



Mark DeHart '84 Directorate Fellow Nuclear Science & Technology Directorate Idaho National Laboratory



Multiphysics Modeling in Support of NASA Nuclear Thermal Propulsion Designs

**Texas A&M University** 

October 5<sup>th</sup>, 2022



INL/MIS-22-69498

### **Overview**

Introduction to Idaho National Laboratory

 Specific Work Opportunities of Potential Interest

▶ Nuclear Thermal Propulsion

- Background on Griffin
- >>>>Analysis Workflow
- Malysis Approach
  - Cross section generation
  - Mesh generation
  - Fuel element modeling

Validation using SIRIUS measurements in TREAT

(time permitting)

- Closing Remarks
- Internship Opportunities



SIRIUS-1 Fuel Test Specimen



IDAHO NATIONAL LABORATORY

2

### **National Laboratories**



### Addressing the world's most challenging problems





- Nuclear fuels and materials
- Nuclear systems design and analysis
- Fuel cycle science and technology
- Nuclear safety and regulatory research
- Advanced Scientific Computing



#### Advanced Test Reactor Complex

- Steady-state neutron irradiation of materials and fuels
- Naval Nuclear Propulsion Program
- Industry
- National laboratories and universities



#### Materials & Fuels Complex

- Transient testing
- Analytical laboratories
- Post-irradiation examination
- Advanced characterization
- Fuel fabrication
- Space nuclear power and isotope technologies



#### Energy & Environment S&T

- Advanced transportation
  - Environmental sustainability
- Clean energy
- Advanced manufacturing
- Biomass



#### National & Homeland Security S&T

- Critical infrastructure
  protection and resiliency
- Nuclear nonproliferation
- Physical defense systems

# Advanced reactors are coming – a key opportunity for reactor physics capabilities



#### **Griffin: Advanced Reactor Physics Tool** Workhorse of Reactor Physics Methods and Analysis Dept. FHR, SFR, MSR PROTEUS Neutronics Argonne SAM Pronghorn Sockeye **Opportunities**: +Internships, January post-doc, 2020 115 full-time AMMOTH RELAP-7 **BISON Multiapp** Coupling by Design **Micro-Rx Strong Coupling HTGR** Westinghouse 200 Canadian Nuclear Laboratories • Los Alamos Fuel Particl framatome OKLO NASA Fuel Kerne Low Density Graphite Buffer Fuel Annulus BWX High Density Graphite Surface AEROSPACE Silicon Carbide Outer Pyrocarbon Sub-app 4-1 Sub-ap 4-2 **IDAHO NATIONAL LABORATORY** 6

### **INL's Thermal Fluids Methods and Analysis Department**

#### RELAP5-3D

- Modeling air ingress scenarios in High Temperature Gas Reactor (HTGR)
- Simulating steam generator tube rupture and steam ingress in the primary side (HTGR)
- Sodium natural circulation during transients (SMR)

*Contacts*: Theron.<u>Marshall@inl.gov</u> Connie.Stevens@inl.gov

#### **Computational Fluid Dynamics**

- Modeling coupled fluid flow and heat transfer including coupled effects such as oxide layer growth and nucleate boiling
- Simulating 3D flow induced vibration and analyzing risks of multi-axial mechanical fatigue
- Development of the INL CFD code







#### **Multiphysics**

- Modeling flow-accelerated corrosion and tracking species in Molten Salt Reactor (MSR)
- Coupled neutronics thermal hydraulics thermomechanics simulations (MSR & microreactors)
- Multiphysics analysis of bowing in liquid-metal cooled reactors involving thermomechanical deformation and coupled thermal hydraulics effects

#### **Opportunities**:

Internships, post-doc, full-time

#### **Code Development**

- Code coupling to model dynamic and complex systems for advanced reactors
- Python scripting for material property generation, analytic solutions, and input/output processing

### **Nuclear Propulsion for Interplanetary Travel**

- >> NASA plans to launch a manned mission to Mars by the end of this decade.
  - Interplanetary travel will be fueled by nuclear propulsion up to half the travel time
  - Two options are being considered:



directly. Nuclear electric propulsion (NEP), where a nuclear reactor is used to generate electromagnétic fields to accelerate ions that are used to generate thrust.

