Complex System Simulation: Interactions of NOM Molecules, Mineral Surfaces, and Microorganisms in Soils

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Abstract

Natural organic matter (NOM) is a heterogeneous mixture of organic molecules that is ubiquitous in terrestrial and aquatic ecosystems. NOM plays a vital role in many ecological and biogeochemical processes. NOM, microorganisms, and mineral surfaces can interact to form a complex system with emergent properties, i.e., system properties not present in the parts, but present in the whole system. To better understand these complex systems and the mechanisms leading to emergent properties, we are developing a Web-based stochastic simulation of NOM, mineral surfaces, and microbial interactions, starting with a simple model soil system. Individual molecules, their transport through soil pore waters, adsorption to surfaces, various reactions, chemical and physical attributes and behaviors are simulated using the Java programming language and the SWARM agent-based modeling library (open source software developed at the Santa Fe Institute), Molecules and micro-organisms are modeled as heterogeneous agents with individual properties and behaviors. Molecular properties modeled include elemental composition and major functional groups. Currently 10 first-order and second-order reaction types, sorption to and from mineral surfaces, diffusion, and aqueous transport are the types of behaviors modeled. The simulation is configured, started, and monitored from standard Web-browser pages over the Internet. Configuration of the system includes selecting from standard predefined NOM molecule types and using a "molecular editor" to define new molecular configurations. Each scientist using the simulation has access to a workspace in which every simulation setup, stored molecular configurations, simulation events, and results are stored in a database, and analyzed using standard query commands. Queries can be applied against one or more simulations and reported both in alphanumerical and graphical output. We are designing an online collaboratory built around a data warehouse in which collaborating researchers will merge their simulation data and use data-mining techniques for knowledge discovery, including the discovery of self-organizing emergent phenomena. We use Java Server Pages, Servlets, and Java Database Connectivity protocols to build the Web interface. Our ultimate goal is to make the simulation widely available over the Internet, for interactive use. To provide for scalable reliable service, a loosely coupled infrastructure of application servers and database servers using failover, checkpointing, and automatic restart is implemented.