A Practical Method to Model Complex Three-dimensional Geometries with Non-Uniform Material Properties Using Image-based Design and COMSOL Multiphysics

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Abstract: Multiphysics modeling of complex three-dimensional geometries is a challenge. Image-based computer aided design (CAD) is a practical alternative to reconstruct complex geometries from cross-sectional images. Nevertheless, incompatibilities between different CAD file formats and simulation software can occur, especially when dealing with multipart geometries that require assembling. Our objective was to develop a practical method to use complex geometries with heterogeneous material properties in COMSOL Multiphysics without the challenge of assembling multiple parts. The proposed method involved the use of X-ray computed tomography (CT) images to reconstruct the entire geometry as a unit, and of each of its parts representing different materials. A custom algorithm to label geometry nodes with corresponding materials was developed. Then, interpolation functions of COMSOL Multiphysics were used to define material properties as a function of mesh coordinates. Such method allowed incorporating complex geometries with heterogeneous material properties in COMSOL Multiphysics without the difficulties that may arise when assembling complex multipart geometries.

Keywords: Imaged-based mesh generation, 3D modeling; CT-scanning; geometry assembly; Materialise Mimics.

1. Introduction

Constructing high quality and accurate meshes of complex three-dimensional (3D) geometries for multiphysics modeling remains a challenge. The challenge is greater when such geometries involve assembling of parts with different material properties (e.g., chicken carcass with bone, skin, and meat sections). Multiphysics models for biomedical and food processing applications would likely involve such complex multi-part geometries. A common approach to minimize geometry complexity is to approximate using basic shapes such as bricks, cylinders, or ellipsoids. Another common strategy is to consider the multipart geometry as a single unit having homogeneous material properties. The later strategy is commonly used for geometries reconstructed from 3D surface scanners (e.g., laser scanners, contact scanners). However, such simplifications may compromise the accuracy of the model.

1.1 Image-based Mesh Generation

Image-based computer aided design (CAD) is a practical alternative to reconstruct complex geometries from cross-sectional images of an object1,2. Said et al. (2007, 2008) developed image-based multi-part meshes for a human head model, and for a piece of pork bacon using Simpleware Software (namely ScanIP and +ScanFE)3,4. A similar approach was used by Hermans et al. (2009) to develop a multi-part mesh of a human thorax5. The resulting meshes were fully compatible with Comsol Multiphysics models.

1.2 Challenges with the Traditional Material Assignment Approach

Modeling heterogeneous geometries typically requires the geometry to be defined as a set of multiple parts, each part representing a different material. The material properties are assigned to each individual part subsequently.

Nevertheless, there are situations in which assembling or defining the individual parts of highly complex geometries can be non-trivial.
Incompatibilities between different CAD file formats and simulation software can occur. Such problems are generally caused by inconsistencies that are difficult to control when assembling highly complex geometries. For instance, nodes on interfaces between neighboring subparts of the geometry may be displaced and/or not fully connected, creating voids or overlapped regions. When these types of inconsistencies occur, importing geometry CAD files into COMSOL Multiphysics can be complicated due to face parameterization and geometry decomposition errors (Figure 1).

Our objective was to develop a practical method to mesh complex geometries of heterogeneous materials and to assign non-uniform material properties in COMSOL Multiphysics without the challenge of assembling complex multipart geometries.

2. A Practical Method to Model Complex Multipart Geometries in COMSOL

The proposed method involves the following steps:

1. Scanning and 3D reconstruction
   1.1 Scan the object
   1.2 Define a mask for the object as a unit
   1.3 Define a mask for each sub-part of the object representing a different material
   1.4 Use mask of step 1.2 to construct a 3D surface geometry of the object as a unit
   1.5 Use masks of step 1.3 to construct a 3D surface geometries of each individual sub-parts of the object

2. Meshing
   2.1 Create a volume mesh for the object as a unit using the 3D surface geometry of step 1.4
   2.2 Create volume meshes for each subpart of the object using the 3D surface geometries of step 1.5. Use a finer refinement level compared with the mesh of step 2.1
   2.3 Export the meshes of steps 2.1 and 2.2 as COMSOL native mesh files (.mphxt)

3. Material labeling
   3.1 Use algorithm described in Figure 5 to map the nodes of the mesh of the object as a unit (mesh from step 2.1) that interface with the nodes of the meshes of the object subparts (meshes from step 2.2)
   3.2 Create look-up table with the list of nodes of the mesh for the object as a unit and their corresponding material properties