heated to high (~3000 K) temperature to provide thrust

- NTP is more technically mature, and NASA is focused on it for rocket design.
- >> A mission to Mars will use a space or lunar base to assemble interplanetary engines and vehicles, nuclear engines will not launch from Earth.
- The US Department of Defense is also pursuing development of NTP engines for cis-lunar operations (Space Force) under the "Demonstration Rocket for Agile Cislunar Operations (DRACO)" project.







Conceptual NTP design. Crew cab is on far right. Golden tanks are for hydrogen, and most will be jettisoned during the mission.



**IDAHO NATIONAL LABORATORY** 



### Why NTP?

The value of NTP was recognized in 1947 and large experimental programs pursued NTP engine design in the1950s and 1960s.

NTP has several advantages over chemical H<sub>2</sub> + O<sub>2</sub> engines

- First and foremost, a factor of 2-3 gain over performance (specific impulse,  $I_{sp}$ , analogous to MPG in a car).
  - The I<sub>sp</sub> represents the <u>time</u> over which 9.81 kilograms (or one Newton of weight on Earth) of propellant can produce one Newton of thrust.
  - The larger the I<sub>sp</sub>, the longer the engine can operate with a given mass of fuel.
  - For chemical engines the  $I_{sp}$  is about 450 s. For  $H_2$  in an NTP engine, the ISP is about 900 s. This is related to the molecular mass of the propellent.
- Can cut transit time to Mars in half (reduced radiation exposure)
- Large abort window relative to chemical system
- Potential for doubled payload (but with increased transit time)



unclear inermal propulsion



INL support for NASA Marshall Flight Center and Glenn Research Center

- Development of Griffin model NASA nominal plant design
  - 2D single assembly
  - 3D single assembly
  - 3D full core
  - Multiphysics simulations
    - Neutronics
    - Thermal-fluids
    - Heat transfer
    - Structural mechanics
    - Transient simulations
- Simulation of SIRIUS series of experiments in TREAT

IDAHO NATIONAL LABORATORY

11

(U,Zr,Nb)C fu

Metal hydrid

### **The MOOSE Herd**



### What is Griffin and Why is it important?

Griffin is a generalized tool for reactor physics for non-LWR reactors

- Multiphysics-oriented
  - Provides native coupling to all MOOSE-based tools
  - Takes advantage from common investment in framework
- Flexible and Extendable
  - Regular and unstructured geometries
  - Various types of calculations (variable fidelity)
  - Easy addition of functionality
- Robust
  - Consistent with NQA-1 process
  - Strict software development cycle
- NRC's designated non-LWR neutronics code
- 50/50 partnership between INL and ANL



### **Homogenization Equivalence Methods 101**



Equivalence-corrected library

Monte-Carlo corrected cross-sections to use an *accurate* diffusion scheme for *transients* 

#### In-house meshing-tools Cubit NTP (and TREAT) Analysis Workflow Homogenization overlay file Build mesh (Cubit) and Serpent model\* Reference k-eff Exodus mesh file Serpent PAlign detectors (tally regions) in Serpent model with corresponding regions in mesh for cross Multigroup cross section and flux tallies section assignment.\* Calculate k<sub>eff</sub> and fluxes in cross section regions ISOXML with Serpent (reference solution) tallied over MG Multigroup cross section energy groups library in xml format Perform a Super-Homogenization (SPH) Griffin-sph calculation using Griffin to find energy-dependent correction (SPH) factors that will match multigroup Multigroup cross section fluxes. library with SPH factors Update cross section library to add SPH factors\* Griffin-eigenvalue Repeat for each state point (typically temperature, control element position)\* Steady-state solution Run steady state calculation, confirm agreement \*These processes are largely automated with reference Run transient simulations **IDAHO NATIONAL LABORATORY**

### **Cross Section Preparation with Serpent**

What is Serpent? A Monte-Carlo code created for reactorphysics calculations.

