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A Methodology to Generate a Patient Specific High Quality Structured Computational Domain from Medical Imaging Data.

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Abstract
In this study a methodology for shape reconstruction and multi-block structured grid generation of patient-specific human organs is proposed. Starting from data obtained by a medical imaging examination a high quality multi-block structured grid that conforms to the geometry of human organs is generated. In order to assess the quality of the produced grid, the methodology is applied to two medical cases of great interest, the Abdominal Aorta Aneurism (AAA) and the iliac bifurcation. Furthermore a brief comparison between computational grids produced by the method unstructured tetrahedral grids produced by commercial meshing software are presented. The proposed methodology may be combined with several Computational Mechanics (CM) models and may be a step towards an accurate, patient specific, medical diagnosis and prognosis framework.

Keywords: Patient-specific approach, structured grid, CFD, Bifurcation geometries, Abdominal Aorta Aneurism

Introduction
In recent years there is a growing interest in the simulation of biomechanical applications such as air flow through the respiratory system, particle deposition in the lung\cite{1,2} and blood flow in the cardiovascular system\cite{3,4,5,6,7} in terms of Computational Fluid Dynamics (CFD). The modern approach in this type of simulations is the patient-specific modeling. For the implementation of accurate CFD simulations of patient specific flows an accurate reconstruction of realistic human organ geometry and a robust grid generation technique able to reproduce the complex shapes of human organs are necessary.

In patient specific CFD simulations the most common approach is the extraction of the patient specific geometry starting from medical imaging data and the generation of an unstructured computational domain by the use of commercial meshing software\cite{5,6}. The use of unstructured computational grids is often preferred for its ability of effortless grid generation in complex domains combined with preservation of the geometrical shape.

Although unstructured grids are generally considered to provide less accurate solutions than structured grids due to a number of factors, including poor alignment with the primary flow direction and increased numerical diffusion\cite{8,9}. A quantified comparison between structured and unstructured grid performance on an air flow simulation with the use of an idealized geometry model may be found in previous studies\cite{1,2}.

The above mentioned study concluded that structured grid domains used for the simulation of that type of applications are better than the unstructured. The use of structured grid ensures the strict alignment of the grid elements with the predominant flow direction concluding to lower numerical diffusion, provide a mesh independent flow solution with fewer elements and reduces run time by a factor of 3.

Furthermore a structured grid allows one to obtain fine grid resolution on the computational domain boundaries using fewer grid elements than a similarly sized unstructured grid. Additionally the prior knowledge of the exact shape and dimension of the matrices formed by the system of the physical equations, may lead to the operation of memory and time efficient solving techniques.

The present study proposes an approach, for the generation of multi-block structured computational grids on patient-specific geometries. The structured grid generation technique is applied to data obtained by medical imaging examination, concluding to a surface conforming, high quality, multi-block structured grid of the patient specific geometry.

The method starts from a surface triangulation constructed by the reconstruction of medical imaging data and through an isomorphic reparametrization\cite{10}.
concludes to a planar triangulation. The next step is the projection of a planar isomorphic mapping [11] over the planar triangulation and the production of the surface structured grid. At the last step the structured hexahedral volume grid is produced and grid enhancement is carried out.

The methodology is utilized in two applications that are of a great interest among biomedical community.

The first application is the Abdominal Aorta Aneurism (AAA). In this application the high quality of the produced grid, the high element alignment with the primary flow direction combined with the ability of clustering hexahedral elements near the wall, certified that the use of the grid generated by the proposed methodology provide more accurate computational results, especially near the artery wall [12]. In the present manuscript some additional details about the AAA case are presented.

The second application is a patient specific bifurcation study. The presence of series of branching geometrical shapes inside the human body, along with the observation that the distributed flows may be responsible for the development of complicated phenomena, renders the patient specific modeling of branching geometries an important task. In this application the produced structured grid, provide more accurate computational results with a computational domain with 4 times less mesh elements than the unstructured computational domain produced by commercial meshing software.

In both applications for the evaluation of the grid produced by the method a flow field comparison between the multi-block structured grid produced by the method and unstructured grids produced by commercial meshing software are carried out.

