Task 12

Radiation Transport Modeling using Parallel Computational Techniques

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BACKGROUND

One of the most significant tools available for the design and analysis of accelerator-driven systems, such as the systems proposed for transmutation, is the high-energy particle transport code MCNPX. The MCNPX code suite, developed by the national laboratories, allows researchers and engineers to model the complex interactions of high-energy particles with the target and related systems, including the spallation reaction and subsequent neutron multiplication expected in the accelerator targets.

The next stage in the development of the MCNPX code suite is to validate the code by comparing the theoretical predictions from the models with experimental observations. Additionally, the nuclear database, particularly the cross sections (i.e., reaction probabilities) for high-energy particle interactions, needs to be revisited to reduce the uncertainties associated with key nuclear properties.

The Department of Energy, through its national laboratories, has initiated several experiments geared towards removing uncertainties in the MCNPX libraries, with more in the planning stages. These experiments utilize the proton and neutron beam lines at the LANSCE proton accelerator at the Los Alamos National Laboratory to irradiate a target, producing a pulse of neutrons which are observed by the experimenters. The results of these experiments are then compared against the predictions from the MCNPX models of the system. By comparing the predicted system behavior to the data acquired from the experiments, the experimenters will be able to validate the MCNPX code and its nuclear data libraries.

Through this project, UNLV researchers are involved in support of these experiments by developing the system models in MCNPX and benchmarking/validating the models against the experimental results. UNLV students have also been involved in conducting experiments at LANL and in assisting researchers in designing new experiments.

RESEARCH OBJECTIVES AND METHODS

The second year of this project involved modeling several aspects of the LANCSE beam experiments:

- Modeling targets of varying diameter in air, in a vacuum, and in the presence of humid air;
- Modeling various proton beam profiles;
- Modeling the effects of off-axis proton beam impingement on the target;
- Modeling the asymmetry introduced by the steel table below the target;
- Modeling the effect of varying ratios of Pb to Bi and the effect of impurities; and
- Modeling the system, including other structures within the test room.

With the experience gained through modeling these systems, the UNLV researchers plan, with the assistance of their national laboratory collaborators, to develop a benchmark program for the neutron leakage tests and other tests related to transmuter development. A comprehensive three-dimensional computer-aided design (CAD) image of the LANSCE experiments was prepared using ProEngineer to help benchmark the experiments and provide accurate geometric data for MCNPX modeling.

RESEARCH ACCOMPLISHMENTS

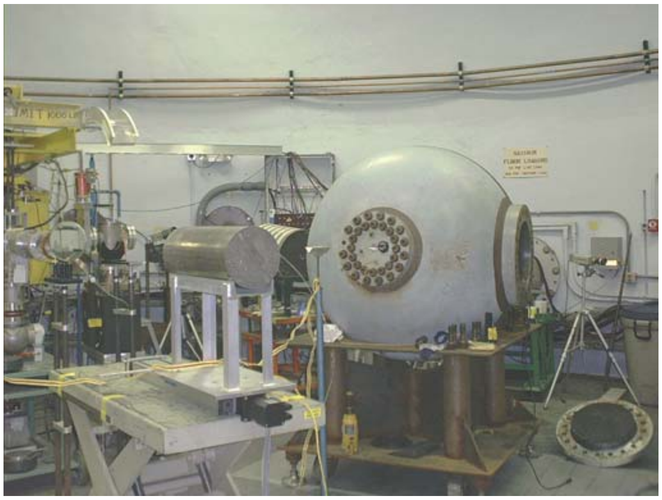
Undergraduate student Daniel Lowe worked on neutron spallation tests at the LANSCE facility (Summer 2002). He performed MCNPX runs and worked on calculations for initial benchmarking data. His early MCNPX calculations helped the experimenters determine where foil packets should go and what types of neutron flux to expect from these foils. He also prepared foils to determine neutron flux from the experiment and assisted in radiation counting of the foils. Mr. Lowe completed Solid Works CAD models of the Blue Room at LANSCE and conducted MCNPX simulations of the summer experiments when he returned back to UNLV. His MCNPX runs included estimations of the effect of the proton beam striking the target at positions slightly off of the centerline. He also estimated the neutron energy spectra expected from the time-of-flight neutron detectors.

Through MCNPX simulations of the neutron leakage from lead-bismuth targets, the UNLV team was able to assist in the design of the experimental configurations for the LANCSE experiments. These models were also used to predict the results for the experiments, and assist in positioning detectors for measuring the leaking. Similar computational support was also provided for proton activation experiments in sodium coolant.

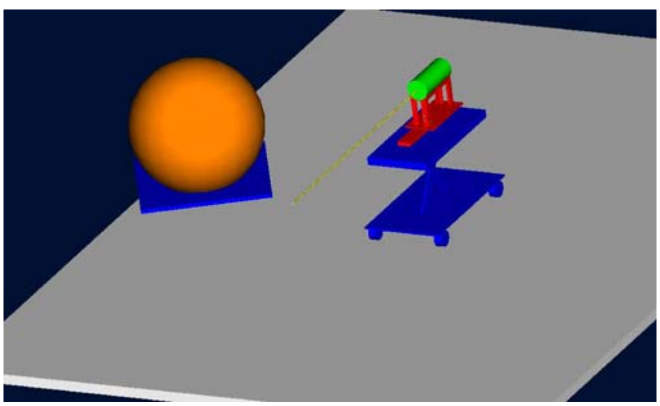
Extensive studies on how MCNPX performs with respect to MPI (Message Pass Interface) and PVM (Parallel Virtual Machine) have been run. PVM will no longer be supported by the LANL team after 2005, hence more emphasis is being put on how MCNPX runs with MPI on Beowulf system.

Parallelization of MCNPX for a Parallel Virtual Machine was completed. Efforts began to resolve Message Passing Interface (MPI) bugs and compiling problems.

Analysis of linearization characteristics on a Beowulf cluster was completed. Work was then focused on characteristics of the Supercomputing Center and the linearization of criticality studies.



Experimental facility at LANSCE, Los Alamos, NM.



Schematic of the experimental facility at LANSCE used for modeling.

HIGHLIGHTS

- "Properties of Photo-neutron Sources for Accelerator Driven Sub-Critical Systems" presented at the ANS Conference, San Diego, CA, June 1-5, 2003.
- "Measurements from Activation Foils of a Proton Irradiated Lead-Bismuth Target" presented at the ANS Conference, San Diego, CA, June 1-5, 2003.
- "MCNPX on Heterogeneous Clusters Using PVM and MPI" presented at the ANS Student Conference, Madison, WI, April 1-4, 2004.
- "Benchmarking Photo-Neutron Predictions from MCNPX" presented at the ANS Student Conference, Madison, WI, April 1-4, 2004.
- A 16-processor LINUX cluster, coupled to a 4-processor system, was developed. This system will be used to run the parallelized version of MCNPX.

FUTURE WORK

The primary focus of the ongoing work in this project consists of the continued benchmarking and optimization of MCNPX to run on multiple platforms. This insures that the user will not be limited to a specific system type when running simulations. In addition, the MCNPX simulations of planned and future experiments will continue. Along with the work to implement MCNPX on multiple platforms, user guides will be developed for future users.

They will describe how to implement an optimized version of MCNPX on a heterogeneous cluster using a Message Passing Interface. Efforts to increase the speed of MCNPX on parallel clusters of computers will be initiated. Researchers will also begin the preliminary development of a graphical user interface (GUI) for MCNPX, using open source code and tools. Codes developed for this program will be made available to Advanced Fuel Cycle Initiative researchers.

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