

## ADVANCES IN REACTOR FLUENCE AND DOSE EVALUATIONS

### 4. Advanced Three-Dimensional Deterministic and Monte Carlo Codes for Simulation of Real-Life Complex Nuclear Systems, *A. Haghghat (Penn State), G. E. Sjoden (USAF Academy), J. C. Wagner (ORNL), invited*

In the past 10 yr, the Penn State Transport Theory Group (PSTTG) has concentrated its efforts on developing accurate and efficient particle transport codes to address increasing needs for efficient and accurate simulation of nuclear systems.

The PSTTG's efforts have primarily focused on shielding applications that are generally treated using multigroup, multi-dimensional, discrete ordinates ( $S_n$ ) deterministic and/or statistical Monte Carlo methods. The difficulty with the existing public

codes is that they require significant (impractical) computation time for simulation of complex three-dimensional (3-D) problems. For the  $S_n$  codes, the large memory requirements are handled through the use of scratch files (i.e., read-from and write-to-disk) that significantly increases the necessary execution time. Further, the lack of flexible features and/or utilities for preparing input and processing output makes these codes difficult to use. The Monte Carlo method becomes impractical because variance reduction (VR) methods have to be used, and normally determination of the necessary parameters for the VR methods is very difficult and time consuming for a complex 3-D problem.

For the deterministic method, we have developed the 3-D parallel PENTRAN (Parallel Environment Neutral-particle TRANsport) code system that, in addition to a parallel 3-D  $S_n$  solver, includes pre- and postprocessing utilities. PENTRAN (Refs. 1, 2,

TABLE I  
Highlights of Problems Solved with the PENTRAN Code System

Problem	Type of calculation	Size(cm <sup>3</sup> )/ Number of meshes/ Number of groups/ Sn/Pn	Notes	Solution <sup>a</sup>	Computer/ Number of processors/ Par. Alg. (A/G/S) <sup>b</sup>	Time
VENUS-3 benchmark facility	Fixed source, forward neutron	65x65x70 84,784 26 S8/P3	Complex geometry, Partial length assemblies	Agrees with experimental results	IBM SP2 <sup>c</sup> 32 8/1/4	82 min
BWR core shroud	Fixed source, forward neutron and gamma	295x295x345 265,264 67 S8/P3	Complex geometry, large problem	Within 5-15% of continuous energy Monte Carlo; similar to TORT results	IBM SP2 <sup>d</sup> 48 8/1/6	14 hours
PGNAA device	Fixed source, adjoint gamma	35x38.9x36.48 27730 1 S14/P3	Localized source, moving detector	Agrees with experimental results	LIONX PC-cluster <sup>e</sup> 8 8/1/1	240 sec
X-ray room	Fixed source, forward photon ( $\leq 80$ KeV)	575.95x549.19x287.02 131,000 4 S4/P1	Large geometry, angular dependent source, group dependent albedos	Agrees with experimental results	SPARKY cluster <sup>f</sup> 2 2/1/1	111 min
Kobayashi voided duct benchmarks, e.g., problem 3 with $C^g = 0$	Fixed source, forward neutron	60x100x40 8,000 16 S12/P0	Zero scattering, voided duct	Largest difference from analytical results is $<20\%$ at $\sim 9$ mfp from the source	LIONX PC-cluster 1 1/1/1	88 sec

<sup>a</sup>Variable meshing and adaptive differencing strategy is used.

<sup>b</sup>Angular, energy, and spatial domain decomposition, respectively.

<sup>c</sup>"Wide" nodes with 512 megabytes of memory per processor (DOD high-performance computing).

<sup>d</sup>San Diego Supercomputing Center, each node has 256 megabytes of memory.

<sup>e</sup>Penn State PC-cluster, each PC has two processors with 500-MHz clock-cycle and 1 gigabyte of memory.

<sup>f</sup>Two PCs, each PC has a 380-MHz AMD K6-z processor with 192 megabytes of memory.

<sup>g</sup>Zero scattering.

TABLE II  
Highlights of Problems Solved with the A<sup>3</sup>MCNP Code System

Problem	Type of Calculation	Size(cm <sup>3</sup> )/ Cross-section	Notes	Deterministic Calculation (Mesh/Sn/Pn/#group/time)	Ratio of FOM(A <sup>3</sup> MCNP) to FOM(MCNP)	Speedup, Ratio of CPU(A <sup>3</sup> MCNP) <sup>a</sup> to CPU(MCNP)
PWR PV	Cavity dosimetry, forward neutron	R=350 cm, $\theta = [0,45]$ / continuous energy	Deep penetration, localized detector	r- $\theta$ DORT with a Z cosine shape (8500/S8/P3/47/15 min)	~50,000	~50,000
BWR core shroud	DPA at core shroud weld, forward neutron	300x300x368 continuous energy	Deep penetration, localized detector	x-y-z TORT (10800/S8/P3/47/40.8 min)	~2945	~2005
Shipping cask	Surface dose, forward gamma	180x180x840 continuous energy	Deep penetration, whole surface	x-y-z TORT (32256/S8/P3/18/20.7 min)	~9632	~8277
Kobayashi voided duct benchmarks, e.g., problem 1b	Flux value, forward neutron	60x100x40 1 group	Purely absorbing, deep penetration, localized flux tallies	x-y-z TORT (1000/S16/P0/1/2 sec)	~222	~222

