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OSIRIS: A MODERN, HIGH-PERFORMANCE, COUPLED, MULTI-PHYSICS CODE FOR NUCLEAR REACTOR CORE ANALYSIS

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ABSTRACT

To meet the simulation needs of the GNEP program, LLNL is leveraging a suite of high-performance codes to be used in the development of a multi-physics tool for modeling nuclear reactor cores. The **Osiris** code project, which began last summer, is employing modern computational science techniques in the development of the individual physics modules and the coupling framework. Initial development is focused on coupling thermal-hydraulics and neutral-particle transport, while later phases of the project will add thermal-structural mechanics and isotope depletion. **Osiris** will be applicable to the design of existing and future reactor systems through the use of first-principles, coupled physics models with fine-scale spatial resolution in three dimensions and fine-scale particle-energy resolution. Our intent is to replace an existing set of legacy, serial codes which require significant approximations and assumptions, with an integrated, coupled code that permits the design of a reactor core using a first-principles physics approach on a wide range of computing platforms, including the world's most powerful parallel computers. A key research activity of this effort deals with the efficient and scalable coupling of physics modules which utilize rather disparate mesh topologies. Our approach allows each code module to use a mesh topology and resolution that is optimal for the physics being solved, and employs a mesh-mapping and data-transfer module to effect the coupling. Additional research is planned in the area of scalable, parallel thermal-hydraulics, high-spatial-accuracy depletion and coupled-physics simulation using Monte Carlo transport.

Key Words: nuclear reactor modeling, multi-physics simulations, high performance computing

1. OVERVIEW AND MOTIVATION

The Global Nuclear Energy Partnership (GNEP) is designed to address national energy needs and improve national security through the development of a closed nuclear fuel cycle, as well as safe and efficient next-generation nuclear reactors. The initial phase of the program is focused on the development of an advanced burner reactor for the transmutation of spent nuclear fuel, and separation and reprocessing technologies to permit the reuse of nuclear fuel in a multi-pass fuel cycle. Meeting the design challenges for this initiative requires the availability and use of advanced simulation tools that are based upon first-principles physics. Such tools are essential for a detailed understanding of the complex physical phenomena within reactor cores, and to enable the design of new, innovative reactor systems.

The motivation for the development of an advanced reactor simulation code becomes clear when one examines the current state of practice in reactor design. The existing methodology is largely based upon lumped-parameter modeling. This approach replaces a detailed, first-principles description of the reactor with a reduced-complexity, approximate model, in order to provide a tractable problem for solution. This results in a lack of detailed understanding of phenomena at unresolved scale lengths.

Current design methodology also relies upon multiple, successive coarse-resolution averaging steps over both space and neutron energy. Consider the successive energy-group collapsing steps employed during reactor modeling. A typical approach to modeling a light water reactor starts with the calculation of pin cells with fine energy resolution (continuous energy or hundreds of energy groups), followed by assembly calculations using a coarse energy-group structure (tens of groups), and finishing with full core calculations using a very coarse group structure (typically two groups).

In addition, the current state of practice makes significant use of empirical or semi-empirical approximations. The reliance on empirical approximations is, in large part, due to the limited simulation capability that has been available to reactor designers. Current modeling efforts utilize codes that were developed in the 1960s through the 1980s, which have little (if any) high-performance computing capabilities. As a result, modeling methodologies have been developed that use up to 100 different codes to solve individual portions of the overall design process [1]. Neutronics modeling of a reactor core could utilize three separate codes, each of which models a portion of the core, where the results from each computational step are averaged over space and neutron energy, before proceeding to the next step. While the nuclear reactor industry in the United States has lagged behind those in France, Japan and Korea over the last two decades, this type of modeling methodology is routinely applied around the world.

Numerous limitations in nuclear reactor design are inherent in the use of current design codes and models. As a result, conservative safety factors, or margins, are built into the reactor design to account for the lack of fine-scale spatial/energy resolution. In addition, expensive component and scaled-plant experiments are required to provide numerical values for empirical models, especially for the design of new reactors which do not have a previous operational history from which to obtain the required data. Based upon these limitations, participants at a recent workshop on simulation and the nuclear fuel cycle concluded that coupled, multi-physics reactor design codes are grand challenge applications that are required for accurate modeling of future reactor systems [2].

