

**PENTRAN™ (Parallel Environment Neutral-particle TRANsport)
CODE SYSTEM**

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ABSTRACT

1. **Program Name and Title:** PENTRAN™ Code System: Parallel Environment Neutral-particle TRANsport Code System.
2. **Computer for Which Program is Designed and Other Machine Versions Available:**
Distributed-Memory and Distributed Computing Environments: IBM SP2, Linux PC Cluster, SUN mutiprocessors (SMP), SGI ORIGIN 2000;
Single processor: PCs, Workstations, etc.
3. **Problem Solved:**
Benchmarking: Performance and accuracy of PENTRAN has been benchmarked¹⁻³ against other production codes, mainly TORT (Ref. 4) and THREEDANT (Ref. 5) codes. We have simulated the VENUS-3 benchmark facility in 82 minutes on a 32-processor SP2, and calculated reaction rates at 370 experimental locations.⁶ The relative difference between the calculated and experimental results are within ~5% at 258 locations, within ~5% and ~10% at 97 locations, and within ~10% and ~15% at 15 locations. We have simulated the Kobayashi 3-D benchmark problems with pure absorber and void ducts/regions (e.g. dog-leg problem). Even for these problems, we have obtained relatively accurate solutions; the largest difference from the analytical solutions is ~20% that is observed at more than 9 mfps from the source. The reason for achieving such accurate results is combination of PENTRAN's unique formulations and features.⁷
Applications: Thus far, PENTRAN has been used for simulation of a BWR core shroud of size ~300x300x350 cm³ using a 67-group, P3 coupled neutron and gamma cross section library, and a level-symmetric S8 quadrature set.⁸ PENTRAN solves for a 3-D, 67-group flux distribution on 48 processors of an IBM SP2 in 14 hours. These flux

distributions are in excellent agreement with the TORT results that are obtained using 100 hours. Further, calculated reaction rates are within 5-15% of a continuous energy A³MCNP (Ref. 9) results; this difference can be attributed to the use of multigroup cross sections. We have used PENTRAN for simulation of the Westinghouse PGNAO device¹⁰ and an x-ray room¹¹. Both calculations yield results that are within the experimental uncertainties. Currently, we are using PENTRAN for simulation of a CT scanning device as well as a shipping cask.

4. **Method of Solution:** PENTRAN solves the linear Boltzmann equation for fixed-source and eigenvalue problems in "forward" and "adjoint" modes. It is based on the discrete ordinates (S_n) method with the source iteration (SI) approach. It uses different iterative techniques including Block Jacobi and Red-Black with alternate directions sweep (ADS). It includes an adaptive differencing strategy that allows for the use of different differencing schemes at different regions of a calculation domain. Currently, the available differencing schemes are Linear Diamond (DD), Directional Theta-Weighted (DTW)¹², Exponential Directional Weighted (EDW)¹³, and Exponential Directional Hybrid (EDH). Based on the problem physics, PENTRAN can automatically select an appropriate differencing scheme, however, the user can over-ride the code's selection. To be able to handle a variable grid density, PENTRAN uses the TPMC formulation¹⁴ to project angular fluxes from a coarse grid onto a fine grid. For parallel processing, PENTRAN allows for spatial, angular, and energy domain decomposition algorithms, or any hybrid combinations of them. For spatial decomposition, it includes Block-Jacobi and Red-Black with alternate direction sweep (ADS) approach. For angular domain decomposition, different sets of angles can be processed in parallel. For energy decomposition, two options are available: i) multigroup; ii) the Hiromoto-Wienke one-pass approach.¹⁵ For acceleration of the SI iteration, PENTRAN includes the coarse-mesh-rebalance (CMR), partial current rebalance (PCR), and different spatial and angular multigrid algorithms.¹⁶
5. **Restrictions on the Complexity of the Problem:** It is restricted by the available memory on each processor; typically, at least 256 Mb is required per processor. Most 3-D problems require between 2 and 8 processors, depending on the memory per processor and/or problem size.
6. **Typical Running Time:** Running time varies from seconds to hours depending on the problem size and complexity, and the available number of processors and allocatable memory per processor.
7. **Unusual Features of the Program:** PENTRAN is a 3-D parallel S_n code designed for distributed-computing and distributed memory environments with decomposition possible among the angular, energy, and spatial variables. For small problems or for a machine with large memory, serial version of the code can be used. PENTRAN has several unique numerical techniques and formulations developed to obtain highly accurate solutions, while achieving a large parallel efficiency. This is accomplished by development of the adaptive differencing strategy with DTW, EDW, and EDH differencing schemes, the Taylor projection mesh coupling (TPMC), full phase space

domain decomposition with different iterative techniques, several acceleration schemes, memory partitioning, and parallel I/O.

8. **Related and Auxiliary Programs:** PENTRAN code system includes pre- and post-processing software. For pre-processing, it uses PENMSH (Ref. 17) (for generation of mesh, material and source distributions) and PENINP (for automatic generation of a PENTRAN input file). For post-processing, it uses PENDATA (for preparation of data tables from the PENTRAN output files) and PENPRL (for calculations of flux value at any arbitrary point within the calculation domain).
9. **Status:** PENTRAN has been successfully benchmarked and used for solving several real-life complex problems. For benchmarking, the Kobayashi 3-D problems with void duct and absorber, and the VENUS-3 3-D experimental benchmark facility are used. Thus far, PENTRAN has been used for solving several real-life complex problems including a BWR core shroud, the PGNAA assaying device, as well as an x-ray room. Currently, it is being used for simulation of a CT scanning device and a shipping cask.
Availability: PENTRANTM can be purchased from the H & S Advanced Computing Technologies Inc, (H&SACT) at <http://www.hsact.com>. For further information you may contact Professor A. Haghghat at ali@hsact.com or haghghat@psu.edu.
10. **References:**
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11. **Hardware Requirements:** The hardware requirement is dependent on the problem size and complexity. PENTRAN can readily operate on most serial and parallel systems without modification.
 12. **Programming Language(s):** PENTRAN is written in ANSI FORTRAN 90 with dynamic memory allocation. Problem-dependent array sizes are determined by the PENINP code and incorporated into the standard PENTRAN input file. For parallel processing, it uses the MPI (message passing interface) library. Currently, PENTRAN is comprised of 223 subroutines and ~32,000 lines of code.
 13. **Operating System:** PENTRAN is written in a standard FORTRAN, and does not have any machine specific instructions or routines. Thus far, it has been implemented on the Microsoft Window (using POWERFortran), LINUX (using Portland Group Fortran with MPI), IBM AIX (using mpixlf and xlf), and SUN Solaris (using FORTRAN 77 and High Performance Computing (HPC) environment).
 14. **Other Programming or Operating Information or Restrictions:** None.
 15. **Name and Affiliation of Author or Contributor:** Authors: Glenn E. Sjoden (US Air Force) and Alireza Haghghat (Penn State University, PSU); Contributor: Vefa N. Kucukboyaci (PSU)

16. **Material Available:** Code manual, executable code, and numerous papers discussing PENTRAN's formulations, applications, and performance.
17. **Category:** Reactor shielding, Reactor Core Physics, Criticality Safety
Keywords: Three-dimensional neutral particle transport, Sn method, Parallel Processing, Complete Phase Space Domain Decomposition
18. **Sponsor:** H&S Advanced Computing Technologies, Inc.