Project Continuation Proposal

Project Title:

Radiation Transport Modeling using Parallel Computational Techniques

Principal Investigator (PI): William Culbreth, Ph.D.
Department of Mechanical Engineering, UNLV
4505 Maryland Parkway
Las Vegas, NV 89154-4027
(702) 895-3426
FAX: (702) 895-393, culbreti@clark.nscee.edu
http://www.nrcc.unlv.edu

Collaborators (LANL): Laurie S. Waters
Los Alamos National Lab
P.O. Box 1663, Los Alamos
NM 87545
(505) 665-4127
FAX: (505) 665-2897
lsw@lanl.gov

Collaborators (UNLV): Trevor Wilcox, M.S. Math, M.S. Mech. Eng.
Research Associate & Systems Analyst
wilcox@nrcc.unlv.edu

Suresh Sadineni, M.S. Mech. Eng.
Suresh@nrcc.unlv.edu

Daniel Lowe
Research Assistant
lowe@nrcc.unlv.edu

Mechanical Engineering
Department of Mechanical Engineering, UNLV
4505 Maryland Parkway
Las Vegas, NV 89154-4027
(702) 895-1331
FAX: (702) 895-3936
http://www.nrcc.unlv.edu

AFCI Research Area: Transmutation Sciences

Requested Funds: $101,247 (Year Three)

Radiation Transport Modeling Using Parallel Computational Techniques

Abstract:

The Advanced Fuel Cycle Initiative (AFCI) program will rely on the use of accurate calculations and simulations of criticality and shielding for the separation process of the long-lived isotopes that present a significant safety hazard in commercial spent fuel. To help design and verify the safety of the separation process, the neutronics code MCNPX will be used to model the distribution of neutron flux within the fuel blanket and to determine the neutron multiplication, k_{eff}. However, the cross section libraries and computational methods used by MCNPX at these neutron energies still have some uncertainty and will require validation.

Over the past two years, the faculty and students on this project have worked with researchers at Los Alamos National Laboratory (LANL) and the Idaho Accelerator Center (IAC) to use MCNPX in support of the work on the Transmutation of Nuclear Waste. During this effort, our students have traveled to LANL and the IAC to support projects on neutron production using both proton and electron accelerators. A parallel cluster of 20 computers has been assembled at UNLV to support these MCNPX simulations.

Currently MCNPX relies on a hand created input deck, which can be time consuming to produce and prone to errors. One way to solve this problem is to create a graphical user interface (GUI) to help the user create the input deck. Also, to achieve accurate results in a short period of time there is a need to increase the efficiency of the parallel version of MCNPX. We propose to involve UNLV students and faculty in this endeavor to create a GUI, to increase the speed of MCNPX on parallel clusters of computers, and to continue application of MCNPX to solve practical AFCI problems.

Fig. 1 Researcher Trevor Wilcox and the UNLV MCNPX Computer Cluster

Work Proposed for Academic Year 2003-2004, Goals and Expected Results:

The project proposed for year three of the project will consist of three parts:

- Optimization and validation of MCNPX on multiple platforms using Message Passing Interface (MPI).
- Create a graphical user interface (GUI) to help users generate input files for MCNPX.
- Continue MCNPX simulations in support of AFCI work.

The UNLV team working on these topics is composed of Suresh Sadineni, a doctoral mechanical engineering student, Danny Lowe, a senior in ME, Trevor Wilcox, a special graduate student in ME, and Dr. Culbreth.

MCNPX problems can require significant computer type to produce acceptable uncertainty. The software has been parallelized using PVM and MPI to provide high processing speeds on clusters of computers. Problems still exist in extending MCNPX to clusters of computers running different operating systems. To optimize and validate MCNPX using MPI, three different platforms will be used: Linux, Sun, and SGI. MCNPX will be compiled on each and any bugs in the compile and install scripts will be fixed and forward to the MCNPX team. After MCNPX is successfully installed on each platform, work will begin on implementing MPI between the different platforms. Once these tasks are completed, the optimization and validation portion of the project can commence. The results will be published on the research team's website at: http://www.nrcc.unlv.edu to benefit other MCNPX users in the use of the software on parallelized clusters of computers.

