PARTISN

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ABSTRACT

1. Program Name and Title: PARTISN (PARallel, TIme-Dependent SN)

2. Computer for Which Program is Designed and Other Machine Versions Available: The current release is designed for UNIX-like systems. The specific computers supported fall into two categories - long word and short word. The program has been implemented on the long word Cray J90 and T90 computers. It has also been implemented on SGI, IBM RS6000, HP9000, and DEC Alpha short word workstations. The workstation versions use double precision arithmetic. The program has been run in parallel on clusters of SGI workstations (ASCI Blue Mountain) and the IBM SP2 (ASCI Blue Pacific). The ASCI Red machine at SNL is also supported. An older version of the program has also been run on the Cray T3D.

3. Problem Solved: PARTISN solves the linear Boltzmann transport equation for neutral particles using the deterministic (SN) method. Both the static (fixed source or eigenvalue) and time-dependent forms of the transport equation are solved in forward or adjoint mode. Vacuum, reflective, periodic, white, or inhomogeneous boundary conditions are solved. General anisotropic scattering and inhomogeneous sources are permitted. PARTISN solves the transport equation on orthogonal (single level or block-structured AMR) grids in 1-D (slab, two-angle slab, cylindrical, or spherical), 2-D (X-Y, R-Z, or R-T) and 3-D (X-Y-Z or R-Z-T) geometries.

4. Method of Solution: PARTISN numerically solves the multigroup form of the neutral-particle Boltzmann transport equation. The discrete-ordinates form of approximation is used for treating the angular variation of the particle distribution. For curvilinear geometries, diamond differencing is used for angular discretization. The spatial discretizations may be either low-order (diamond difference or Adaptive Weighted Diamond Difference (AWDD)) or higher-order (linear discontinuous or exponential discontinuous). Negative fluxes are eliminated by a local set-to-zero-

and-correct algorithm for the diamond case (DD/STZ). Time differencing is Crank-Nicholson (diamond), also with a set-to-zero fixup scheme. Both inner and outer iterations are accelerated using the diffusion synthetic acceleration method. The diffusion solver uses the conjugate gradient or multigrid method and Chebyshev acceleration of the fission source. First-collision source treatment options are provided for the elimination of primary ray effects in fixed-source calculations. The angular source terms may be treated either via standard PN expansions or Galerkin scattering. An option is provided for strictly positive scattering sources. Parallelization is performed via a 2D spatial decomposition, which retains the ability to invert the source iteration equation in a single sweep.

5. Restrictions on the Complexity of the Problem: The code is thoroughly variably dimensioned, with memory requirements determined from the input parameters. At present, no out-of-core (i.e., disk) storage capability is provided.

6. Typical Running Time: Running time on a single processor is directly related to problem size and to central processor and data transfer speeds. On a SGI R10000, a four-group eigenvalue calculation of an X-Y-Z model of the Fast Test Reactor (FTR) took 9 seconds. The calculation used transport corrected P0 cross sections, an S8 angular quadrature, DD/STZ spatial differencing, and a 14x14x30 spatial mesh. Running time on parallel platforms is sensitive to the latency and topology of the interconnect, as well as the single processor performance.

7. Unusual Features of the Program: PARTISN is modularly structured in a form that separates the input and output (edit) functions from the main calculational (solver) section of the code. The code makes use of binary, sequential data files, called interface files, to transfer data between modules. Standard interface files whose specifications have been defined by the Reactor Physics Committee on Computer Code Coordination are accepted, used, and created by the code. A free-field card-image input capability is provided for the user. The code provides the user with

considerable flexibility in using both card-image or sequential file input and in controlling the execution of modules.

8. Related and Auxiliary Programs: PARTISN is the evolutionary successor to DANTSYS. User input is very similar to that of the DANTSYS code.

9. Status: The current PARTISN release is 1.66. Updates are made approximately three times a month.

10. References:

"DANTSYS: A Diffusion Accelerated Neutral Particle Code System", LA-12969-M, Los Alamos National Laboratory (1995).

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Computation, Reactor Physics, and Env. Analysis in Nucl. Applications, **1**, 377, Madrid, Spain (1999).

"Automatic Mesh Coarsening for Discrete Ordinates Codes", Scott A. Turner, *Proc. of the Joint Intl. Conf. on Mathematics and Computation, Reactor Physics, and Env. Analysis in Nucl. Applications,* **2**, 1423, Madrid, Spain (1999).

11. Hardware Requirements: The virtual machine memory must be large enough for the problem being executed. On many architectures, stack size limits must be large enough to allow the placement of temporary arrays on the stack.

12. Programming Languages: The program is written in standard F90 with a few C language routines used to interface to the Unix operating system. Parallelization is performed using MPI 1.1.

13. Operating System: The program is designed to port to any UNIX-like operating system with minimal effort. Where available, POSIX routines are used to obtain the machine name, cross section path, and access rights. Otherwise, system-specific routines must be used.

14. Other Programming or Operating Information or Restrictions: In addition to compilers, program building requires GNUmake (Version 3.74 or later), GNUawk (Version 3.0 or later), and cpp. A Readme file in the top program directory contains complete build instructions.

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16. Material Available: The PARTISN source code (~80,000 lines), although available through LANL (contact Randal Baker, rsb@lanl.gov), is export controlled.

17. Categories: B, C, F, and J.

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