<sup>a</sup>Includes CPU for the deterministic calculation.

and 3) provides for full phase-space decomposition, memory partitioning, and parallel input/output to provide the capability of solving large problems in a relatively short time. Besides having a modular parallel structure, PENTRAN has several unique new formulations and features that are necessary for achieving high parallel performance. These include an adaptive differencing strategy; variable grid density along all spatial axes; Taylor Projection Mesh Coupling<sup>3,4</sup> (TPMC) for projection of coarse-mesh angular fluxes onto fine meshes; new differencing schemes, including directional theta-weighted<sup>5</sup> and exponential directional weighted<sup>6</sup>; new iterative techniques for space, energy, and angular decomposition; and new acceleration techniques.

In addition to being an efficient and accurate transport solver, PENTRAN incorporates the PENMSH (Ref. 7) and PENINP tools for preprocessing, and PENDATA and PENPRL for postprocessing. PENMSH prepares a 3-D mesh distribution and projects a given arbitrary source distribution onto the 3-D mesh. Using output files from PENMSH, PENINP automatically prepares a complete PENTRAN input file. PENDATA prepares various tables of flux, material, and source in ASCII format by merging parallel output files generated by different processors. PENPRL is used to extract flux values at any arbitrary position by performing a 3-D linear interpolation.

Thus far, we have used PENTRAN for simulation of several problems including the VENUS-3 benchmark facility,<sup>8</sup> a boiling water reactor (BWR) core shroud,<sup>9</sup> the PGNAA waste assaying device,<sup>10</sup> an X-ray room,<sup>11</sup> and the Kobayashi 3-D voided duct problems.<sup>12</sup> Table I highlights the important aspects of each problem.

For the Monte Carlo method, the major difficulty currently facing most users is the selection of an effective VR method and its associated parameters. For complex problems, generally, this process is very time consuming and may be complicated due to the possibility of biasing the results. In an attempt to eliminate this problem, we have developed the A<sup>3</sup>MCNP (automated adjoint accelerated MCNP) code<sup>13-15</sup> that automatically prepares parameters for source and transport biasing within a weight-window VR approach based on the  $S_n$  adjoint function. A<sup>3</sup>MCNP prepares the necessary input files for performing multigroup, 3-D adjoint  $S_n$  calculations using TORT (Ref. 16). For this, A<sup>3</sup>MCNP prepares a mesh distribution and the corresponding mixtures with

their identification numbers and densities. Note that almost all of this information is extracted from the normal MCNP input. Only six additional cards are needed to specify the meshing, multigroup cross-section library, and other controlling parameters. Upon completion of the adjoint  $S_n$  calculation, A<sup>3</sup>MCNP (a) reads the adjoint function variable spatial mesh, and energy group structure from the standard  $S_n$  code binary output file, (b) superimposes the variable spatial mesh and energy grid onto the MCNP problem, (c) couples the original source distributions with the adjoint function to generate dependent source-biasing parameters and weight window lower bounds, and (d) performs the transport calculation using the superimposed grids and calculated parameters. The grids facilitate the use of the detailed space- and energy-dependent importance function and do not impose any limitation on the transport of particles.

A<sup>3</sup>MCNP has been used for simulation of a few real-life problems including a pressurized water reactor (PWR) pressure vessel (PV) and cavity dosimetry,<sup>17</sup> a BWR core shroud,<sup>18</sup> a shipping cask,<sup>19</sup> and the Kobayashi 3-D voided duct problems.<sup>20</sup> Table II highlights capabilities and performance of using A<sup>3</sup>MCNP for each problem.

As presented in Table I, PENTRAN yields very accurate results in a short computing time. For example, the VENUS-3 problem was solved in 82 min on a 32-processor SP2, and calculated reaction rates were consistent with the experimental values at all experimental locations (i.e., 370). The relative difference between the calculated and experimental results are within  $\pm 5\%$  at 258 locations, within  $\pm 5\%$  and  $\pm 10\%$  at 97 locations, and within  $\pm 10\%$  and  $\pm 15\%$  at 15 locations. The larger differences are consistent with the larger experimental errors. Both PGNAA and X-ray problems yield results within experimental uncertainties. Even for the Kobayashi benchmark with pure absorber and voided duct (e.g., dog-leg problem), PENTRAN has resulted in a relatively accurate solution; largest difference ( $\sim 20\%$ ) from the analytical solution occurs at more than 9 mean free paths from the source, within the pure absorber. This can be attributed to the unique formulations and features of PENTRAN, including the adaptive differencing strategy, TPMC, and variable meshing. Table II demonstrates that for different real-life problems, A<sup>3</sup>MCNP can yield significant speedups (several orders of magnitude) over the unbiased cases. This is even true for

media with pure absorber and void regions, where the discrete ordinates ( $S_n$ ) method, because of the limited number of directions, has difficulty with the “ray effect.”

In conclusion, PSTTG has developed highly efficient and accurate deterministic and Monte Carlo transport theory codes for the simulation of complex 3-D nuclear systems. Currently, PSTTG is developing a methodology for automatic mesh generation and examining approaches for generating effective multi-group cross sections for A<sup>3</sup>MCNP.

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