Neutronics Modeling Activities in FY 2010

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Neutronics Modeling - Summary

- Objectives
  - Develop high-fidelity neutronics solvers for the reactor IPSC code SHARP
- Main Accomplishments in FY2010
  - Multigroup Cross Section Generation Code MC^2-3
    - Integrated unit cell calculation capabilities of the legacy code SDX into MC^2-3
    - Extended fine group (230 groups) transport calculation of SDX to ultrafine (~2000) and hyperfine (~300,000) group levels
    - Developed a practical hyperfine group calculation scheme based on the iteration between ultrafine group eigenvalue calculations and hyperfine group fixed source calculations
  - Even-Parity Discrete Ordinate Solver SN2ND
    - Has been demonstrated to scale well up to 294,912 (April 2010)
      - Good performance on BlueGene/P (ANL & JSC) and XT5 (ORNL)
    - Replaced P_N scattering source operations with S_N algorithm
      - Required to maintain >75% strong scaling in angle with anisotropic scattering
      - Required to create a time dependent version of the algorithm

Neutronics Modeling – Summary (cont'd)

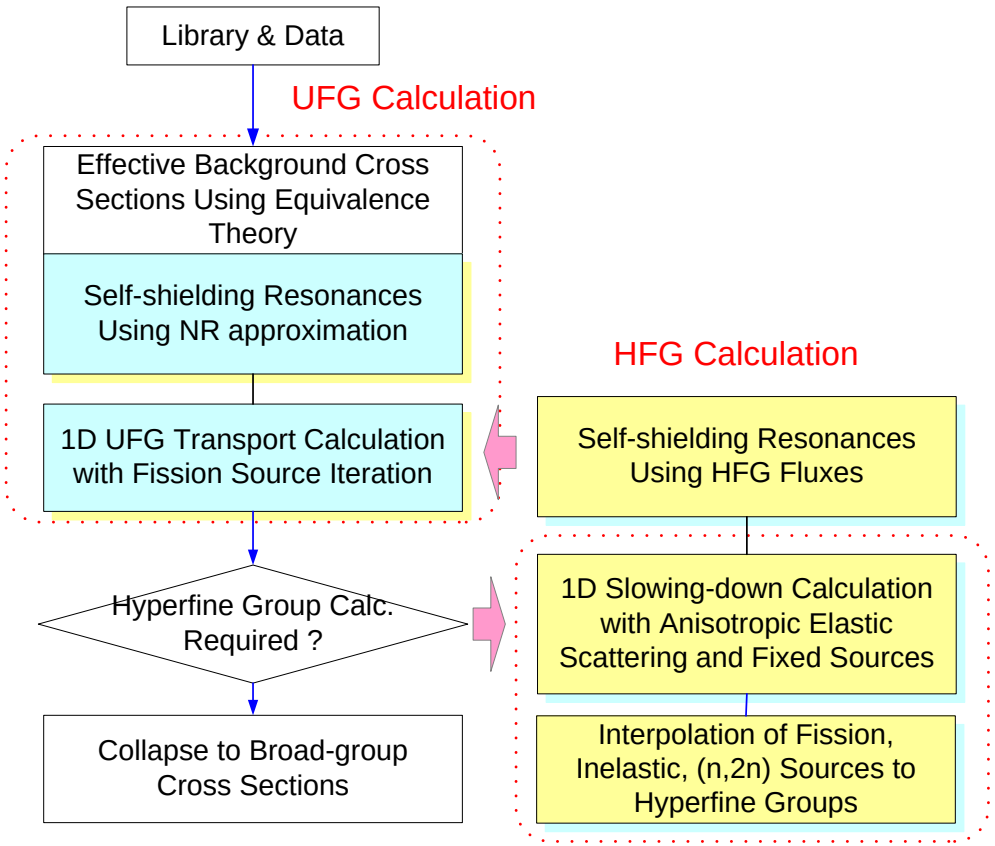
- Main Accomplishments in FY2010 (cont'd)
  - First Order MOC Solver MOCFE
    - Identified and resolved numerous parallel ray tracing issues
      - Developed a scalable back projection algorithm for 3-D
    - Formalized the algorithmic basis of the dynamic error controller
    - Large scale parallel testing is in progress
      - 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)
    - Implemented angular domain decomposition scheme to enhance parallel computation capability
    - Implemented a coupled neutron and gamma heating calculation capability
  - Verification and Validation Tests
    - Extensive verification and validation tests of MC^2-3 against over 30 benchmark problems in the ICSBEP and IRPhEP handbooks
    - Combined validation tests of MC^2-3 and UNIC against ZPR-6/7 experiments
      - Criticality and foil activation measurements for four core loadings
    - Verifications tests of DeCART against HTTR and VHTRC benchmark problems

Neutronics Modeling – Summary (cont'd)

- Main Accomplishments in FY2010 (cont'd)
  - 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
- Milestones/Deliverables
  - 09/15, Report on UNIC Code Development and Associated Verification and Validation Tests (M3)
  - 09/30, Report on Multigroup Cross Section Generation for UNIC and Associated Verification (M2)
  - 03/31, Enhanced Iteration and Parallel Solution Methodologies for VHTR Simulation (M3, VHTR M&S)
  - 06/30, Verification and Validation Studies of Advanced VHTR Modeling and Simulation Code (M2, VHTR M&S)
  - 09/30, Status Report on High-Fidelity VHTR Modeling and Simulation (M2, VHTR M&S)

