SAND2008-4718P

Proposal to the GNEP Advanced Fuel Cycle FOA

Simulation, Optimization, & Uncertainty Quantification of the Advanced Fuel Cycle

Summary of Proposed Project

Description: This project will provide the capability to perform systems level simulation, optimization, & uncertainty quantification on the Advanced Fuel Cycle**.** The proposed project will leverage our Omega Sandia-developed software development tool which allows us to rapidly produce systems analysis simulators for specific customer applications. In addition, we will make use of a recently-developed robust optimization methodology intended to be placed within the Sandia's DAKOTA optimization toolkit. The first year's work will focus on building a simplified Advanced Fuel Cycle system simulator using Omega, introduction of robust optimization & uncertainty methods into DAKOTA for discrete-event and agent-based systems, and a demonstration to simulate, optimize, and perform uncertainty quantification on a simplified Advanced Fuel Cycle system.

Relevance to FOA: This project addresses one of the seven elements in the FOA (Advanced Fuel Cycle Systems Analysis). In particular, the resulting software will provide the underlying capability to model the Advanced Fuel Cycle System with respect to safety, security, waste management, economics, long-term-sustainability, and affordability. In addition, robust optimization and uncertainty quantification will be an integral part of the software package. The success of GNEP will hinge on the development of optimal (or near-optimal) system implementations which are safe, economically attractive, physically realizable, can be integrated into the existing electric power infrastructure, acceptable to the public, and present a minimum risk of proliferation despite the substantial uncertainties in almost all aspects of the model.

Project Director: Ken Sorensen/JD Smith

Principal Investigator: John Siirola

Team Members: Bill Hart, James Overfelt, JD Smith

Potential Recipient: Sandia National Laboratories

FY09 Budget: $500K

Technical Approach

General Technical Approach: The proposed project will utilize our Omega software development tool allowing us to produce a systems analysis simulator for the Advanced Fuel Cycle. Sandia's DAKOTA optimization toolkit will then be used to provide the capability to optimize and perform uncertainty quantification on the Advanced Fuel Cycle. We plan to make use of agent-based optimization (ABO) which provides a very robust optimization methodology for the present problem. As part of this work, we will add ABO to the set of optimization methodologies residing within DAKOTA which will also extend DAKOTA's uncertainty quantification capability.

Omega: The Sandia developed Omega software development environment supports general discrete-event (DE), systems dynamics (SD), and or agent-based (AB) modeling paradigms. Omega provides a modular GUI-driven environment designed specifically for modeling networks of complex, hierarchically defined components. Individual modules containing AB, SD or DE representations may be created and removed from the model along with changes in network connectivity during the course of a simulation. This greatly facilitates the ability to represent evolutionary and dynamic behaviors of a system. As a result of the inherent modularity, explicit model hierarchy, and dynamic system configuration, models based on Omega are flexible and can easily expand both in scope and complexity as warranted by application needs. For the present demonstration, the Omega modules will be populated by component models that represent a simplified Advanced Fuel Cycle system. It is anticipated that the demonstration model will be a hybrid mix of SD and AB modules where the SD models represent highly aggregated phenomenon and the AB models more fine-grained behavior.

DAKOTA: The Sandia developed Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) toolkit provides a flexible, extensible interface between analysis codes and iterative systems analysis methods. DAKOTA contains algorithms for optimization with gradient and nongradient-based methods; uncertainty quantification with sampling, reliability, and stochastic finite element methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study capabilities. These capabilities may be used on their own or as components within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty. Part of the present project will be to introduce agent-based optimization (ABO) and related uncertainty methods into DAKOTA. ABO provides a capability needed for DE and AB simulations since other optimization and uncertainty methods are not very robust in dealing with the discrete nature of AB and DE formulations.

ABO: In agent-based optimization, individual agents embody different optimization strategies. By interacting and sharing potential solutions the individual agents build on each other's successes. In this sense, ABO leverages many of the concepts from conventional hybrid optimization strategies, but on a much larger scale. This produces a system which is much more robust than the individual member-agents and can solve problems that could have otherwise been intractable for any of the member-agents individually. ABO systems scale well in parallel and can leverage massively-parallel high-performance computing resources to efficiently solve both complex single- and multi-objective optimization problems.

Summary: The project goal is to provide a simplified but extensible systems simulator for the Advanced Fuel Cycle (AFC), provide necessary enhancement of capability to the DAKOTA toolkit, and demonstrate multi-objective optimization under uncertainty for a simplified Advanced Fuel Cycle systems model.

FY09 Project Milestones

Task 1: Develop a simplified extensible systems simulator for the AFC
Task 2: Provide necessary enhancement of capability to the DAKOTA toolkit
Task 3: Demonstrate multi-objective optimization under uncertainty for simplified AFC

Team Members

John Siirola who will serve as the project PI is the principle developer of Omega and an expert on ABO, James Overfelt has experience in developing customer applications using Omega, Bill Hart has a working knowledge of both ABO and DAKOTA, and J D Smith is an expert on nuclear energy systems modeling.