

Biosystems Simulation/Modeling

Research:

Greg Burgreen – Mississippi State University

Development of next-generation CFD analysis and design framework

Advanced object-oriented CFD software is being developed. The concept innovatively integrates geometry, analysis, and design using a forward-looking approach. The ultimate goal is to develop a robust framework that CFD researchers can plug into and develop their own specialties and interests as well as any contractual deliverables (multi-phase, aero-elasticity, sens. analysis, turbulence transition, multi-physics). Recent progress has been made in developing non-manifold topology, novel polyhedral mesh representations, and basic discretization classes for convection, diffusion, and source terms. This software will be used in the computational modeling component of the NSF ESPCoR project.

Development of numerical models of platelet activation

This NSF sponsored project is a joint computational/experimental project with the University of Mississippi Medical Center. The goal of this project is to develop new understandings and models of platelet activation subjected to pathophysiological levels of shear stress typical of biomedical prostheses and cardiovascular disease states. We have acquired novel datasets of experimental information that is currently being reduced to mathematical models.

Biomedical fluid simulation for industry and academia

Commercial biomedical devices (blood pumps of Thoratec, Inc. and JarvikHeart, Inc; artificial lung device of ALung Technologies, Inc.) were analyzed using CFD. These results revealed new details of the flow characteristics of these devices to the clients. These efforts are designed to bring attention to MSU at a national level. The long-term goal is to establish the SimCenter as a center of excellence for biofluid computing as our reputation and funding levels grow over the years.

Development of G1-continuous representations of discrete geometry models

Discrete geometry models derive from a variety of sources, e.g., structured and unstructured finite-element mesh generation, computer graphics tessellations, and stereolithography models. Such models are simply a collection of faceted entities that include discrete points, edges, faces, and cells. Like CAD entities, these discrete entities have both a topological and a geometric interpretation and function. However, compared to CAD entities, the topological and geometric roles of discrete entities are much more intertwined. We are implementing techniques to decompose and classify a discrete model into its topological and geometric definitions. We also are developing methods to treat discrete geometric models as an alternative geometry kernel for mesh generation and

simulation purposes. To this end, we assign a triangular quartic Bezier patch to each facet to enable a smooth (G1-continuous) description of a discrete faceted surface.

Keisha B. Walters – Mississippi State University

In Situ Neutron Reflectivity Studies of Tethered pH-Responsive Polymer Layers

Atomic transfer radical polymerization (ATRP) is being explored as a method to develop a chemically and architecturally well-defined series of amine-based polymers. Synthesis and characterization with NMR, ellipsometry, FTIR spectroscopy, and XPS are on-going. Within the next six months, these samples will be analyzed using neutron reflectivity (NR) at Oak Ridge National Lab (ORNL) to ascertain the pH-dependent polymer density profiles as a function of chemistry, architecture, grafting density, and molecular weight.

Development of Bioplastics from Biomass

Polyesters have been produced by condensation polymerization using malonic acid and 1,3-propane diol. Efforts currently focus on optimizing the reaction conditions, including reaction time, temperature, and catalyst. By using the waste products from biofuel production processes as the monomers, bioplastics can be produced with commercially viable bulk and surface properties.

Separation of Specialty Chemicals from Bioenergy Processes

Phospholipids are present in the FAME biodiesel production process. These materials are currently separated and disposed since phosphorous can poison the catalyst and also lead to fouling of biodiesel during long-term storage. We have developed a reaction scheme which cleaves the fatty acids from the phospholipids. This produces free fatty acids which can then be recycled back to the biodiesel feedstock. It also produces a polar head group which we are using to synthesize polymers with novel properties.

Encapsulation of Trace Impurities in Biodiesel through Nanotechnology

Heavy metal contaminants are present in the feedstock used for biodiesel production. These contaminants can poison the transesterification process and must be removed for the biodiesel to reach ASTM specifications. We have developed a novel mechanism for making these heavy metals inert by encapsulation. As the metals are inert, they no longer have a negative impact. The encapsulation process creates nanoparticulates that may be removed by settling, magnetic, or electrophoretic means.

David S. Thompson - Mississippi State University

Enhanced vortex detection and characterization

We have developed the automated capability to extract a vortex, in terms of its core line and the extent of its core region, from large scale computational fluid dynamics

simulation data. Our approach is designed specifically to work with realistic engineering simulation data, which typically involves many data points and only marginally resolved features. Our technique avoids potentially noisy gradient computations to determine the position of the core line and is able to identify distinct branches of complex merging vortex topologies.

Our vortex detection and characterization techniques facilitate visualization of large-scale simulations of complex vertical flows. We are currently using them to study the vortex dominated secondary flows in the small bronchial tubes. A better understanding of these flows will impact our understanding of the deposition of particulates in the lungs.

Robert Hester - University of Mississippi Medical Center

QCP Model

The current QCP model has been enhanced within the past year and the work is supported by this EPSCOR grant. QCP is being converted to XML language and at this time approximately 3000 of the 4000 equations have been converted to open source human readable XML. This software has been continually tested during the conversion process to verify the accuracy of the modeling effort.

We expect that the XML version of QCP will be posted on our web site by Jan 1, 2007. We will continue to translate the remaining variables within the next 3-6 months. This will allow other investigators to add to the model to start our multiscale modeling effort.

David Marcum - Mississippi State University

Geometry Framework

Physics based computational simulation enables scientists and engineers to predict physical behavior. To accomplish this, a numerical representation (computational mesh) of the geometry for all of the objects or articles being simulated is required. Creation of the representation is typically a tedious and time-consuming process for the complex geometry of physical systems. A generalized geometry framework was developed that simplifies and reduces the time required to generate computational meshes for physics based simulation.