Whole Core Multiphysics Simulations Enabled Through Pin Resolved Transport

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INTRODUCTION

Significant advances in multi-core, multi-node computing clusters over the past several years have enabled the development of practical numerical methods for solving the Boltzmann Transport Equation (BTE) to calculate fuel-pin-resolved neutron fluxes in full 3D nuclear reactor cores. Historically, the nuclear reactor industry has relied upon a two-step procedure to solve for full-core power distributions – by using pre-generated few-group cross sections, homogenized over a fuel assembly, and low-order 3D nodal diffusion approximations to obtain neutron flux distribution throughout the reactor. Then, the detailed fuel pin powers (required for core design and safety analysis) are determined by post-processing the whole core neutron diffusion solution and utilizing pre-computed shape functions, to reconstruct the detailed intra-assembly flux and power distribution. For several decades, these methods – which provide reasonable accuracy and require limited computing resources – have been the workhorse of the nuclear industry.

The use of more accurate full-core pin-resolved neutron transport methods to model the reactor requires significant additional computational resources [1–3], which are made available through the use of leadership-class computing facilities such as the U.S. Department of Energy INSITE program, which are capable of supporting applications using more than 100,000 compute cores and occasionally hardware accelerators such as GPUs. However, in order to deploy whole core transport methods to the nuclear industry, a methodology is needed that can run on industry-class computing clusters, which are typically between 500 and 5000 compute cores.

In this paper we will look at the impact of having full core, pin resolved neutron transport and the requirements for multiphysics coupling to realize new simulation capabilities that impact both the current fleet of operating nuclear reactors as well as advanced reactors that are currently being proposed.

WHOLE CORE PIN RESOLVED TRANSPORT

During the last few years, the Method of Characteristics (MOC) has become a nuclear industry standard for solving the transport equation for fuel assembly-sized problems [4,5], to generate the few-group homogenized cross sections for whole-core nodal diffusion methods [6]. Because of the computational appeal of MOC and the familiarity of the industry with this method, several researchers investigated the extension of MOC to larger 3D reactor problems [7,8,2]. However, it became evident that even with leadership-class computing platforms, the MOC method is too costly for these problems. A group of Korean researchers then investigated "2D/1D" methods, which utilize MOC in the 2D radial (xand y) directions and a lower-order transport solution in the 1D axial (z) direction [9,10]. This approach was motivated by the fact that most of the material heterogeneity in Light Water Reactors (LWRs) occurs in the radial directions, whereas the axial material heterogeneity is comparatively minimal.

The first 2D/1D method was introduced as the "2D/1D Fusion" method in the CRX code [11], which utilized a 2D MOC solution radially with a discrete-ordinates solution axially. Specifically, the radial 2D MOC method was discretized on a "fine" radial grid (in which each pin cell is divided into 50–100 "fine" spatial cells or "flat source regions"), while the axial solution was discretized on a "coarse" radial cell (consisting typically of one pin cell). The second major implementation of the 2D/1D method was in the DeCART code, developed at the Korean Atomic Energy Research Institute (KAERI) [9]. This method differed from the 2D/1D fusion method in that the axial solver was based on the diffusion approximation (and later, on SPN) [10]. A more recent implementation of the 2D/1D method in DeCART has been the nTRACER code [12]. In the KAERI codes, the 2D MOC methods are also discretized on a fine radial grid, and the axial methods on a coarse radial grid. During the past few years, the KAERI 2D/1D methods have achieved success for practical reactor applications [13].

However, significant limitations in the numerical stability and accuracy were observed in DeCART, particularly when refining the axial mesh. None-the-less, the general concept of a 2D/1D method for whole-core reactor methods research provided a useful starting point when the U.S. Department of Energy (DOE) initiated the Nuclear Reactor Simulation Hub, CASL, in 2010. The first step in this development was to derive the 2D/1D equations directly from the 3D transport equation and to formalize the sequence of approximations used in the derivation. The result of this work was a numerically robust 2D/1D method that provided the foundation for the MPACT computer code [14,15] – which has become the whole-core deterministic neutron transport solver for the CASL core simulator VERA-CS. The purpose of this paper is to describe the principal features of the 2D/1D method in MPACT.

MPACT is a 3D whole-core transport code based on the 2D/1D method. It provides pin-resolved flux and power distributions, which are important for the "challenge problems" in CASL. This fine spatial resolution is achieved by obtaining transport solutions for heterogeneous reactor problems in which the detailed geometrical configuration of fuel components, such as the pellet and cladding, is explicitly retained. The cross-section data needed for the calculation is obtained directly from a multigroup microscopic cross section library, similar to libraries used in lattice physics codes that generate the few-group cross sections for the full-core nodal simulators. Because MPACT involves neither a priori homogenization nor group condensation for the core spatial solution, it represents a significant advance in the fidelity and accuracy of the full-core flux solution, without compromising the stability and robustness required for industry applications.