4. Define material properties in COMSOL
   4.1 Import single mesh of the object as a unit (mesh from step 2.1)
   4.2 Create interpolation functions for each material property based on nearest neighbor method
   4.3 Use interpolation functions to define material properties as functions of mesh coordinates

Figure 1. Potential errors when importing complex multi-part geometries in COMSOL Multiphysics.
2.1 Step 1 - Scanning and 3D Reconstruction

Step 1.1 - Three-dimensional geometries can be reconstructed from a series of two-dimensional (2D) cross-sectional images of the object of interest. Medical imaging techniques such as X-ray computed tomography (CT) and Magnetic Resonance Imaging (MRI) are commonly used to obtain high-resolution images (sub-millimeter scale) (Figure 2).

Steps 1.2 and 1.3 - Processing necessary to go from a series of 2D-images (typically presented as Digital Imaging and Communication in Medicine or DICOM format) to a high quality 3D geometry is not always trivial. It involves multiple steps including: subsampling, segmentation, 3D reconstruction, and quality improvement.

Subsampling involves the selection of the specific images in the series of 2D-images to be used for the 3D image reconstruction. MRI and CT scanning allow capturing cross-sectional images at less than 1-mm intervals. However, there may be regions of the geometry in which such high resolution may not be required. Therefore, certain cross-sectional images can be skipped to avoid creation of redundant nodes in the geometry that may lead to very small size mesh elements. Unnecessary small size elements may increase computational time and generate numerical errors when solving the multiphysics model.

The segmentation process allows identifying the regions of the image corresponding to each subpart of the object representing a different material (Figure 3). In general, different materials can be visualized in the images by different grayscale values. Image processing software (e.g., Materialise Mimics, 3D-Doctor, ScanIP) provide tools to define what pixels belong to each subpart of the object. The segmentation process typically starts by selecting regions of the images using thresholding tools (automatic selection based on a minimum and maximum pixel value). The defined regions are commonly referred to masks. The individual masks can be edited and smoothed to minimize noise. Individual masks should be created for the object as a unit, and for each of its subparts representing different materials.

Steps 1.3 and 1.4 - Once masks are defined, 3D reconstruction can be easily performed by image processing software. The result of this process is a set of 3D surface geometries representing the object as a unit, and each of the object subparts separately. The 3D surface geometries are presented as CAD file formats such as STL and VRML. Quality of the 3D surface geometries is crucial to ensure the quality of the volume meshes. Image processing and/or CAD software (e.g., Materialise 3-matic, Hyperworks, +SCANFE, Pro/ENGINEER, SolidWorks, SpaceClaim) can be used to verify and improve quality of 3D surface geometries. Techniques such as smoothing, wrapping, filling holes, stitching, and triangle reduction can be used to refine and improve 3D surface geometries. The idea is to make sure to eliminate all potential bad edges, inverted normals (i.e., faces are inside out or not pointing the correct way), bad contours, planar holes, noise shells, overlapping triangles, and intersecting triangles.
2.2 Step 2 - Meshing

Steps 2.1 and 2.2 - Three-dimensional (3D) surface geometries can be used to generate individual volume meshes for the object as a unit, and for each of its subparts representing different materials as illustrated in Figure 4. Volume meshing can be performed by importing individual 3D surface geometries in COMSOL Multiphysics and meshing them separately. Meshing software such as Materialise 3-matic, Hypermesh, and +SCANFE can also be used to generate high quality volume meshes. Mesh quality is important for the accuracy of the simulation. Recommended mesh quality indicators for finite element analysis include Height/Base ratio > 0.4, aspect ratio > 0.4, skewness < 0.4, and maximum geometrical error < 0.5. The maximum triangle edge length can be used to control mesh refinement level.

2.3 Step 3 - Material Labeling

Step 3.1 - COMSOL native mesh file format (.mph.txt) provides the Cartesian coordinates of each of the nodes of the mesh. Since the meshes generated using the procedure described in Step2 share the same Cartesian plane origin, a mapping between the nodes of the mesh for the object as a unit, and the nodes of the meshes for the subparts representing different materials can be performed. Figure 5 describes an algorithm that can be used to label each node of the mesh for the object with its corresponding material.