The results of both simulations fortified the evidence that the structured grid provide more accurate results, in terms of convergence, flow field detail and near the wall computational accuracy. Furthermore both cases underline the accuracy improvement that the use of a high quality structured computational domain may provide to CFD patient specific simulations.

2. Method description

The purpose of the methodology is the generation of an advanced patient specific computational domain of a human organ shape starting from medical imaging data.

This procedure comprises of the following steps:

- Medical imaging data processing and segmentation of the volume of interest. Creation of a 3D shell of the volume of interest.
- Generation of a surface structured grid over the 3D shell of the human organ geometry.
- Generation of the volume grid and grid enhancement.

A more detailed description of the previous steps follows.

The first step in the methodology is the manipulation of the medical imaging data file by a medical data visualization and image analysis program.

Currently almost all the medical imaging machines (magnetic resonance imaging (MRI), computed tomography (CT), medical ultrasonography (MU) etc.) handle, store, print, and transmit information through Digital Imaging and Communications in Medicine (DICOM) format. A DICOM file consists of a set of greyscale images of planar cross sections through the spatial dimensions and often through time. In Fig. 1 a typical case of medical imaging data visualization is illustrated. DICOM information reading and human organ geometry reconstruction from DICOM data sets is considered to be a routine task today and is utilized by locally customized codes or commercial software. In the presented methodology, the highly efficient and reliable open source software 3DSlicer® [13] is used for accessing the medical imaging data and for the segmentation of the volume of interest (VOI).

![Fig.1 Left: A typical DICOM data visualization process along the segmentation of the volume of interest. Right: The reconstructed surface by the medical data visualization and image analysis program.](image)

A considerable step in the geometry reconstruction process is the segmentation of the volume of interest. Due to the heterogeneous nature of signal intensity distribution and quality of the DICOM images, this procedure can not be automated. A certain degree of user intervention is always required during the segmentation, mainly in the identification of the vessel's bounds.

Moreover in plenty of medical cases considering the cardiovascular system the segmentation of the volume of interest tends to be even more difficult task due to the presence of thrombus [14]. The thrombus develops in the inner vascular wall of arteries and the optical separation between thrombus and the outer vascular wall has to be done. The separation between vascular wall and thrombus is achieved due to the difference in the biochemical synthesis that causes different optical result. Hence, by using luminescence thresholds it is possible to distinguish thrombus from the outer vascular wall and segment the volume of interest.
After the segmentation of the volume of interest, the medical data visualization and image analysis software produces a 3D surface cell by combining the data of every planar image. The typical result of this combination is a reconstructed volume of interest geometry exported as an STL file (STL is a file format native to the stereolithography CAD software). An STL file describes an arbitrary geometry by an unstructured triangulated surface. In the methodology, an STL file was used as the origin file containing the geometrical information of the patient specific volume of interest. Nevertheless, the methodology is applicable to every triangle-based description of a surface. In Fig. 1 a reconstructed patient specific iliac bifurcation surface is shown.

The essence of the methodology is the production of a high quality surface structured grid with absolute respect to the patient specific volume of interest shape. This procedure is done by an in-house code developed for the needs of the methodology. The surface grid generation process has the ability to produce multi-block structured grids of high quality with controlled refinement over a triangulated surface.

The surface grid generation procedure is comprised of two steps:

- **The creation of an isomorphic parameterization for the surface triangulation.**
  
  From a surface triangulation in 3D, a planar triangulation in 2D is formed inside a predefined 2D domain, with a one-to-one correspondence between nodes, edges and faces. This is done by solving a linear system of equations that expresses the conservation of a convex combination factor for every triangle of the 3D triangulation to the newly calculated 2D triangulation.

