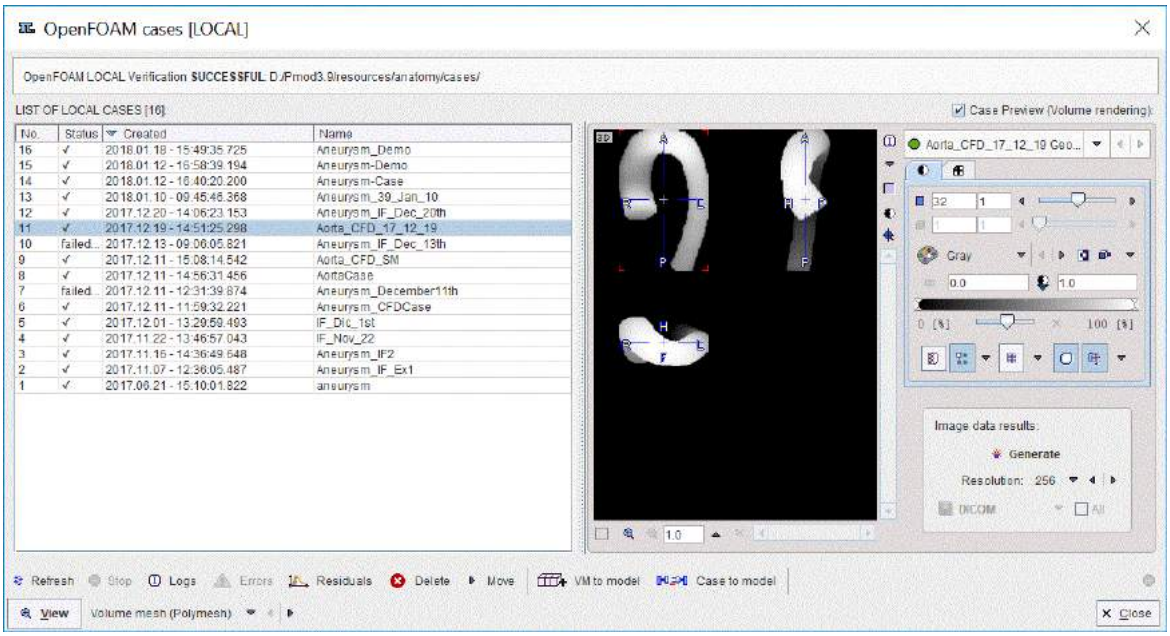
Refresh	Allows refreshing the case list
Stop	Allows stopping a running case on the list.
Logs	Allows visualizing the logs file of the cases in the list. Its activation opens a window like illustrated below:  The window is organized on pages which content can be **Copy to Clipboard** and paste in a text file.
Errors	Allows visualizing the error logs. Its activation opens a dialog window as shown below:

	 The window is organized on pages which content can be **Copy to Clipboard** and paste in a text file.
Residuals	Allows visualizing the residuals for the case selected in the list. A dialog window opens and shows the plotted residuals as illustrated below:  In this example the residual becomes flat after approximately 30 iterations meaning that solution is converged.
Delete	Allows deleting the selected case from the list
Download	Allows downloading the selected case from the list. Optionally, the case can be deleted from the OpenFOAM server enabling the **Delete** checkbox aside the **Download** button. When activated a confirmation dialog appears as illustrated below:  It shows the location where the file will be saved. Please note that this setting is configured locally within the PGEM interface as explain above 8.

The *AortaCase* was selected for download.

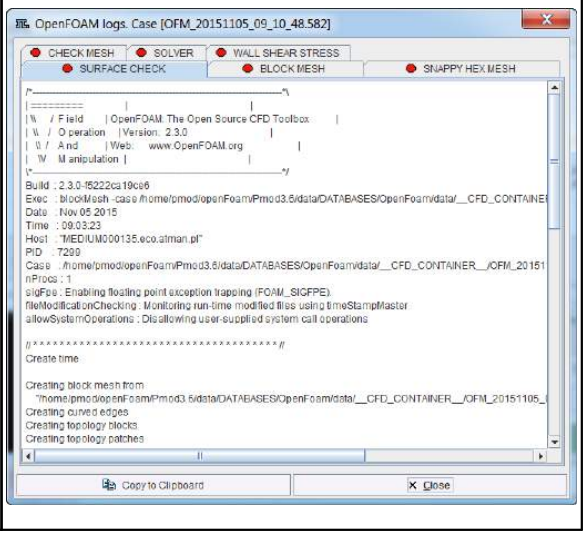
5.2.6 Management of the OpenFoam Local Cases