The UNLV team will work in conjunction with researchers at LANL to develop an open source GUI for creating input files for MCNPX. The foundation of the program will be an Initial Graphics Exchange Specification (IGES) file reader that can be exported by most CAD packages. After successfully developing code to import an IGES file, work will begin on a GUI that will display the geometry in 3D. Next, an interactive interface to accept user input would be created, where by a user can input the necessary MCNPX parameters. Finally the geometry and user input would be post processed to create a usable MCNPX input deck. Results will also be available through the team's website.

Suresh Sadineni, a team member and doctoral mechanical engineering student, recently completed his thesis titled "Benchmarking Photoneutron Production of MCNPX Simulations with Experimental Results" based on his work at the Idaho Accelerator Center. We propose to extend his work to the simulation of a subcritical reactor that is augmented by a pulsed neutron source. This simulation will be based on research currently underway by Dr. Culbreth and Jason Viggato on simulation of the Oklo nuclear reactors. These simulations will complement work planned at IAC to demonstrate that a pulsed electron accelerator can be used to produce sufficient neutrons in a subcritical blanket to maintain steady-state operation. Continued collaboration with LANL for MCNPX simulations of their LANSCE experiments will also remain a priority.

Funding Profile:

Academic Year:	2001-2002	2002-2003	2003-2004
Total (K$)	*$105,534*	*$101,532*	*$101,247*

Background and Rationale:

Currently all MCNPX input files must be created by hand. This requires the user to remember (or have to lookup) geometry formats, material properties, and a myriad of possible inputs. After the input deck is created by hand, the user can use a 2-D viewer provided with MCNPX, as shown in Figure 2 to view the geometry. However, the viewer does not allow the user to interactively change any parameters of the input file.

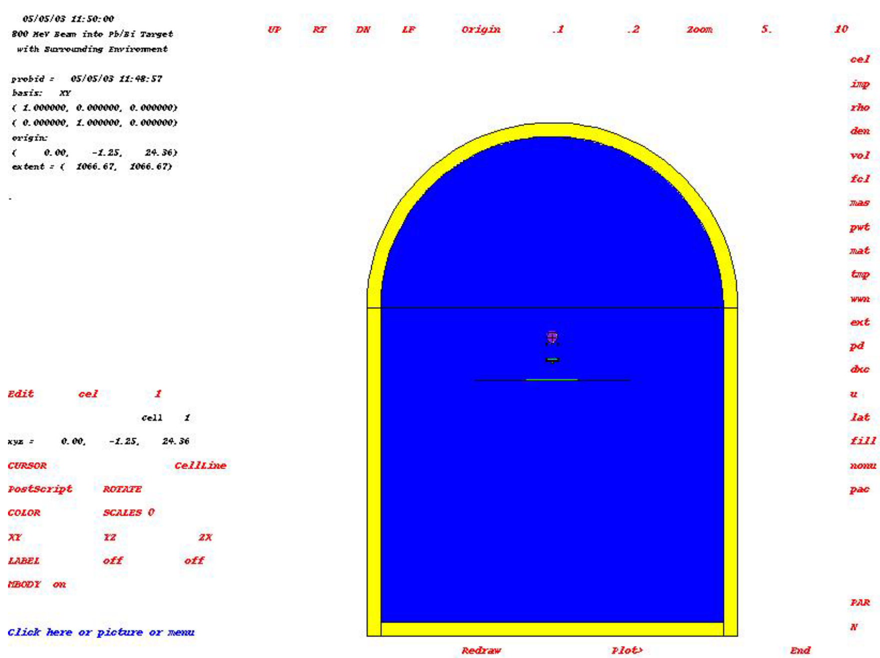

Fig. 2 MCNPX Output of a Problem Geometry
(LANSCE Blue Room with Spallation Target)

By creating a GUI the user can create geometry using a CAD package and then import the IGES file, eliminating the need to hand input geometry and reducing possible errors. As seen in Figure 3 a 3D modeler allows the user to see different views of the model. In addition, the user will be able to change parameters on the MCNPX input deck through the GUI as needed.