MULTIPHYSICS COUPLING MECHANISMS

While accurate solutions of the BTE can greatly inform our understanding of the local flux distribution and fission source in a reactor, the integration of this capability with other physics is crucial to understand the behavior of operating power reactors. MPACT directly addresses this need by integrating the concept of feedback from other physics directly into its solution sequence [16]. Such feedback operations include; coupling to thermal hydraulics to provide the impact of temperature and density changes on the cross-sections, the computation of equilibrium Xenon and Samarium concentrations, and coupling with coolant chemistry and mass transport to understand how constituents move with the coolant and their impact on reactor behavior.

For the applications shown here, the thermal-hydraulic feedback comes from CTF [17]. CTF is a subchannel code which solves the flow in every channel in the core accounting for cross-flow between pins. This closely matches the fidelity in which MPACT is solving for the flux in the reactor. The MPACT-CTF coupling forms the core of a standard reactor core simulator which is capable of accurately simulating multiple cycles of operation of commercial reactors [18, 19].

CRUD INDUCED POWER SHIFT SIMULATIONS

A long-standing challenge within the nuclear industry is the prediction of the evolution of nickel ferrite ($NiFe_2O_4$) "crud" on cladding surfaces and the precipitation of lithium tetraborate($Li_2B_4O_7$) in the PWR cladding. As crud forms on the water-side surface of the cladding near subcooled nu-cleate boiling sites, as a result of metals in the coolant, the temperature in the adjacent cladding and fuel increases. Because of the boron in the coolant used to control reactivity in a PWR, lithium tetraborate can precipitate within the porous crud and trap a significant amount of boron at that location on the fuel rod. This localized boron in the upper half of the core can absorb neutrons and thus cause the power to shift to the lower half of the core, leading to a crud-induced power shift (CIPS).

The MAMBA code [20] is developed to simulate the crud growth and precipitation of lithium tetraborate on a surface. This capability is tightly coupled with CTF to perform a detailed thermal-chemical solution on the surface of each fuel pin in the reactor. All of the shared data have direct feedback into the physics of the problem. High power in a location will cause higher surface temperatures in CTF, which in turn will cause an increase in the local steaming rate, resulting in more crud deposition. The increased crud deposition will reduce the local moderation around the pin, and the thicker crud will provide locations at which boron can precipitate in the form of lithium tetraborate. The result of the reduced moderation and boron precipitation will be suppression of reactor power. This entire process must be captured to adequately simulate CIPS. [20]

The high fidelity multiphysics simulation is a key driver in understanding and predicting CIPS. The pin-by-pin resolution of MPACT and CTF uniquely provides a capability that can consider the crud growth on a rod-by-rod detail along with the lithium tetraborate deposition in the crud layer. The feedback of the changing boron concentration in the crud layer is propagated into the neutronics solve which will have a direct impact on the power shape. Without this effect on the pin-wise level, it would be difficult to predict CIPS.

MOLTEN SALT REACTOR SIMULATIONS

The US Department of Energy and industry have shown significant interest in advanced reactors, as evidenced by over 1.3 billion dollars of private investments in companies to develop advanced reactor concepts [21]. More than seven of these advanced reactor concepts use molten salt reactor (MSR) technology. The extension of a capability like MPACT and CTF to solve molten salt reactors involves understanding and characterizing new physics, enhancing underlying data and property models, and expanding the geometric flexibility of the codes.

The flowing fuel introduces a few new feedback mechanisms that need to be included but they all tie into a

tight coupling with a passive species mass transport model. Since the fuel and the fission products are flowing with the salt, care must be taken to account for the motion of each constituent. Of key interest is the motion of delayed neutron precursors and the impact on reactivity. The half-life for delayed neutron emission is grouped on the order of milliseconds to minutes and it is important to know exactly where these delayed neutrons are emitted. Typically, the neutrons are emitted significantly down stream from the original fission site and potentially completely outside of the core region.
Likewise, the motion of other isotopes can be important for a range of reasons; neutron poisons, decay heat release, corrosion, noble metal plating, and off-gas considerations. Work is underway to identify which elements and isotopes are crucial to track and groupings of these isotopes to reduce computational burden. For the remaining isotopes, a well-mixed assumption is sufficient over the time scales that are of concern for steady state analysis of these reactors.

Another key area for molten salt reactors is understanding the thermochemistry as the fuel constantly changes. While the salts of interest are fairly well qualified for beginning of life conditions, the addition of fission products creates a complex mixture of elements and it is crucial to understand both the change in thermophysical properties but also the phase and chemical state of the salt for the full temperature range of the reactor. Also understanding the chemical potential of the salt is important to control corrosion in the reactor materials.

High fidelity simulation capability allows the analysis to easily understand the complex behavior of these advanced reactors without the need for upfront cross-section functionalization, develop approximate transport and coupling models which could take years to accurately develop models that work in all situations. While the whole core transport capability will take more time to run, it saves significant development time into new methods and tools.

CONCLUSIONS

In this paper, we demonstrated the benefits of whole core pin-resolved neutron transport for coupled multiphysics problems. For CIPS, the pin-resolved coupled neutron transport, thermal-hydraulic and crud chemistry compoents were crucial to solve together to capture the power shift. In molten salt reactors, new complex physics require advanced modeling and simualtion capabilities to understand the behavior over time. Additionally, high fidelity tools reduce methods development time to determine robust and accurate low-fidelity models to solve these reactors which could take several years to develop and demonstrate.

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