Multi-group Cross Section Generation Code MC^2-3

- One-dimensional HFG unit cell calculation capabilities
  - Intermediate group unit cell calculation capability was extended to ultrafine group
  - Further extended to hyperfine group calculations with anisotropic scattering sources
    - Eliminate the equivalence theory approximation used to prepare self-shielded ultrafine group cross sections



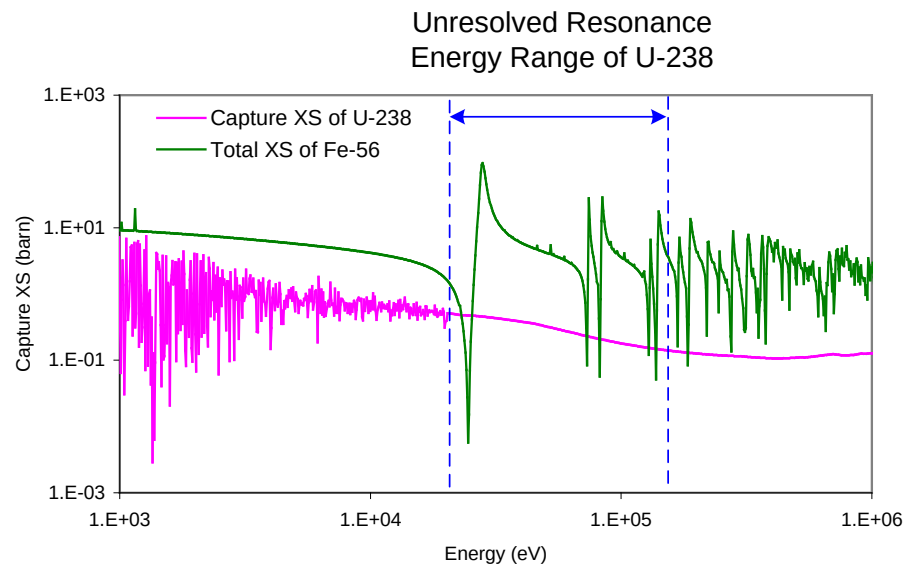
  - However, one-dimensional hyperfine group eigenvalue calculation with anisotropic scattering sources requires a prohibitive computational time
  - A practical hyperfine group calculation scheme was developed based on the iteration between ultrafine group eigenvalue calculations and hyperfine group fixed source calculations

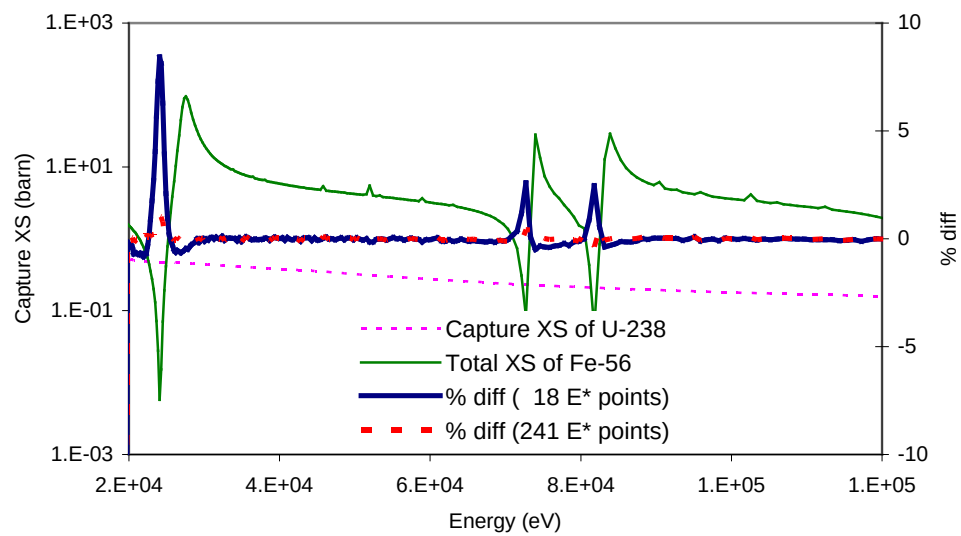
Improved Self-Shielding of Unresolved Resonances

- The number of energy grid points for evaluating self-shielded cross sections in the unresolved energy range was increased from those given in ENDF/B data to the UFG energy grid
  - E.g., 18 to 241 points for U-238