Because MCNPX simulations can take a considerable amount of time (days, months) to achieve accurate results, there is an increasing need to run them on parallel systems. Currently MCNPX implements two types of parallel processing Parallel Virtual Machine (PVM) and MPI. As seen in Figure 4 the UNLV team has made progress in implementing PVM on a parallelized cluster of 20 computers. For this proposal the UNLV team will be concentrating on the use of MPI. Due to the diversity of many computing systems there is a need to implement MCNPX on heterogeneous systems. In this effort, the UNLV team in conjunction with the MCNPX team at LANL will implement and debug the install of MCNPX on a heterogeneous system. In addition efforts to optimize MCNPX on each platform will be made.

Fig. 3 CAD Rendition of the LANSCE Blue Room Using SolidWorks

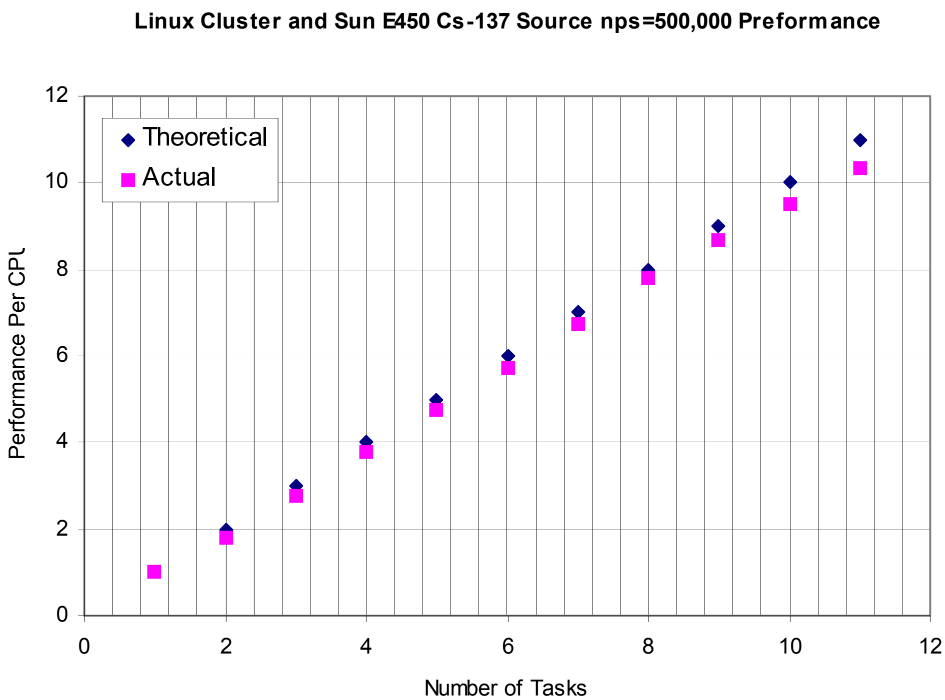

Fig. 4 LINUX Cluster Performance Comparison (Theoretical Performance to Actual Performance)

Research Objectives and Goals:

During the third year of the project, the goals include:

<u>Optimization and validation of MCNPX on multiple platforms using Message Passing Interface (MPI)</u>

- Acquire the latest version of MCNPX that is MPI aware.
- Successfully compile the obtained code on Linux, SGI, and Sun.
- Implement MPI on a Linux, SGI, and Sun heterogeneous cluster.
- Perform an optimization study on each of the systems.

