Securing the Atom – Using Advanced Simulation to Look Ahead to 21st Century Nuclear Energy

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Nuclear energy could grow rapidly in the coming decades, driven by two major factors – - expanding energy demand occurring in developing nations and requirements for emission-free energy production derived from regional or global environmental needs.

Historical data indicate that energy use is linked to prosperity. Typically a nation has reached a "developed" state when its per capita annual electricity use is several thousand kilowatts[1]. In the future an increasing number of nations could meet "prosperity" conditions and simultaneously have significant populations. In the developing world, in addition to China and India, nations such as Brazil, the Philippines, Indonesia, Mexico, Turkey, Thailand, Iran, Columbia (among others) could reside in the top-twenty most populous nations and could achieve energy usage characteristic of developed nations by mid century[2].

Under such scenarios, nuclear energy, nuclear materials and nuclear materials technology could exist in environments very different from that of the past forty years. At issue are what types of nuclear technologies could lead to achieve even higher levels of proliferation resistance, safety, economics, and environmental performance required in the future? What are technology routes and tools that could help create needed nuclear energy and fuel cycle systems optimized for 21st Century needs and implementation?

Meeting requirements of the types indicated above place strains on the nuclear energy infrastructure present in the United States and other developed nations. Nuclear facilities (laboratories, nuclear materials processing, test reactors, and critical assemblies) are often old, in a state of decline, and a significant number have ceased operation. Student populations in areas associated with nuclear energy (nuclear engineering and physics, materials science, actinide chemistry,…) are also decreasing.

At the same time, capabilities in advanced simulation and massive computational power have grown substantially. Nuclear weapons stockpile certification, a technology area having major parallels to the nuclear energy area, has adopted massive simulation (through the Advanced Simulation and Computing Initiative (ASCI)) as a means of meeting its needs in the absence of nuclear testing. The simulation philosophy of the ASCI program is to incorporate detailed models of processes and systems on a multidimensional scale (microscopic, macroscopic, to full systems levels) that are then run on large, massively parallel computers. A similar approach could be developed and employed for nuclear energy system design and nuclear materials control. Two example areas are presented.

Enhanced integration and optimization of proliferation resistance and safeguardability into fuel cycle facilities and operations

Future nuclear energy demand scenarios could lead to larger-scale and more widespread implementation of closed fuel cycles (ones where spent reactor fuel is reprocessed to recover plutonium and higher actinides which are further consumed in reactors). For the first half of the 21st Century, thermal reactors (light water, heavy water, or gas-cooled) will probably represent the mainstay for nuclear energy production. At the same time, recovery of plutonium and higher actinides, as well as certain long-lived fission products, followed by their burning or transmutation, could see widespread implementation as a means to reduce the number of geologic repositories required for a once-through nuclear fuel cycle (as presently implemented in the United States). In closed cycle systems, inherent proliferation resistance and safeguardability attributes protect against nuclear materials theft, materials diversion, and/or national efforts to acquire materials from civilian nuclear energy facilities and/or technology.

The past development and construction of nuclear materials facilities have often approached safeguardability as an "add on" -- *ie* detection and material control systems are implemented once a design has been largely developed. Two simulation-based approaches can be used to integrate and optimize, in an *a priori* fashion, facility operations and safeguards. The first is detailed facility simulation models that include features describing

- The tracking of materials (plutonium, uranium, …) inventories through all processes;
- microscopic materials separations flowsheets;
- all relevant process operations including equipment performance description, material inventories, and transfer lines; and
- measuring instruments performance and expected data; and
- a wide variety of process logic options.

Earlier [3] versions of such nuclear material facility simulators have been used to assess the performance of facilities such as the Rokkasho reprocessing plant under construction in Japan. Newer approaches, based upon dynamic systems simulation, that utilize commercially available platforms such as EXTEND™, offer the potential for expanded capabilities and flexibility.

A second promising method lies in the utilization of multimillion-dollar gaming industry engines to create true-to-scale interactive, virtual environments. Such approaches (for example the Virtual Interaction Simulation and Inspection Tool (VISIT)[4]) allow development of three-dimensional interactive architectural and outside-world representations that can be true to scale and operation. These methods can provide visual details and simulated processes for replication of real physical locations (equipment, facilities, buildings) and environments, and can allow multiple users to interact in the same virtual environment.

The development and use of such tools could provide increased confidence in the operability and safeguardability of future nuclear material facilities by exploring computationally the effects of alternative processing methods on the operating characteristics of a proposed facility, by computationally evaluating nuclear material inventories and associated detection systems, and by allowing evaluation of "what if" scenarios to maximize resistance of facilities to materials diversion and misuse.

Advanced Simulation - The Numerical Reactor

Future implementation scenarios for nuclear energy will place increased emphasis on the operational performance of nuclear reactors and associated systems. Safety will be continue to be of paramount importance as the number of reactor operating years increases worldwide. Traditional reactor safety requirements may have to extend well beyond traditional limits to include situations where deliberate actions (terrorist, insider threat) could maximize negative impacts normally associated with a severe reactor accident. Today a number of uncertainties exist pertaining to the description and assessment of severe reactor accidents. They include the interaction of fission products with the reactor vessel and containment, core melting and subsequent interaction between a molten core and concrete, containment response and failure modes, and, overall, the validation of diverse computer codes used to model complex sequences of events.

Advanced simulation, coupled with modern computational power, could provide powerful tools to further enhance the robustness of future reactor systems. For example, reactor safety codes were largely written in the 1970's when supercomputers were one-thousand times slower and had roughly one-thousands of the memory of today's supercomputers. Such computers (and codes) use approximation algorithms to solve necessary partial differential equations for representation of two-phase flow. These approximations create numerical errors, violate energy conservation, etc. Modern computers and numerical methods can allow simultaneous, and accurate, solution of non-linear, coupled sets of partial differential equations describing two-phase flow with conservation of mass, momentum, and energy in both phases.

In analogy with the ASCI example mentioned earlier, a virtual or numerical reactor simulation system could be created having the following features:

- the description in three dimensions (plus time-dependent behavior) of microscopic processes involving particle transport, materials response, chemical kinetics, and time-dependent nuclear data;
- meso and macroscopic descriptions of thermal hydraulics, radiation damage, fuel performance and burn, subsystems including heat exchangers, safety and control, and power conversion as well as system interfaces and feedback processes;
- systems levels descriptions including containment structure performance and creation of "virtual" assessment environments.

"Models" currently exist that point to the end product for such a simulation system (or for key components). One example is the MCNP Monte Carlo particle transport code[5] that operates within state-of-the-art parallel computing environments and allows computation of transport phenomena within sophisticated geometrical environments. Another recent, and very pertinent model for a numerical reactor simulation system is the multinational REVE (Reactor Virtual Experiment)[6] effort. This project aims at quantitative simulation of irradiation effects in materials, thus complementing and eventually replacing presently-used empirical approaches. An eventual computational system, benchmarked with suitable experimental data, could reliably move simulation from interpolation between known data to prediction into performance areas lacking in experimental data.

These two examples illustrate the power and potential of advanced computing and simulation as applied to advanced systems for nuclear energy and nuclear materials control. Developing and applying results of such systems could engage and attract new talent into an important national and international need area. Equally important, such capabilities could be a cornerstone for the development of safe, secure, and cost-effective nuclear energy systems needed for the 21st Century.

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