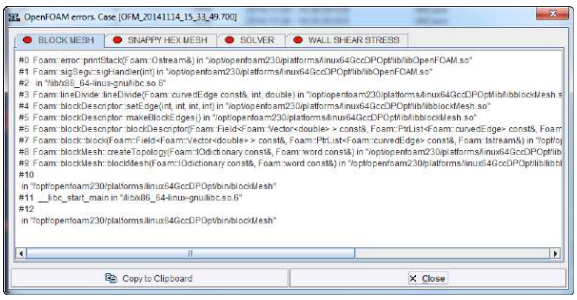
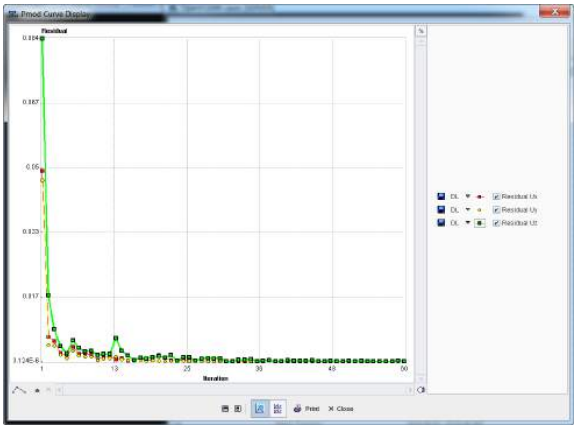
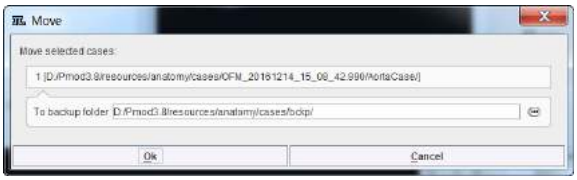
Activate the **Manage OpenFOAM Local cases** button from the lateral task bar. The local cases dialog window is illustrated below:

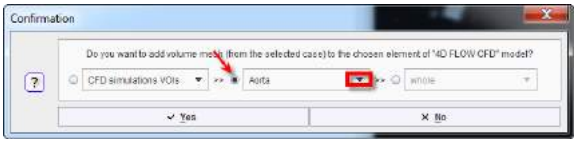
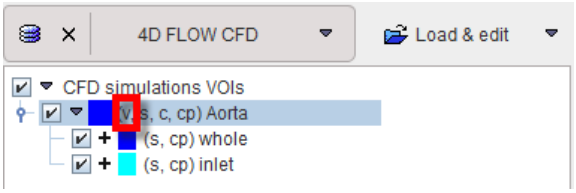
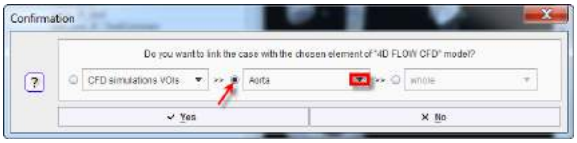
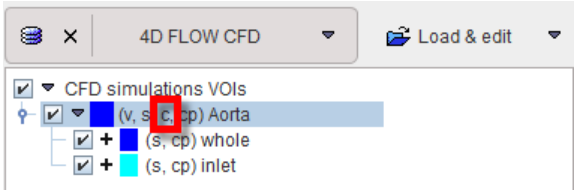


The left side shows the list of the available local cases. The list allows selecting one of the local cases for visualization and inspection in the 3D page. With the **Case Preview** box enabled, the result of the selected case is shown in the image port. The general image manipulation panel is available on the right hand side. It allows changing the appearance of the image in the viewport. The CFD results previewed in the viewport can be converted into images with the specified **Resolution** using the **Generate** button in the **Image data result** panel. The images series are saved in the specified format using the **Save** button.

The functionality of the action buttons available under the local cases list are summarized in the table below:

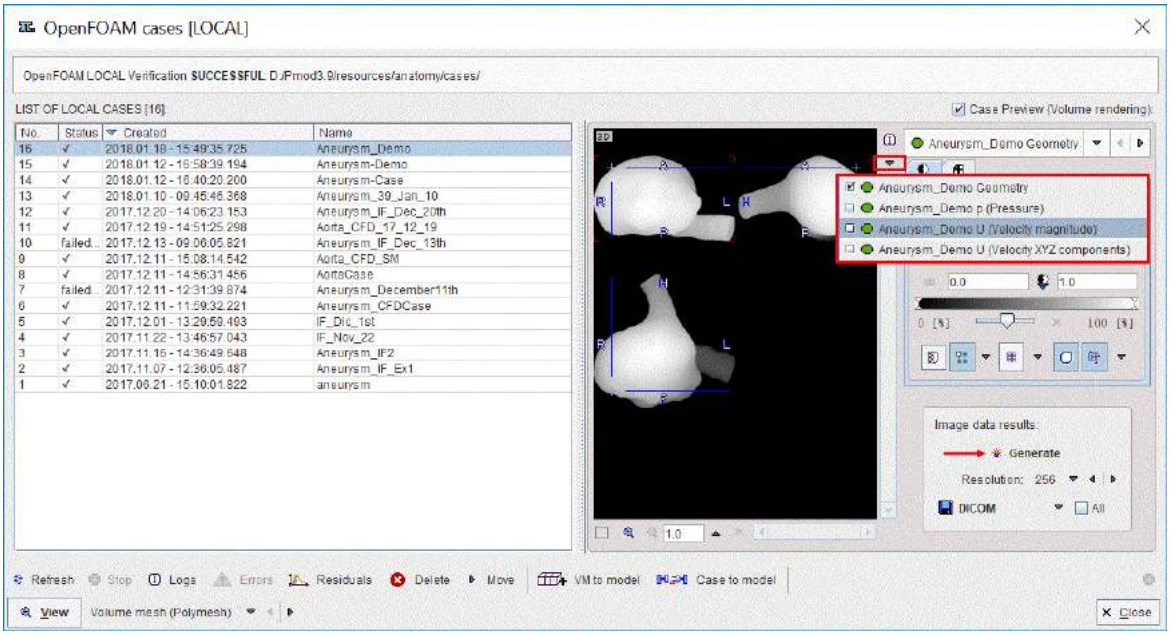
Refresh	Allows refreshing the case list
Stop	Allows stopping a running case on the list.
Logs	Allows visualizing the logs file of the cases in the list. Its activation opens a window like illustrated below: 

