

## From Desktop to Large-Scale Model Exploration with EMEWS

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The increasing use and complexity of computational modeling and simulation in biomedical research has led to the need to augment the workflows involved in the development, calibration, analysis, validation and eventual use of these models. As many of these workflows utilize repeated ensembles of simulation runs, computational constraints can limit the scale and scope of such investigations, and therefore we propose a framework, Extreme-scale Model Exploration with Swift (EMEWS) that can automate the process of carrying out very large-scale simulation experiments while utilizing computational capabilities of modern and forthcoming high-performance computing (HPC) resources. EMEWS enables the combination of existing capabilities for model exploration approaches (e.g., model calibration, metaheuristics, data assimilation) and simulations (or any “black box” application code) with the Swift/T parallel scripting language to run scientific workflows on a variety of computing resources, from desktop to academic clusters to Top 500 level supercomputers. We present two use-cases for EMEWS: 1) examination of the factors and patterns of mutational events of oncogenesis in population level simulations of a mechanism-based ABM of colorectal cancer (CRC), and 2) a complex adaptive parameter space workflow for calibrating a colorectal cancer model (CRC-SPIN) with the use of Incremental Mixture Importance Sampling (IMIS). The tutorial for EMEWS can be found at <http://www.mcs.anl.gov/~emews/tutorial/>.