PARCS: PURDUE ADVANCED REACTOR CORE SIMULATOR

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1. Program Name and Title: Purdue Advanced Reactor Core Simulator (PARCS).

2. Computer for Which Program is Designed and Other Machine Versions Available:

Table I: Platforms tested with PARCS.

Processor	Operating System	Compiler
x86	Windows	DVF 6.1, CVF 6.5
x86	Linux	Intel 5.0.1 NAGWare 4.2 Lahey/Fujitsu 6.0
IBM RISC6000	AIX 4.3	AIX HPF 1.4.0.2
DEC Alpha	OSF1 V4.0 1091	V5.2-171-428BH
Sun UltraSparc	Solaris 8	Sun WorkShop 6.2
HP	HP-UX 10.20	HPUX F90 v1.0
SGI	IRIX64	MIPSpro 7.3.1

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3. Problem Solved:

PARCS is a three-dimensional reactor core simulator that solves the steady-state and time-dependent neutron diffusion or SP_3 transport equations to predict the dynamic response of the reactor to reactivity perturbations such as control rod movements, boron concentration or changes in the temperature/fluid conditions in the reactor core. The code is applicable to both PWR and BWR cores loaded with either rectangular or hexagonal fuel assemblies. Multigroup diffusion or a SP_3 kernel can be used for the rectangular geometry option. The multigroup diffusion kernel is used for the hexagonal geometry option. Currently under development is a multigroup SP_3 capability method for cylindrical geometry. Kernel options available for different geometry types and their solution methods are summarized in Table II.

The PARCS code was chosen by the U.S. Nuclear Regulatory Commission (NRC) as its best estimate core neutronics code, and PARCS is coupled directly to the U.S. NRC thermal-hydraulics systems codes TRAC-M and RELAP5 using a message passing interface. The thermal-hydraulic solution is incorporated into PARCS as feedback into the few group cross sections. A depletion capability has also recently been added to PARCS that includes cross section interface capability to lattice physics codes such as HELIOS.

The major features in PARCS include the ability to perform eigenvalue calculations, a transient (kinetics) calculation including decay heat and xenon and samarium treatment, the adjoint calculation and the depletion calculation. The primary use of PARCS involves a 3D calculation model for the realistic representation of the physical reactor. Numerous sophisticated spatial kinetics calculation methods have been incorporated into PARCS in order to accomplish the various tasks with high accuracy and efficiency.

Table II: Solver types available in PARCS.

Geometry Type	Kernel Name	Solution Method	Energy Treatment	Angle Treatment	Comments
Cartesian 3D	CMFD	FD	2G	Diffusion	
	ANM	nodal	2G	Diffusion	
	FMFD	FD	MG	SP3	
	NMG	nodal	MG	SP_3	
Hexagonal 3D	CMFD	FD	2G	Diffusion	
	TPEN	nodal	MG	Diffusion	
Cylindrical 3D	CMFD	FD	2G	Diffusion	
	FMFD	FD	MG	Diffusion	Under development.

A. Eigenvalue Calculation

In order to establish the initial steady state, PARCS performs the eigenvalue calculation using the Wielandt eigenvalue shift method. In addition to the standard k_{eff} calculation for a given reactor configuration, the critical boron concentration search function is available for PWRs and a critical control rod search function is available for BWRs. The solution of the Coarse Mesh Finite Difference (CMFD) problem is obtained using the Krylov linear solver, Bi-Conjugate Gradient Stabilized (BiCGSTAB), which utilizes a BILU3D preconditioner.

B. Transient (Kinetics) Calculation

One of the primary functions of PARCS is solution of the time-dependent neutron diffusion or SP_3 equation involving both delayed and prompt neutrons. The 2^{nd} order temporal differencing based on Crank-Nicholsen (theta method) and enhanced with an exponential transform results in a transient fixed source problem (TFSP) at each time step. The TFSP is solved using the CMFD method with a conditional nodal update. In order to speed up the transient, the conditional nodal update scheme activates the higher order solution only when there are substantial local cross section changes. For spatial discretization, any of the kernels described in Table I is available in transient mode as well.

A conventional quasistatic treatment of xenon and samarium transients is used which employs the eigenvalue problem solver instead of the transient fixed source problem. The number densities of Xe/Sm are updated by solving the respective balance equations using the fluxes resulting from the eigenvalue calculation. Equilibrium Xe/Sm and no Xe/Sm option are available as well.

A simplified decay heat model involving six groups of decay heat precursor groups is employed in PARCS. The 6 group decay heat precursor equation is treated in the same way as the delayed neutron precursor equation. The solution of the precursor equation is thus nodewise and provides at each time step the decay heat to be summed with the fission power in order to determine the total power produced in each node. Default values of the precursor fraction and decay constant of the 6 groups are based on UO_2 fueled cores operated for a long period of time, but the user can specify alternate values.

A one-dimensional (1D) modeling feature is available in PARCS to support faster simulations for a group of transients in which the dominant variation of the flux is in the axial direction, which is the case for several BWR applications. The 1D feature also allows PARCS coupled to TRAC-M to execute existing TRAC-B input decks with no modifications to the input.

C. Adjoint Calculation

The adjoint flux is needed for the reactivity edits during the transient calculation. For this purpose, the adjoint calculation is performed at the end of the steady-state calculation with the transpose of the converged CMFD coefficient matrix.