	The window is organized on pages which content can be **Copy to Clipboard** and paste in a text file.
Errors	Allows visualizing the error logs. Its activation opens a dialog window as shown below:  The window is organized on pages which content can be **Copy to Clipboard** and paste in a text file.
Residuals	Allows visualizing the residuals for the case selected in the list. A dialog window opens and shows the plotted residuals as illustrated below:  In this example the residual becomes flat after approximately 30 iterations meaning that solution is converged.
Delete	Allows deleting the selected case from the list
Move	Allows moving selected cases to the back-up folder (path set in PGEM configuration as explain above 8.). The back-up folder is not scanned, therefore the local cases dialog will open up faster. When activated a dialog appears as illustrated below: 

	It shows the location where the file will be saved.
VM to model	Allows adding VM from the selected case to one of the model components as illustrated below:  The active radio button and the selection in the list indicate the component in the model tree where the VM will be added. This information is encoded with **v** in the component name: 
Case to model	Allows linking the selected case with the selected element in the model tree as illustrated below:  The active radio button and the selection in the list indicate the component in the model tree where the case will be linked. This information is encoded with **c** in the component name: 

5.2.6.1 Conversion of CFD Resuts to Images

The **Generate** button in the **Image data results** panel allows creating image data with the specified **Resolution.**

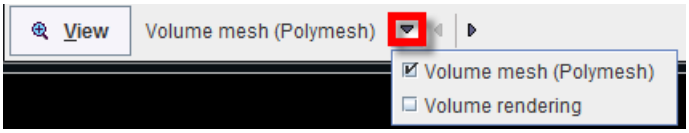


Four image series are created: **Geometry**, **p (Pressure)**, **U (Velocity magnitude)**, **U (Velocity XYZ components)**.

Use the **Save** icon to save the currently shown series in any of the supported formats. If the **All** box is checked, all image series are saved in separate files with the specified resolution.

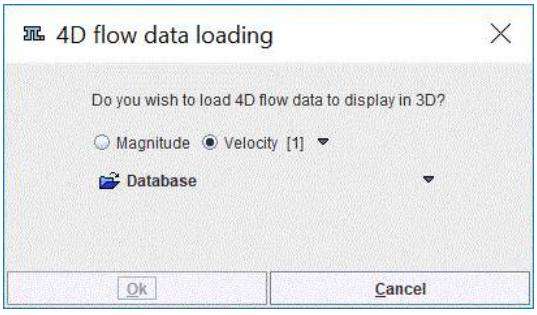
5.2.6.2 Visualization of the CFD Results

The View button allows displaying the results of the CFD case selected in the list in a 3D window. There are two options for visualization of the CFD results: as **Polymesh** or as **Volume rendering**:



