INL/MIS-21-64799-Revision-0

Multiphysics Modeling in Support of NASA Nuclear Thermal Propulsion Designs

October 2021

Changing the World's Energy Future

Mark D DeHart

Idaho National Laboratory

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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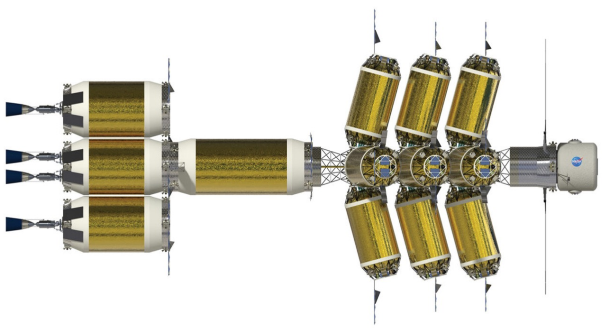
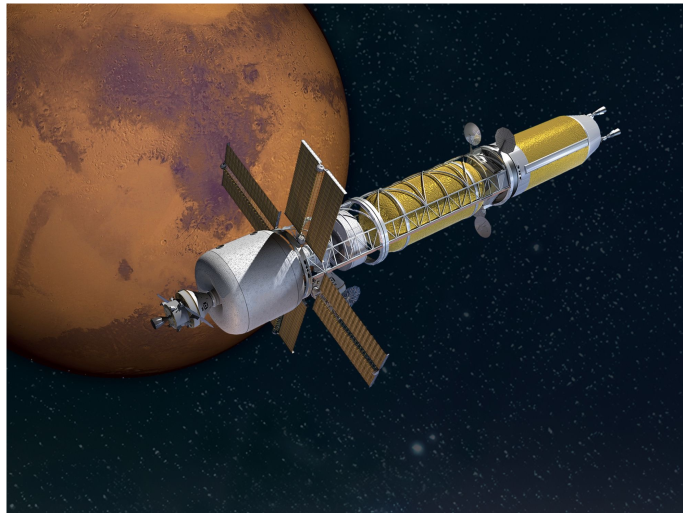


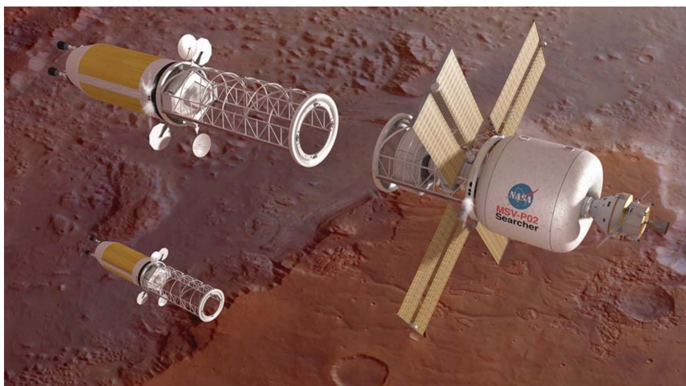


Mark DeHart

Directorate Fellow

Nuclear Science &
Technology Directorate

Idaho National Laboratory



Multiphysics Modeling in Support of NASA Nuclear Thermal Propulsion Designs

The Ohio State University

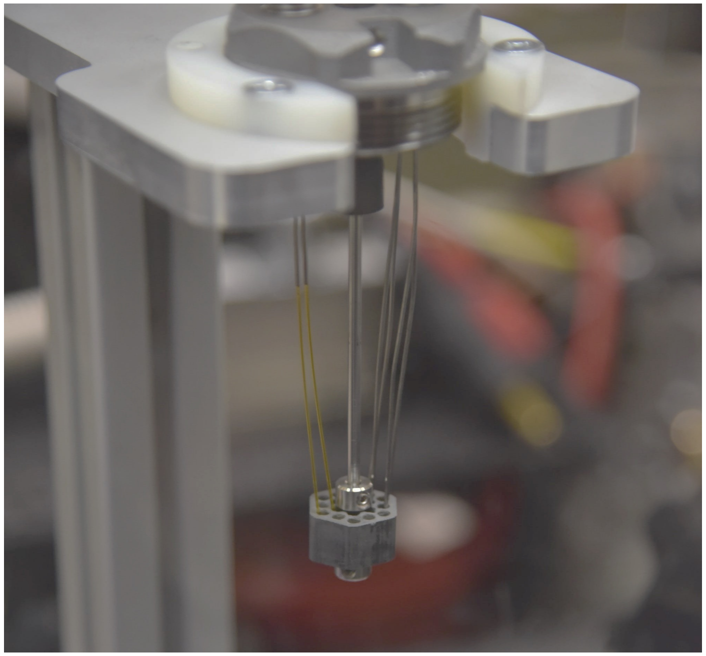
October 13th, 2021

INL/MIS-21-64799

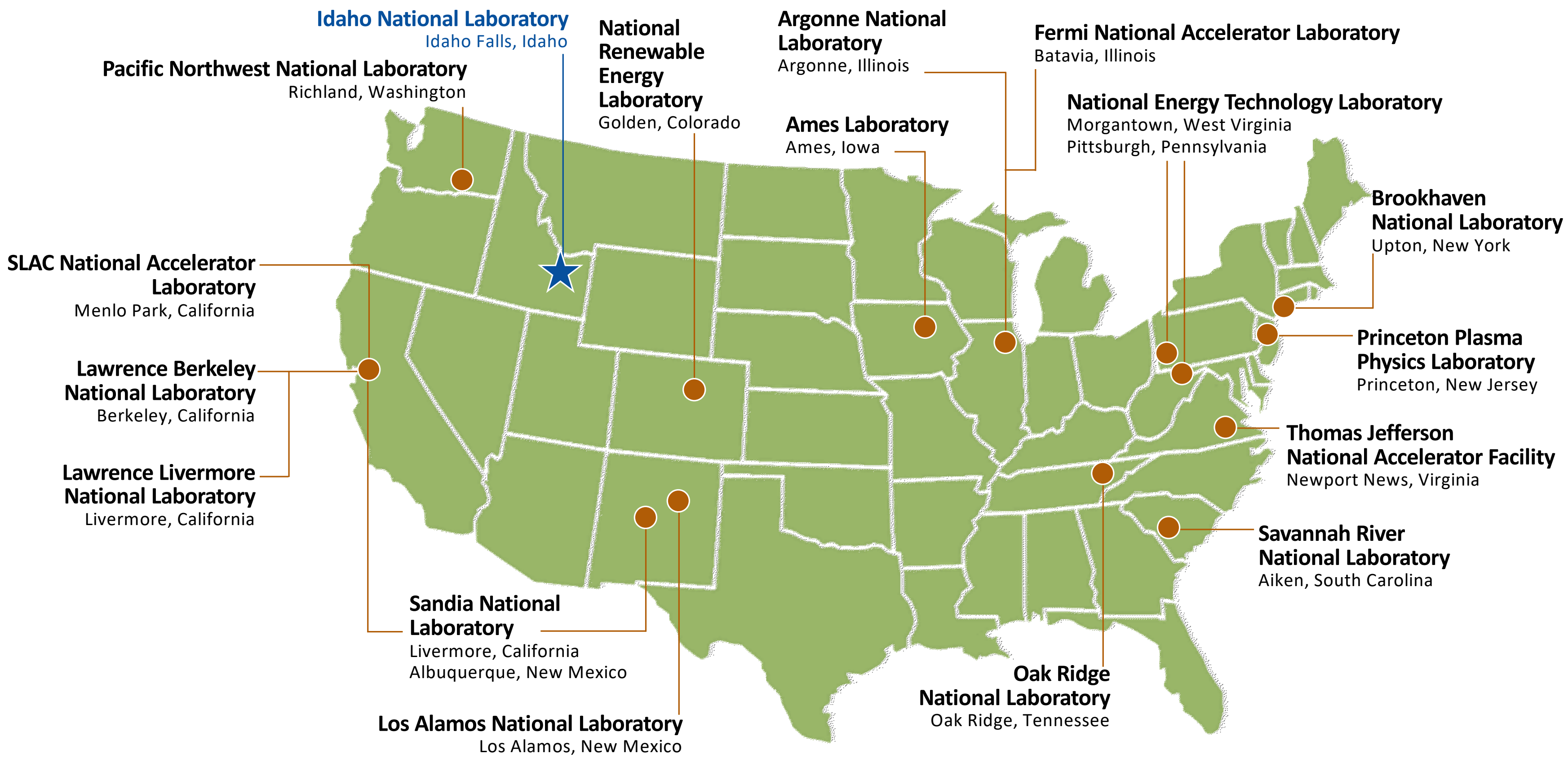
Idaho National Laboratory

Overview

- Introduction to Idaho National Laboratory
- The Reactor Multiphysics Team
- MOOSE Background
- Griffin
- Nuclear Thermal Propulsion
- Analysis Workflow
- Analysis Approach
  - Cross section generation
  - Mesh generation
  - Fuel element modeling
  - Validation using SIRIUS measurements in TREAT
  - Full Core Modeling
- TREAT experiment simulations (time permitting)
- Closing Comments