Bottom line: it creates nuclear cross sections for us!

- Monte Carlo method:
  - Stochastic transport method
  - Highly accurate in energy resolution
  - Slow & mostly limited to steady-state
- Griffin:
  - Deterministic transport method
  - Uses few-group cross sections
  - Designed for multiphysics transients
- We use Serpent's built-in cross section tallying, energy collapsing and spatial homogenization to generate cross sections in a userspecified group structure



Serpent NTP core calculation

IDAHO NATIONAL LABORATORY

Serpent

Model

### **Mesh Generation for the Neutronics Model**

- Needs to occur before developing Serpent models to define homogenization zones in Serpent
- Homogenization: Average nuclear cross sections over heterogeneous regions
  - Pro: Saving in computational resources
  - Con: Loss of fine resolution
- Often thermal-hydraulics drive uncertainties despite homogenization
- Homogenization equivalence and reconstruction mitigate loss of fine resolution









Axial homogenization





Quantity	Value
Av. Fuel T [K]	2188
Inlet Moderator T [K]	410
Max. T [K]	3033
Outlet Moderator T [K]	2656





- Neutronics: Griffin
- Heat Transfer: Griffin (MOOSE Heat Conduction module)
- Structural Mechanics: Griffin (MOOSE Tensor Mechanics module)
- Convection Cooling: Griffin (MOOSE Thermal Hydraulics Module)

### **Full-Core Model Overview**

- ▶ 61 Fuel Elements in 5 rings
- 18 Control Drums in Be reflector to adjust reactivity/power
- In most current simulations all the drums are simultaneously rotated with the same rotation angle
- Griffin allows independent drum rotation (e.g., for a simulated reactivity insertion accident)

#### New CERMET/CERCER NASA/BWXT NTP concept





### **Coupled NTP Full-Core Model**





Using MOOSE control logic, we have created a software proportional-integral-derivative (PID) controller

- Requires less trial and error than manual control
- Eurrently ignores any limitation on drum rotation (speed, etc.)

### **SIRIUS experiment series**

- Experimental campaign for transient testing of new NTP Fuel candidates: UN-CERMET & UN-CERCER
   Experiments are performed in TREAT
- Challenges of NTP fuel:
  - Very hot: 2600-2850 K
  - Fast heat rates: 100 K/s
  - Strong temperature gradient (~25 K/cm)
- SIRIUS series progresses in complexity:
  - SIRIUS-1: UN-CERMET proof of principle
  - SIRIUS-2: Series of different materials, fab. processes, CERMET (and a CERCER experiment in the works)
  - SIRIUS-3: Stack of 16 fuel specimens with 7 gas channels
  - SIRIUS-4: first hydrogen-cooled experiment, 10 stacked specimens of CERMET
  - SIRIUS-5: second hydrogen-cooled experiment, CERCER stack of specimen





### **Multiphysics Simulations of SIRIUS-CAL**

Calibration experiment for SIRIUS-1



- Fuel element containing safety control rod
- Fuel element containing compenstation control rod
- Non-fueled source element
- Zirc-clad non-fueled graphite element Zirc-clad slotted graphite block
- Experiment region
- Half-width zirc-clad slotted element
- Half-width zirc-clad non-fueled graphite element



#### SIRIUS-CAL Insert Assembly SIRIUS-CAL Insert Assembly .....

### **Multiphysics Model of SIRIUS-CAL**

- Multiphysics model uses 2-step process: Serpent cross section, Griffin diffusion with SPH equivalence
- Transient is a coupled Griffin neutronics + thermal model



### **SIRIUS-CAL Multiphysics Results**

SIRIUS-CAL reactivity insertion is 0.55% dk/k

We currently adjust control rod motion to match TREAT initial period – ongoing work to be fully predictive for TREAT transients