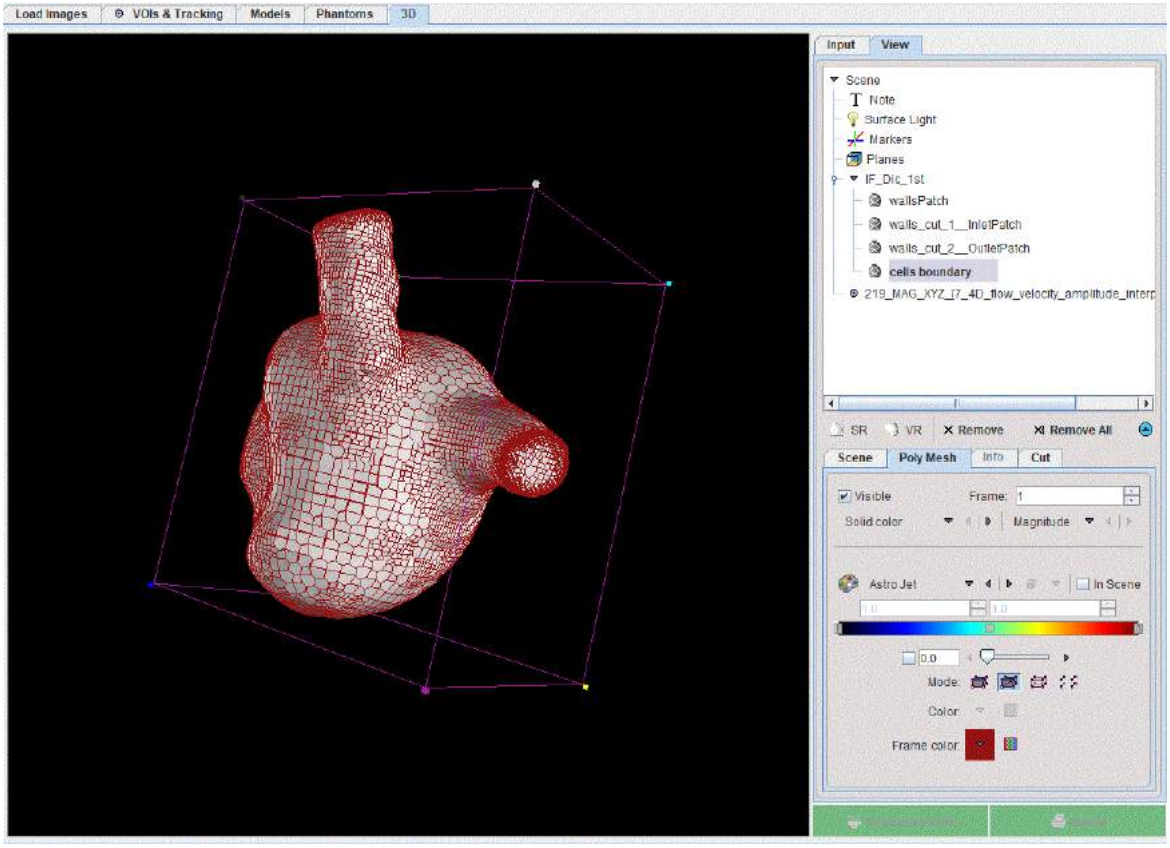
5.2.6.2.1 As Polymesh

Select the **Volume mesh (Polymesh)** option in the list and activate the **View** button to transfer the CFD results to the **3D** page. An intermediate dialog window allows selecting the original 4D Flow data:

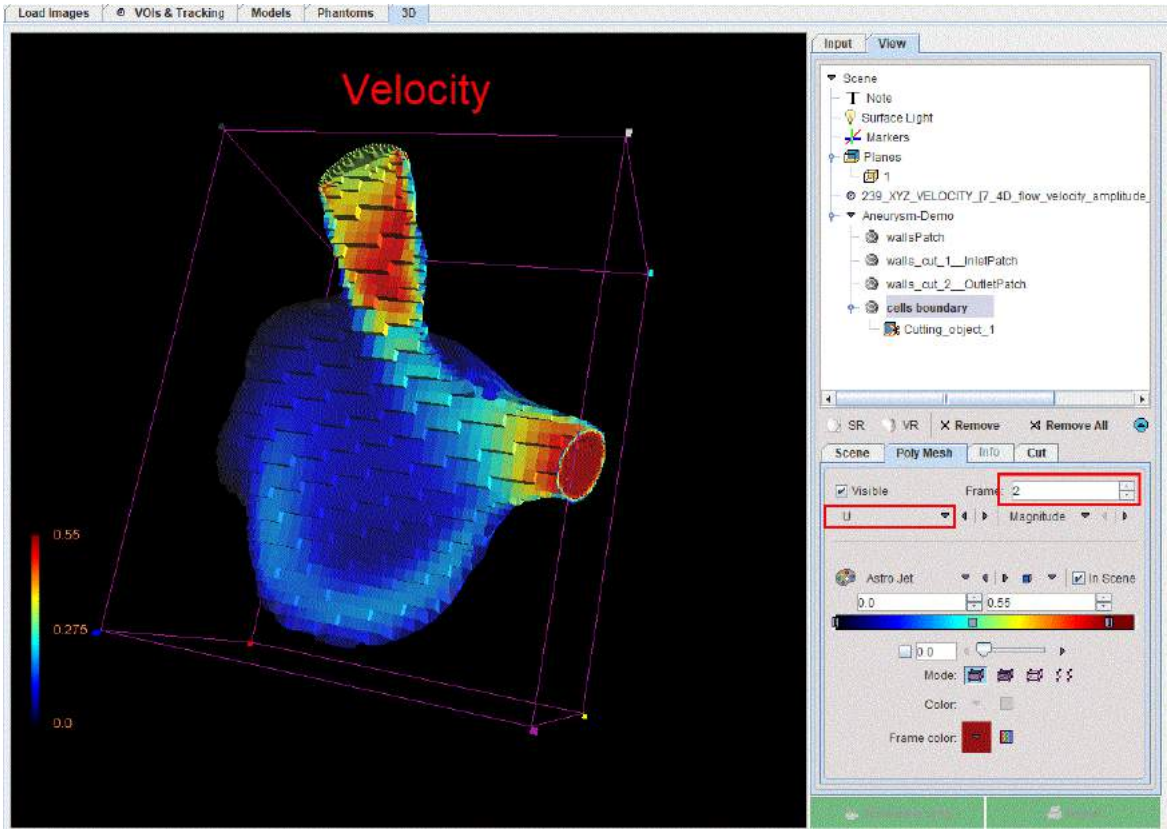


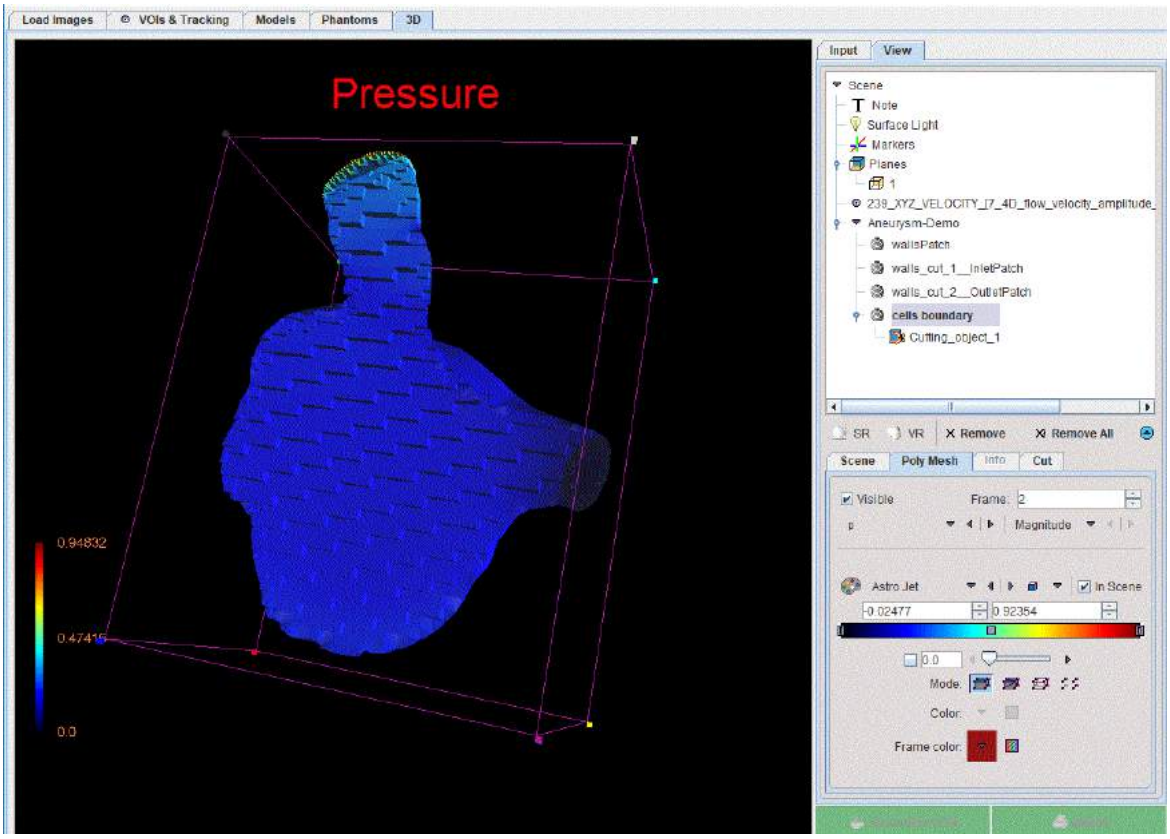
The selected image series may be used for texturing in the 3D interface only if the same data were used to create the geometric model used for the simulation.

The result for a Brain Aneurysm data is illustrated below:



For further visualisation, an oblique cutting plane is applied to the aneurysm CFD results, to reveal internal values for velocity and pressure:

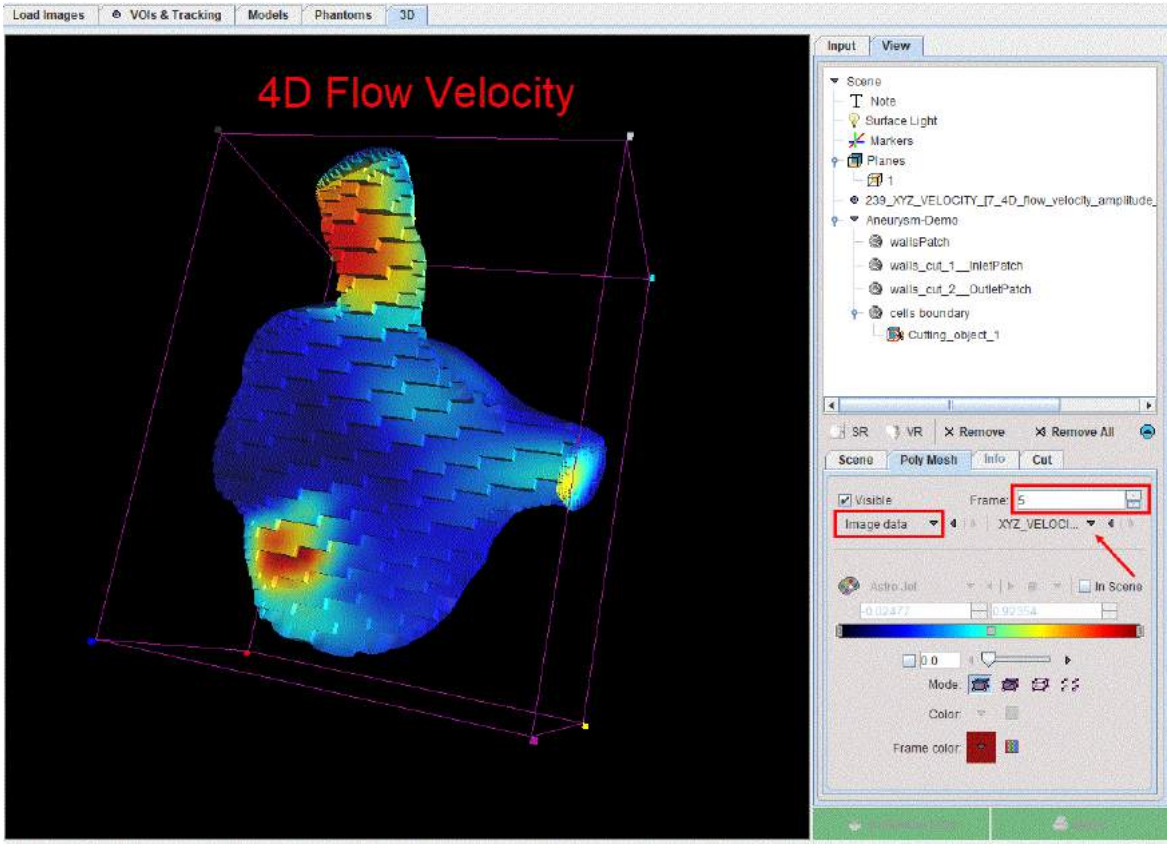




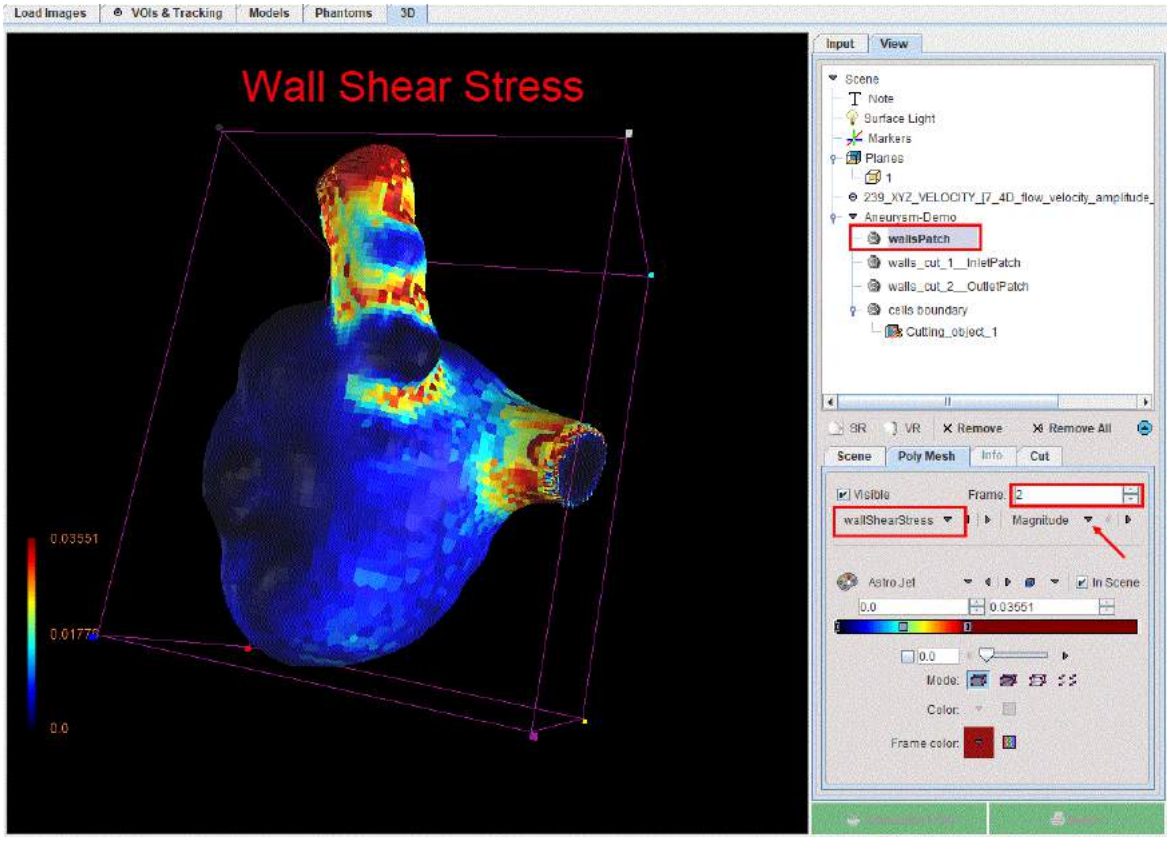
The following settings were used for visualization:

1. All the objects in the **View** tree were set to **Solid**.
2. The **wallsPatchVisible** box was switched OFF.
3. An oblique plane was used to cut the **cells_boundary**. After cuttin, the plane **Visible** box was set to OFF.
4. The **p** (pressure) and the **U** (velocity) **Magnitude** selected on **Frame** 2 were used to texture the **cells_bounday** object.