![Algorithm for labeling materials](https://example.com/algorithm.png)

Each of the nodes of the subpart meshes is matched to a node in the object mesh. The matching can be determined by the nearest neighbor method. For instance, the nearest neighbor of the subpart node (namely nodeA) corresponds to the node i in the object mesh having the minimum Euclidean distance (ED) to nodeA.

$$ ED = \sqrt{(x_{nodeA} - x_i)^2 + (y_{nodeA} - y_i)^2 + (z_{nodeA} - z_i)^2} $$

where x, y, z represent the nodal coordinates.
At the end of the matching process, all nodes of the object mesh should have been labeled with a particular material (or subpart). To make sure all nodes are labeled properly, meshes for the subparts must have a higher level of refinement compared with the mesh for the object as a unit.

**Step 3.2** - The output of the suggested algorithm (Figure 5) is a look-up table containing the list of nodes coordinates of the mesh for the object as a unit, and their respective material properties. It can be presented as a spreadsheet or text file, which can be subsequently imported in a COMSOL model.

### 2.4 Step 4 - Defining Material Properties by Interpolation

**Step 4.1** - Comsol Multiphysics does not currently allow importing multiple meshes that may intersect with each other. Hence, only the volume mesh for the object as a unit should be imported into the COMSOL model.

**Steps 4.2** - The look-up table obtained in Step 3.2 can be used to create interpolation functions of material properties using mesh coordinates as arguments and the nearest neighbor interpolation method as illustrated in Figure 7.

**Steps 4.3** - Material properties should be defined as functions of \((x, y, z)\) mesh coordinates as illustrated in Figure 8.

Consequently, even though the model has only a single domain, heterogeneous material properties can still be defined.
3. Case Study - Modeling a Chicken Carcass in COMSOL Multiphysics

Volume meshes of a chicken carcass, and each of its subparts (i.e., muscle, rib bone, round bone, and internal cavity air sections) were built following the methodology described in Section 2. The chicken carcass was scanned using a General Electric LightSpeed VCT 16 Slice CT-scanner (Advanced Medical Imaging, Lincoln, NE). CT cross-sectional images at 0.625-mm intervals were used to reconstruct the 3D surface geometries for the carcass as a unit, and for each of its subparts using software for image processing (Materialise Mimics 16.0). Volume meshes consisted of 4-node tetrahedral elements and 3-node triangular boundary elements were constructed with Materialise 3-matic 8.0.

The algorithm described in Figure 5 was implemented in Java™ (Java Platform JDK 7u13, Oracle) to label each node of the mesh for the carcass as a unit with the corresponding material (i.e., muscle, rib bone, round bone, and internal cavity air).

Only the mesh for the chicken carcass as a unit was imported in a COMSOL model to simulate heat and mass transfer during air-cooling of chicken carcasses. The modules of Heat Transfer in Solids and Transport of Diluted Species, as well as the LiveLink for MATLAB were used to carry out the simulations.

Interpolation functions were created to define specific heat \( C_p \), thermal conductivity \( k \), moisture diffusivity \( D_m \), and density \( \rho \) as a function of mesh coordinates. Then, material properties corresponding to different sections of the carcass were easily defined without the need of assembling or defining the carcass subparts in the geometry (Figure 9).

The heat and mass transfer model was successfully validated in a local poultry processing facility. Predicted temperatures and moisture losses were in agreement with observed values (Figure 10).

4. Conclusions

The proposed method uses image-based mesh generation, a custom algorithm, and interpolation features of COMSOL Multiphysics to define heterogeneous material properties of complex geometries without the difficulties associated with assembling complex multipart geometries. Hence, the method is a practical alternative to avoid the need of critical geometry simplifications that may compromise model accuracy for certain applications (e.g., industrial food processing applications). The basics of this method can be potentially implemented as features in future versions of COMSOL Multiphysics to increase geometry definition and meshing flexibility.
5. Acknowledgements

A contribution of the University of Nebraska Agricultural Research Division, supported in part by funds provided through the Hatch Act, USDA. The authors recognize the valuable support provided by Santosh Reddy Velugoti and MBA Poultry. Special acknowledgements to Dr. Namas Chandra and Shailesh Ganpule for providing access to image processing software. Mention of a trade name, proprietary products, or company name is for presentation clarity and does not imply endorsement by the authors or the University of Nebraska.

6. References


Excerpt from the Proceedings of the 2013 COMSOL Conference in Boston