- **The use of the isomorphic mapping to produce a structured surface grid.**
  
  In order to produce a produce a structured surface grid a planar structured grid is overlapped over the planar triangulation. In Fig. 3 an overlap of the planar structured grid and the planar triangulation used in the interpolation process is shown. After the interpolation the barycentric coordinates for each structured grid vertex inside every triangle are calculated [15].

\[\text{Fig.3 a) The planar triangulation. b) The 2D multi-block structured domain that is interpolated. c) Both grids inside the predefined 2D domain.}\]

Due to the isomorphic transformation, the barycentric coordinates are unvaried in the 3D surface triangulation. Using that information, along with a back projection, a surface structured grid over the triangulated surface is obtained. In Fig. 4 the surface structured grid obtained by the methodology and the starting surface triangulation are illustrated.

\[\text{Fig.4 a) The initial surface triangulation in 3D. b) The multi-block structured domain generated over the triangulation.}\]

When this methodology is applied to a branching shape, a more sophisticated approach has to be followed. The interpolated structured grid has to be multi-block and with a predefined topology capable to receive the one to one unification of the two branches.

In the iliac bifurcation case a multi-block structured planar domain, is objected to the full planar triangulation. The result of that procedure is a multi-block structured grid with a structured block formed at the place where the branch was formerly united. As a result the formed computational domain has a one block per branch topology. A simple one block per branch topology has the advantage of effortless grid generation and the ability to
create multiple branching geometries without grid resolution limitation that more complicated topologies have. The cost of the simplicity of the selected topology is the production of computational domains that contain a few skewed elements in the block corners. Complementary, the methodology may be combined with more complicated topologies.

An additional advantage of the proposed methodology is the ability to control the grid clustering. This is done by the application of different multi-block structured grid projections. The application of the method may provide computational grids with clustering near the domain bounds or even more near a specific domain area that may represent a specific spot of interest by the variation of the grid clustering and topology of the interpolated 2D structured grid.

For the methodology to conclude to a computational domain, the creation of an initial 3D grid has to be done. The inner initial grid is produced by the use of a linear transfinite interpolation (TFI) method [8]. The quality of the inner grid may be further improved with the use of a Sorensen algorithm [8] by an in-house grid enhancement code. This algorithm makes possible to control the distance of the first element vertex from the bounds and by the application of it on the produced computational domain the irrational shape of the elements in the topology corners is avoided.

3. Applications—results

In order to evaluate the computational domain that is formed by the methodology, two highly interesting biomechanical simulations along with comparison between approaches based on different grid generation techniques are briefly presented.

For the AAA case, two different computational domains, a multi-block structured with clustering near the wall generated by the methodology and a similar resolution unstructured generated by the commercial software Ansys ICEM, are compared. Both domains are depicted in Fig. 5.

As a comparison simulation a steady flow corresponding to the maximum inflow velocity at the systolic phase of the cardiac cycle [4] is selected.

The flow field is calculated by the Ansys CFX® software and the blood is simulated as an incompressible, homogenous and Newtonian fluid. The blood density was assumed equal to 1056 kg/m2 and the dynamic viscosity equal to 3.1 \times 10^{-3} \text{ Pa s}. As boundary conditions, a constant velocity profile was selected giving a Reynolds number equal to 2000, while the outlet pressure was selected equal to 112 mmHg. The walls were considered smooth and the no slip condition was applied. The performed CFD simulation, for both domains, predicted a pressure and velocity distribution in the physiological range and corresponded to the expected values reported in previous studies [4].

In order to quantify the difference of the flow fields developed inside the two different computational domains, a relative error measurement is done. For that purpose, equation (1) calculates the formula of the relative error variable at selected geometrical points and equation (2) calculates the root mean square value of the same variable ($E_{\text{rms}}$) [1].

\[
E = \frac{u_{\text{coarse}} - u_{\text{fine}}}{u_{\text{fine}}} \quad (1)
\]

\[
E_{\text{rms}} = \sqrt{\frac{1}{180} \sum_{i=1}^{180} E^2} \quad (2)
\]

For the estimation of the relative error a line consisting of 180 points close to the vascular centerline is
selected. The formula is comparing the values of the same geometrical points in both computational domains. The results of the computed velocity coordinates X and Y are depicted on Fig. 6 and Fig. 7 as graphs. In the flow field of the AAA simulation the primary flow direction is towards the Z axis. The two coordinates were selected not to be the dominant flow direction coordinates in order to better estimate the ability of the computational domain to simulate the secondary flows inside the AAA.

