

Madey, G. R., University of Notre Dame, Notre Dame, USA, gmadey@nd.edu
Huang, Y., University of Notre Dame, Notre Dame, USA, yhuang3@nd.edu
Xiang, X., University of Notre Dame, Notre Dame, USA, xxiang1@nd.edu
Chanowich, E., University of Notre Dame, Notre Dame, USA, echanowi@nd.edu
Cabaniss, S., University of New Mexico, Albuquerque, USA, cabaniss@unm.edu
Maurice, P., University of Notre Dame, Notre Dame, USA, pmaurice@nd.edu

Agent-Based Simulation of Biocomplexity: NOM, Mineral Surfaces, and Micro-Organisms

Natural organic matter (NOM) is a heterogeneous mixture of organic molecules found in terrestrial and aquatic environments – from forest soils and streams, to coastal rivers and marshes, to the open sea. NOM plays a vital role in ecological and biogeochemical processes. NOM, micro-organisms, and mineral surfaces can interact to form a complex system with emergent properties. To better understand these complex systems and the mechanisms leading to emergent properties, we develop a Web-based stochastic simulation of NOM, mineral surface, and microbe interactions. Individual molecules, their transport through the soil and in solution, adsorption to mineral surfaces, reactions, chemical and physical attributes and behaviors are simulated using the SWARM agent-based modeling tool. The simulation is configured, started, and viewed from Web-browser pages. Simulation events are stored in a data warehouse, and analyzed using data-mining techniques.