CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: Joint International Topical Meeting on Mathematics & Computations and Supercomputing in Nuclear Applications (M&C+SNA 2007)
Project No. 20.06002.01.212; AI No. 06002.01.212.706

DATE/PLACE: Monterey, California, April 15–19, 2007

AUTHOR(S): Scott Painter

PERSONS PRESENT: S. Painter, Center for Nuclear Waste Regulatory Analyses (CNWRA), and several hundred attendees from various countries

BACKGROUND AND PURPOSE OF MEETING/TRIP:

The M&C+SNA 2007 meeting showcased the role of high-performance scientific computing in all aspects of design and development of nuclear systems. The conference was sponsored by the American Nuclear Society. The Nuclear Energy Agency of the Organization for Economic Cooperation and Development and the Computational Science and Engineering Division of the Atomic Energy Society of Japan were international cosponsors.

S. Painter attended the conference on April 19th to

- Present a paper authored by CNWRA staff
- Co-chair a session on Computational Methods in the Nuclear Fuel Cycle
- Attend presentations addressing various computational issues relevant to the high-level waste program

SUMMARY OF PERTINENT POINTS:

All five papers in the session Computational Methods in the Nuclear Fuel Cycle were related to geological disposal of nuclear waste. The session was organized by S. Mohanty of CNWRA.

H. Umeki of the Japan Atomic Energy Agency presented the paper A Challenge for Computing in the 21st Century: Radwaste Knowledge Management. His presentation, a short version of the one he made at CNWRA on Friday, April 13, 2007, summarized recently initiated efforts to develop a knowledge management system to accommodate the vast amounts of information being generated in studies of radioactive waste disposal.

Two of the papers were from French research groups. A. Genty (Atomic Energy Commission of France) presented Radionuclide Transport Calculations from High-Level Long-Lived Radioactive Waste Disposal in Deep Clayey Geologic Formation Toward Adjacent Aquifers. That work uses a spatial discretization scheme based on the finite-volume method with multipoint flux approximation. A massively parallel approach based on domain decomposition is being used to resolve highly heterogeneous three-dimensional regions with a fine spatial grid. M. Dymitrowksa from Institute of Radioprotection and Nuclear Safety also presented large

three-dimensional radionuclide transport calculations using domain decomposition. Her simulations used the finite-element/finite-volume method and were executed on a small cluster of workstations.

K. Tsujimoto (Mitsubishi Materials Corporation) presented the paper Uncertainty Analysis of Multiple Canister Repository Model by Large-Scale Calculation. The work investigated the possibility of explicitly resolving an entire site-scale fracture network in a flow/transport simulation. The simulations were performed on the Earth Simulator computer—a hierarchical system with vector processors at the lowest level. Several vector processors are grouped together in a shared-memory configuration to form one of many nodes. Parallelization within each node was performed by the compiler, and parallelization across the nodes was by domain decomposition with explicit message passing. Even with this leadership-class computer, transport in the full three-dimensional domain could not be simulated without homogenizing part of the discrete fracture network. The magnitude of this computational challenge underscores the need for efficient algorithms and carefully designed computational strategies when considering transport in sparsely fractured rock that may be difficult to represent with continuum transport models.

S. Painter (CNWRA) presented Sensitivity of Repository Thermal-Hydrological-Chemical Simulations to Choice of Numerical Algorithms. That work was coauthored by J. Myers and A. Sun (CNWRA) and L. Sabido (subcontractor to CNWRA). That presentation described systematic investigations of methods for coupling transport and reactions for strongly nonisothermal systems. These investigations are part of ongoing work to understand the anticipated near-field conditions for the potential repository at Yucca Mountain, Nevada. Advantages and disadvantages of various coupling methods are well understood for isothermal systems, but relatively little work has been done on similar considerations for systems that reach above-boiling temperatures. The studies demonstrate that split operator methods, which are often used for their relative computational efficiency, are inadequate for strongly nonisothermal systems. For example, the split operator methods were characterized by significant numerical artifacts and generally failed to reproduce mineralization patterns produced by more accurate fully coupled simulations. The studies demonstrate that ongoing MULTIFLO simulations should continue to use the more computationally expensive fully implicit numerical schemes.

The plenary session of April 19th contained two presentations of interest. Professor P. Turinsky (North Carolina State University) presented Improving Nuclear Power Economics Via Utilization of High Performance Computing. He noted that current practice uses multiple conservative assumptions in calculations of fuel centerline temperatures to avoid computationally demanding simulations. The use of multiple conservative assumptions to bound mutually uncorrelated uncertainties results in extremely conservative operating limits on reactor power output, which significantly affects reactor economics. Professor T. Downar (University of California, Berkeley) presented High Performance Computing in Nuclear Systems: Lessons Learned from Some Recent LWR Applications. Multiscale and multiphysics simulation was a theme in that presentation.

A session on multiphysics simulation was held on the afternoon of April 19th. Many of the presentations addressed generic computational issues of interest to CNWRA/NRC work. Particular attention was devoted to strategies for coupling different processes in multiphysics codes.

SUMMARY OF ACTIVITIES:

S. Painter presented NRC-funded work, co-chaired a session, and attended various presentations on computational methods.

IMPRESSIONS/CONCLUSIONS:

The Fuel Cycle session was sparsely attended relative to other parallel sessions, with 5 papers from 3 countries and an audience of approximately 20. The session did provide a useful perspective on different computational approaches taken by different high-level waste programs. More generally, two generic issues addressed by many of the presentations, multiscale and multiphysics simulations, are highly relevant to high-level waste repository program, and it was useful to see how researchers in other fields are approaching these issues.

PROBLEMS ENCOUNTERED:

None.

PENDING ACTIONS:

None.

RECOMMENDATIONS:

Continued participation in this and similar computationally oriented topical meetings is recommended.

REFERENCES:

None.