Reactor IPSC FY-10 Overview

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Argonne National Laboratory

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Outline

- Motivation
- Budget
- Overview of FY10 Reactor IPSC work
  - Neutronics
  - Thermal hydraulics
  - Systems/safety
  - UQ
  - Framework
- FY11 plans

Motivation and Objectives

- Apply modern, high-performance techniques to nuclear reactor modeling
  - Improve turn-around time for reactor design iterations
  - Understand and reduce uncertainty of computational models
  - Use advanced simulation tools to improve safety, reduce cost, explore advanced designs
- We are using a balanced approach
  - Allow for both rapid-turnaround reactor-scale calculations (desktop) and detailed, high-fidelity simulations to augment experiments (petascale & beyond)
  - Deliver near-term capability and insight while also developing next-generation tools and integrated capabilities
- Extensive leveraging with other projects
  - INCITE, SciDAC, ASC programs provide computing infrastructure and tools
  - Argonne LDRD to develop methods for validation data collection and comparison

- FY10 emphases:
  - GenIV VHTR work folded into Reactor IPSC program
  - VVUQ across all physics modeling activities
  - Intermediate-fidelity modeling, coupling
  - Scalability of high-fidelity tools

NEAMS Reactor IPSC
FY10 Budget: $5M

- In FY10, Reactor Simulations effort moved from FCR&D to GenIV
  - Scope increased to include previously separate $1M VHTR project from FY09 and additional VHTR milestones to reflect funding sources.
- Neutronics: ($2.1M - includes $450K for VHTR T/H)
  - 1000k (ANL): UNIC development/modeling, MC^2 development
  - 1000k (ANL): DeCart/Star-CCM+ coupling, VHTR modeling
  - 100k (LANL): MCNP coupling to UNIC/SHARP
- T/H: ($1.25M)
  - 1050k (ANL): Nek development/modeling, Star-CCM+ modeling
  - 200k (LBNL): Visualization support
- Systems/Safety: ($550K)
  - $450k: Systems Level Safety Analysis
  - $100k: Uncertainty Quantification
- Framework: ($1.1M)
  - 1000k (ANL): Geometry & meshing development/application, coupling, UQ
  - 100k (LLNL): Longer-term viz development
- University collaborations funded out of specific areas
  - UIdaho: RANS for VHTR/SFR design (T/H)
  - UMich: Monte Carlo (neutronics)
  - UWisc: 2-phase flow in LWRs (T/H), geometry/mesh tools support (framework)

Neutronics Modeling

- Objectives
  - Develop high-fidelity neutronics solvers for the reactor IPSC code SHARP
- Multigroup Cross Section Generation Code MC^2-3
  - Fine group (230 groups) ultrafine (~2000) and hyperfine (~300,000) group levels
- Even-Parity Discrete Ordinate Solver SN2ND
  - Demonstrated scaling on BlueGene/P (294,912 procs) and XT5
  - Replaced the P_N scattering source operations with S_N algorithm
- First Order MOC Solver MOCFE
  - Scalable back projection, dynamic error controller
  - 83% spatial strong scaling from 64 to 1024 cores of BG/P (SN2ND is 95%)
- First Order MOC Solver DeCART for Thermal Reactor Analyses (VHTR M&S)
  - Angular domain decomposition, coupled neutron and gamma heating
- Coupled Neutronics and Thermo-fluids Analysis of VHTR
  - Improved the DeCART/STAR-CD coupling scheme for consistently coupled neutronics and thermo-fluids analysis of prismatic VHTR cores
- Verification and Validation Tests
  - Extensive V&V tests of MC^2-3 against over 30 benchmark problems
  - Combined validation tests of MC^2-3 and UNIC against ZPR-6/7 experiments
  - Verifications tests of DeCART against HTTR and VHTRC benchmark problems
- Reactor IPSC Talk #1: Won Sik Yang, “Neutronics Modeling & Simulation”