Based on the two graphs we may suggest that the use of the structured grid provided more smooth flow fields. The unstructured grid shows evidence of high numerical diffusion with the occurrences of curly lines and rough velocity transition over neighboring geometrical points. Furthermore the unstructured grid computed the secondary flow velocity coordinates (Velocity_X and Velocity_Y) with lower magnitude. In terms of $\varepsilon_{\text{rms}}$ the Velocity_Y is underestimated by an $\varepsilon_{\text{rms}}$ equal to 2.05 while the Velocity_X is underestimated by an $\varepsilon_{\text{rms}}$ equal to 4.15. Those facts lead the structured grid to be more accurate in the simulation of secondary flows and resolve more secondary vortices inside the flow field. Furthermore, the result of the underestimation of the secondary velocities by the use of the unstructured domain, may lead to a calculation of lower vertical pressure on the wall and a shear strain rate underestimation.

A visual confirmation of our conclusions may be observed in Fig. 8 where contours of the velocity magnitude for the same transverse plane for both domains are depicted. It is visually evident that the structured grid produced by the methodology calculated a more detailed flow field of the similar resolution unstructured grid generated by a commercial software.

The second application that will be presented is an iliac bifurcation flow field simulation. For that simulation two different computational domains, a multi-block structured generated by the methodology and an unstructured computational domain generated by the commercial software Ansys ICEM®, are briefly compared. The unstructured grid was created to be a finer grid consisting of 891,557 tetrahedral elements while the structured grid consisted of 198,768 hexahedral elements. In Fig. 9 the two computational domains are depicted.
For the comparison a steady flow corresponding to a Reynolds number equal to 800 was selected. The flow field is calculated by the Ansys CFX® software for both computational domains. As in the previous application the blood is simulated as an incompressible, homogenous and Newtonian fluid with density equal to 1056 kg/m² and dynamic viscosity equal to 3.1 \times 10^{-3} \text{ Pa s}.

The conclusions that arising out, after a brief comparison, are similar with the previous application. As it is depicted in Fig. 10 the structured grid computed a flow field with smoother velocity and pressure transitions and with a higher velocity magnitude than the unstructured grid.

In order to quantify the differences, a relative difference measurement using the $\varepsilon_{\text{rms}}$ formula was done. The comparison was done over a test volume near the branch of the patient specific geometry consisting of 1560 points. In Fig. 11 a visualization of the test volume is illustrated.

The result is the multi-block structured computational domain calculated a higher velocity magnitude near the distribution area with $\varepsilon_{\text{rms}}$ equal to 8.3%.

Based on the difference in the flow field calculation, the use of a tetrahedral unstructured grid in similar simulations may cause inaccurate flow field calculations, mainly near the area where the flow is distributed, and lead to uncertain conclusion about thrombus formation and the development of complicated phenomena.

The observed differences and the visualization of the flow fields obtained by the different computational grids is in agreement with conclusions reported by previous comparison studies \cite{6,16}, considering the structured grid capable to provide more accurate flow field solutions at similar grid resolution.

**Conclusions**

In this study a new technique is developed for shape reconstruction and multi-block structure grid generation of patient-specific human organs. The method is utilized over surface triangulations representing patient specific geometries obtained by a medical imaging examination and reconstructed by a medical data visualization and image analysis program.

The application of this methodology to two medical cases and a brief comparison against unstructured tetrahedral meshes produced by commercial meshing software, underlines the superiority of the structured grid against tetrahedral unstructured meshes.

As a future task, different topologies for the computational domain will be studied to conclude to the highest quality grid with the use of the fewer elements possible. Finally the application of the method for the grid generation of a patient specific aorta shape, including
series of bifurcations and the performance of blood flow simulations is also a future task.

Overall, the proposed methodology is able to generate high quality multi-block structured grids that may be used for a series of Computational Mechanics (CM) simulations of biological systems, including but not limited to CFD, Finite Elements Method (FEM), Fluid Structure Interaction (FSI), approaching various biomechanical problems. The methodology presented in this study may be a step towards the development of an advanced patient specific model, which may provide an accurate, patient specific, medical diagnosis and prognosis framework.

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