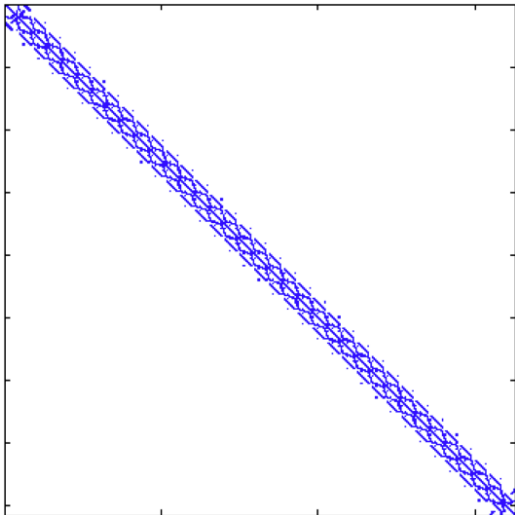
$$\bar{\sigma}_x^i(E^*) = \sum_{k\in i} \bar{\sigma}_{x_k}^i(E^*) = \sum_{k\in i} \sigma_b < \Gamma_{x_k} J_k^* > /(< D_k > f)$$

- The method used to represent the fission spectrum as a function of incident neutron energy was also improved by directly importing the fission spectrum matrix data of all fissionable isotopes from the ENDF/B files





SN2ND: Even-Parity Discrete Ordinates



SPD spatial stencil for all energy groups and angles

$$\left(\sum_{k,l=1}^{3} \frac{\Omega_k^n \Omega_l^n}{\Sigma_{t,g}} \otimes P_{k,l} + \Sigma_{t,g} I \otimes F + BCs \right) \Psi_{g,n}^{+} = b$$

$$\begin{bmatrix} * & & & & & \\ & * & & & & * \\ & & * & & & \\ & & & * & & \\ & & & & * & \\ & * & & & & * \end{bmatrix}_{N \times N}$$

SPD stencil for each space-angle system

$$\begin{bmatrix} * & & & & & \\ * & * & & & & \\ * & * & * & & & \\ * & * & * & * & & \\ & * & * & * & * & \\ & & * & * & * & * \end{bmatrix}_{G \times G}$$

Lower triangular energy structure

Very clear path to peta-scale computing capability

SN2ND Iteration Scheme

Fission source (power) iteration for the eigenvalue (or time-dep. or fixed source...)

Gauss-Siedel iteration over energy groups

Scattering iterations for the within-group scattering system

Conjugate gradient over the whole space-angle system

PETSc preconditioned conjugate gradient for each discrete ordinate

- Parallel hierarchy proceeds as energy, angle, and space in descending order
- At the lowest level, PETSc uses SSOR-preconditioned CG to solve the full spatial domain for a given angle and group. This requires distributed sparse matrix storage of each SPD matrix.
- We are developing a multi-grid preconditioner at the fourth level to reduce sparse matrix storage requirements
- We use DSA at the 3rd level to accelerate the scattering iterations
- We use Chebychev acceleration to reduce the outermost number of iterations
- Each level has dynamic error control to minimize effort in the calculation.

SN2ND Parallel Performance used for Gordon-Bell Nomination

- Strong spatial scaling of 94% on BlueGene/P-ANL

Total Cores	Vertices/ Process	Total Time (seconds)	Parallel Efficiency
8,192	7,324	2,402	100%
16,384	3,662	1,312	92%
24,576	2,441	873	92%
32,768	1,831	637	94%

Mainly measurement of PETSc

Strong scaling in angle is <75%

Diffusion equation needs further partitioning

- Weak angle scaling of 75% on XT5. 76% on BlueGene/P **294,912** cores JSC

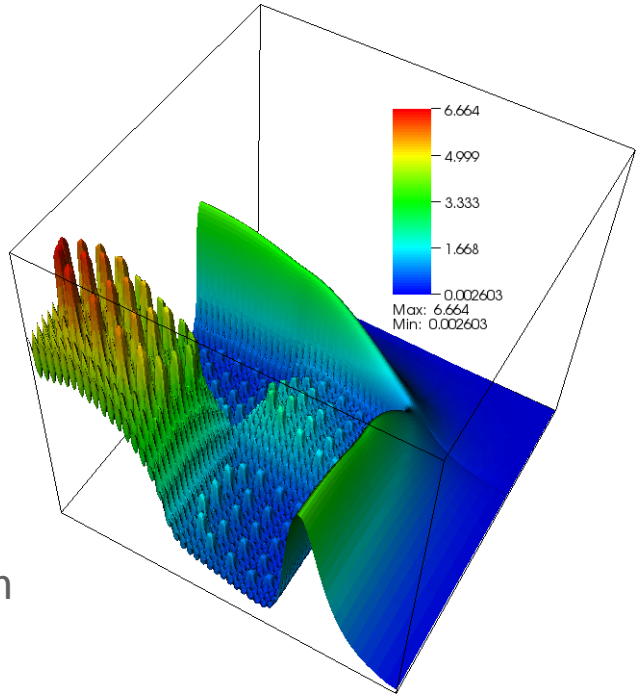
Total Cores	4π Angles	Total Time (seconds)	Weak Scaling
16,512	32	1891	100%
37,152	72	1901	99%
66,048	128	1829	103%
103,200	200	2050	92%
148,608	288	2298	82%
222,912	432	2517	75%