2. A HIGH-PERFORMANCE TOOL FOR REACTOR DESIGN

Responding to this challenge, our team is leveraging its proven expertise in code development and our suite of existing codes to produce a high-performance, coupled, multi-physics reactor design tool. This code has been named **Osiris** after the Egyptian god of death, rebirth and fertility: a direct analogy to the history of the nuclear power industry in the United States. **Osiris** will be applicable to the design of existing and future reactor systems through the use of first-principles physics models of flow, heat transfer, structural mechanics and neutral-particle transport, with fine-scale spatial resolution in three dimensions and fine-scale particle-energy resolution. The use of modern computational science methods will enable high-fidelity, efficient calculations on high-performance, parallel computing platforms.

As a result, highly resolved calculations of reactor-core operational and transient scenarios will be possible without resorting to lumped-parameter approximations. This new code will permit full-core calculations of flux and power profiles, with reasonable energy resolution and a sufficient number of cells which spatially resolve flux distributions across the fuel pins and within the flow channels. The high-fidelity, first-principles-based calculations enabled by the **Osiris** code will permit a reduction of conservative operating margins, and will reduce the need for costly component-based and pilot plant experiments.

Our intent is to replace an existing set of legacy codes, which require significant approximations and assumptions, with an integrated, coupled code that permits the design of a reactor core using a first-principles physics approach. This will greatly simplify the reactor-core design process, and increase the productivity of reactor designers. In addition, the high performance capabilities of **Osiris** will enable routine calculations at scales which are impossible for the current modeling methodology.

2.1. Technical Approach

Our team is currently performing the algorithmic research and development necessary to create the prototype version of the **Osiris** code. This code will be used to model complex reactor systems through the use of first-principles physics models of flow, heat transfer, structural mechanics and neutral-particle transport, with fine-scale spatial resolution in three dimensions and fine-scale neutron-energy resolution. The use of modern computational science methods will enable high-fidelity, efficient calculations on high-performance, parallel computing platforms.

Highly resolved calculations of reactor-core operational and (near-operational) transient scenarios will be possible without resorting to lumped-parameter approximations. **Osiris** will permit full-core calculations of flux and power profiles, with reasonable energy and spatially resolution of the flux distributions across the fuel pins and within the flow channels. The high-fidelity, first-principles-based calculations enabled by **Osiris** will allow for a reduction of conservative operating margins, while the use of first-principles physics models will reduce the need for costly component-based and pilot plant experiments.

Although **Osiris** is a new code, the project having been started in July 2006, it is being built from a solid base of past achievement. Our approach strongly leverages existing LLNL capabilities which have been previously developed with support from other DOE programs, most notably the Advanced Simulation & Computing (ASC) program and the Advanced Scientific Computing Research (ASCR) program. These codes are either currently in production use, or are nearing production status. For the initial version of **Osiris**, we are coupling a thermal-hydraulics code to a suite of neutron transport codes which have modular interfaces, such that data communication can occur via a set of mesh-mapping and "driver" modules. Later phases of the project will add a thermal-structural mechanics module and a depletion-deposition-decay module, as well as extend the capabilities of the mesh-mapping module. High-performance, parallel computations has been one of the key design and development requirements for each of these modules. As a result, **Osiris** will enable large-scale, first-principles calculations of reactor cores through use of a single, integrated code, instead of using multiple codes, each of which is used for a particular modeling phase with a particular level of spatial and energy homogenization (averaging).

As shown in Figure 1, **Osiris** is built around a mesh-mapping and data-transfer module named **Carter** [3], which acts as the conduit for data transfer between the various physics modules.

