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Online Collaboratory for NOM Research: Agent-based Simulations, Data-Mining, and Knowledge-Discovery

Computer and web-assisted research in the sciences, sometimes called e-Science, includes internet-based facilities for communication and sharing data, information, and software tools. We describe the design, implementation, features, lessons learned, and future plans for such an e-Science system for supporting NOM (natural organic matter) research. A core feature of the system includes online stochastic simulators, data visualization, and tools for knowledge discovery using data mining on simulation and experimental data. Large numbers of NOM molecules are simulated as individual heterogeneous entities (agents) with unique properties and behaviors. Unlike equation-based approaches, this agent-based approach may uncover the effects of possible but rare conditions, sensitive dependence to initial conditions, and the effects of far from average entities. These conditions may be the source of unexpected or unexplained phenomenon in geomicrobiological systems. We describe an extensive calibration, verification and validation process for the simulations, and discuss how agent-based simulation complements lab and field research on NOM.

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Coupling Dissolved Organic Matter (DOM) Chemistry and Microbial Activity in Aquatic Ecosystems