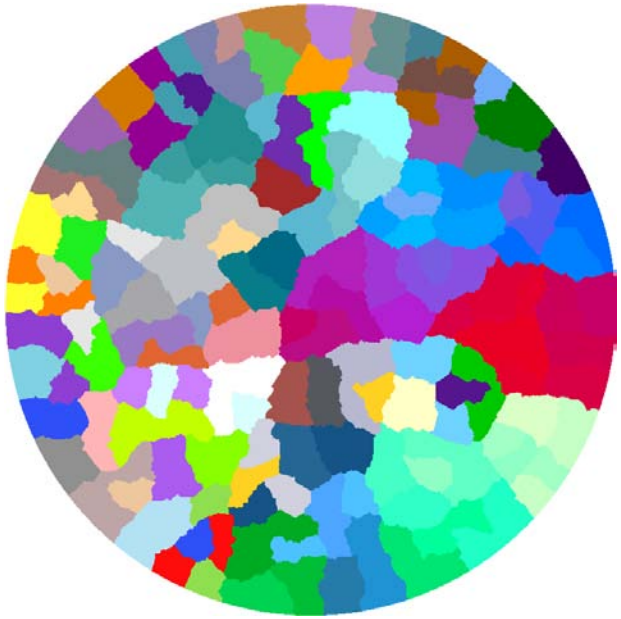
Weak scaling in space means mesh refinement for us

Refinement of bad aspect ratio elements produced >95%

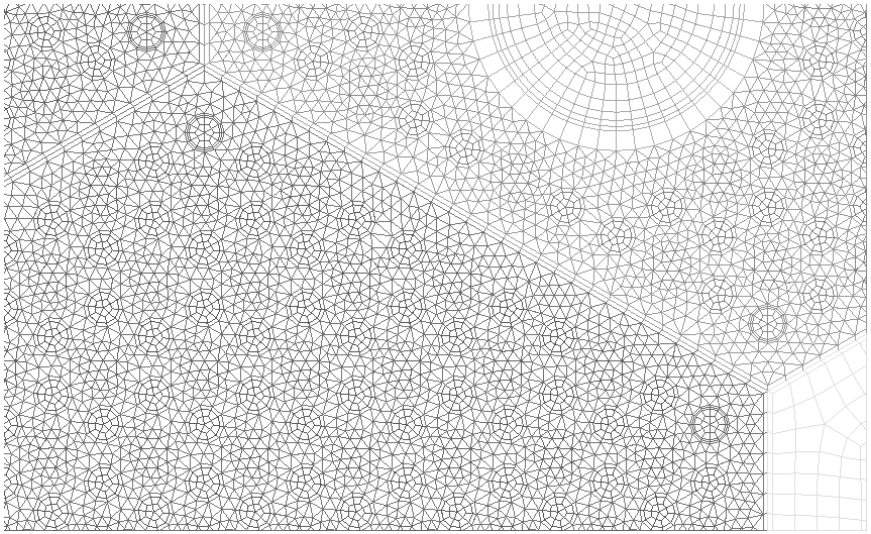
MOCFE Development Path

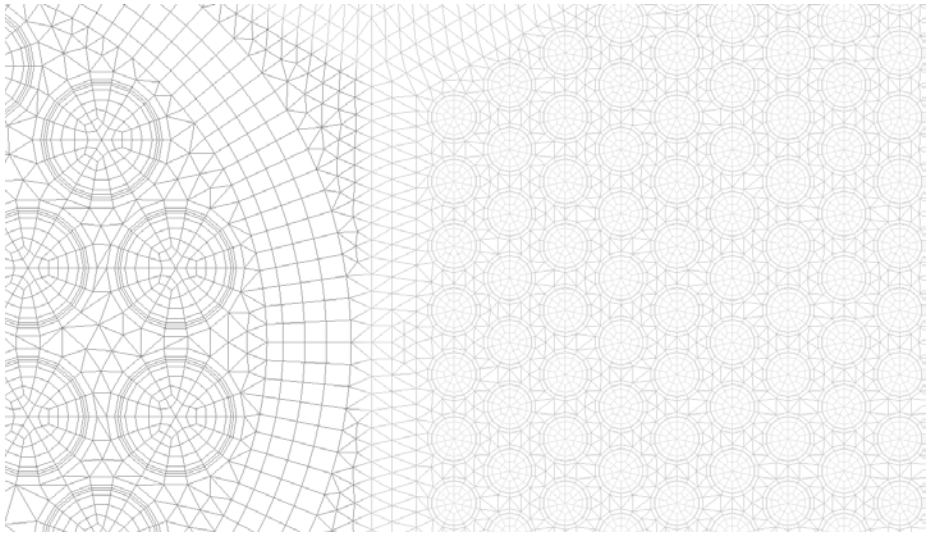
- In 2009-2010 we rebuilt 2D and 3D MOCFE solver
  - About 10 times faster than older version
  - Easier to modify/maintain/develop
  - Faster ray tracing with ability to treat all element types/orders
  - Spatial domain decomposition
    - More appropriate path for large scale parallelism
      - Executed on 65,636 cores of BG/P at ANL
    - Assumes trajectory splitting and communication of trajectory flux
    - Vector space increases as the number of sub-domains increase
    - Needs significant research into preconditioner
  - Flexible to utilize fundamental algorithms as part of multiple solver strategies
    - Lattice geometry cross section generation
    - 2D-1D thermal design tool (replace DeCART)
    - Whole core 3-D transport solver