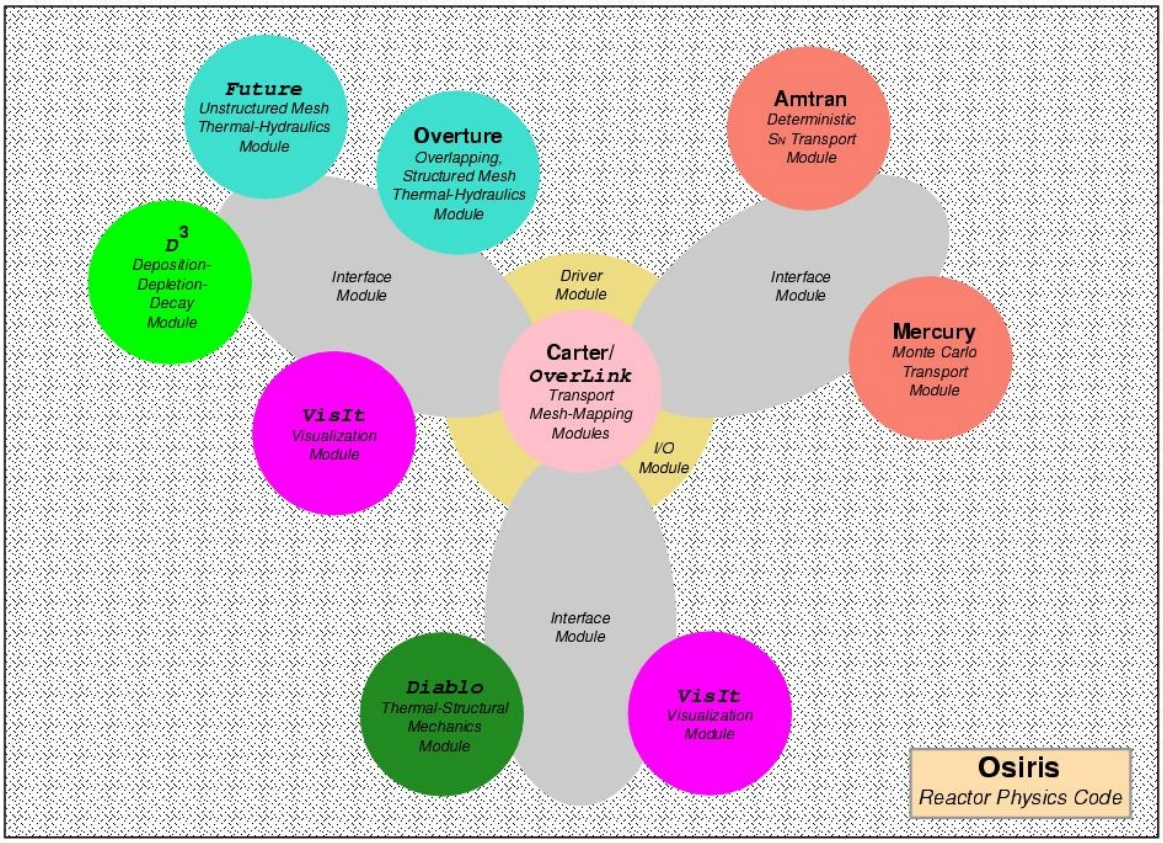


Figure 1. A schematic layout of the **Osiris** reactor analysis code. The the mesh-mapping module **Carter** acts as a data conduit at the hub of this multi-physics code. The thermal-hydraulics module is built upon the **Overture** framework, which is connected to the transport modules, **Amtran** and **Mercury** via **Carter**. Future physics and support modules are shown in *italicized* font. **Osiris** is designed as a single, integrated code that is capable of replacing the use of multiple, legacy codes for the design of nuclear reactors.

The thermal-hydraulics module in **Osiris** has been developed within **Overture** [4], a framework for the solution of coupled PDEs. The ASCR program has funded the development of **Overture** during the past decade. An existing suite of transport code modules is also being interfaced to **Carter**. The **Amtran** discrete-ordinates (S_N), adaptive mesh refinement (AMR), deterministic transport code [5], and the **Mercury** Monte Carlo statistical transport code [6], have been developed over the past decade with support from the ASC program. The same program has also funded development of the **Diablo** thermal-structural mechanics code [7]. These three code modules have a long history of production use within the ASC program at LLNL. The sum total of the development time that has been invested in all of these code modules is approximately 80 person-years.

