MaterialSim: an agent-based simulation toolkit for Materials Science learning

Authors:

Paulo Blikstein, Northwestern University, 2120 Campus Drive, Evanston, IL, 60202, USA
paulo@northwestern.edu
Uri Wilensky, Northwestern University, 2120 Campus Drive, Evanston, IL, 60202, USA
uri@northwestern.edu

Abstract *— Computer modeling and simulation are progressively penetrating the engineering workplace in all fields. However, their use in undergraduate engineering education lags far behind. One of the reasons is that, although there are many commercial simulation packages available, few of them are targeted for learning. Most of these background and "black-box" the actual mathematical models used in the simulation engine, assigning a passive rather than active role to students. That constitutes a considerable drawback for learners, particularly in Materials Science, in which the understanding of basic, atomic-level models is vital. At the other extreme of simulation tools, are generic programming languages. While they are open and "glass-box", they lack the specific tools needed to make modeling in Materials Science feasible for non-programmers. In this work, we present MaterialSim, a multi-agent, cellular-automata based modeling and simulation environment built with the NetLogo language. It occupies a niche between specialized commercial applications and generic programming languages, and is targeted for undergraduate Materials Science courses. On one hand, it provides openness for learners to investigate and redesign specifics of every model. On the other hand, it offers tools that make complex modeling and experiment design approachable for non-programmers. We have implemented libraries to investigate crystallization, solidification, grain growth and annealing, with which students can build their own models and run experiments, or use the sample models provided. One of the main features of the system is to make possible the comparison between real laboratory experiments and computer simulation. This is accomplished with an image import module, which allows the user to import digital pictures of cross-sections of moulds or micrographies as the starting point of the simulation. It also includes various measuring and graphing capabilities, wall and annealing temperature controls, as well as the capability to output data and images for further analysis. Previous research has suggested the benefits of cellular-automata simulation to understand a variety of complex behaviors derived from simple, local rules. MaterialSim offers undergraduate engineering students in Materials Science a new, innovative avenue to investigate and understand complex physical phenomena. Preliminary studies of student use of MaterialSim are being conducted in spring of 2004.*