National Laboratories



Addressing the world’s most challenging problems

Nuclear S&T

- 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



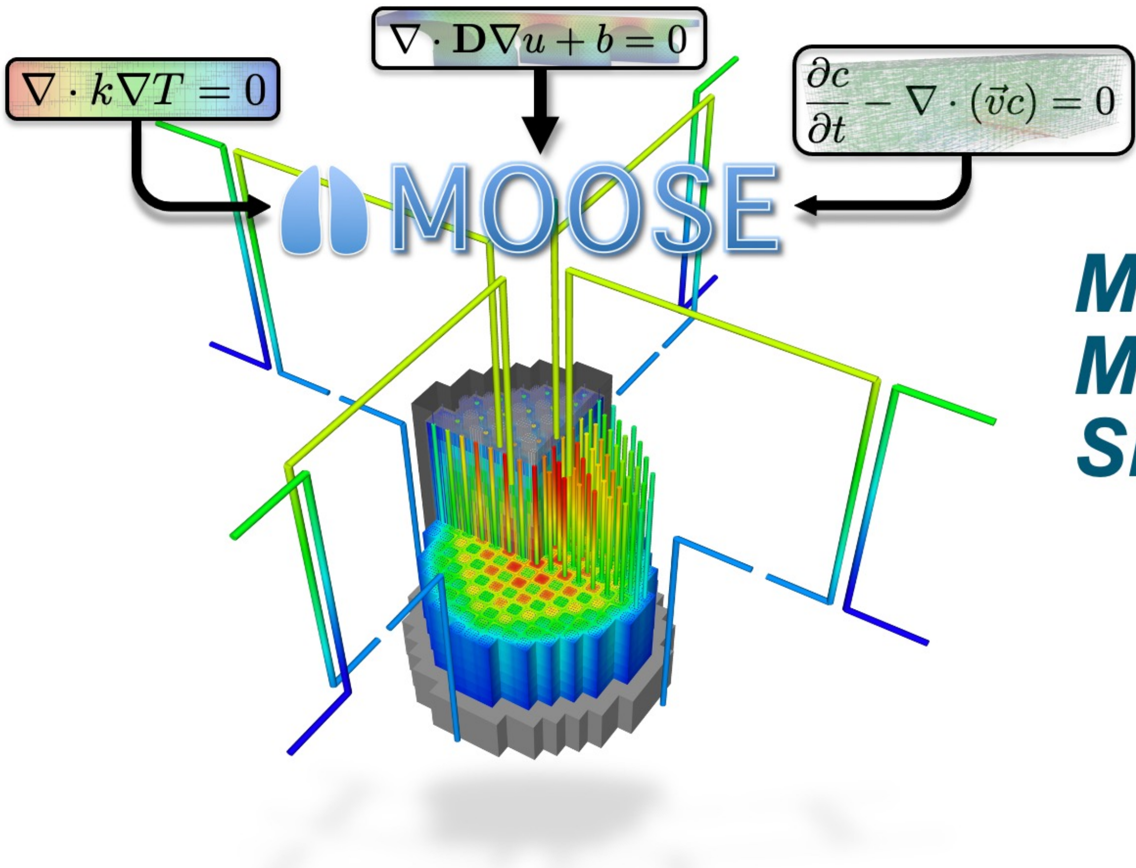

The East Idaho Lifestyle

- Enjoy unparalleled access to the region's world-class 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, and more

The Reactor Multiphysics Team (RMT)

- Primary development of the Griffin (neutronics) and Pronghorn (coarse mesh TH) codes within the DOE/NE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program
- Partnering with several companies on GAIN vouchers and Advanced Reactor Demonstration Project (ARDP) awards
- Advises the US NRC on multiphysics tools for analysis of advanced reactors
- Funded by US NRC, NASA, NEAMS, Nuclear Reactor Innovation Center (NRIC), DOE/NE Advanced Reactor Technology (ART), INL Strategic Thermal Irradiation Program.
- Scope runs the gamut from algorithm development, implementation, to reactor analysis
- Reactors we work on: PBRs, FHRs, MSRs, NTPs, prismatic VHTRs, micro-Rx, and INL's Transient Test Reactor (TREAT), Advanced Test Reactor (ATR) and the Neutron Radiography (NRAD) Reactor

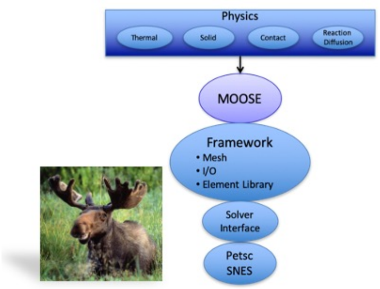
The Reactor Multiphysics Team (RMT)



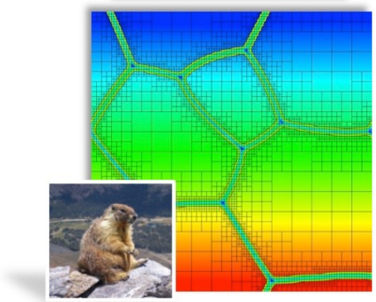
MOOSE Enables Multiphysics Simulation

The MOOSE Herd

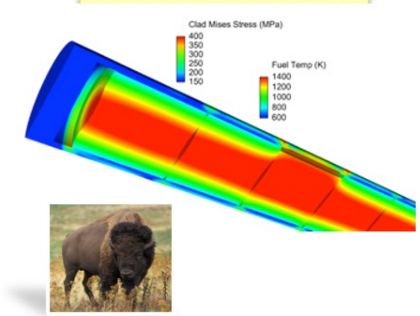
MOOSE
HPC Framework



Marmot
Mesoscale Materials

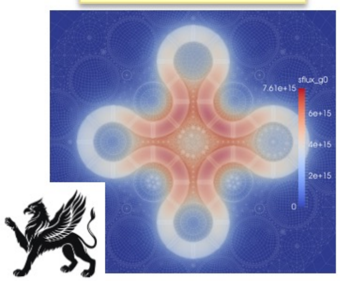


Bison
Nuclear Fuel Performance



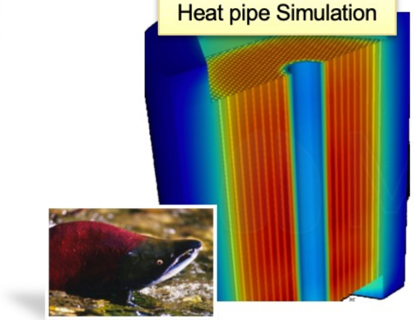
Grizzly
Structural Mechanics for Component Aging

Griffin
Radiation Transport

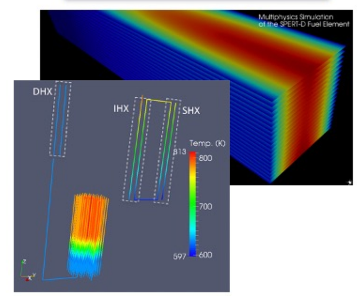


Pronghorn
Engineering Scale Flow

Sockeye
Heat pipe Simulation

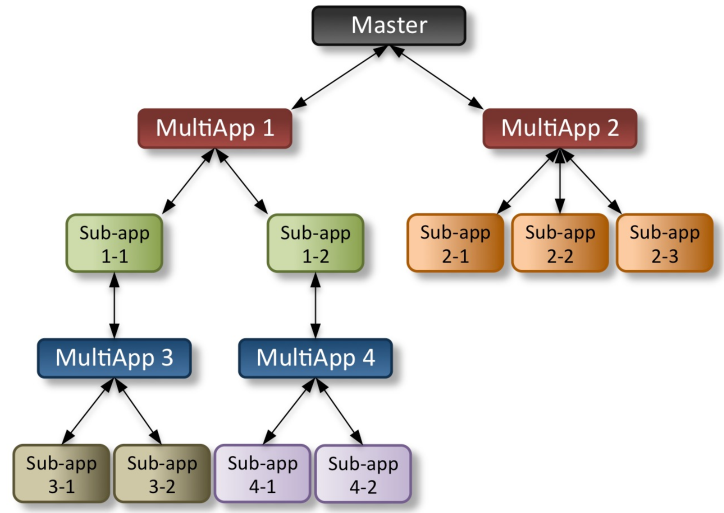


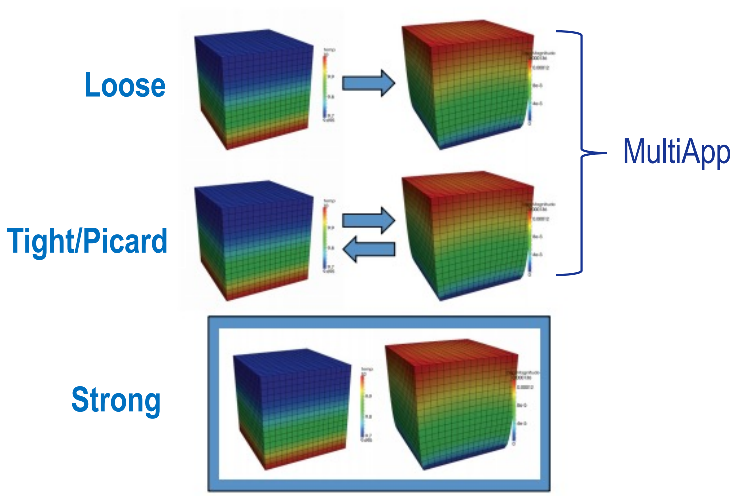
SAM and RELAP-7
Multiscale Multiphysics Systems Analysis



Flexibility by MultiApps

- Master app owns a sub-app
- Recursive: sub-app can own its own sub-app tree
- Information transfer via flexible MOOSE transfers
- Different meshes & dimensionality (different length scales)
- Sub-cycling (different time scales)
- Mixing eigenvalue & transients
- Picard Iterations



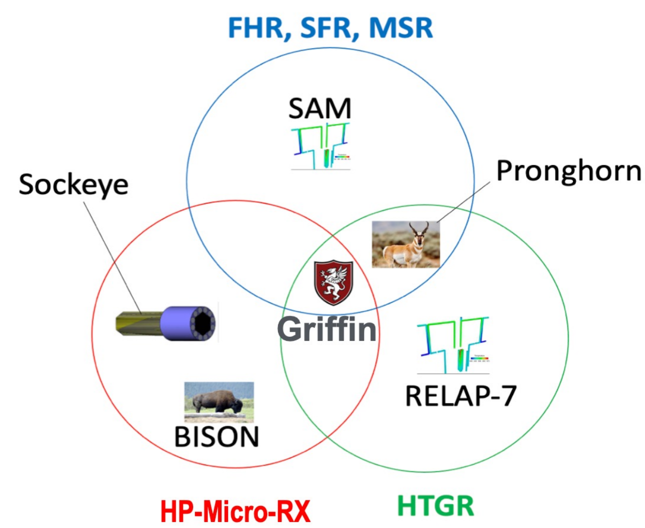


- MOOSE supports loose coupling (operator split) & Picard via MultiApps
- MOOSE supports strongly coupled solves