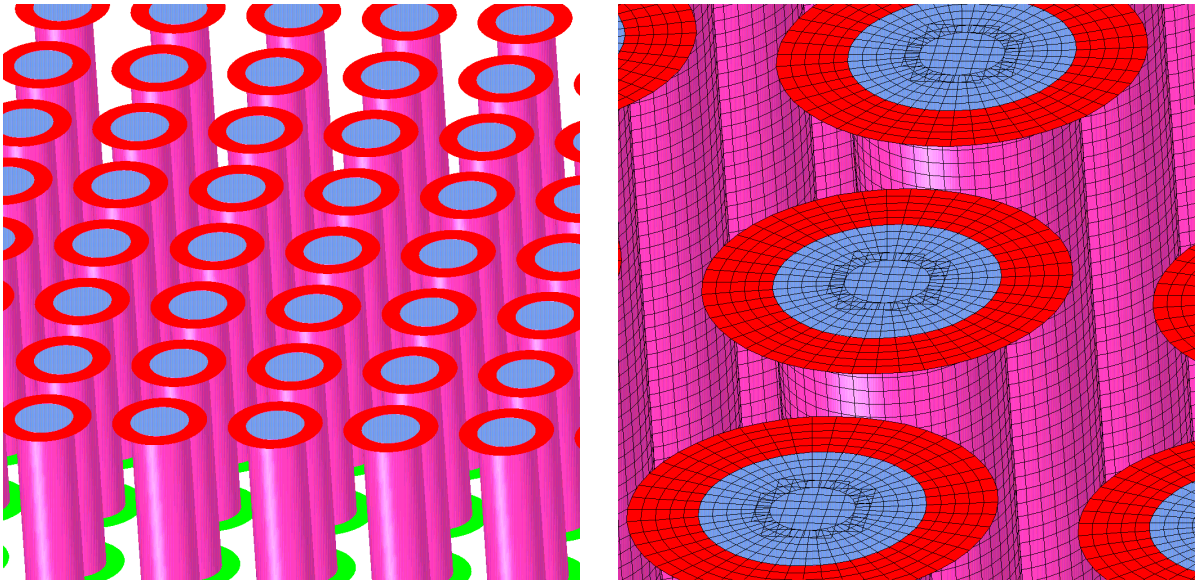
Of course, significant effort must still be expended to produce a production quality reactor design code. While our team has a solid set of physics capabilities on which to build, the overall code system needs to held together with a set of "driver" and interface modules. The driver module serves many functions, which include maintaining module-common data structures, scheduling input/output tasks, and orchestrating the overall execution of the individual physics packages. The interface modules serve to funnel mesh-based data between the peripheral physics/support

modules and the mesh-mapping modules in the central hub. The **OverLink** module [3], which will be added in a later phase of development, is a superset of the **Carter** mesh mapper that supports a more general set of donor-target mesh topologies: unstructured meshes on each end, compared to **Carter** which maps from an unstructured donor mesh to a structured target mesh. Development of the **D^3** module is underway to provide support for flux-based isotope depletion and production, energy deposition and radioactive isotope decay.

2.2. Research and Development Activities

There are numerous algorithmic challenges associated with this development effort. While some are associated with the individual modules, many deal with the requirement to produce a coupled code that operates efficiently in a parallel computing environment.

A key research activity of this effort deals with the efficient and scalable coupling of physics modules which utilize rather disparate mesh topologies. Our approach allows each code module to use a mesh topology and resolution that is optimal for the physics being solved, and employs a mesh-mapping and data-transfer module to effect the coupling. The mapping of mesh-based data through the code's central hub is made rather complex by the variety of mesh topologies supported in the various physics modules. The thermal-hydraulics module in **Overture** uses multiple sets of overlapping grids of various topologies (as shown in Figure 2), the **Diablo** thermal-structural mechanics module employs a "finite element zoo" representation of (degenerate) hexahedra, the **Amtran** transport module uses block-based structured AMR meshes, and the **Mercury** Monte Carlo code supports many mesh-based options, both structured and unstructured, as well as combinatorial geometry. This rather diverse set of meshes has motivated the use of the **Carter** mesh-mapping module for the initial development phase. In this mode of operation, the



(a) *(b)*

Figure 2. Example of an **Overture** overlapping mesh that can be used for a multi-physics computation. There is an overlapping mesh for the region exterior to the cylinders and overlapping meshes (cylindrical plus Cartesian; See Figure 2b) for the interior of each cylinder. This composite mesh could be used for the modeling of a heated pin, with a fluid flowing around each of the cylinders and the heat equation solved within the cylinders.

overlapping-grid (**Overture**) or unstructured (**Diablo**) mesh data is mapped to/from a structured transport mesh. Research is underway to develop an optimal mapping scheme within **Carter** to map data between overlapping meshes and structured/AMR meshes. Full-physics calculations (thermal-hydraulics, thermal-structural mechanics and transport) will require the more general option provided by the **OverLink** mesh-mapper must be employed. In this case, Figure 1 clearly shows that multiple instances of an **OverLink** or **Carter** map will be required to transfer mesh-based data between the different lobes.