<u>Creation of a GUI to help users generate input files for MCNPX</u>

- Acquire an open source CAD package or 3D viewer.
- Acquire the IGES file specifications.
- Develop code to read the IGES file and display it in the CAD package or 3D viewer.
- Develop code to allow the user to input MCNPX specific data in the CAD package or 3D viewer.
- Develop code to output the MCNPX input deck.

<u>Continue Student Doctoral Work on the Simulation of Subcritical Reactor</u>

- Continue collaboration with the IAC to simulate transmuter behavior.
- Continue MCNPX simulation of LANSCE neutron production experiments.

Technical Impact:

Without parallelization MCNPX can be computationally time prohibitive to run. Parallelization will allow users to run computationally intensive simulations in a reduce amount of time. Because of the diversity of computing architectures MCNPX needs the flexibility to run on different platforms. This insures that the user will not be limited in the types of systems they can run simulations on.

Without a coherent GUI the user is force to create each input deck by hand. As the input file size and complexity increases, the probability of errors increases significantly. A GUI allows the user to interactively view and input data for the problem at hand. Also, since the geometry is imported form a CAD file, the time it takes to create an input file is reduced.

Continued UNLV collaboration using MCNPX in support of LANSCE and IAC work will assist in completion of their work under the Advanced Fuel Cycles Initiative.

Research Approach:

The research approach involves the use of MCNPX on a cluster of Linux, SGI, and Sun systems for the testing of MPI and optimization. Also, ProEngineer and Solid Works will be used to create 3D drawings, which are exported as IGES files. Open source software and tools will then be used to create a GUI to write input files for MCNPX. Numerical simulation of reactor (transmuter) operation in a pulsed neutron source will be based on MCNPX and on a Fortran 90 program used to simulate the Oklo natural reactors.

Expected Technical Results:

In collaboration with researchers at LANL and other institutions, a guideline for installing and optimizing MCNPX will be created. Also, potential bugs in implementing the MPI version of the code on a system of heterogeneous platforms will be identified. Finally, an open source GUI will be created that other researches can evolve and contribute.

Capabilities at the University and Los Alamos:

To carry out the proposed work, computer workstations located at UNLV will be utilized. Also, a cluster of heterogeneous systems (including Linux, Sun, and SGI) at UNLV and the National Supercomputing Center for Energy and the Environment at UNLV will be implemented to test parallelization and optimization.

Equipment Requested for AFCI User Labs:

Due to the computational requirements for the proposed work, additional computer workstations are requested to expand the Linux cluster housed at UNLV. The computer workstations will be equipped with microprocessors with at least 2.4 GHz of speed and at least 1 gigabyte of random access memory. The MCNPX software and associated data libraries are available from the Radiation Sciences Information computing Center at Oak Ridge National Laboratory without charge to universities.

Project Timeline:

<u>Timeline Narrative:</u>

Year 1 of this project began in late August 2001 at the beginning of the academic year at UNLV. Students began the year by learning how to use radiation transport codes. During the winter break, students received formal training in MCNPX and visited the Argonne National Laboratory to discuss the research. They also made presentations on their progress at the ANS Conference held in Reno, Nevada.

During Year 2 of this project, Danny Lowe spent two summer months at LANSCE and Suresh Sadineni spent 6 months at the IAC (Idaho Accelerator Center) to conduct work. The student working at LANL assisted in the neutron spallation experiments while conducting simulations using MCNPX. Much of the work scheduled for Year 2 of the project included benchmarking of the experiments conducted at LANSCE, simulation of proposed LANSCE tests, and comparison of experimental results to MCNPX models. Mr. Sadineni's work included experimental verification of the production of neutrons using a lead target and a 25 MeV electron accelerator. He also provided MCNPX simulations in support of the work.

Much of the work scheduled for Year 3 of the project will consist of benchmarking and optimizing MCNPX on a heterogeneous cluster while continuing to provide MCNPX simulations in support of AFCI. As progress is made in this endeavor, user guides will be written on the implementation of an optimized version of MCNPX on a heterogeneous cluster using MPI. Also, preliminary development for a GUI will be pursued using open source code and tools.

