



Discrete Modeling and Simulation

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During the past few years, the modeling community has given much attention to advancing the performance of its models and simulation tools, aiming to help tackle modeling difficulties and resulting computational burden in almost every field of application. Nevertheless, it has become apparent that, in several physical systems, the solution to the underlying modeling problems lies in the nature of the systems themselves. Thus, advancing the modeling community's abilities through computational tools that can capture a system's essential features—where global behavior arises from the collective effect of simple or discrete components that interact locally—is a rather essential and timely task.

Problems to Solve

Although several mathematical tools and advanced solutions do exist and support the tasks of modeling and simulation in many different aspects, computer scientists and their colleagues are still interested in alternatives that can couple the principles of smaller computational burden and complexity with much wider applicability. Consequently, discrete models with nontrivial behavior have successfully proven to be an appealing computational tool for researchers who want to generate and manage complexity using very simple rules of dynamical transitions.

This special issue deals with the application of discrete modeling and simulation tools to problems from different fields, including physics, engineering, environment science, social science, and life sciences. Many of the authors highlighted here examine the computing abilities and principles of discrete models with a focus on their expressive dynamics, their emergent computation, and their inherent parallelism, making them suitable for high-performance computing. Such models can also successfully tackle the computational bottleneck in terms of the complexity inherent in a variety of numerical simulations.

In This Issue

We received a wide variety of interesting articles for this special issue that represent the unique aspects and novelties of discrete modeling and simulation tools and their applications in several interesting computational science domains.

In the first article, “Eliciting Characteristics of H5N1 in High-Risk Regions Using Phylogeography and Phylodynamic Simulations,” Neil Giridharan and Dhananjai Rao propose a computational approach that couples different agent-based modeling methods to simulate ecological characteristics of avian influenza virus (AIV) epidemics, via the development of prophylactic strategies and vaccines. The introduced agent-based simulation methods include epidemiological simulation and phylogeographic annotations to identify high-risk countries, and phylodynamic simulations to elicit AIVs’ evolutionary characteristics in the aforementioned high-risk countries. The resulting analysis can be used to guide time frames for redesigning vaccines for different geographic regions, prevent and contain outbreaks, guide and focus sampling and surveillance efforts of migratory waterfowl in areas with high antigenic drift, and potentially guide surveillance efforts to assess risk of novel strains emerging at the human-animal interface.

In the second article, entitled, “A Scalable Modeling and Simulation Environment for Chemical Gas Emergencies,” Moon Gi Seok and his colleagues propose a scalable and hybrid agent-based simulation (ABS) model that incorporates an interactive computational fluid dynamics gas flow model for designing countermeasures in the event of an uncontrolled chemical gas emergency. The proposed simulation environment’s requirements are twofold: resolve hybrid simulation between discrete-event and continuous simulations,

and support the combination of various simulators in various domains. The proposed ABS model’s scalability is provided via PDEVs, a parallel discrete-event system specification model of human behavior. The authors implemented a distributed, real-time simulation of a chemical gas emergency for parallel execution of a GPU-based game engine and constructive simulators by utilizing multiple GPUs.

In the third article, “Agent-Based Creation and Simulation of Artificial Social Networks and the Analysis of Their Properties,” Marek Zachara and Cezary Piskor-Ignatowicz propose a lively method for artificially creating a social network, utilizing simulation and a multi-agent environment that enables the design and development of networks with properties similar to those observed in the real world. In such a manner, statistical parameters—the likelihood of the relationship distribution to a power-law distribution and the scaling factor of the relationship distribution—have been selected to enhance the resultant network’s resemblance to natural networks. To achieve a network with real-life properties, the agents need not only to have an opportunity to meet each other and form relations, but they must also be allowed to voluntarily choose the other agents they meet, based on shared interests. The number of these voluntary meetings seems to be one of the primary factors influencing the resultant networks’ parameters.

In the last article, “A Conceptual Modeling and Simulation Framework for System Design,” Eric Coatanéa and his colleagues present the dimensional analysis conceptual modeling (DACM) framework, which intends to offer a solid scientific approach to modeling and simulating early design problems. Although initially developed for military use, DACM has been used in several engineering domains, from redesigning a torpedo system to modeling a laser system and its interaction with metal powders. Concepts on how DACM can be enhanced and utilized as a specification tool are becoming apparent through a set of design structure and design mapping matrices, forming a “fingerprint” of the design problem and the conceptual design solutions.

Clearly, the computational scientists who must proceed with modeling and simulations must overcome the constraints caused by their selected methodologies and tools. In some cases, they might even have

to develop their own tools and methods. This special issue should help *CiSE* readers understand the potential of discrete modeling and simulation and to design and develop their own models and tools. ■

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