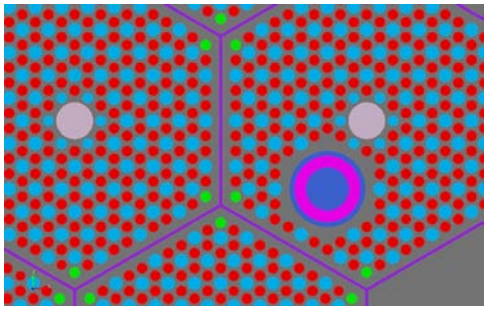




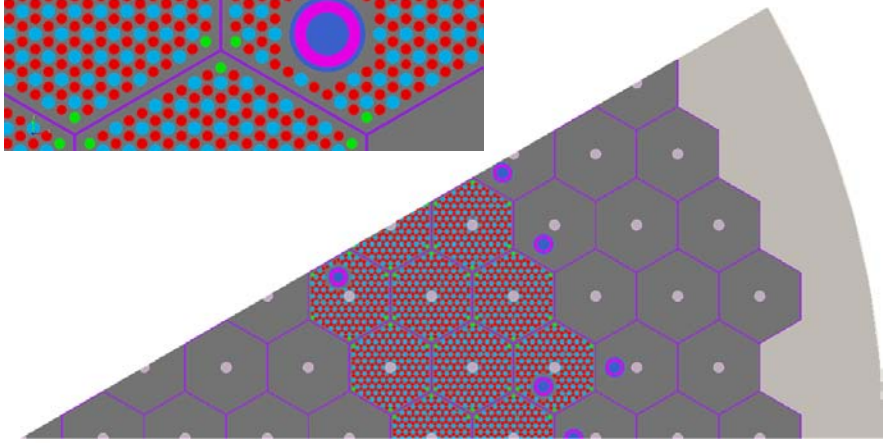
Sample Meshes of MOCFE

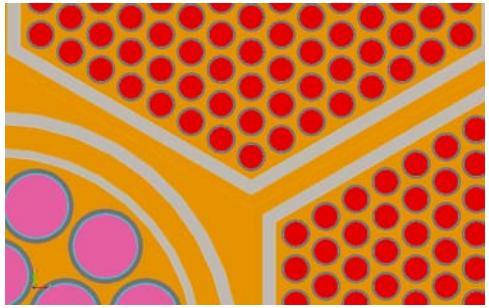




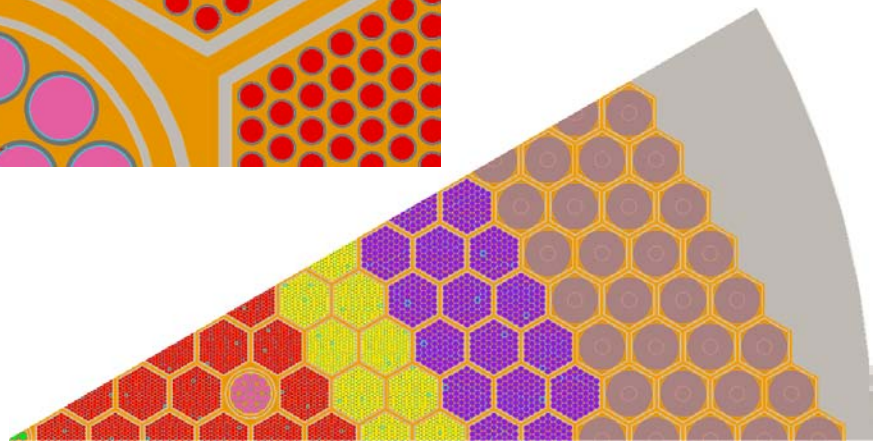


VHTR



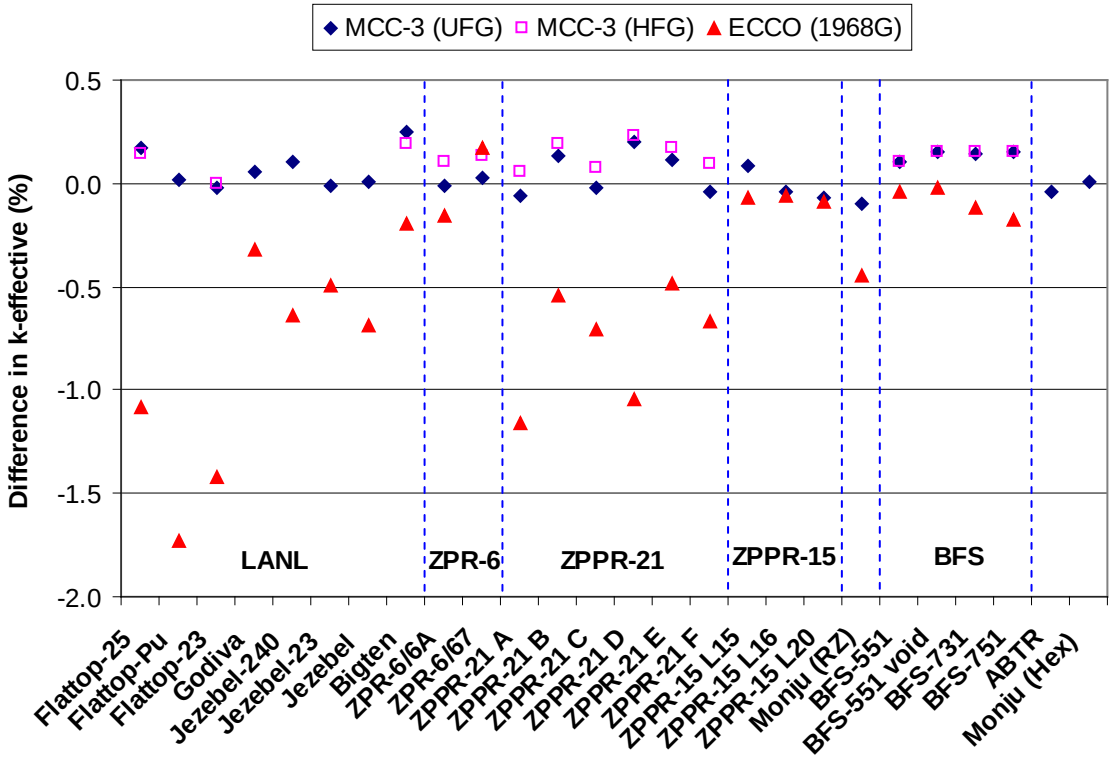


MONJU



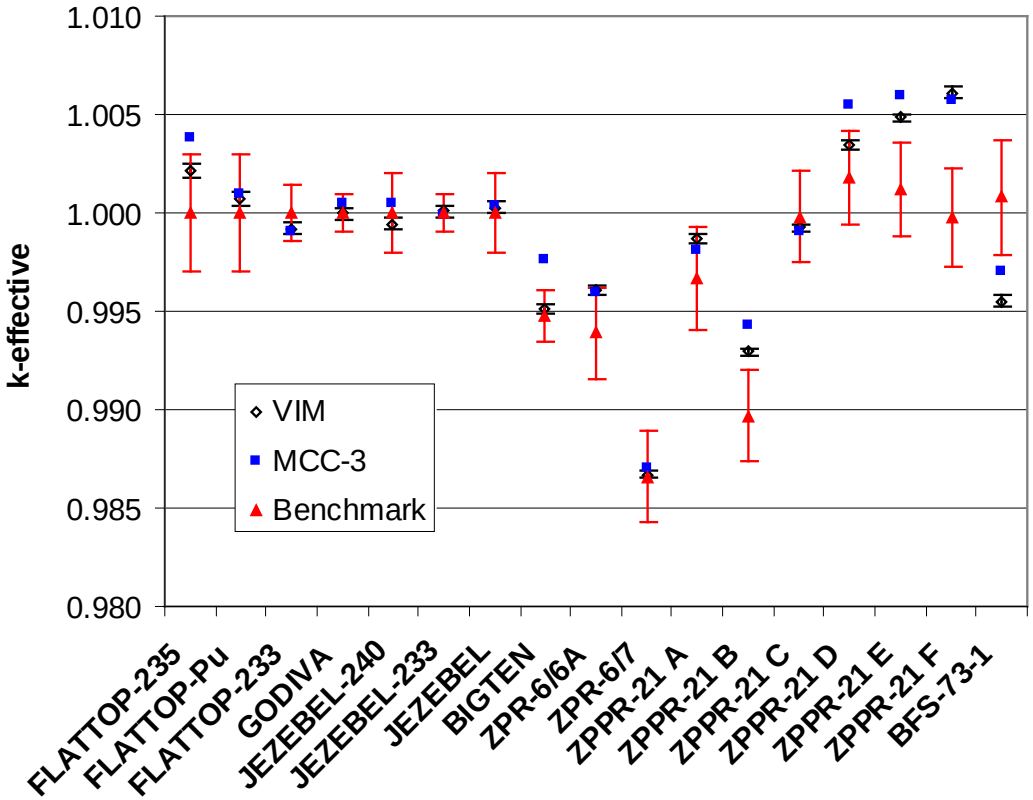
Criticality Benchmarks

- Region-dependent cross sections were generated in a 230-group structure using ENDF/B-VII data
- Whole core calculations were carried out with TWODANT and ERANOS
  - TWODANT $S_{24}P_3$ and VARIANT P_5P_1 with MC^2-3 cross sections
  - ERANOS $S_{16}P_3$ with ECCO cross sections (1968 group slowing-down calculation)
- Deterministic results compared with VIM and MCNP5 Monte Carlo solutions
- RMS difference between MC^2-3/TWODANT and Monte Carlo solutions is 0.14%
- Relatively large differences in ECCO/ERANOS results
  - LANL small critical assemblies with large leakage
  - ZPPR-21 assemblies with no blankets and thick graphite reflector around core



Criticality Benchmarks (cont'd)