The disparate space and time scales associated with the thermal-hydraulics or thermal-structural mechanics (typically long-time/short-space scales) and transport modules (typically short-time/long-space scales) means that care must be taken when developing operator-splitting techniques for parallel execution of the integrated code. While this is an important aspect for static calculations, it is critical that an efficient means is developed for operation of the code in time dependent calculations. We are investigating several techniques for operator-splitting, including the use of sub/super cycling, and will implement a scheme that maximizes the accuracy and stability of the coupled code.

Research and development is also required to enhance our current flow and thermal-transfer capabilities within **Overture**, in order to produce an efficient, accurate and scalable parallel thermal-hydraulics capability. The challenge relates to **Overture**'s use of overlapping grids. Efficient parallelization and load-balancing of algorithms on these meshes is significantly more challenging than for the case of a single non-overlapping mesh. A key development here is the extension of the current 2nd-order accurate multi-grid solver to be both fourth-order accurate and parallel. The use of high-order accurate methods is important for simulating high-Reynolds number flow regimes, and for future extensions that may incorporate LES turbulence models. This multi-grid solver will be used to efficiently solve the elliptic constraint equations associated with the fourth-order accurate incompressible (Boussinesq) and “all-speed” compressible flow solvers. These constraint equations are currently solved using Krylov and algebraic-multi-grid techniques. Serial calculations indicate that the multi-grid solver uses an order of magnitude less memory and is order of magnitude faster that other state-of-the-art linear solvers.

An area of upcoming research will focus on methods for performing isotopic depletion/decay and energy deposition calculations in the context of coupled, multi-physics, time-dependent calculations. This is important, since isotope depletion is rather sensitive to the material temperature, which is coupled in a non-linear manner to neutron transport, and thus, the reactor power level. An important aspect of this work is the development of a high-spatial-accuracy solution of the Bateman equation for modeling the temporal decay of radioactive isotopes. This effort is aimed at reducing discontinuities between zones within fuel pins, in order to provide high-order estimates of the fission-product gradients which induces isotope migration within fuel pins.

Finally, we will investigate the feasibility of using the high-performance Monte Carlo transport methods provided by **Mercury** for the solution of coupled physics problems. The statistical noise associated with the use of Monte Carlo methods in cell-local quantities, such as energy deposits, has led to convergence problems when transport and fluid flow have been coupled [8]. It is not clear whether these problems can be overcome through the use of higher particle counts possible with parallel computations, or whether advanced expected-value tally techniques will be required to make this a viable option.

3. SUMMARY AND CONCLUSIONS

A new effort at LLNL has recently begun to develop a modern, integrated, multi-physics reactor analysis code. Our intent is to produce a single, high-performance modeling tool which is capable of replacing an existing set of legacy codes that are used in a cumbersome, multi-step modeling methodology. The resulting **Osiris** code will permit highly resolved calculations of reactor-core operational and transient scenarios while minimizing the need for lumped-parameter approximations. To achieve this goal, our team is leveraging its proven expertise and suite of modern code modules, which have been developed for use on high-performance computers with funds from other DOE programs.

The short-term focus of this effort is to couple a thermal-hydraulics module to multiple neutral-particle transport modules through a mesh-mapping module, which represents the central hub of **Osiris**' code integration framework. While this approach to code coupling has been used successfully at LLNL in the past, this initial integration step is challenging, since each of the physics modules to be coupled uses a unique description of the mesh topology. A later phase of the project will add support for an existing thermal-structural mechanics, as well as new depletion-deposition-decay and driver modules. This rather capable design tool will require multiple instances of the mesh mapping process to couple the disparate meshes used in the various physics modules.

The anticipated time frame for completion of the prototype version of **Osiris** is three years. During this time, our team will continue to consult with reactor designers in industry and at the national laboratories to ensure that **Osiris** will (eventually) meet their needs when designing future, innovative reactor systems.

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