Table 1 Timeline for Year 3 of the Project

	2003					2004						
Tasks	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul
A. MCNPX MPI and Optimization												
(Wilcox, Lowe, and Culbreth												
MPI												
1. Obtain MPI Version 2.5c												
2. Install individual systems												
3. Implement MPI on cluster												
Optimize												
1. Optimize individual systems												
2. Optimize MPI on cluster												
B. Graphical User Interface (GUI)												
(Lowe, Wilcox, and Culbreth												
1. Survey open source												
2. Obtain appropriate open source												
3. Set up CVS server												
4. Outline development with LANL												
5. Write interface for open source												
6. Develop prototype of GUI												
C. MCNPX Transmuter Simulations												
(Sadenini, Culbreth, and Lowe)												
1. Continue work with IAC												
2. Continue LANL MCNPX work												
3. Develop model of transient reactor												

Expected Technical Results:

The results will include benchmark data and user guides in setting up and optimizing MCNPX using MPI on a heterogeneous cluster. Also, a prototype GUI with user guide will be developed. Codes produced for this project will be made available to AFCI researchers.

Milestones:

The milestones include installation and optimization of MCNPX on a heterogeneous cluster and development of a GUI as shown in Table 1.

Deliverables:

The products of the research will include quarterly reports that detail progress on the research, copies of publications, and summaries of collaboration with the national laboratories. A final annual report will be submitted by the 12th month of the project. Student work, including copies of theses, dissertations, senior design, and user guides reports will also be included with quarterly progress reports.

Review of Accomplishments to Date

Work Completed During 2001-2002

UNLV faculty and students have accomplished a number of tasks during the first year of the project. The project began in late August 2001 and continued through the summer of the first year of the project. During the summer, Daniel Lowe (student researcher) spent 6 weeks at LANSCE and Suresh Sadineni (graduate student researcher) spent 3 months at the Idaho Accelerator Center at their expense with 3 months of additional support under the project. A list of accomplishments in Year 1 of the project were covered in the previous continuation proposal.

Work Completed During 2002-2003

- During the summer of 2002, Daniel Lowe spent 2 months at the LANSCE facility at LANL working on the neutron spallation tests. His work consisted of MCNPX runs in preparation for the tests with R. Klann and M. James. He also prepared foils for the determination of neutron flux from the experiment and assisted in radiation counting of the foils.

- Daniel Lowe completed Solidworks CAD models of the Blue Room at LANSCE and conducted MCNPX simulations of the summer experiments upon his return to UNLV for the fall semester, 2002. 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. Due to changes in funding at ANL and LANL, other planned LANSCE experiments related to the Advanced Fuels Cycles Initiative have been postponed.

- Mr. Lowe presented his work at the recent ANS Conference in Berkeley, California in March, 2003.

- Over the summer, 2002, Suresh Sadineni was employed by Dr. Frank Harmon at the Idaho Accelerator Center in Pocatello, Idaho, to assist in experiments on their lead neutron-production target. Mr. Sadineni ran MCNPX simulations to predict the performance of a lead target exposed to 25 MeV electrons produced by one of their accelerators. Mr. Sadineni also assisted in the experiments. He also took courses in nuclear engineering from UNLV and Idaho State University.

- During the fall semester, 2002, Mr. Sadineni returned to UNLV to defend his master's thesis. In December 2002, Suresh Babu Sadineni completed his masters thesis, ***Benchmarking Photoneutron Production of MCNPX Simulations with Experimental Results***, which directly related to the projects in year 2.

- Mr. Sadineni started the Ph.D. Program in Mechanical Engineering at UNLV in the spring semester, 2003 and will be working on a dissertation related to *sustained operation of a subcritical nuclear reactor using an electron accelerator for neutron production*.

- Trevor Wilcox joined the project during 2002/2003 to assist in the development of a computer cluster to run the parallelized version of MCNPX. He has completed a 16 processor LINUX cluster that works with a 4-processor