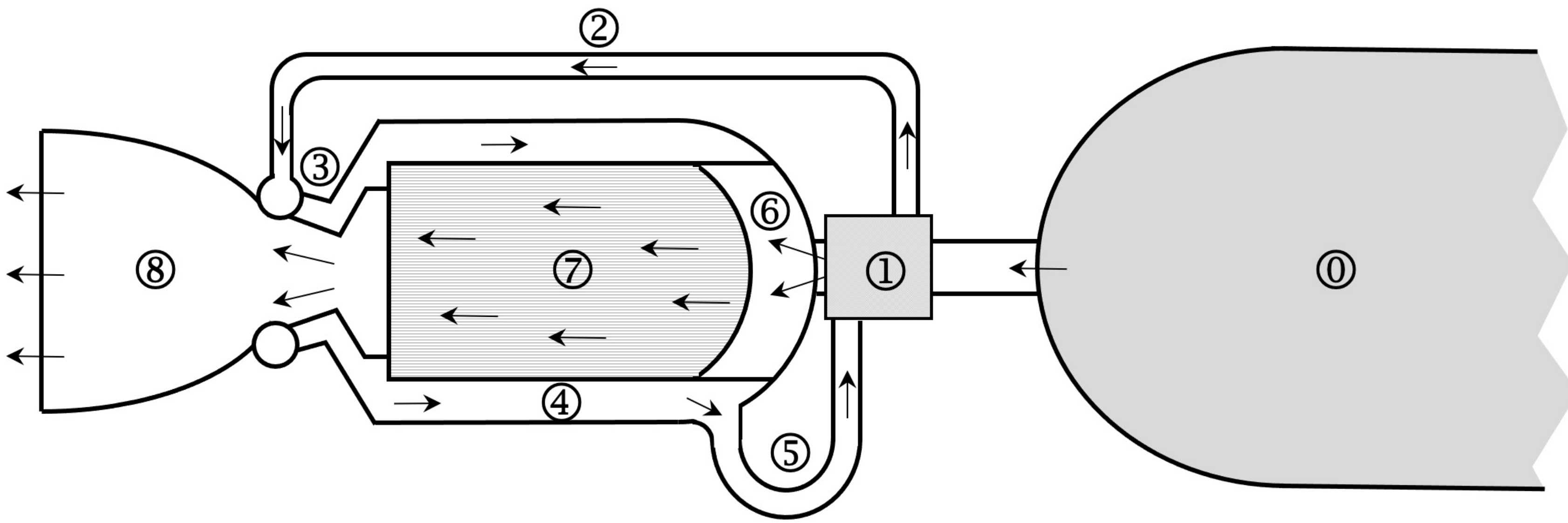
What is Griffin and Why is it important?

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



Nuclear Thermal Propulsion (NTP) Engine

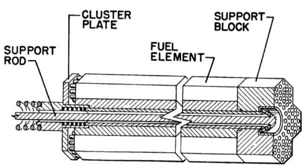


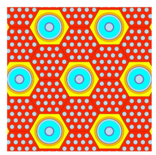
(0) Liquid hydrogen storage tank
(1) Pre-heated-hydrogen-driven turbopump
(2) Flow line from turbopump to nozzle
(3) Nozzle cooling
(4) Pressure vessel/reflector/control drum cooling
(5) Gaseous hydrogen feed to turbopump(s)
(6) Gas plenum above core
(7) Reactor core and hydrogen cooling
(8) Exhaust nozzle

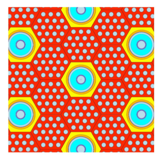
Why NTP?

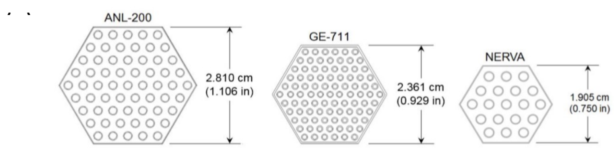
- The value of NTP was recognized in 1947 and large experimental programs pursued NTP engine design in the1950s and 1960s.
- NTP has several advantages over chemical H_2 + O_2 engines
  - First and foremost, a factor of 2-3 gain over performance (specific impulse, I_{sp}, analogous to MPG in a car).
    - The I_{sp} represents the time over which 9.81 kilograms (or one Newton of weight on Earth) of propellant can produce one Newton of thrust.
    - The larger the I_{sp}, 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

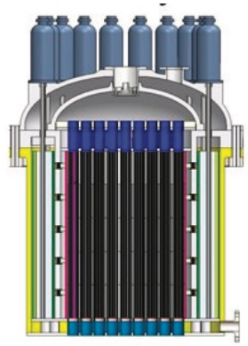
Nuclear Thermal Propulsion Support at INL







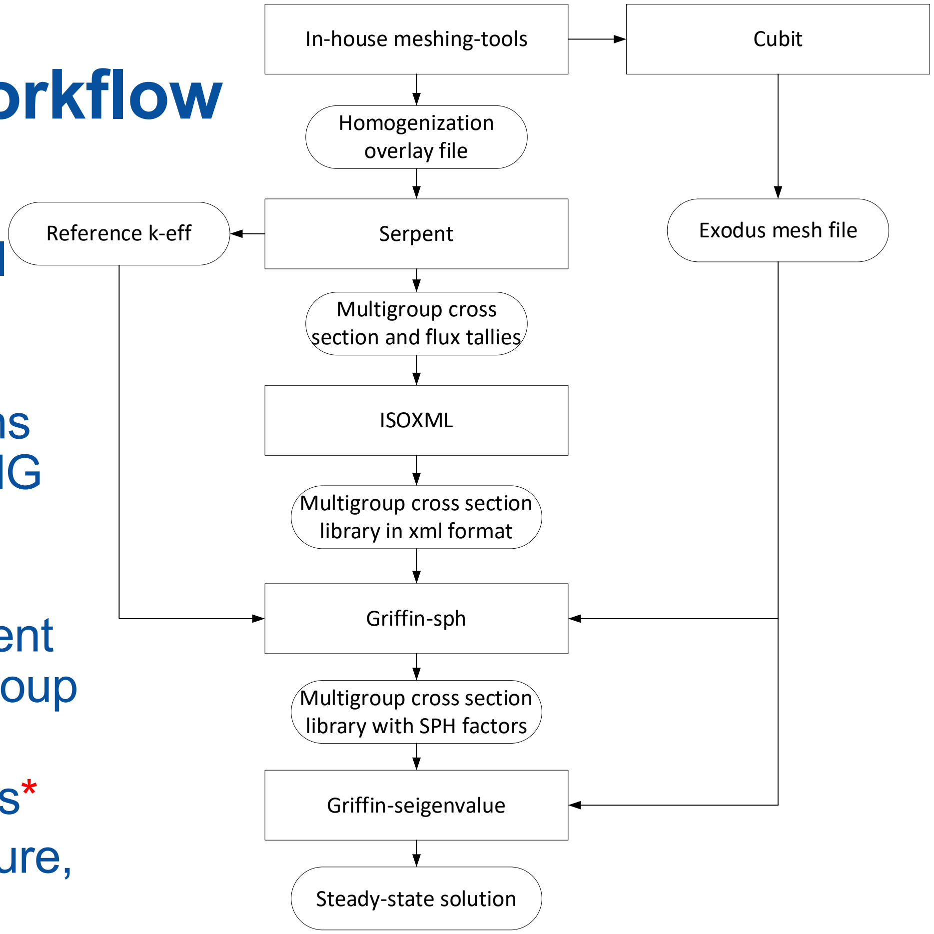




- INL support for NASA Marshall Flight Center and Glenn Research Center
  - Development of Griffin model NASA nominal plant design
    - 2D single assembly
    - 3D single assembly
    - 3D full core
    - Multiphysics simulations
      - Neutronics
      - Thermal-fluids
      - Heat transfer
      - Structural mechanics
      - Transient simulations
  - Simulation of SIRIUS series of experiments in TREAT

NTP (and TREAT) Analysis Workflow

- Build mesh (Cubit) and Serpent model*
- Align detectors (tally regions) in Serpent model with corresponding regions in mesh for cross section assignment.*
- Calculate k_{eff} and fluxes in cross section regions with Serpent (reference solution) tallied over MG energy groups
- Perform a Super-Homogenization (SPH) calculation using Griffin to find energy-dependent correction (SPH) factors that will match multigroup fluxes.
- Update cross section library to add SPH factors*
- Repeat for each state point (typically temperature, control element position)*
- Run steady state calculation, confirm agreement with reference
- Run transient simulations



*These processes are largely automated

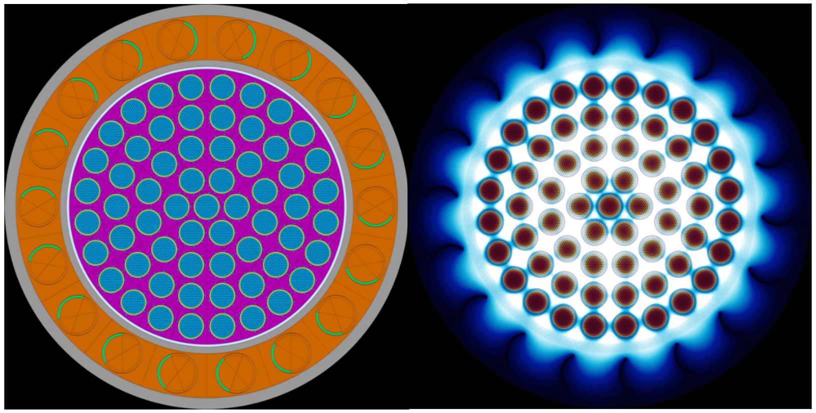
Cross Section Preparation with Serpent

Serpent Model

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

Bottom line: it creates nuclear cross sections for us!

