Argonne National Laboratory's

Simulation Toolset for Reactor Physics and Fuel Cycle Analysis



# Faster and more accurate

Neutronics calculations enable optimum reactor design...

Argonne National Laboratory's powerful reactor physics toolset, PROTEUS,

# ...Reducing costs for designers of fast spectrum reactors.

The PROTEUS toolset can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling. The modeling capabilities within PROTEUS enable accurate and efficient simulation, the key to reducing both design and future construction costs.

## **Simulation Tools** for Reactor Physics and Fuel Cycle Analysis

PROTEUS encompasses the entire set of neutronics simulation tools developed over many years at Argonne, including the widelyused legacy tools for reactor physics analysis, and also the more recently developed code, UNIC. PROTEUS' extensive integrated suite of computer codes provides solutions to the coupled neutron-gamma ray Boltzmann transport equations. These, in turn, are part of a larger multi-physics design and analysis toolset that simulates fuel performance, fluid dynamics and structural mechanisms. Many modules in PROTEUS are also applicable to thermal reactors.

Users can request and/or acquire most of the PROTEUS toolset through the Radiation Safety Information Computational Center (RSICC). Source code, manuals, and sample problems are available to users. While UNIC is not expected to be released to RSICC in the near future, Argonne researchers routinely perform analysis with UNIC for various customers. Argonne maintains the PROTEUS toolset and may be contacted with any requests or questions.



## **PROTEUS'** long history of validation provides confidence in predictive simulations

Argonne's simulation tools have more than 30 vears of validation history against numerous experiments and measurements. The tools within PROTEUS work together, using the same interface files for easier integration of calculations.

### Multi-group Fast Reactor Cross Section Processing: MC<sup>2</sup>-3

No other fast spectrum multigroup generation tool matches the demonstrated accuracy of MC<sup>2</sup>-3. It generates broad-group, cell-average microscopic cross sections from ENDF/B basic nuclear data. MC<sup>2</sup>-3 handles the complicated resonance selfshielding in fast spectrum systems by directly accounting for the resonance interactions in detail and performing calculations (2082 ultrafine group + 400,000 hyperfine group) on conventional lattice cells or simplified R-Z core models. The resulting microscopic cross sections are used for fast reactor design and analysis calculations.

### **Solving Coupled Neutron-Gamma Transport Equations: DIF3D and VIM**

DIF3D, the main engine of PROTEUS, has been used for more than 30 years to solve the multigroup form of the coupled neutron-gamma transport equations using diffusion theory or transport theory. DIF3D provides the steady state reactor multiplication factor as well as flux and power distributions on standard one-, two-, and three-dimensional curvilinear, Cartesian, and hexagonal grids.

VIM solves the neutron and gamma transport equations using the continuous-energy Monte Carlo methodology to produce solutions on parallel computing machines. VIM is used primarily for criticality safety and verifying the accuracy of DIF3D + MC<sup>2</sup>-3 results.



## **Fuel Cycle/Depletion: REBUS**

REBUS, a reactor burnup and fuel cycle analysis code within PROTEUS, uses DIF3D as its flux solver. Modeling nuclide transmutations on a three-dimensional, region-dependent basis, REBUS offers flexibility for specifying operational constraints and fuel management strategies, in-core and ex-core. A unique and powerful technique for simulating equilibrium core characteristics is provided within REBUS as an alternative to discrete, cycle-by-cycle core modeling calculations.

### **Time-Dependent Modeling:** VARI3D, PERSENT and DIF3D-K

The dynamics of a reactor system under design basis and off-design basis operations is a key part of reactor design. Perturbation theory and sensitivity analysis codes VARI3D and PERSENT provide the kinetics parameters deployed in point kinetics models of reactor systems. VARI3D is built around the finite-difference diffusion solver in DIF3D-K, while PERSENT is built around the nodal P, transport solver in DIF3D-K.

detailed geometry models can be used in UNIC analysis.

method.

## SN2ND

PROTEUS also includes more recent work on SN2ND, a parallel neutronics solver for largescale simulations based on an unstructured finite element, multigroup, discrete ordinates formulation of the even-parity transport equation. SN2ND's higher fidelity representations permit the gradual phasing-out of existing modeling simplifications, allowing users to solve more complicated problems in finer detail.

Using SN2ND's parallel computing capabilities, researchers were able to reduce the error on predicted Zero Power Reactor (ZPR) reaction rates from ~15% to within the experimental measurement error (<3%). Future development is focused on extending SN2ND for all reactor types by incorporating a sub-group cross section treatment.

Arying levels of spatial detail are represented in geometry models for Argonne's Zero Power eactor. Homogenized drawer models are blicable to all tools in PROTEUS, and

Drawer Homogenized

DIF3D-K allows users to perform reactor kinetics or dynamics calculations within the geometrical capabilities of the DIF3D solver. DIF3D-K obtains time-dependent diffusion results using either the theta method or the space-time factorization

## **High-Fidelity Tool Development:**

Plate by Plate with Explicit Matrix Tube

## **Finalist for GORDON BELL PRIZE** in Supercomputing

SN2ND, part of the UNIC toolset within SN2ND scales on massively parallel Leadership Computing Facility, allowing researchers to solve more complicated problems in finer detail with fewer approximations. SN2ND was nominated for the prestigious Gordon Bell Prize in Supercomputing for its efficient and scalable algorithms.

 Detailed pin-cell geometry represented in full-core MONJU reactor calculation for UNIC.



# The PROTEUS Toolset: Representing Decades of Innovation

Since the mid-1980s, the PROTEUS toolset has helped scientists and researchers improve the design and safe operation of fast spectrum nuclear reactors. Offering a complete set of neutronics tools, the integrated environment within PROTEUS enables users to create internally consistent analysis projects and provides an additional level of confidence.

Today, PROTEUS enjoys a global audience, with users representing a wide range of industries and academic researchers.



 Thermal group flux distribution for Idaho National Laboratory's Advanced Test Reactor using SN2ND on the Argonne Leadership Computing Facility's Blue Gene/P.

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The PROTEUS development team is led by scientists at the Nuclear Engineering Division of Argonne National Laboratory. Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.



## Seventy years of leadership in nuclear science and technology

Argonne developed and/or built experiments, research reactors or prototypes of nearly every kind of commercial nuclear reactor in the world today, as well as many research and training reactors. An overview of this history can be found at

www.ne.anl.gov/About/ANL-Reactors.shtml

## On the cover

Argonne's UNIC code, part of the PROTEUS toolset, generates detailed pin-by-pin solutions for full core reactor problems. Shown on the cover is the full core fast flux distribution for the Japanese MONJU reactor generated using Argonne's SN2ND code on the Blue Gene/P.