A Stochastic Simulation of Natural Organic Matter and Microbes in the Environment

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Abstract

Natural organic matter (NOM), a heterogeneous mixture of molecules, plays a crucial role in the evolution of soils, the transport of pollutants, and the change of global weather. The evolution of NOM over time is an important research area in biology, geochemistry, ecology, soil science, and water resource. Due to its complexity and the structural heterogeneity, new simulation approaches are needed to help to better understand the structure and the evolution of NOM. We present a new stochastic model which explicitly treats NOM as a large number of discrete heterogeneous molecules. The NOM, micro-organisms, and their environment are taken together as a complex system, and simulated using an agent-based modeling approach. The global properties of NOM evolution over time can be studied by simulating the physical and chemical reactions between individual agents with temporal and spatial properties.

Unlike the previous stand-alone simulation models, the NOM simulation model serves as an example of E-science, in which we do science on the Web by combining recent information technologies (Java 2 Enterprise Edition, J2EE) with a computational approach. An intelligent Web-based interface is developed to allow scientists to access the remote simulation model from a standard Web browser. The Web-based interface enables scientists to remotely provide parameters for their simulations, start and stop the simulations, and view the results.

The initial users of the NOM simulation model includes a geographically separated group of NSF sponsored scientists from different research areas. A prototype of a NOM "collaboratory" is built to promote collaboration among these scientists and allow them to share their data and information across distributed sites. A XML-based Markup Language, NOML, is provided to build the XML-based Web components and facilitate Web services development in the future.