### **PHISICS: New Features and Advancements**

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

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

### I. INTRODUCTION

The PHISICS (Parallel and Highly Innovative Simulation for INL Code System) [1] suite of codes is under an intensive development at INL. In the last months new features have been added and improvements of the previously existing one performed. The modular approach has created a friendly development environment that allows a quick expansion of the capabilities. The spherical harmonics based nodal transport solver [2,3] has been improved while the implementation of a solver based on the self adjoint formulation of the discrete ordinate [4] is in the test phase on structured mesh. PHISICS now includes a depletion solver with the possibility of using two different algorithms for the solution of the Bateman equation: the Taylor development of the exponential matrix and the Chebyshev Rational Approximation Method [5]. The coupling with RELAP5 [6] is also available at least in the steady state search mode. This makes possible coupled neutronics-thermal hydraulics calculations and can also take advantage of the new cross section interpolation module. In this way the coupling could be performed using an arbitrary number of energy groups.

#### **II. INSTANT**

The nodal option, spherical harmonics based, transport solver INSTANT (Intelligent Nodal and Semistrucured Treatment for Advanced Neutron Transport) has gone through a more intensive validation and the thermal iterations have been accelerated by the introduction of the two grid acceleration [7]. The improvement derived by the introduction of such computational scheme is highlighted in Fig. 1. The implementation of the self adjoint discrete ordinate formulation of the transport equation is under way.

#### **III. Depletion Capability**

The previously developed depletion code MRTAU [8] has been integrated in the PHISIC environment. The algorithm initially implemented in the code has been modified and also the possibility of using the CRAM approach has been added. Some challenges in extending the Taylor expansion used by MRTAU (with matrix split between actinides and fission products) to a general order of accuracy has been encountered. For this reason, a more general expansion of the full decay/depletion matrix, the CRAM algorithm, has been adopted and also implemented.

In order to test the code the old implementation has been taken as a reference and compared with the new algorithms. Fig. 2 shows the relative error (CRAM with 3000 time step and 14<sup>th</sup> order as a reference) between CRAM 8<sup>th</sup> order and Taylor second order for different time step. CRAM results to be stable and accurate even for very large time step. Unfortunately, changes in the flux will preclude the usage of so large time step; therefore, the exponential matrix method might be still convenient for core depletion based calculation. In out of core decay or fuel cycle simulation, where the flux could be assumed constant, CRAM seems to be a better option. Further investigation is ongoing to assess computational time comparison and optimization of the Taylor and CRAM accuracy order.

#### **IV. Perturbation Analysis**

The implementation of the adjoint solution for the INSTANT solver has been completed for diffusion and transport. The realization of a module to perform Generalized Perturbation Theory [9] based analysis is ongoing.

# V. RELAP5 Coupling

The coupling with RELAP5 is on progress, and at this time it is possible to run steady state search calculation. The major advantage of replacing the version of NESTLE module of the RELAP5 package by INSTANT is the capability of increasing the spatial approximation arbitrarily and/or the angular approximation. Moreover, the cross section dependence from temperatures of structures, moderator density, control rod insertion, and xenon concentration are treated externally from the RELAP5 allowing the extension to an arbitrary number of energy group. The final implementation of the coupling will include also the implementation of a time dependent driver for INSTANT that is under development. Fig. [3]

shows the thermal group flux distribution with thermal feedback for one of the RELAP5 test cases (PWR rodded).

# **V. CONCLUSION**

The development of the PHISICS suite of codes at INL is continuing on a fast pace. The continuous addition of new features is generating a valuable tool to the reactor designers that it is foreseen to be deployable soon by the community.



Fig.1: Number of thermal iteration by outer. 3D model of the MHTGR350 Benchmark Model with 26 energy group



Fig. 2: Relative error (%) of CRAM  $8^{th}$  order and Taylor  $2^{nd}$  order with varing time step (TS) after 100 days of core burn up(flux costant) and 100 day cooling down.



Fig. 3:  $2^{nd}$  energy group for a PWR rodded RELAP5 test case

## 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

- C. RABITI, Y. WANG, G. PALMIOTTI, H. HIRUTA, J. COGLIATI, A. ALFONSI "PHISICS: a New Reactor Physics Analysis Toolkit," *Proc. 2011 ANS Annual Meeting*, Hollywood, Florida, USA, June 26–30, 2011, American Nuclear Society (2011) (CD-ROM).
- 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," *Proc. International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Rio de Janeiro, Brazil, May 8-12, 2011, .
- 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," *Proc. 2011 ANS Annual Meeting*, Hollywood, Florida, June 26– 30, 2011, American Nuclear Society (2011) (CD-ROM).
- 4. J. E. Morel and J. M. McGhee, "A Self-Adjoint Angular Flux Equation," *Nuc. Sci. Eng.*, **132**, 312 (1999).
- 5. M. PUSA, J. Leppänen "Computing the Matrix Exponential in Burnup Calculations," *Nucl. Sci Eng.*, **164**, 140, (2010).
- 6. RELAP5-3D Development Team, "RELAP5-3D Code Manual, Volume 1," INEEL-EXT-00834, Revision 2.4, Idaho National Laboratory, ID (2005).
- B. T. ADAMS and J. E. MOREL, "A Two-Grid Acceleration Scheme for the Multigroup S<sub>n</sub> Equations with Neutron Upscattering," *Nucl. Sci. Eng.*, 115(1993).
- S. BAYS, S. PIET, A. DUMONTIER, "Fuel Cycle Isotope Evolution by Transmutation Dynamics over Multiple Recycles," Proc. *ICAPP* '10, San Diego, CA, June13-17, 2010, American Nuclear Society (2010) (CD-ROM).
- 9. A. GANDINI, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy* **21**, 755, (1967).