Phisics: A New Reactor Physics Analysis Toolkit

2011 ANS Annual Meeting

- C. Rabiti
- Y. Wang
- G. Palmiotti
- H. Hiruta
- J. Cogliati
- A. Alfonsi

June 2011

The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance



This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint should not be cited or reproduced without permission of the author. This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights. The views expressed in this paper are not necessarily those of the United States Government or the sponsoring agency.

PHISICS: A NEW REACTOR PHYSICS ANALYSIS TOOLKIT

C. Rabiti, Y. Wang, G. Palmiotti, H. Hiruta, J. Cogliati, A. Alfonsi

Idaho National Laboratory: 2525 North Fremont Avenue, Idaho Falls, ID, 83415 cristian.rabiti@inl.gov

The main purpose of this paper is to introduce a newly developed reactor physics toolkit named PHISICS (Parallel and Highly Innovative Simulation for INL Code System). This package is intended to provide a modern analysis tool for reactor physics investigation. It is designed with the mindset to maximize accuracy for a given availability of computational resources. This is obtained by implementing several different algorithms and meshing approaches among which the user will be able to choose in order to optimize his computational resources and accuracy needs.

I. INTRODUCTION

In the last year INL has internally pursued the development of a new reactor analysis tool: PHISICS. The software is built in a modular approach in order to simplify the independent development of modules by different teams and future maintenance. Most of the modules at the time of this summary are still under development (time dependent transport driver, depletion, cross section I/O and interpolation, generalized perturbation theory, uncertainty and sensitivity analysis), while the transport solver INSTANT (Intelligent Nodal and Semi-structured Treatment for Advanced Neutron Transport) has already been widely used^{1, 2, 3, 4}. For this reason we will focus mainly on the presentation of the transport solver INSTANT.

II. INSTANT

As already mentioned INSTANT is the neutron transport solver for PHISICS. The code is based on two different discretizations of the transport equation. The first one implemented is the Variational Nodal Method⁵ and correspond, as shown in reference 1, to hybrid finite element in space and spherical harmonics in angle. The discretized equations are formulated in three different form and solved respectively using: iterative multi-color scheme, CG (Conjugate Gradient), or the GMRES

(Generalized Minimum Residuals). The three different solution schemes provide the user with three different trade off options depending on high speed/high memory (multi-color) and low speed/low memory (GMRES) available machines. These three solution algorithm are implemented on Cartesian 2/3D, hexagonal, Z-hexagonal, 2D triangular (structured/unstructured) and Z-triangular. The Variational Nodal method, based on the P_N second order formulation is ill suited to deal with fine unstructured mesh while very effective for node size typical of one assembly³. However, the implementation of an unstructured mesh will be useful in conjunction of the soon available new discretization method based on the self adjoint form of the second order S_N equation⁶. This form of discretization should be well suited to deal with the flux discontinuities arising when using a detailed description of the core (e.g., pin by pin). The variational nodal method has been implemented also in a parallel² computing environment with good results. We expect the implementation of self adjoint S_N equation to achieve a good level of scalability.

Table 1 shows the results for the Takeda 4 benchmark⁷ that are well in agreement with the results previously obtained with this methodology. Figure 1 and 2 show respectively a detail of the triangular mesh for the C5G7 2D benchmark and its solution using the hybrid FEM approach³.

TABLE I. Takeda Benchmark*: control rod in			
Space	Surface	Angular	K _{eff}
polynomial	polynomial	order	
order	order		
5	0	1	0.85866
6	1	3	0.87846
6	1	5	0.88176
7	2	7	0.87963
7	2	9	0.87983

*Reference value: 0.88001 ± 0.00038 (GVMP, Monte Carlo)

Reactor Analysis Methods—II

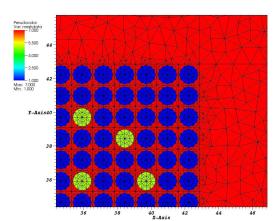


Fig. 1. C5G7 mesh detail (total 89426 elements).

