A Simple Artificial Chemistry Experiment System

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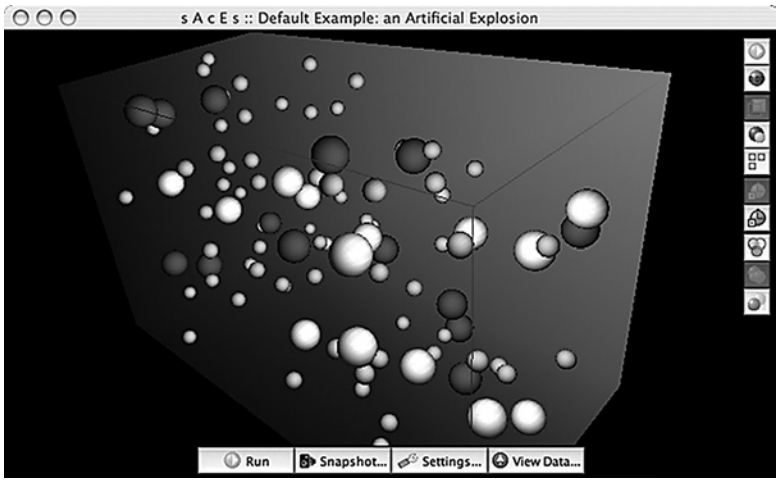
'saces' is a simple tool written in Java which visualizes chemical processes using 3D animation of molecules. It is intended as both an application in artificial chemistry and as an educational tool for students and teachers in chemistry. An artificial chemistry is a man-made system that is similar to a real chemical system. There is a population of molecules, a set of reaction rules and an algorithm which executes the reactions. With artificial chemistry many applications are possible: artificial life, chemistry modeling, massively parallel execution of finite automata, and modeling how to solve NP-complete problems.

'saces' is a simple educational tool which visualizes chemical processes and reactions using 3D animation of molecules. The paradigms of artificial chemistry are helpful when considering a compromise between costly physics based real-time calculations and a more abstract approach to modeling. Artificial chemistry is also in itself a fascinating and important subject.

Adleman demonstrated that computations can be carried out using molecules and solved a “Traveling Salesman” problem using real DNA in 1994. An artificial chemistry can be designed to model DNA computing and their operations. Other applications of artificial chemistry are parallel execution of finite automata, graph rewriting, artificial life, and chemical and biology modeling.

Molecules in artificial chemistry need not always represent physical molecules. Strings, graphs, bit vectors, etc., are also good candidates for artificial molecules. Reaction rules then recombine them in diverse ways. Artificial chemistry is therefore more about speculative thinking than it is an attempt to model chemistry with physical realism. The Conway Game of Life can be viewed as an extremely abstracted form of artificial chemistry.

Despite the level of abstraction dictated by artificial chemistry, 'saces' uses a more concrete model. The molecules are hard, colored spheres which move as an ideal gas in a rectangular reaction vessel. They may collide with each other. If a reaction applies upon collision, the educt molecules are removed from the simulation and the product molecules added. Physical preservation laws for mass, energy and momentum can be modeled where neccessary. A few sample experiments are available: an abstract explosion, a simplified detonating gas explosion, Brownian movement, and others.



Running an ‘artificial’ explosion

More general-purpose experiments are possible. A Lotka-Volterra system models predator-prey interaction. The Lotka-Volterra experiment fluctuates as expected: The number of prey molecules decreases as the number of predators increases. The predators in turn begin to die out when most of the prey has been eaten, giving the prey species a chance to recover. The cyclic nature of predator-prey can therefore be visualized. A finite automaton experiment is also included. The states and the letters of the input alphabet are modeled as molecules. State transitions are reactions of which the new state is the product.

'saces' is developed using Java 5 and JOGL (Java OpenGL) and is available for Windows, Mac OS X and Linux. JOGL is a native wrapper which provides hardware-accelerated 3D graphics to Java applications. Experiments are saved as XML files and validated with XML Schema.

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