- Monte Carlo method:
  - Stochastic transport method
  - Highly accurate in energy resolution
  - Slow & 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 user-specified group structure

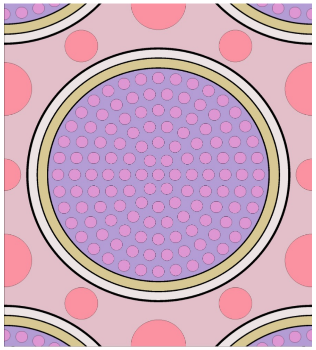


Serpent NTP core calculation

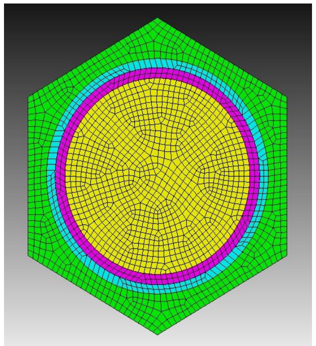
Mesh Generation for the Neutronics Model

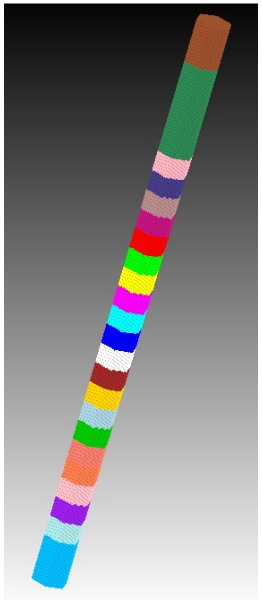
Mesh Generation

- 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



Geometry → Griffin

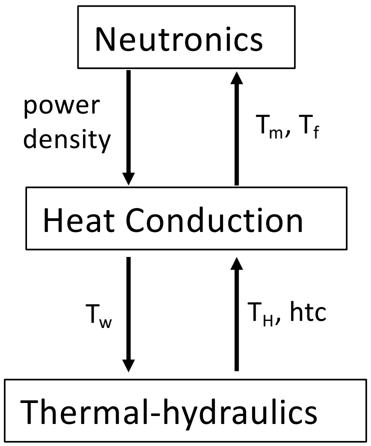




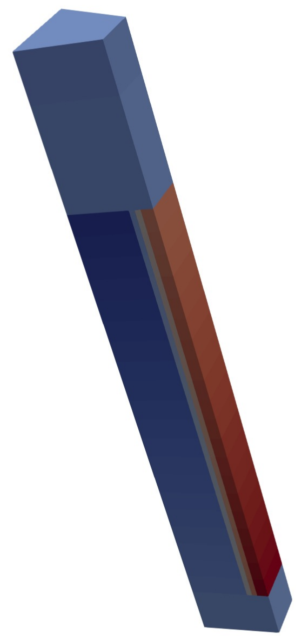
Axial homogenization

Coupled Fuel Element - Overview

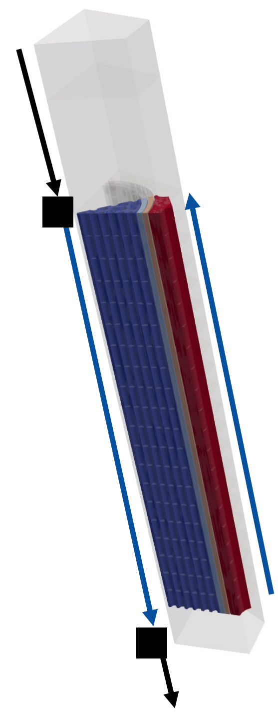
- Neutronics geometry: 90-degree, fuel + axial reflectors
- Heat conduction: active fuel region, 30-degree
- Thermal-hydraulics: representative fuel and moderator flow channels



Neutronics: primary app

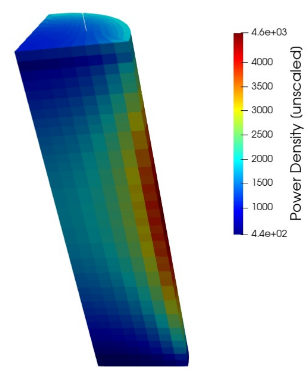


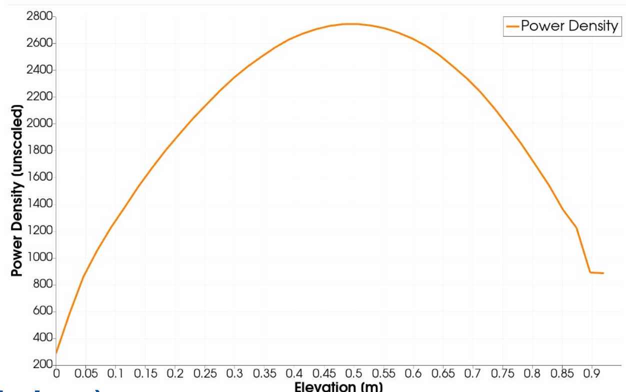
Heat conduction: sub-app 1
TH channels: sub-app 2

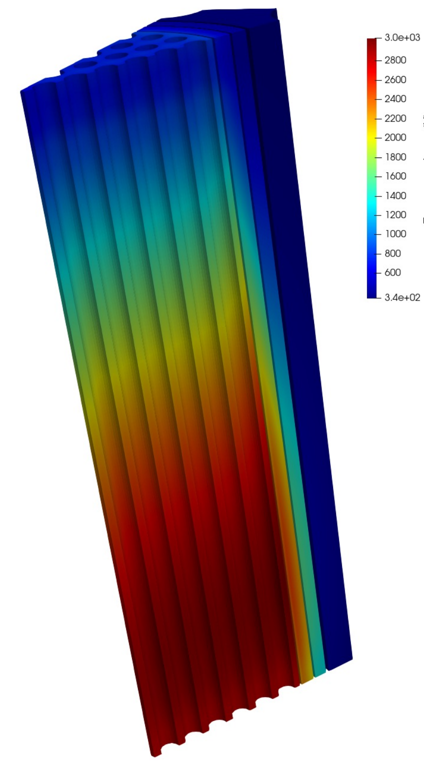


Coupled Fuel Element Steady-state – Results

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





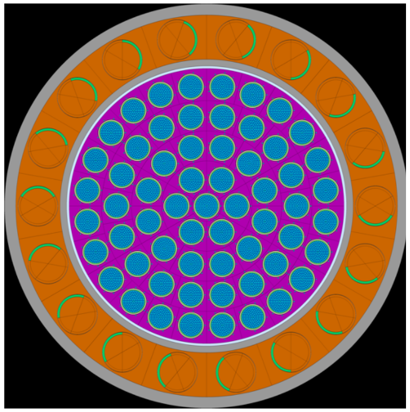


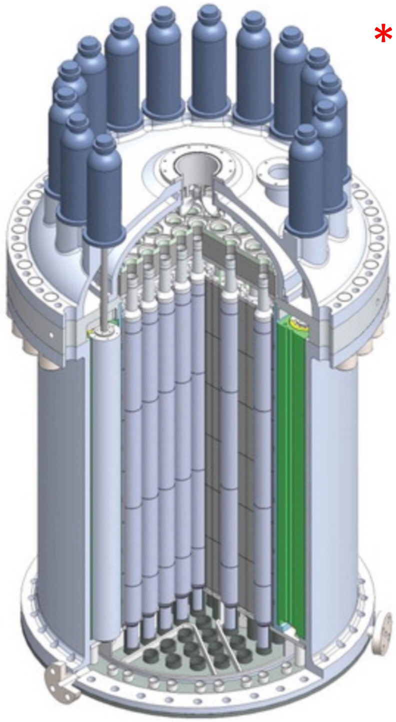
- Neutronics: Griffin
- Heat Transfer: Griffin (MOOSE modules)
- Structural Mechanics: Griffin (MOOSE modules)
- Convection Cooling: RELAP-7

Full-Core Model Overview

New CERMET/CERCER NASA/BWXT NTP concept

- 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 rotation (e.g., for a simulated reactivity insertion accident)