The resulting velocity field and pressure can be compared visually to the known velocity from 4D Flow. To this purpose the loaded I**mage data** with **XYZ_velocity** selection was overlaid on the **cells_boundary** object:



The wall shear stress maps can also be assessed in the 3D environment. For this purpose the **wallsPatchVisible** box is enabled and the **wallShearStressMagnitudeFrame 2** selected as texture. The scene is updated as illustrated in the capture below:



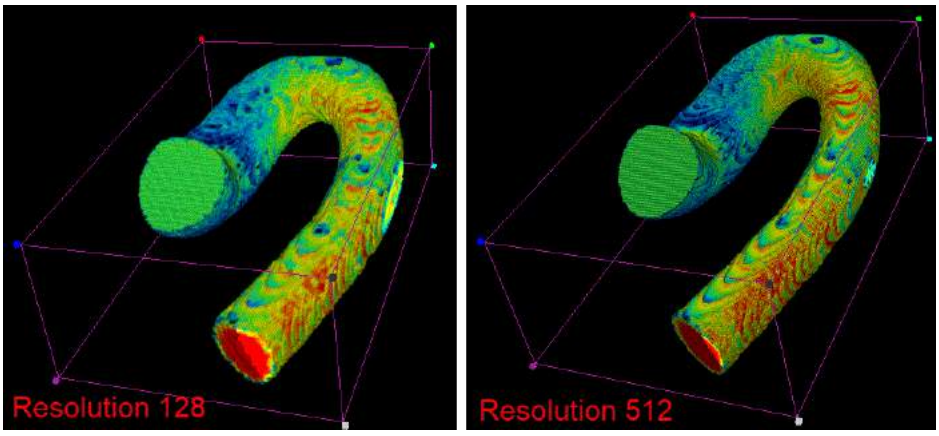
Note: Please refer to the *PMOD 3D Rendering Tool Users Guide* for any further information about the cutting planes and texture of the scene.

5.2.6.2.2 As Volume Rendering

Visualization of the CFD Results as Volume Rendering

With the **Volume rendering** selection additional settings are available, as illustrated below:

The settings are summarized in the following table:

Resolution 128	Allows setting the image resolution. The following selection is available: **64**, **128**, **256** and **512**. The selected number indicates how many cubes will be rendered in each direction. Each cube stores the information about the variable field from one cell of the volume mesh. The higher the resolution the better the precision, but the memory requirements grow significantly. The rendering results for two different resolutions (**128** and **512**) are illustrated below for the velocity magnitude estimated for the Aorta model: 

Note:

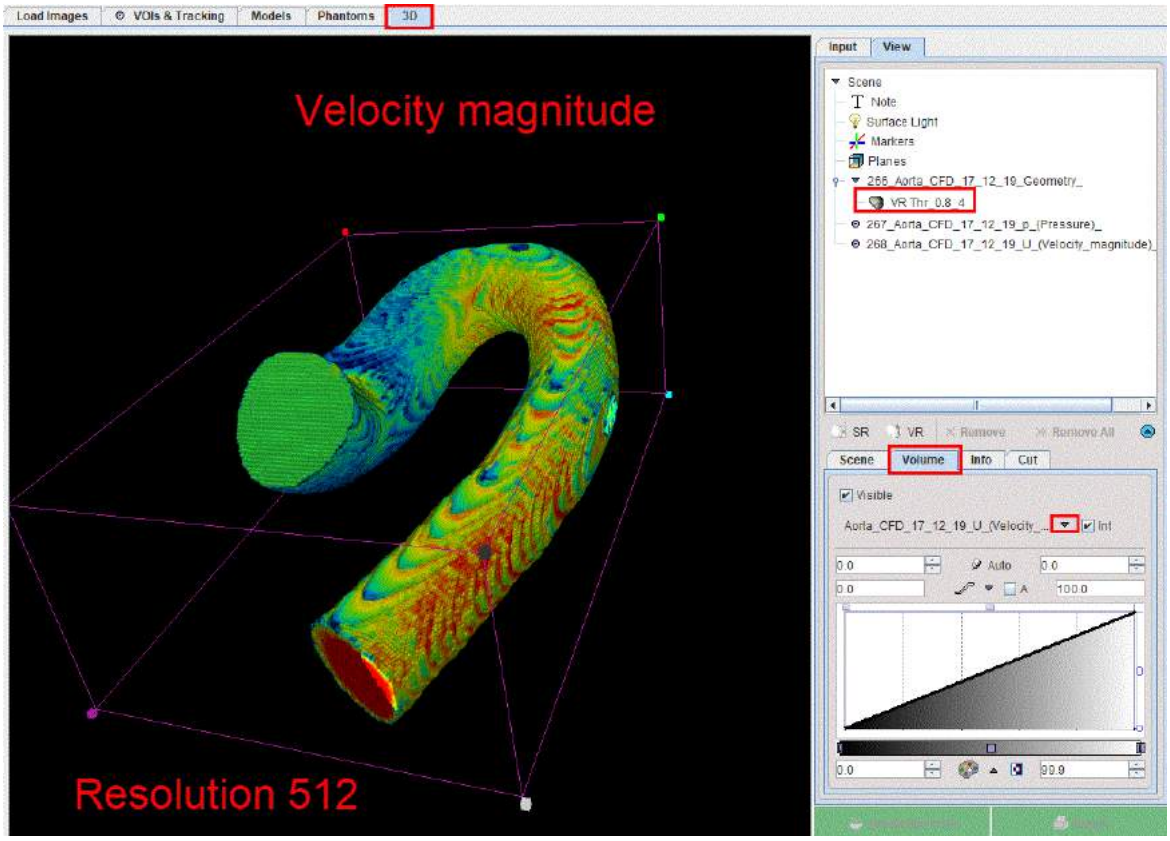
In the 3D scene the cubes will be drawn in the positions which represent the centers of the volume mesh cells.

