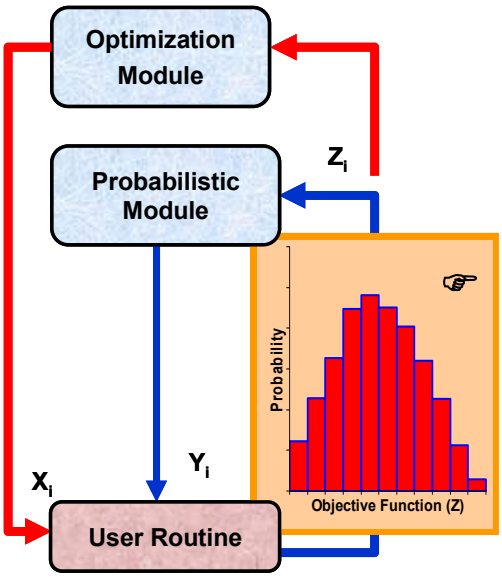
OAK RIDGE NATIONAL LABORATORY FACT SHEET
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Scientific Computing Within the ORNL Modeling and Simulation Group: SuperCode - Problem Solving Environment for Optimization and Uncertainty Analysis

The ORNL Modeling and Simulation Group (MSG) develops sophisticated numerical solutions for a wide range of scientific, engineering, and operational applications. MSG's core competency is computational physics and engineering, and within this context we must frequently quantify problem uncertainties and identify optimal solutions for both *continuous* and *discrete* figures-of-merit. Classes of worked problems within this focus area include non-linear constrained optimization, statistically-independent uncertainty analysis, as well as coupled optimization and uncertainty analysis. Applications include technical and economic studies for design of fusion energy reactors, advanced thermodynamic analysis, pharmacokinetic optimization, pollutant fate and transport, and neutron-source subsystem design. The primary software tool developed by MSG for conducting such analyses on small to medium sized problems is ***SuperCode.*** ***SuperCode*** is a robust software suite for conducting optimization and probabilistic analysis in support of systems design and programmatic decision-making. It combines a sophisticated analysis capability with an extremely flexible problem-solving environment. On a macroscopic level, it permits one to integrate user-supplied process models, programmatic objectives and constraints, and technical uncertainties into a coherent analysis framework. Microscopically, it allows the user to conduct a wide range of sophisticated analysis to characterize problem physics. This multi-level functionality is derived from three major features: an upper-level driver shell, the ability to utilize problem-specific user-supplied process models, and a unique library of optimization and uncertainty-analysis modules. These capabilities are briefly described below.

- The object-oriented interactive programmable driver shell permits (a) real-time problem formulation without recompiling process models, (b) coupling process models to the internal optimization and uncertainty modules, and (c) iterative execution and results visualization.
- Non-linear optimization capabilities include (a) a large number of bound or unbound variables and constraints, (b) equality or inequality constraints, (c) the ***VMCON*** Lagrangian algorithm for *local* evaluations and the ***GALIB*** genetic algorithm for *global* evaluations, and (d) the ***OPTQUEST*** commercial genetic optimization package.
- Uncertainty analysis capabilities include (a) a large library of statistically-independent probability distribution functions as well as (b) Monte Carlo and Latin HyperCube sampling techniques.
- Coupled optimization and uncertainty analysis to evaluate the impact of uncertainties on optimal designs. These unique capabilities include *(a) uncertainty-constrained optimization* which defines an optimum objective function with either a specified level of uncertainty **or** a minimum uncertainty, and (b) *uncertainty with sub-optimization* which defines a probability distribution for the objective function where each value in the distribution is an optimum point.

SuperCode is a mature, robust, and extremely versatile modeling and simulation resource for systems-design and programmatic decision making for a broad range of R&D, industrial, homeland defense, and military applications. We welcome the opportunity to discuss your potential applications and ways ***SuperCode*** can contribute to a solution.



MSG developed SuperCode for optimization & uncertainty analysis to support system design & programmatic decision making

POC: David M. Hetrick
(865)576-7556/hetrickdm@ornl.gov
http://computing.ornl.gov/cse_home/cms/cmshome.shtml