Toward Coupled Multiphysics Models of Hemodynamics on Leadership Systems

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The goal of this project is to develop a method to simulate flow of realistic levels of cells through the circulatory system, thereby gaining insight into mechanisms that underlie disease progression and localization, or to inform the design of next generation drug delivery systems. Building a detailed, realistic model of human blood flow is a formidable mathematical and computational challenge requiring large scale fluid models as well as explicit models of suspended bodies like red blood cells. This will require high resolution modeling of ~20-30 trillion cells in the blood stream, and necessitate significant computational advances. To date, we have efficiently scaled our algorithms to run on up to 294,912 processors and are working to extend this scalability to allow the study of large regions of the circulatory system. Building on HARVEY, a parallel fluid dynamics application designed to model hemodynamics in patient-specific geometries, we are working to further validate the results through rigorous comparison with in vivo and in vitro measurements. Through the Early Independence Award, we are working to expand the scope of projects to address not only vascular diseases, but treatment planning and the movement of circulating tumor cells in the bloodstream. Development of a precise understanding of cell movement through the vascular system and the likelihood of penetration of the vessel wall is likely critical to achieving the ultimate goal of reliably predicting the vascular regions most likely to incur secondary tumor sites on a per-patient basis. A patient-specific method to predict these patterns will assist in cancer staging, enable identification of unknown primary sites, and inform next-generation treatment therapies that target cancer cells in circulation. We have developed a multiscale computational fluid dynamics model for assessing hemodynamics in image-based arterial geometries, and demonstrated its ability to accurately predict macroscopic quantities related to disease localization and progression. Based on this preliminary data, we hypothesize that (1) cell deformability impacts movement through the vasculature; (2) *in vitro* measurements can both quantify the range of cell-specific parameters and physiological states that should be used in assessing likely metastatic patterns and validate the computational models; and (3) case-specific simulations can assist in the prediction of vascular regions at risk for secondary tumor sites. Here, we will present the current application of HARVEY to the study of cardiovascular disease and discuss the aims designed to test the aforementioned hypotheses as focus is shifted to the study of cancer metastasis and full body circulatory simulations.