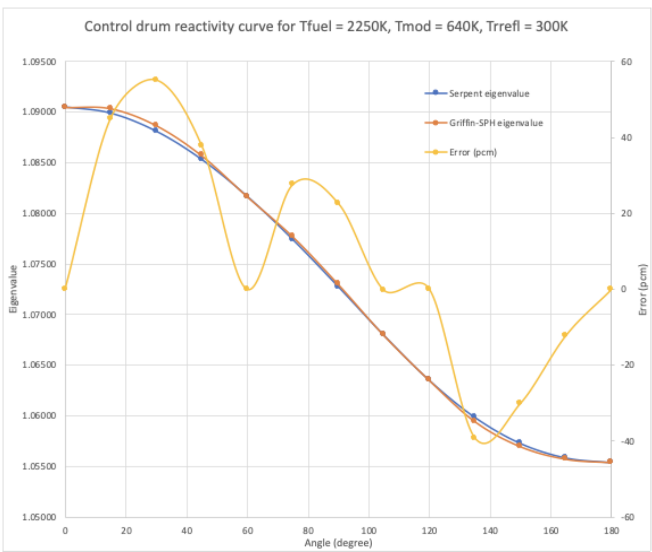




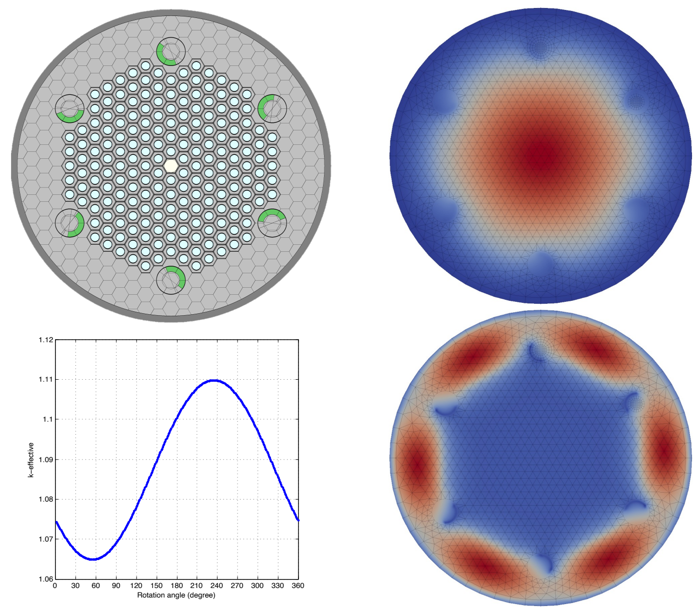
*

Control Drum Worth with Griffin Cusping & SPH

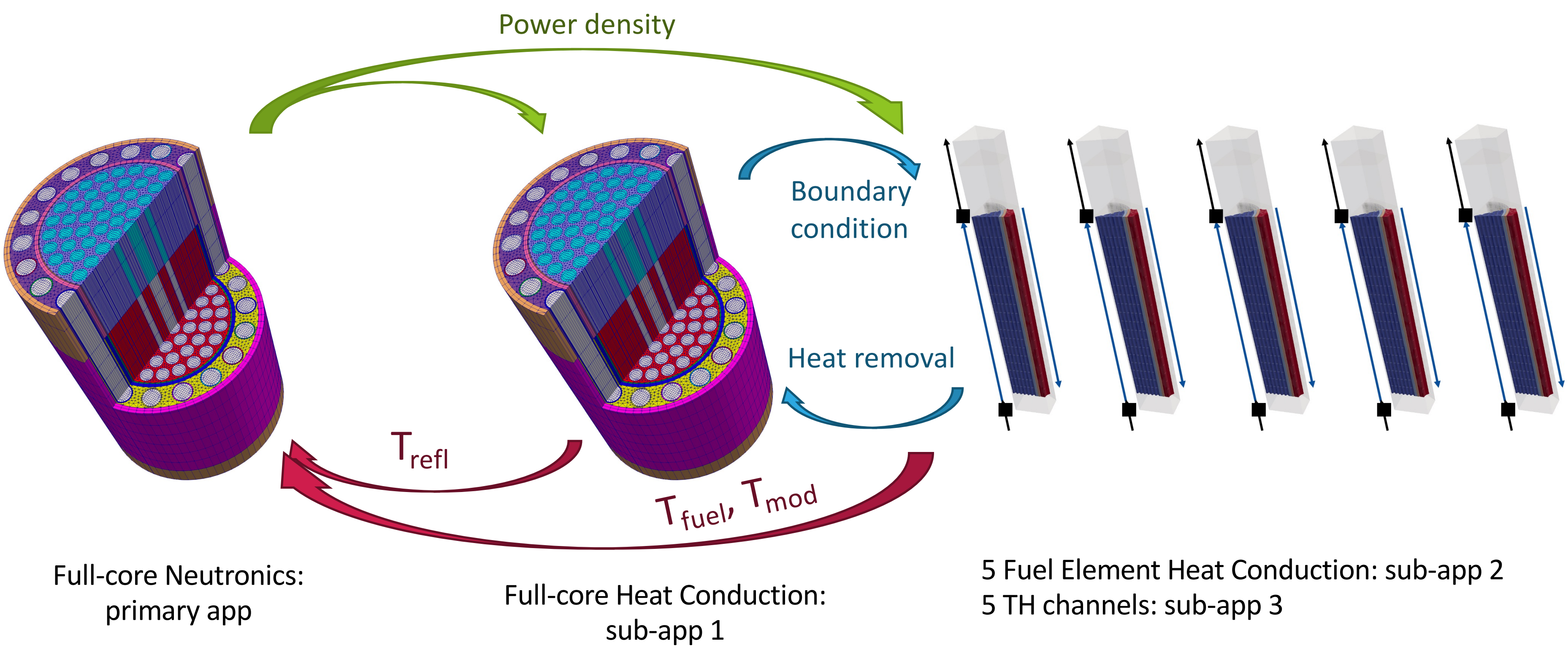
- At state points (0, 60, 120, 180), eigenvalue and power profile exactly reproduced
- Between state points, cusping treatment from Griffin is utilized
- Bias between -40 and +60 pcm
- Series of eigenvalue calculation in both Serpent and Griffin are in good agreement.



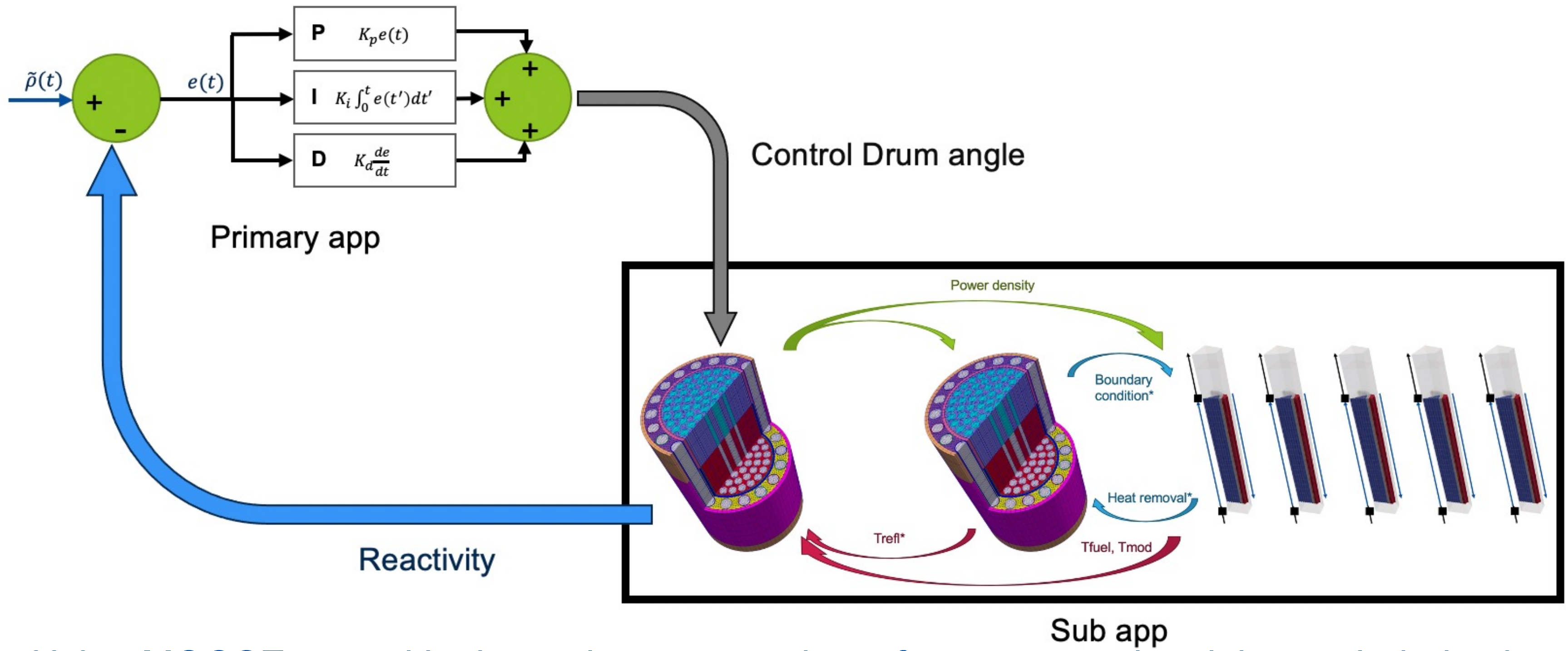
Control drum treatment



Coupled NTP Full-Core Model

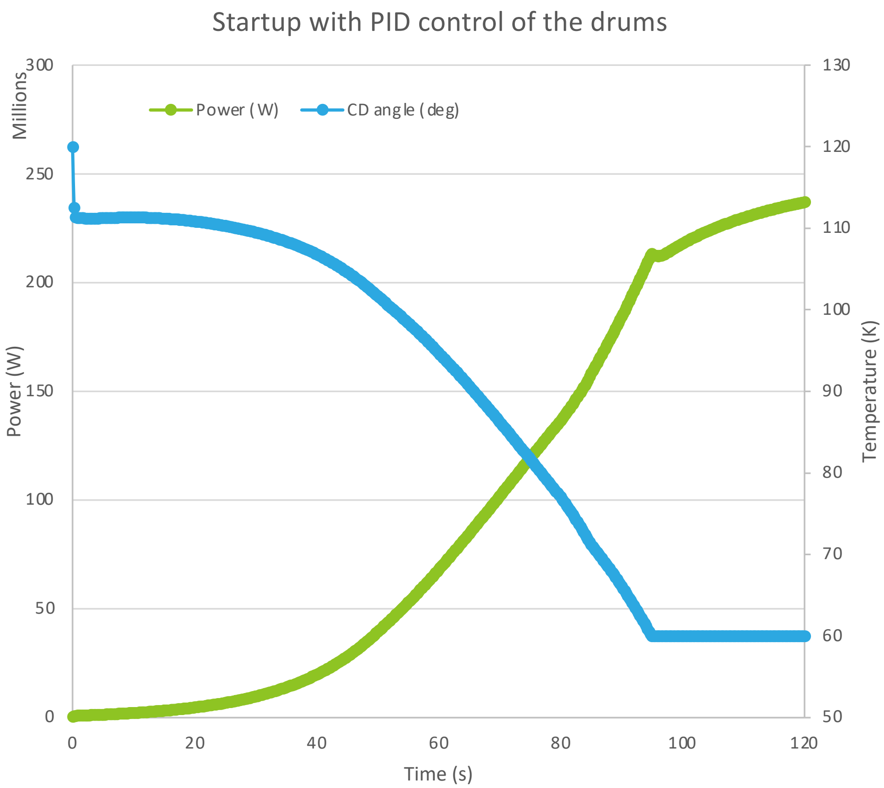


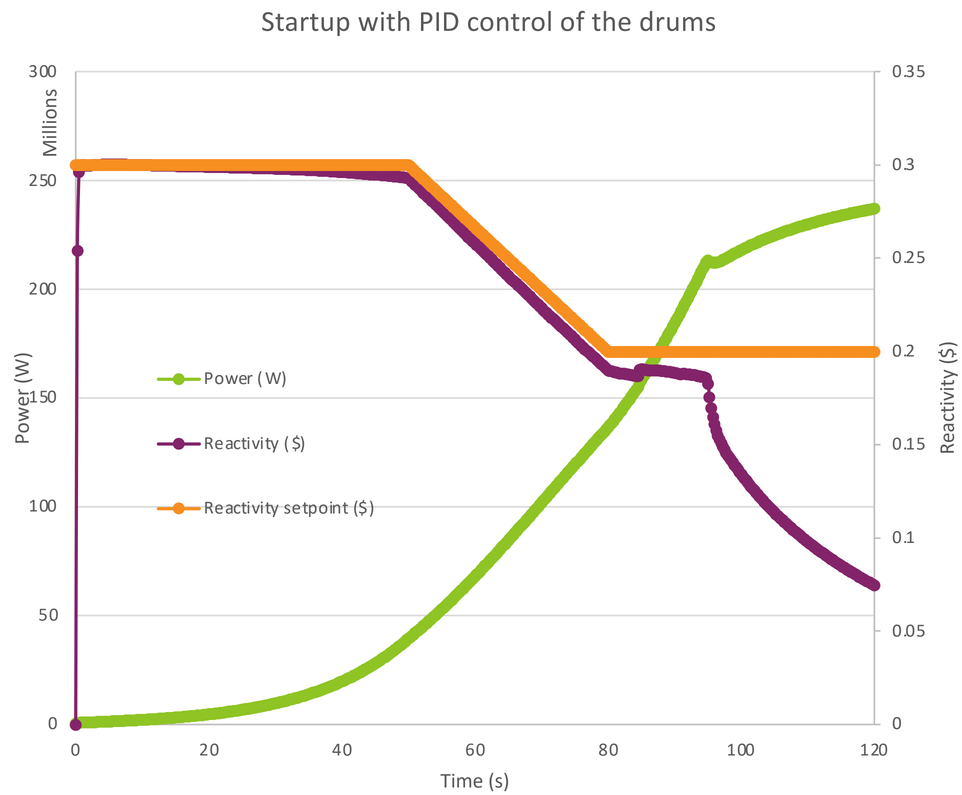
PID Control of Drums



- Using MOOSE control logic, we have created a software proportional–integral–derivative (PID) controller
- Requires less trial and error than manual control
- Currently ignores any limitation on drum rotation (speed, etc.)