Thermal Hydraulics Modeling - Summary

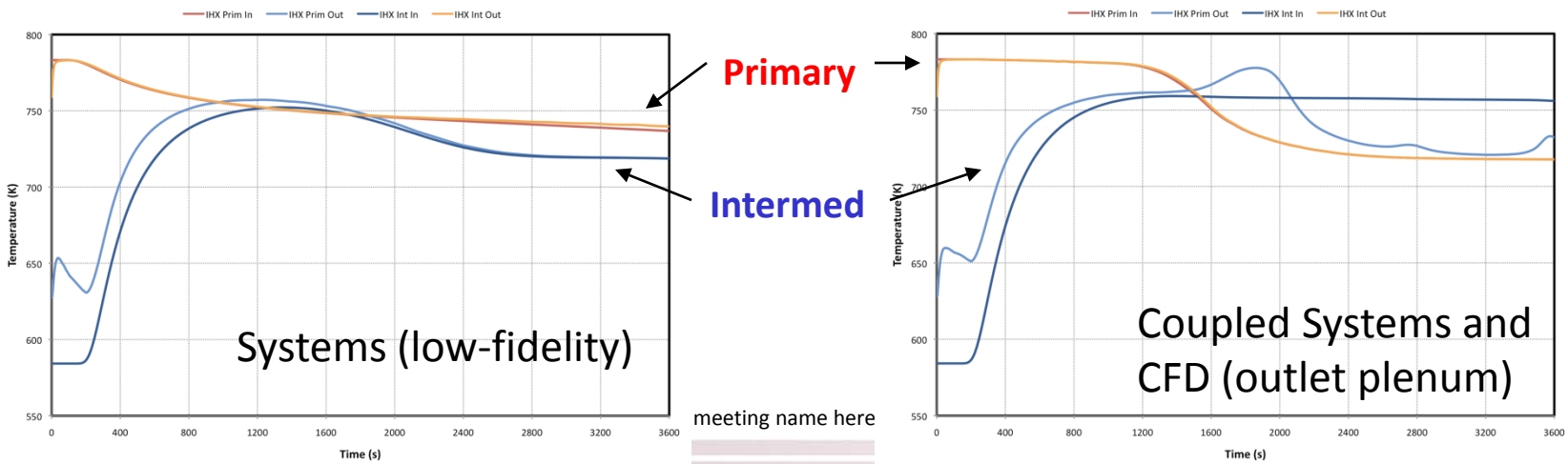
- Objective: develop high-fidelity thermal-hydraulics modeling for the reactor IPSC code SHARP
- V &V effort
  - Established automated code testing based on buildbot
  - Developed a working V&V document providing detailed comparison with analytical / experimental test cases for hundreds of points in input parameter space.
  - Submitted T-junction study to NEA/OECD blind benchmark
  - Nek5000 and Star CD comparison against outlet plenup mock-up (ANL MAX experiment)
- Scalability
  - Nek5000 benchmark scaled to 294912 Blue Gene/P cores (Jülich)
    - Up to 7 billion grid points
    - Sustained 172 TFLOPS on 262144 cores (20% of peak)
- Algorithm Development
  - Developed a new dynamic Smagorinsky implementation that gives superior wall-shear stress predictions for Nek5000, targeting 10,000 < Re < 100,000.
  - POD-based reduced-order model developed and tested in 2D
- Published simulation results
  - 217-pin RANS/LES comparison (Best paper award, Kyoto Fast Reactor Conference)
  - T-junction mixing
  - Impact of contact line/gap
  - etc.
- Reactor IPSC Talk #2: Paul Fischer, “Advances in SHARP Thermal Hydraulics Modeling, Verification, And Validation”

Polynomial Regression with Derivative Information (PRD) for UQ of Nuclear Engineering Applications

- PRD is a new approach for uncertainty quantification
  - Hybridizes Monte Carlo with sensitivity approaches
  - Requires far fewer model simulations for the construction of the system response to uncertainty
- How can sensitivity information be obtained in an efficient manner?
  - Automatic differentiation of nuclear engineering code may succeed to this end even when some legacy components are present
  - The approach was demonstrated on a subset of SAS4A/SASSYS-1.
- Is the uncertainty conclusion robust when PRD is used?
  - Investigated sufficient conditions for this and determined ways to chose the polynomial basis
  - Resulted in better approximations with fewer elements.
- Future work: quantifying uncertainties and validating very large scale codes
- Reactor IPSC Talk #3: Mihai Anitescu, “Polynomial Regression with Derivative Information for Uncertainty Quantification in Nuclear Reactors”

