VMCS – The Virtual Microbial Cell Simulation Framework

Harold Trease*, Pacific Northwest National Laboratory

Summary

This project combines microbial cell biology and SciDAC technology to build a virtual microbial cell simulation framework, called VMCS. The application for the VMCS is the modeling and simulation of individual microbial cells and communities of microbial cells (i.e., biofilms, flocs, etc.) applied to the bioremediation of heavy metal radioactive waste products. The computational technology for building the VMCS is based on interoperable mesh generation and discretization technology developed by the SciDAC TSTT (Terascale Simulation Tools and Technology) Center, component technologies from the CCA (Common Component Architecture), and solver technology from PETSc.

This project focuses on the development of a computational biology simulation framework, called the VMCS, which supports the modeling and simulation of microbial systems for the bioremediation of heavy metal waste. The overall concept of the VMCS is to combine continuum computational biophysics modeling with discrete metabolic network analysis to simulate the metabolic state of microbial cells within a community by using fundamental biology models that interact with realistic environments. The continuum biophysics algorithms (i.e., reaction, diffusion and hydrodynamics) are used to model the spatial and temporal scales and processes, whereas discrete graph-based network algorithms are used to model the state of the metabolic network for each microbial cell within the community. The metabolic networks are derived from genome-scale metabolic pathway reconstructions. Fig. 1 shows several images of Shewanella microbes interacting with heavy metal substrates and Fig. 2 shows a Shewanella floc containing thousands of individual cells.

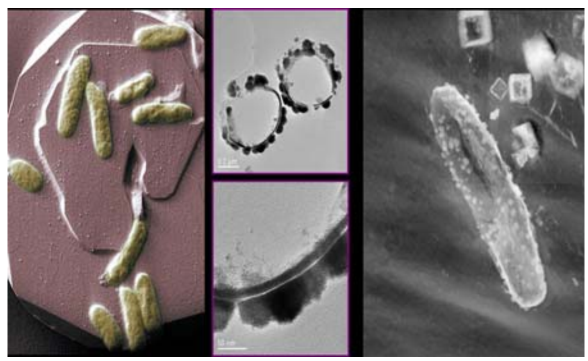

Figure 1. Images of Shewanella microbes and a single Shewanella MR-1 microbe (about 2 um long) with its reconstructed geometry(right) with Uranium crystals attached to it's surface.

The VMCS makes use of the TSTT interoperable mesh capability to combine unstructured mesh generation from NWGrid (PNNL) with the mesh optimization from the Mesquite code (SNL, LLNL) and front-tracking algorthms in FronTier code (SUNY Stoney Brook, BNL). An example computational mesh for the microbial floc in Fig. 2 is shown in Fig. 3.

* 509-375-2602, het@pnl.gov

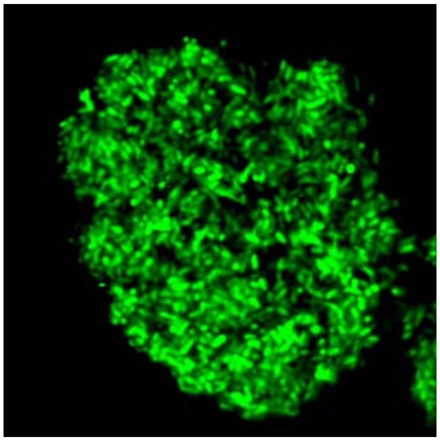

Figure 2. Reconstruction of a floc of Shewanella from confocal micrographs.

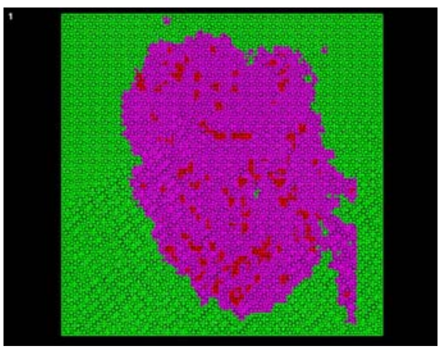

Figure 3. A mesh representation of a floc of Shewanella (right) where each red and magenta nodes represent a Shewanella microbe.

The computational problem to be solved predicts the spatially dependent metabolite flux distribution of each microbe within the community and the distribution of substrate and metabolite fluxes throughout the community volume, based on boundary flux conditions. The solution method is based on a global Flux Balance Analysis method. Fig. 4 shows a calculation of a reaction/diffusion front propagating through a floc of Shewanella. Simulations such as these have provided computational biologists with new insight into the behavior of microbe communities in oxygen rich environments.

Combining fundamental microbial cell biology with state-of-the-art mesh generation and discretization plus advanced, parallel solver technology and other SciDAC technology allows DOE computational biologists to simulate complex microbial systems in a way that was previously difficult or impossible to do.

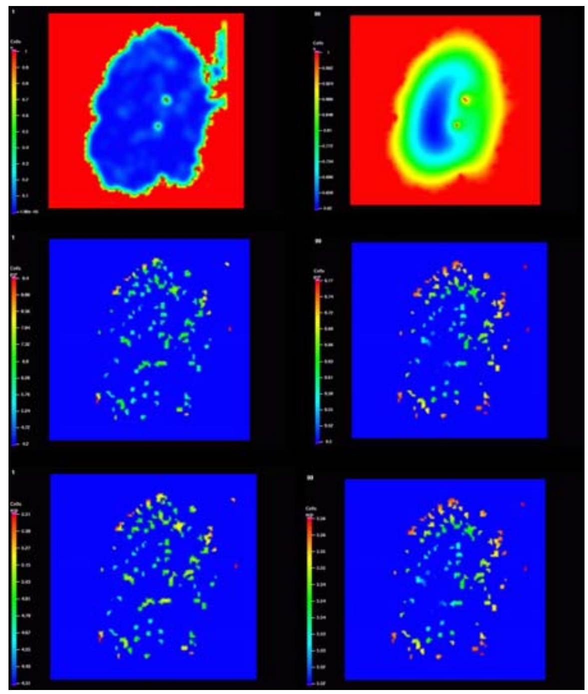

Figure 4. Calculations from VMCS show the propagation of a reaction/diffusion front through a Shewanella floc, initial conditions (left) and final solution (right).

For further information on this subject contact:
Dr. Anil Deane, Program Manager
Mathematical, Information, and Computational Sciences Division
Office of Advanced Scientific Computing Research
Phone: (301) 903-1465
deane@mics.doe.gov