

The DAKOTA software package from Sandia National Laboratories has a large selection of algorithms in its library that can be used for performing sensitivity analysis, optimization, and uncertainty quantification. The package can be coupled to a simulation by providing inputs to the simulation and analyzing the outputs. We have applied DAKOTA's analysis to a random walk to the minimum of the Rosenbrock Test Function $f(x, y) = 100(y - x^2)^2 - (1 - x)^2$. We have also examined DAKOTA's capability to analyze a Markov Chain Monte Carlo (MCMC) process that is used to simulate the Ising Model. This code generates a probability distribution of the energy and magnetization of the macrostate using MCMC and parallel exchanges. Additionally, we will use DAKOTA to solve a problem in geometry about sphere packings on the surface of a cylinder. We want to wrap strings of spheres around the surface of a cylinder. These strings start from the same point, can vary in length, and are wrapped at different angles around the cylinder, essentially making two helices around the cylinder. The distance between the last sphere in each string can be measured as the error, which can be minimized by DAKOTA, eventually making the two strings into one continuous loop. DAKOTA, when run as an executable, will treat a user's simulation as a "black-box", with no access to the source code of a simulation. However, when running DAKOTA this way, it must use external files to communicate. Thus, we take advantage of DAKOTA's direct application interface to couple the algorithms more directly to the simulation and avoid this I/O bottleneck. This mode comes with other improvements, especially when run on a supercomputer. In this poster, we will present the results of the analysis from these examples, and illustrate how DAKOTA can be run on Darter, a supercomputer available at the National Institute for Computational Sciences (NICS).