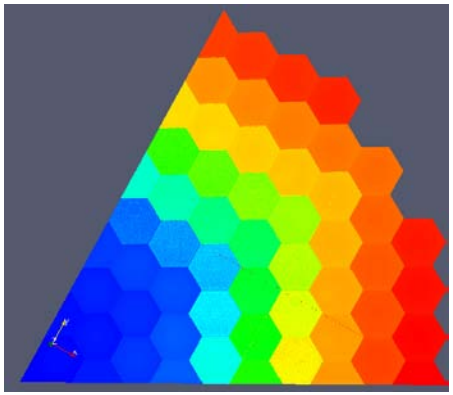
Safety (Systems) Simulations

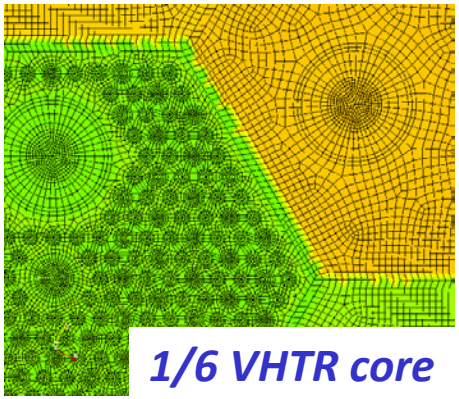
- Objective
  - Develop high-fidelity, whole-system safety analysis models for integration into an advanced simulation code framework.
  - Near-Term: couple safety simulations with high-fidelity modeling to quantify safety-related phenomenon in advanced reactor designs.
- Examples of safety-related phenomenon that can benefit from advanced simulation capabilities:
  - Fuel/cladding temperatures during steady-state and anticipated transients
  - Natural convection cooling and decay heat removal during active or passive shutdown
- Accurate determination of these (and other) phenomenon in relation to design options can be used to quantify performance gains for advanced concepts.
- Example: coupling to high-fidelity outlet plenum model indicates flow stratification



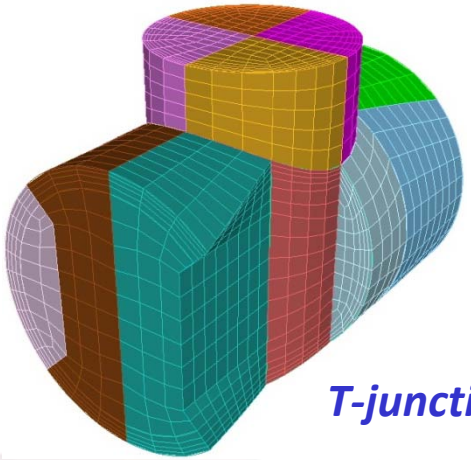
Framework

- Objectives
  - Support existing neutronics, thermal hydraulics, safety simulations with geometry, mesh, coupling services
  - Develop framework-based tools for coupled simulations for next-generation tools
- Development of Reactor Geometry (& mesh) Generator tool
  - Generation of core model as lattice of assemblies (lattices of fuel/other rods)
  - Text-based system simpler, faster
  - Example: VHTR core, 12M hexes, 29 mins to generate
  - Developing 28M element mesh for Kaeri benchmark
- Solution transfer
  - Required for coupled physics simulations
  - Flexibility needed to couple diverse physics models
  - FY10: accuracy, scalability of MOAB-based solution transfer
- Geometry, mesh support
  - CGM port to Open.CASCADE engine
  - CGM, MOAB update to CUBIT 12.x
  - Vettenfal T-junction benchmark support





1/6 VHTR core



T-junction core

Reactor IPSC L2 Milestone Reports

- Neutronics:
  - Verification and Validation Studies of Advanced VHTR Modeling and Simulation Code (6/30)
  - Status Report on High-Fidelity VHTR Modeling and Simulation (9/30)
  - Report on Multigroup Cross Section Generation for UNIC and Associated Verification (9/30)
- T/H
  - Report on SHARP Thermal-Hydraulics code development and associated verification and validation tests for SFR (6/30)
- Systems
  - Uncertainty Quantification for Nuclear Engineering Applications (9/28)
- Framework
  - Mesh Copy/Move Tool for VHTR Applications (4/30)

Reactor IPSC FY11 Plans
Total Budget: $5.5M

- T/H: $1025k (ANL), $200k (LBNL)
  - T/H improvements, R7 integration, viz support, fuels collaboration report
- Neutronics: $1625k (ANL), $200k (INL), $100k (LANL)
  - DIF3D-K+Variant, UNIC, MC2-3, Pronghorn into SHARP, MCNP into SHARP
- Structural Mechanics: $100k (LLNL)
  - Diablo into SHARP
- Systems: $725k (ANL), $200k (INL)
  - Intermediate fidelity tool, SHARP driver, R7 integration, R7 report
- Seismic modeling: $200k (LLNL)
  - Seismic model development in ALE3D
- Framework: $925k (ANL), $100k (LLNL)
  - Mesh generation development/support, solution coupling, long-term viz
- VU: $100k (ANL) (+ $100k FY10 carryover)
  - Reactor IPSC VU report

Reactor IPSC Talks

- Reactor IPSC Talk #1: Won Sik Yang, “Neutronics Modeling & Simulation”
- Reactor IPSC Talk # 2: Paul Fischer, “Advances in SHARP Thermal Hydraulics Modeling, Verification, And Validation”
- Reactor IPSC Talk # 3: Mihai Anitescu, “Polynomial Regression with Derivative Information for Uncertainty Quantification in Nuclear Reactors”