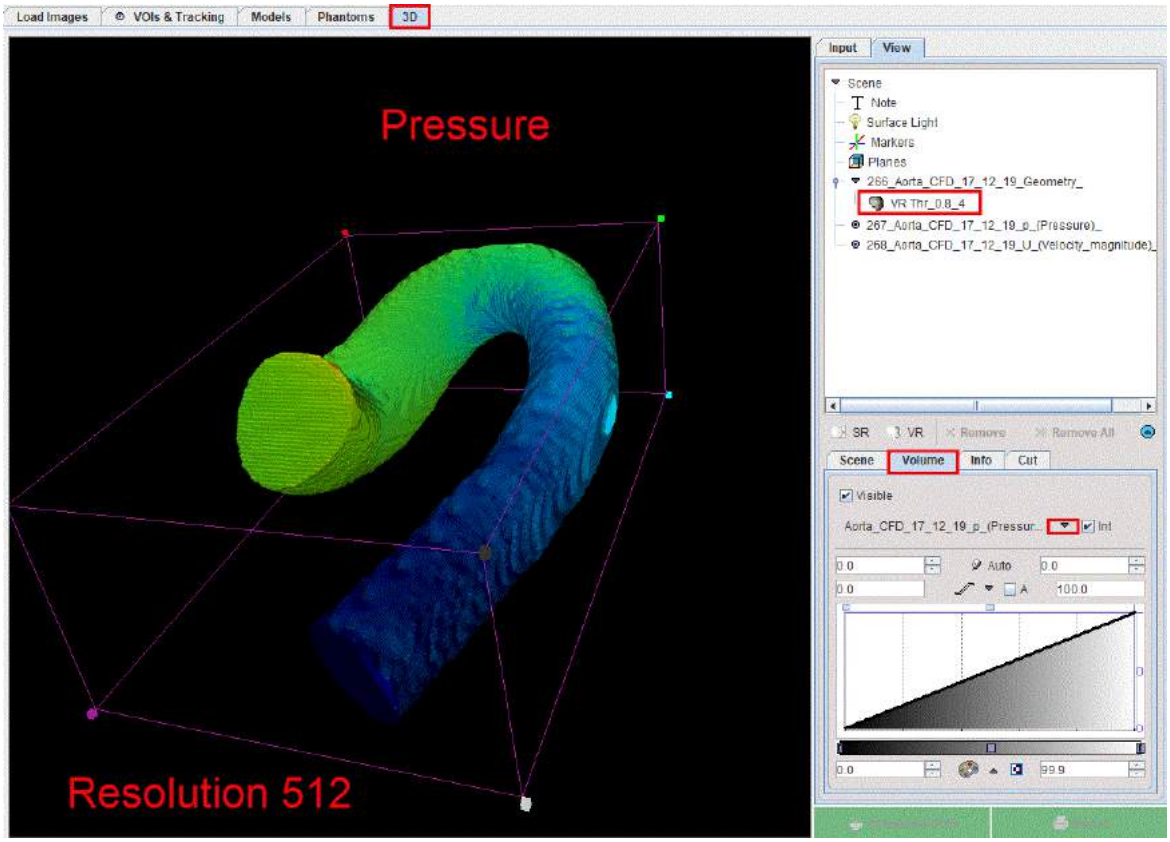
The following settings were used for visualization:

1. The resolution was set to 512.

The simulation results are transferred to the **3D** page activating the **View** button. They are available as images on the **Input** tab of the **3D** page. In the **View** tree, the **CFD_Geometry** is available as the volume render object, the **CFD_p_(Pressure)** and **CFD_V_(Velocity_magnitude)** as images for the texture.

The two physical variables, velocity and pressure, are visualized as textures on the same geometry as illustrated below:





In addition, plane elements can be defined for composing a meaningful scene. The planes serve for defining the parts to be cut out of a VR object.

Please refer to the *PMOD 3D Rendering Tool Users Guide* for any further information about the rendering.

6 References

1. Roy van Pelt, Anna Villanova. Understanding blood-flow dynamics: new challenges for visualization. IEEE Computer. 2013;46(12):60-67.

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