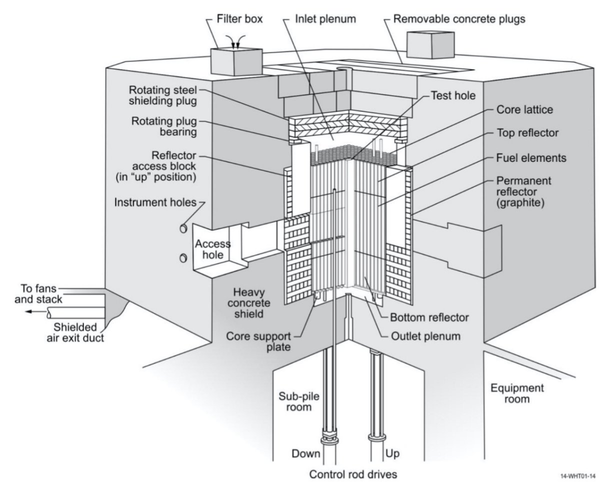
Start-up Transient with PID





SIRIUS experiment series

- Experimental campaign for transient testing of new Nuclear Thermal Propulsion Fuel: 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 (~25K/cm)
- SIRIUS series progresses in complexity:
  - SIRIUS-1: UN-CERMET – proof of principle
  - SIRIUS-2: Series of different materials, fab. processes, CERMET & CERCER
  - SIRIUS-3: Stack of 20 fuel specimens
  - SIRIUS-4: first hydrogen-cooled experiment, 10 stacked specimens CERMET
  - SIRIUS-5: second hydrogen-cooled experiment, CERCER stack of specimen



Multiphysics Simulations of SIRIUS-CAL

- Calibration experiment for SIRIUS-1

TREAT core configuration

Z	Z	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	Z	S
Z	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	Z
F	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	F
F	F	F	F	F	CS	F	F	F	S	F	F	F	CS	F	F	F	F	F
F	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	F
F	F	F	CT	F	F	F	F	F	S	F	F	F	F	F	CT	F	F	F
F	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	F
F	F	CT	F	F	CC	F	F	F	S	F	F	F	CC	F	F	CT	F	F
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F	F	F	F	F	F	F	F	F	EX	F	F	F	F	F	F	F	F	F
F	F	F	F	F	F	F	F	F	ZH	F	F	F	F	F	F	F	F	F
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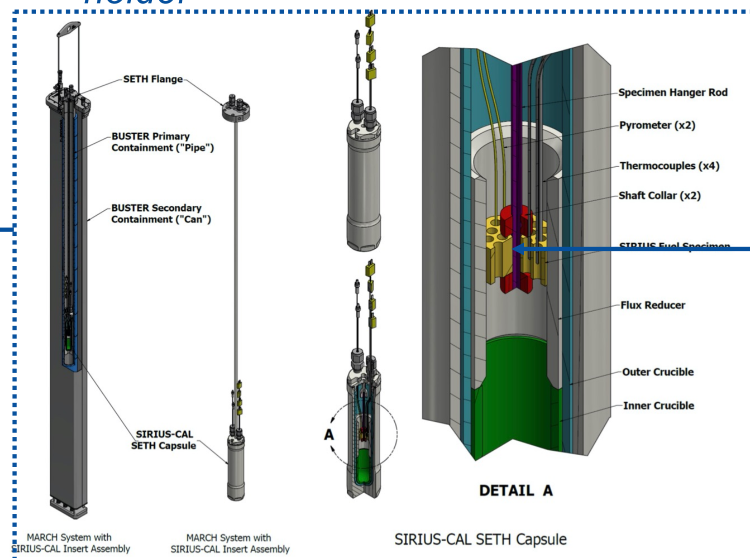
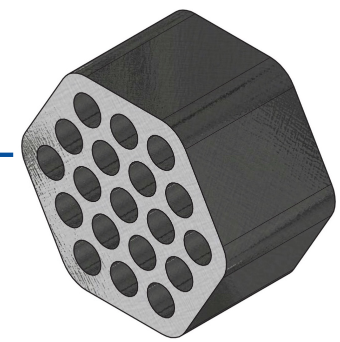
F	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	F
Z	F	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	F	Z
Z	Z	F	F	F	F	F	F	F	S	F	F	F	F	F	F	F	Z	Z

F	Fuel element
CT	Fuel element containing transient control rod
CS	Fuel element containing safety control rod
CC	Fuel element containing compenstation control rod
S	Non-fueled source element
Z	Zirc-clad non-fueled graphite element
S	Zirc-clad slotted graphite block
EX	Experiment region
SH	Half-width zirc-clad slotted element
ZH	Half-width zirc-clad non-fueled graphite element

Experiment vehicle and sample holder



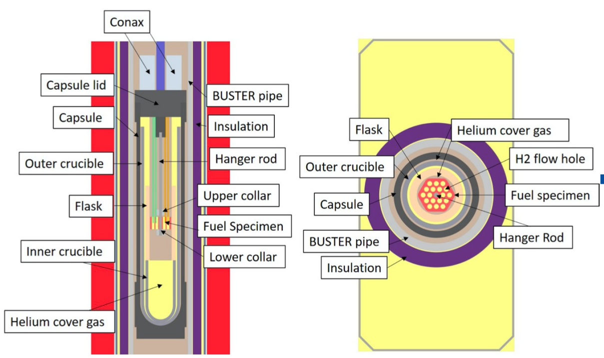
Sample (size of a quarter)



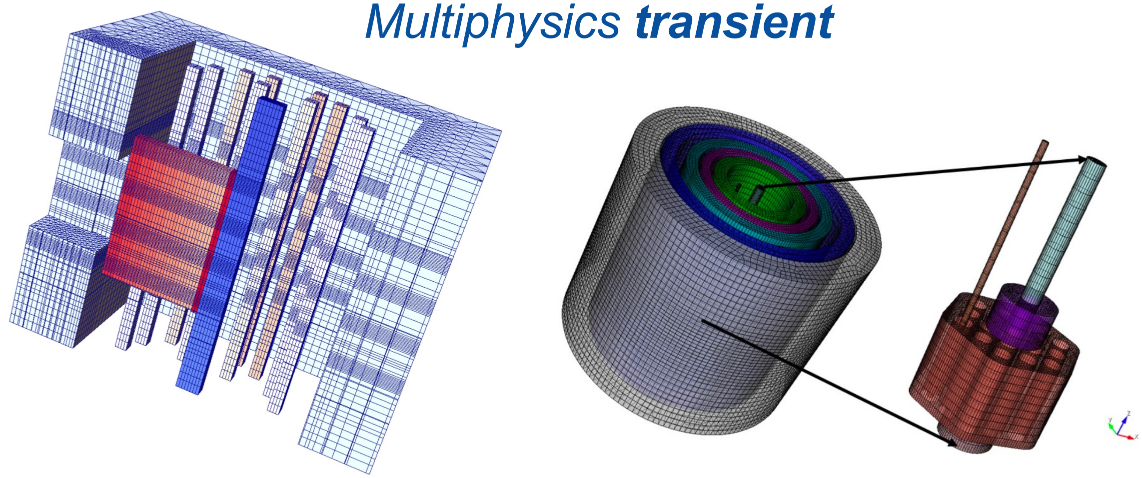
Multiphysics Model of SIRIUS-CAL

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

*Serpent **steady-state** for XS*



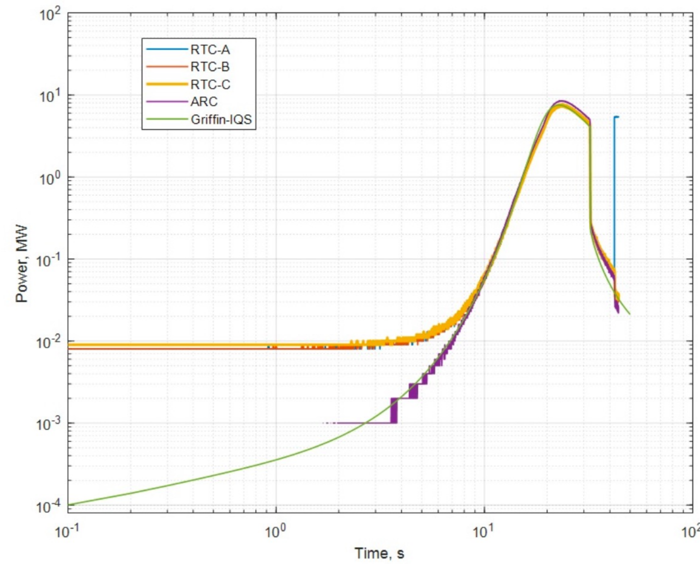
Griffin (Diffusion + SPH)
*Multiphysics **transient***