D. Depletion

The depletion capability was implemented using the same basic general interface design used to couple PARCS to TRAC-M and RELAP5. An external depletion module, DEPLETOR, was developed that communicates with PARCS using PVM. This design had the advantage of minimizing changes to the PARCS code and simplifying code maintenance, since each code solves a different set of equations and performs a separate function. The PARCS code is used only to perform eigenvalue calculations, all depletion functions are performed in DEPLETOR and all temperature/fluid field solutions are performed in RELAP5 or TRAC-M.

E. Pin Power Calculation

The primary dependent variables in PARCS nodal kernels are the node average fluxes and interface currents. In order to obtain local pin power distributions from the nodal kernel, it is thus necessary to "reconstruct" pin powers. This is performed in PARCS by multiplying the heterogeneous power form functions with the homogeneous intranodal flux distribution. The homogeneous intranodal flux is calculated by performing an analytic solution of a 2 group, 2D fixed source problem in which the surface average currents are specified at the four boundaries. The surface average currents are obtained from the converged node average flux distribution at a given state. Pin power reconstruction is performed for both the steady-state and transient conditions. Corner discontinuity factors can be used to enhance the accuracy of the pin power distribution. In order to save computing time for the pin power calculation, only certain fuel assemblies can be selected for the pin power calculation.

F. Other Features

One of the distinct features of the output system is the on-line plotting feature, which is based on XMGR graphics software for UNIX and the QuickWin graphic package for Windows. Some of the primary transient calculation results such as reactivity, core power, peaking factors and coolant and fuel temperatures can be displayed on-line as the calculation proceeds. Current work involves integration with the U.S. NRC Symbolic Nuclear Analysis Package (SNAP), which will provide a unified graphic interface for all of the NRC's reactor analysis codes. Other features of PARCS include a boron criticality search, a control rod cusping correction and an automatic mapping routine that couples PARCS neutronics nodes to RELAP5 or TRAC-M thermal-hydraulics nodes.

4. Method of Solution: PARCS solves the multigroup time dependent diffusion and SP_3 equations with either assembly or cell-by-cell spatial discretization. The nodal options include both the analytic nodal method (ANM) and the nodal expansion method (NEM). In addition, the triangle-based polynomial expansion nodal (TPEN) method is available for hexagonal geometries. The cell-by-cell finite difference option (FMFD) accepts pin cell homogenized cross sections in an arbitrary number of energy groups. The multigroup SP_3 transport option is available in both the NEM and FMFD kernels.

5. Restrictions on the Complexity of the Problem: The problem size is restricted by available memory. The angular approximation is restricted to diffusion and SP_3. The finest level of group constant homogenization is at the pin cell level. There is no restriction on number of energy groups for the NEM and FMFD options.

6. Typical Running Time: Execution times will vary depending on the solution kernel chosen, however, 2 group nodal diffusion solutions for typical LWR transients (e.g. control rod ejection) are on the order of minutes on a current generation PC.

7. Unusual Features of the Program: A BILU3D preconditioned Krylov solver (BICGSTAB) is used to solve the coarse mesh finite difference problem in PARCS. A threads based parallel computing capability has also been added to PARCS for UNIX machines (see paper presented at this conference).

8. Related and Auxiliary Programs: None.

9. Hardware Requirements: See Table I. Because of dynamic memory allocation, the program size is problem dependant. Small problem (2D, 2 group nodal diffusion) takes up about 1 MB. Large problem (3D, 8 group fine mesh SP_3) takes up to 1GB. Typical PWR core transient with 2 group nodal diffusion takes up about 20 MB.

10. Programming Language(s): Fortran 90.

11. Other Programming or Operating Information or Restrictions: None.

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13. Appendix: Validation and Verification.

PARCS has successfully been verified with a number of benchmarks. The eigenvalue benchmarks in rectangular geometry include IAEA 3D PWR problem and NEACRP L336 Case 5 pin power benchmark. In hexagonal geometry, VVER-1000, VVER-440, SNR 4G and BFS 9G have been used to confirm solution method and functionality. The cylindrical geometry solver has been verified using an analytic solution and is currently being verified further with a HTR-10 benchmark. The FMFD SP_3 option in PARCS has been verified using the VENUS-2 MOX critical experiment, and an OECD MOX transient benchmark is currently being developed to validate the FMFD SP_3 transient capability.

PARCS transient benchmarks that are already available include those that use an internal T/H solver (limited to typical PWR T/H conditions) and those that use an external T/H code such as RELAP5 and TRAC-M. The benchmark problems solved with the internal T/H in Cartesian geometry are NEACRP PWR A1, A2, C1 and RWA problem. The hexagonal geometry problem with internal T/H used to verity PARCS solution are VVER-1000 CRE at 10% power and SMART-300 CRE with 12, 7, 4 and 2 group cross sections.

The transient coupled problems with an external T/H code include OECD MSLB benchmark, coupled with TRAC-M and RELAP5, OECD PBTT benchmark, coupled with TRAC-M, NEACRP BWR CWI, coupled with RELAP5 and AER VVER-440 CRA at HZP, coupled with RELAP5. There is ongoing work on the PWR Oconee plant model and BWR Ringhals stability benchmark, both coupled with TRAC-M. The 1D kinetics option has been verified with Brown's Ferry steady-state model coupled to TRAC-M.

The depletion module has been verified with a number of problems, including comparisons with KAERI's MASTER code and the Studsvik Scandpower HELIOS code. In addition, the depletion of the GE Simplified Boiling Water Reactor (SBWR) was performed with the results comparing favorably with the GE calculations reported in the SSAR.