BLUE WATERS ANNUAL REPORT 2017

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PI: Arif Masud<sup>1</sup>

Collaborators: Soonpil Kang<sup>1</sup>, Elizabeth R. Livingston<sup>1</sup>, Daniel R. Sheehan<sup>1</sup>, Naveed Adoni<sup>2</sup>, Tor Jensen<sup>1,2</sup>

<sup>1</sup>University of Illinois at Urbana-Champaign <sup>2</sup>Carle Foundation Hospital

# **EXECUTIVE SUMMARY**

Modern computational technology provides a platform to take Magnetic Resonance Imaging (MRI) and Computed Tomography (CT) images and construct patient-specific geometric models for high-performance computing (HPC) as well as for 3D printing. Computed data obtained from numerical simulations can be converted into graphical images and used for clinical diagnostics as well as for vascular surgical planning. Geometric models can be used for developing STereoLithography (STL) files for 3D printing and generating patient-specific prototypes. In this project we focused on HPC aspects and extended and applied our methods [1,2] for blood flow modeling to patient-specific geometries.

### **RESEARCH CHALLENGE**

The basic scientific and medical question that this research is aimed to address is to determine if computational models can provide insights into identifying regions of significant atherosclerotic plaque, luminal narrowing, and loss of wall elasticity. An important aid in the vascular access decision-making process in Transcatheter Aortic Valve Replacement (TAVR) patients is the ability of reproducing three-dimensionally the aortic, iliac, and femoral artery bifurcations from the data obtained from CT angiograms. This research helped in developing

software to generate STL files for use in 3D printing. A third facet of investigation was to investigate if CT scan-based virtual models can serve as a "Virtual Patient" and provide an inside view of the arteries, which otherwise is available only through angiography.

#### **METHODS & CODES**

Automated generation of patient-specific models from CT scan images for cardiovascular models and blood flow analysis is still a bottleneck in the application of HPC to clinical applications. This research was focused on developing a framework and software that can take CT scan images to create high-fidelity patient models. Since patient-specific calculations involve uncertainty in the data, a series of numerical simulations were carried out based on statistical distribution of the data. Furthermore, blood artery interaction models are computationally expensive and therefore Blue Waters resources were needed to further explore the mathematical attributes of our non-Newtonian constitutive models as well as the coupling schemes for blood—artery interaction.

CT-Scan Images for Patient Specific Model Construction: Fig. 1 shows CT scan images of the femoral arteries of a TAVR patient. Students in Masud's group developed a computer program that identifies arteries and veins in these cross-sectional abdominal scans. Once they are identified and registered in a given scan, the

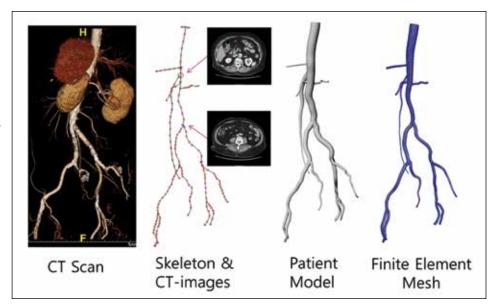


Figure 1: This is the CT Image of the branch structure created using the program developed by students, surface model of the patient, and the computational grid.

program automatically picks a continuation of an artery or a vein in the subsequent image via an algorithm that is based on close proximity of the geometric object to its corresponding image in the previous scan. Once the data is read from the CT scans, a program written by Elizabeth Levingston uses the point cloud method for developing patient-specific arterial tree models that are then used to generate 3D geometric models and Finite Element (FE) meshes. Various stages in the process of development of the model are shown in Fig. 1(c) and 1(d).

Simulation and visualization of patient-specific models: The patient-specific model was solved on the Blue Waters supercomputing platform. Spatial distribution of the pressure field for two time points during the cardiac cycle are shown in Fig. 2. A key step in assignment of outlet boundary conditions is the prescription of unique resistance values for each outlet, based on the morphometry laws. Masud and colleagues have developed dynamic resistance boundary conditions [2] that can accommodate patient-specific clinical data of flow rate distal to the region of interest, into the mathematical model. These boundary conditions help embed clinically measured patient-specific pressure variation into the computational model for a clinically relevant blood flow simulation.

*Employing Data Mining techniques:* Using open source software developed by Sandia National Labs, Daniel Sheehan developed a graphical visualization package that takes the large amount of computed data and converts it into time-dependent images and movies for easy visualization by doctors and clinicians.

3D Printing of Patient Geometry: Soonpil Kang developed a postprocessing capability that takes patient-specific models that are used in virtual modeling and develops STL files for 3D printing of the model. This feature is important for physical experimentation in the lab, thus providing an insight into blood flow rheology in patient specific models that was not possible before.

### **RESULTS AND IMPACT**

Recent advances in computational fluid dynamics and image-based modeling permit determination of flow and pressure from CT scans, without the need for additional imaging, modification of acquisition protocols, or administration of medications. To analyze the massive amount of data in HPC one needs simulation-based images for clinical diagnostics. The software developed by Sheehan can help bring HPC and patient modeling for use by clinicians and surgeons.

## **WHY BLUE WATERS**

Blue Waters was critical for both the development of cuttingedge software and the application of this software to perform large-scale biomechanics simulations. From a computational and algorithmic perspective, the newly developed coupled hierarchical multiscale methods tremendous benefit HPC by exploiting its large local resident memory on the processing nodes in favor of reducing the size of the global problem to be solved.

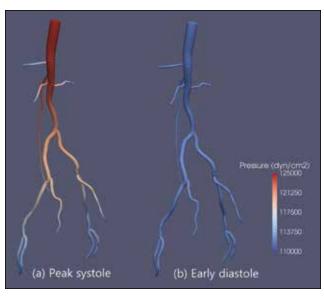


Figure 2: This is the pressure field at two instants in a typical cardiac cycle: (a) peak systole, (b) early diastole.

#### **PUBLICATIONS AND DATA SETS**

Weddell, J.C., J. Kwack, P.I. Imoukhuede, and A. Masud, Hemodynamic Analysis in an Idealized Artery Tree: Differences in Wall Shear Stress between Newtonian and Non-Newtonian Blood Models. *PLoS ONE*, 10:4 (2015), DOI: 10.1371/journal. pone.0124575.

Kwack, J., A. Masud and K.R. Rajagopal, Stabilized Mixed Three-field Formulation for a Generalized Incompressible Oldroyd-B Model, *International Journal for Numerical Methods in Fluids*, 83:9 (2017), pp. 704–734.

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