Goal is validation for SIRIUS-CAL

Thermal fluxes in steady-state



Measured and simulated power traces



### **System Description**

#### SIRIUS-2

SIRIUS-2a: UN CERMET SIRIUS-2a: UN CERMET

**Purpose**: Investigate impacts of temperature ramp rate and operating temperature on cermet fuel performance

#### Specimen Geometry:

- Single 0.5" thick fuel wafer
- Hexagonal geometry
- Cermet: Mo-30W matrix
- Angular uncoated kernels
- 7 flow channels
- No flow tubes

### Test Environment: Static safe gas

### **SIRIUS-3**

#### **UN CERMET**

**Purpose**: Investigate impacts of temperature ramp rate and operating temperature on subscale fuel element

#### Specimen Geometry:

- 8" long stack of 0.5" wafers
- Unbonded wafers
- Circular geometry
- Uncoated angular or spherical fuel kernels
- 19 flow channels
- Unbonded Mo flow tubes

Test Environment: Static safe gas

### SIRIUS-4 (PRIME-1) UN CERMET Flowing H<sub>2</sub>

**Purpose**: Investigate integrity of cermet fuel + moderator unit cell in flowing hydrogen

#### Specimen Geometry:

- 20" long stack of 0.5" wafers
- Unbonded wafers
- Circular geometry
- Fuel, moderator, and insulator materials
- Coated spherical fuel kernels
- 19 flow channels

### Test Environment: Flowing hydrogen

### **Closing Remarks**

- **INL** is the nation's premier nuclear science and technology laboratory
- The reactor multiphysics team works at the forefront of solving some of the most challenging modeling problems for advanced reactors
- Our work relates directly to the nation's energy future via ARDPs, private/public partnerships, & reactor demonstrations
- I only talked about nuclear thermal propulsion systems, but this team is engaged in many types of advanced reactor analysis

>>> Which is a perfect segue to...





### **Internships**

- Paid opportunities available in a wide range of STEM and other fields for both undergraduate and graduate students
- Internship opportunities enable collaboration with experienced scientists and engineers to develop innovative solutions for challenging, real-world projects



of time spent participating in enrichment & professional development activities (workshops, networking, etc.)

20%





2021 Top 100 Internships



### The East Idaho Lifestyle

- Enjoy unparalleled access to the region's worldclass skiing, hiking, camping, climbing, mountain biking, hunting, fishing, and much more
- Live close to some of the country's greatest natural wonders: Yellowstone National Park, Grand Teton National Park, Craters of the Moon National Monument, Jackson Hole, Glacier National Park and more



### Want to learn more?

Visit inl.gov/inl-initiatives/education/

For Internships, Postdocs & INL Graduate Fellowships: <u>academic@inl.gov</u>

For Full-time Careers: <u>careers@inl.gov</u>

Drop your email address in the event chat





WWW.INL.GOV

### **SIRIUS-3: Heat Transfer Challenges**



# Griffin Capabilities





Micro-reactors

#### Advanced Test Reactor (ATR)



### **MARVEL - Test Microreactor**

Microreactor Application Research, Validation and EvaLuation Project

Key Design Features	
Thermal Power	100 kW
Electrical Power	20 kWe (QB80 Stirling Engines)
Weight	< ~10 US ton
Primary Coolant	Sodium-Potassium eutectic
Intermediate Coolant	Lead-Bismuth eutectic
Coolant Driver	Natural Convection, single phase
Fuel	HALE(UZrH), 304SS clad, end caps
Moderator	Hydrogen
Neutron Reflector	Graphite, Beryllium (S200), Beryllium oxide
Reactivity Control	Radial Control Drums, Central Absorber
Primary Coolant Boundary	SS316H



## **Molten Chloride Reactor Experiment (MCRE)**

Parameter	MCRE
Rated Thermal Power	200 kW
Fuel Salt Mass Flow Rate Range	25-100 kg/s
Fuel ΔT	10°C
Nominal Fuel Temperature	650°C
Design Temperature	700°C
Design Pressure	500 kPa
Fuel Salt Composition	NaCl-UCl <sub>3</sub> (67-33mol%)
Fuel Salt Mass	1225 kg
HEU Mass	630 kg
Heat Removal Method	Gas-Cooled Vessel















TerraPower