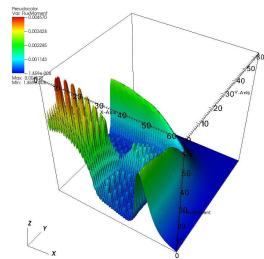


Fig. 2. Thermal flux C5G7 (P5 solution).

II. MODULES UNDER DEVELOPMENT

II. A. Time Dependent Driver

As part of the PHISICS toolkit a time dependent driver for INSTANT is ongoing. The practical realization of the driver follows closely the algorithm and the implementation shown in reference 8. This will allow a quick verification of results by comparison with already existing codes.

II. B. Depletion Module

In order to provide the depletion capability we are in the process to adapt the MRTAU code⁹. MRTAU is a depletion code that has been used insofar for fuel cycle analysis and developed at INL.

II. C. Perturbation Module

One of the major tasks that PHISIC should be capable to perform is the sensitivity and uncertainty quantification connected to the uncertainty in the input parameter. Fundamental step of this task is the implementation of the Generalized Perturbation Theory¹⁰ (GPT). This effort is also already ongoing and the implementation of the adjoint solution is already present in INSTANT.

II. D. Medium and Long Term Future Developments

In the medium term a thermal hydraulics capability (at the beginning based on a subchannel approximation) will be added to PHISICS. This will allow coupled calculations with sensitivity/uncertainty capability. For the long term the addition of a cell code capable of treating all type of reactor spectra is foreseen.

III. CONCLUSION

PHISICS capabilities are quickly increasing; its modular approach allows parallel development and we foreseen this toolset to become soon available to the reactor physics community in order to provide a modern analysis tool. The embedded adjoint capability in conjunction with its scalability between different accuracy levels of the simulation will be the strength of this new toolset.

ACKNOWLEDGMENTS

This work is supported by the U.S. Department of Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

REFERENCES

- 1. Y. WANG, C. RABITI, G. PALMIOTTI, "Krylov Solvers Preconditioned with the Low-Order Red-Black Algorithm for The Pn Hybrid FEM for The Instant Code," Submitted to *Proc. International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Rio de Janeiro, Brazil, May 8-12, (2011).
- 2. Y. WANG, C. RABITI, G. PALMIOTTI, "Parallelization of the Red-Black Algorithm on Solving the Second-Order PN Transport Equation with the Hybrid Finite Element Method," Submitted to *Proc. 2011 ANS Annual Meeting*, Hollywood, Florida, USA, June 26–30, (2011).
- 3. Y. Wang, H. Zhang, R. Szilard and R. Martineau, "Application of the INSTANT-HPS PN Transport Code to the C5G7 Benchmark Problem," Submitted to *Proc. 2011 ANS Annual Meeting*, Hollywood, Florida, USA, June 26–30, (2011).

Reactor Analysis Methods—II

- J. Ortensi, J. J. Cogliati, M. A. Pope, J. D. Bess, R. M. Ferrer, A. A. Bingham, A. M.Ougouag, "Deterministic Modeling of the High Temperature Test Reactor," INL/EXT-10-18969.
- 5. E. Lewis, C. B. Carrico and G. Palmiotti: "Variational Nodal Formulation for the Spherical Harmonics Equations", *Nucl. Sci. Eng.*, **122**, (1996).
- 6. J. E. Morel and J. M. McGhee, "A Self-Adjoint Angular Flux Equation," NUC. SCI. ENG., 132, (1999).
- T. Takeda and H. Ikeda, "3-D Neutron Transport Benchmarks," NEACRP-1-300 OECD/NEA, Organization of Economic Cooperation and Development/Nuclear Energy Agency, March, (1991).
- C. Rabiti, A. Rineiski, "Extension of KIN3D, a Kinetics Capability of VARIANT, for Modeling Fast Transient in Accelerator Driven Systems," Proceeding PHYSOR-2004, Chicago, Illinois, USA, April 25-29, American Nuclear Society (2004).
- 9. S. Bays, S. Piet, A. Dumontier, "Fuel Cycle Isotope Evolution by Transmutation Dynamics over Multiple Recycles," Proceedings of *ICAPP* '10, San Diego, CA, USA, June13-17, (2010).
- A. Gandini, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy* 21, p. 755, (1967).