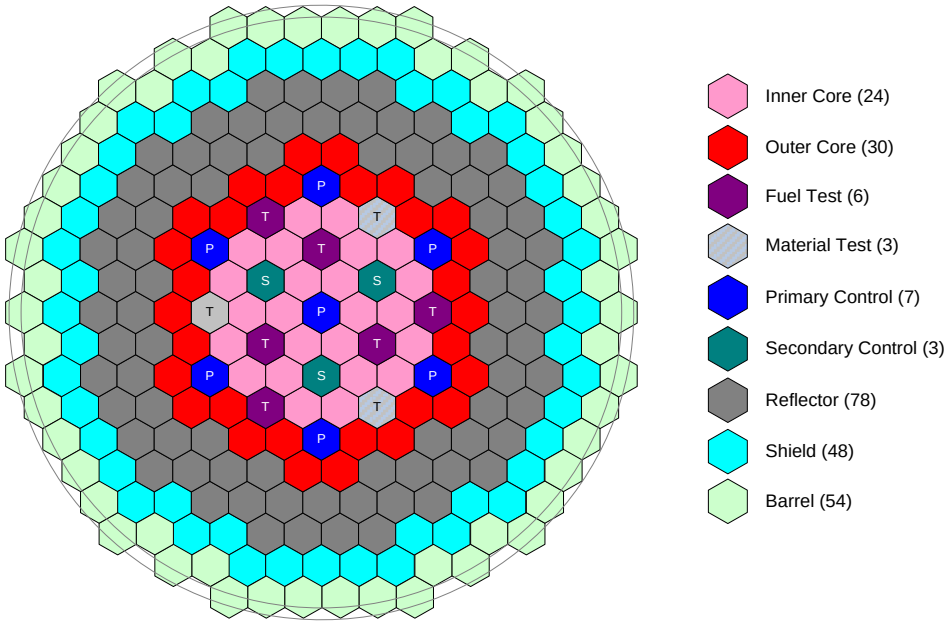
- Comparison with the specified benchmark k-effective values with 1-σ uncertainties



	VIM	MC^2-3
< 1σ	13	10
1σ - 2σ	3	5
2σ - 3σ	1	2
Total	17	17

Advanced Burner Test Reactor Benchmark

- 250 MWt numerical benchmark problem
- 230G cross sections were generated with MC^2-3
- VARIANT calculations up to P_5P_3
- Excellent agreement in the core multiplication factor between MC^2-3/VARIANT and MCNP5

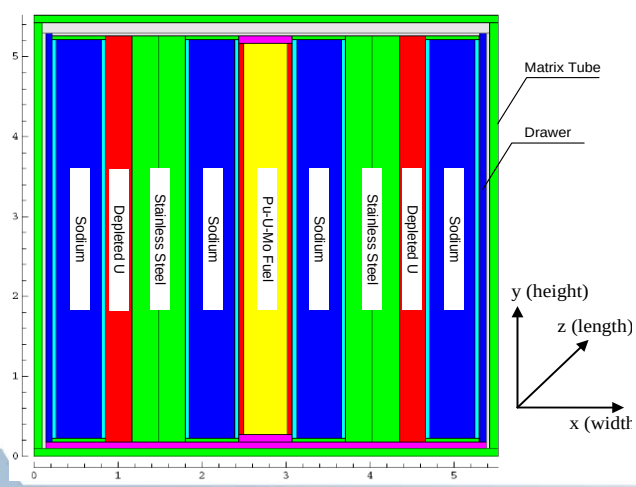


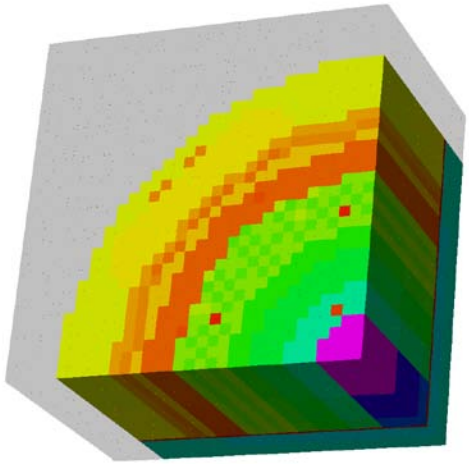
MCNP5 k-eff (a)	MC^2-3 / VARIANT			
	Order	k-eff (b)	Δk (P_N–P_{N-1})	Δk (b – a)
1.03457 ± 0.00025	P_3P_0	1.03370		-148
	P_3P_1	1.03293	-77	-226
	P_3P_3	1.03320	27	-199
	P_5P_0	1.03541		22
	P_5P_1	1.03454	-88	-65
	P_5P_3	1.03477	23	-42

Criticality Benchmarks (Cont'd)

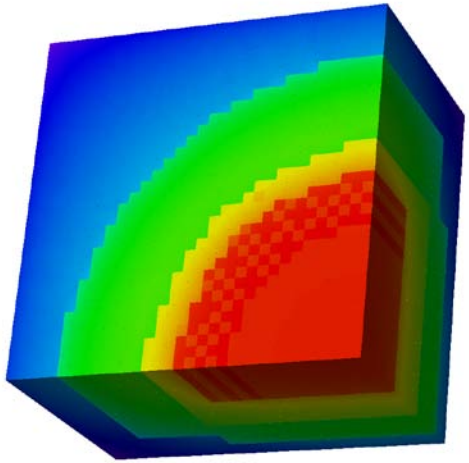
- ZPPR-15 Loadings 15, 16, and 20
  - Drawer averaged 230 group cross sections from MC^2-3 1D slab calculations
  - UNIC calculation with L3T3 (32 directions for 4π) and P_3 anisotropic scattering
- HFG cross sections resulted in better agreements of k-effective with MC solutions