Neutronics *Thermal*

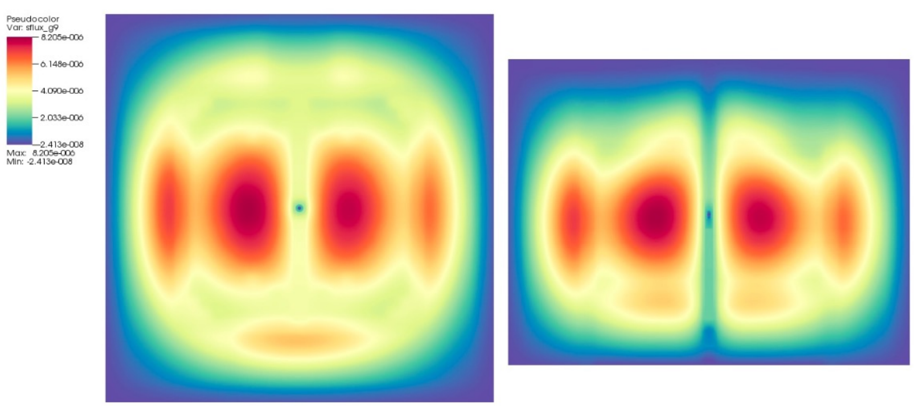
SIRIUS-CAL Multiphysics Results

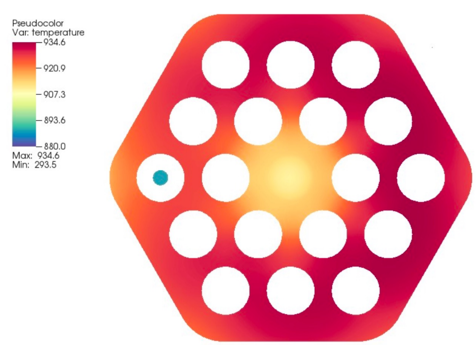
- SIRIUS-CAL reactivity insertion is 0.55% dk/k
- We currently adjust control rod motion to match TREAT initial period – ongoing work to be fully predictive for TREAT transients
- Goal is validation for SIRIUS-CAL



Measured and simulated power traces

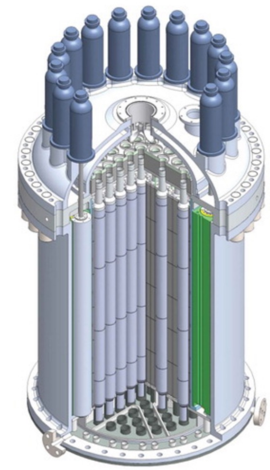
Thermal fluxes in steady-state



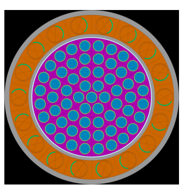


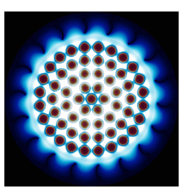
Temperature distribution in the specimen

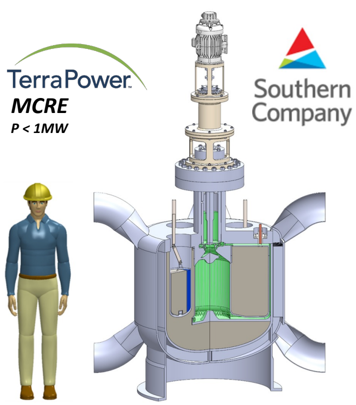
Closing Remarks

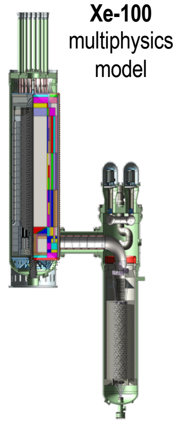


- INL is the nation's premier nuclear science and technology laboratory
- The reactor multiphysics team works at the forefront of solving some of the most challenging modeling problems for advanced reactors
- Our work relates directly to the nation’s energy future via ARDPs, private/public partnerships, & 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…









Technology maturation with Marvel

Modeling autonomous fission batteries

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

80%	20%
of time spent working on projects and applying what you learned in the classroom to solve real work-related challenges	of time spent participating in enrichment & professional development activities *(workshops, networking, etc.)*

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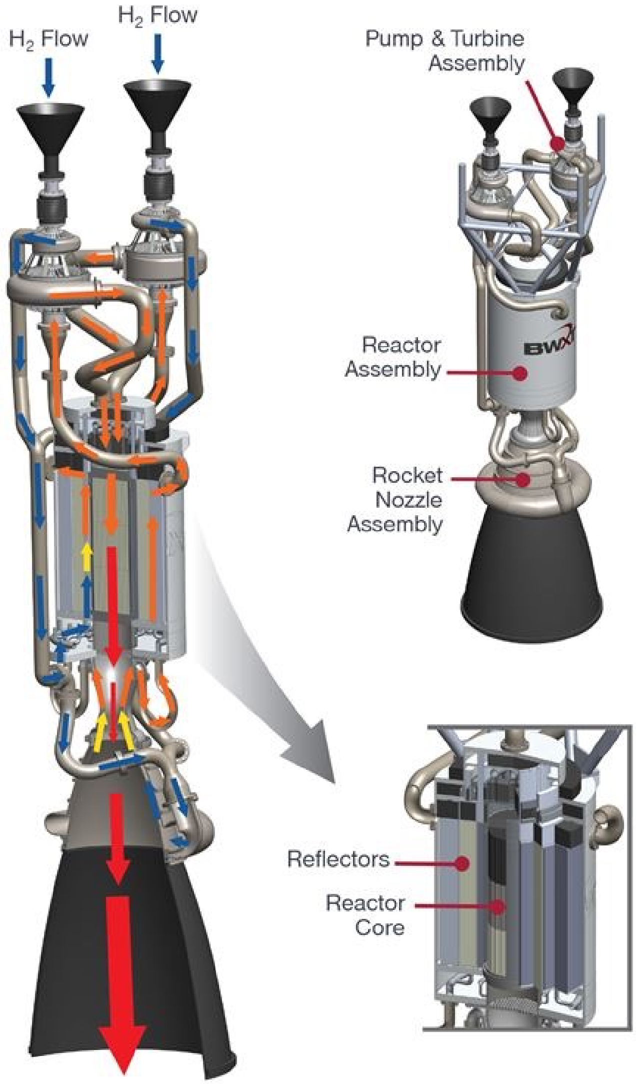


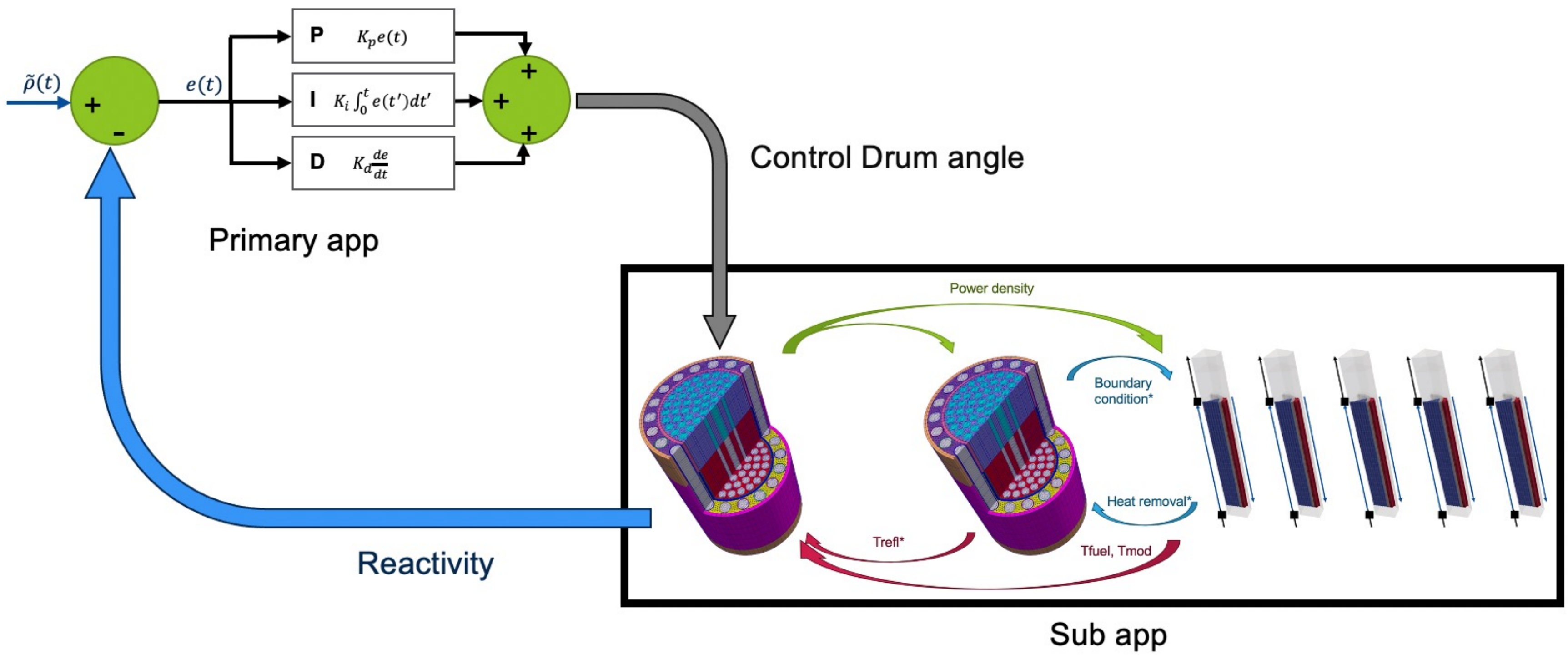
Extra Material

Start-up Transient Assumptions

- *Goal: go from low power to full power in a few minutes*

- Currently, we assume 100% H_2 flow rate established at the beginning of the transient
- Assume initial temperature:
  - Tfuel = 500 K
  - Tmod = 270 K
  - Trrefl = 300 K
- Initial power: 610 kW (10 kW/fuel element)
- Initial CD angle $\theta_i = 120°$
- Final CD angle $\theta_f = 60°$
- Drum rotation determined by PID controller

PID Control of Drums



- For now, ignores any limitation on drum rotation (speed, etc.)

