

Verifying Parameterized Software Models in Computational Data Science against Behavioral Specifications

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Abstract

Computational data science uses a variety of numerical software models to understand, predict and control the evolution of complex systems. For example, computational systems biology employs multi-scale mechanistic stochastic rule-based models while culturomics uses detailed agent-based models. Because of the inherent uncertainty involved in precisely measuring natural systems, software models employed in computational data science include a number of unknown or imprecisely known parameters. A fundamental problem in developing such software models is to discover the set of parameter values that enable a computational model to satisfy a given set of behavioral specifications. In this talk, we will present a new massively parallel extreme-scale parameter discovery algorithm for complex intelligent software models. We will discuss preliminary results obtained using a parallel implementation of the algorithm on a small 1,792-core CUDA cluster. The talk will also identify opportunities for future research in verifying numerical software being deployed by computational data scientists.