PID: Remarks

- If only proportional term is included in PID:

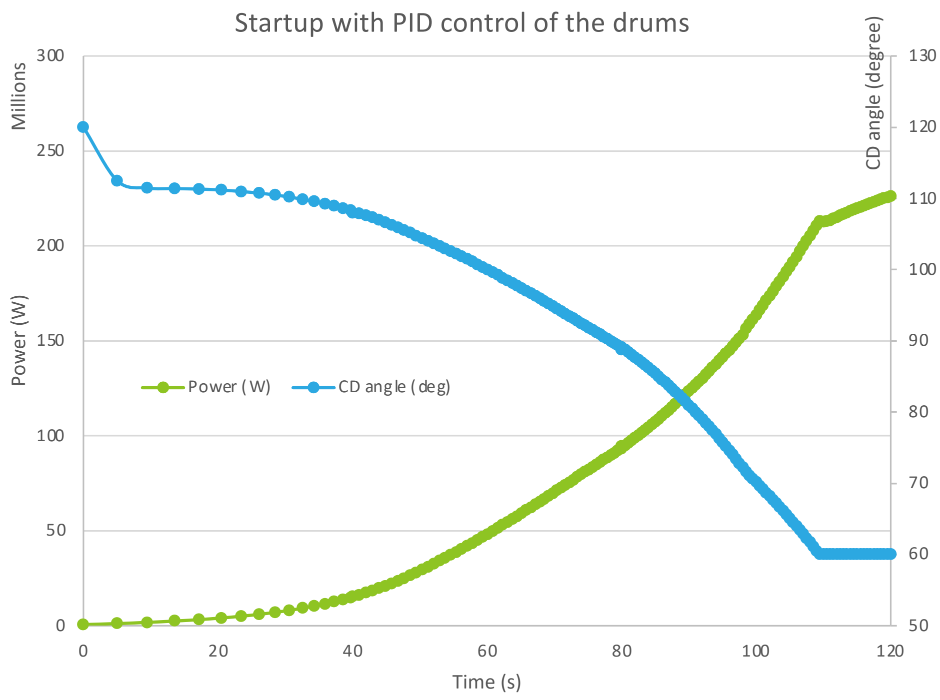
$$K_p = \frac{\Delta\theta}{\Delta\rho}$$

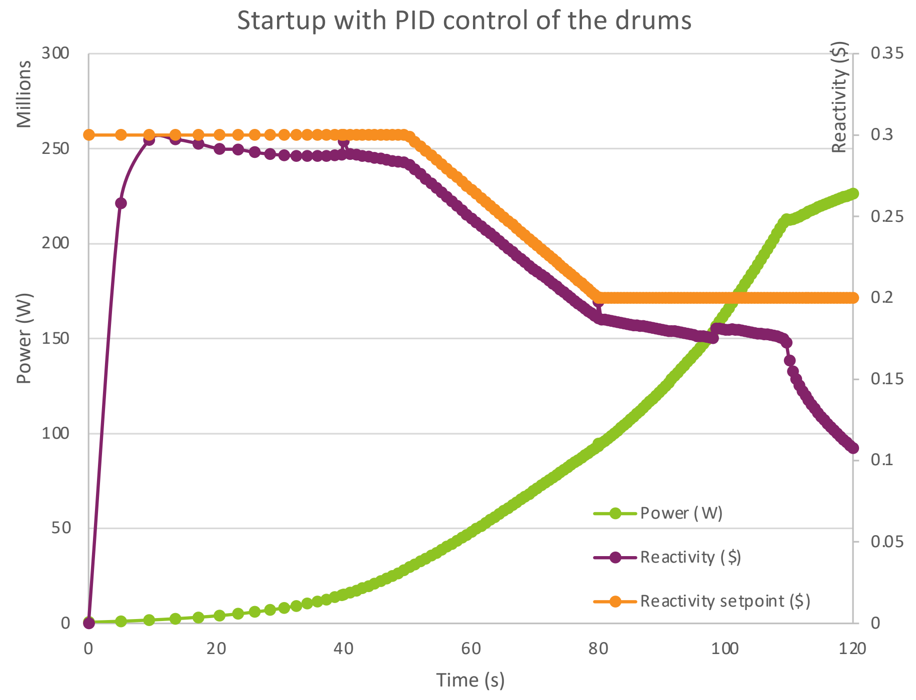
- For the CD angle between $60°$ to $120°$, CD worth ~ 25-30 pcm/° or 24-30 °/$

- $K_p = 25$ °/$ should be reasonable

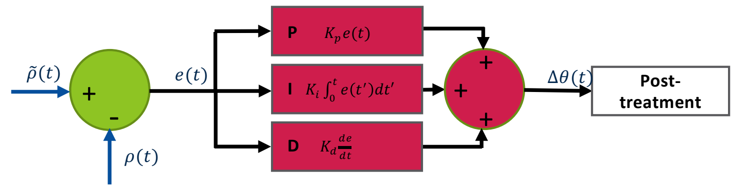
- Direct correlation between reactivity and CD angle: this is why we choose to rotate drums based on reactivity and not power (time delay between reactivity and power)

Start-up Transient with PID: $K_p = 25, K_i = K_d = 0$





Changing K_i

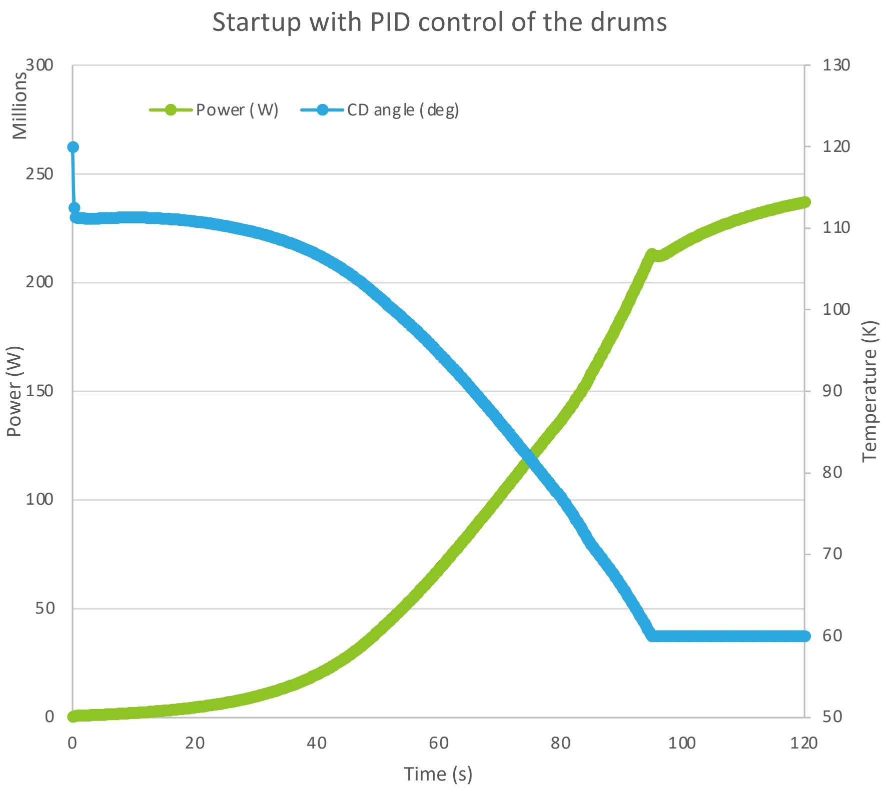


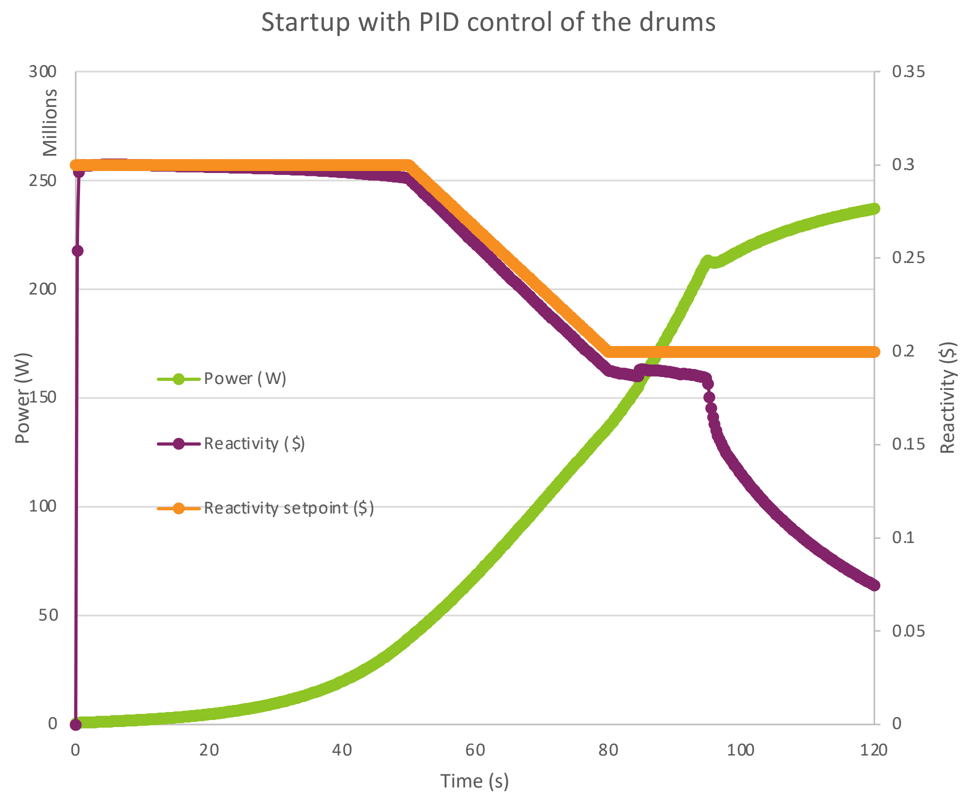
- Increasing temperature creates negative feedback not captured by 'proportional-only' PID
- Integral term can capture the persistent lag behind the setpoint
- During the early stages the transient,

$$\frac{\int_0^t e(\tau)d\tau}{e(t)} \approx 100 - 200 \ \ s$$

- Thus, we pick: $K_i = \frac{K_p}{100} = 0.25 \ \ °/(\$\text{–}s)$

Start-up Transient with PID: $K_p = 25, K_i = 0.25, K_d = 0$





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