ZPPR-15 Loading	VIM (V)	SD	MCNP5 (M)	SD	MC^2-3 UFG		MC^2-3 HFG	
					M–(V)	M–(M)	M–(V)	M–(M)
L15	0.99981	12	0.99956	22	-346	-321	-193	-168
L16	0.99571	21	0.99523	24	-351	-303	-197	-149
L20	0.99780	12	0.99741	23	-313	-274	-158	-119





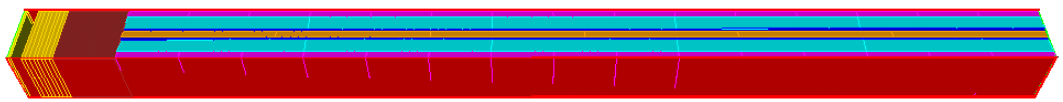
Composition Loading

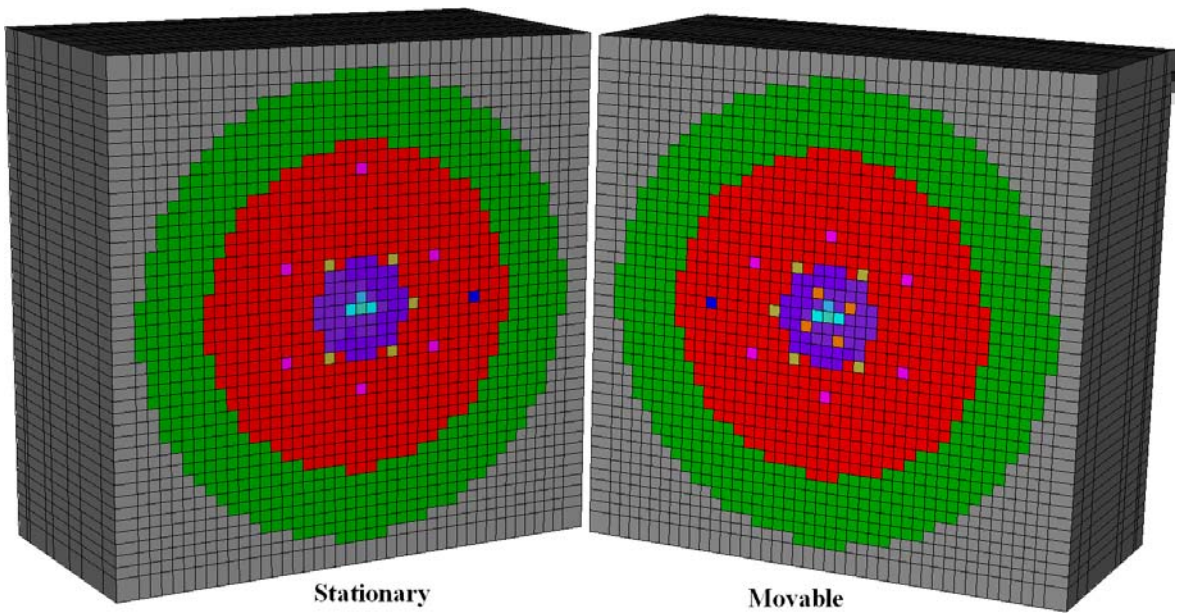


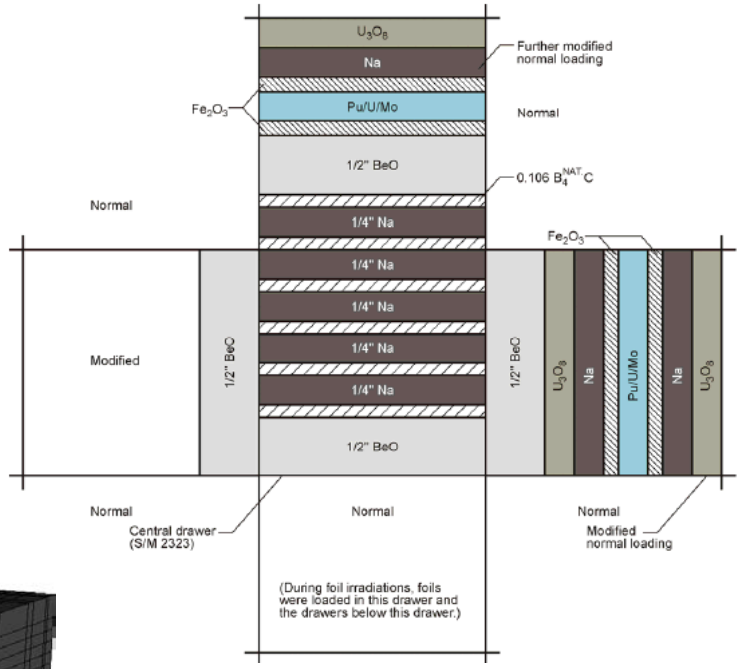
Power Distribution

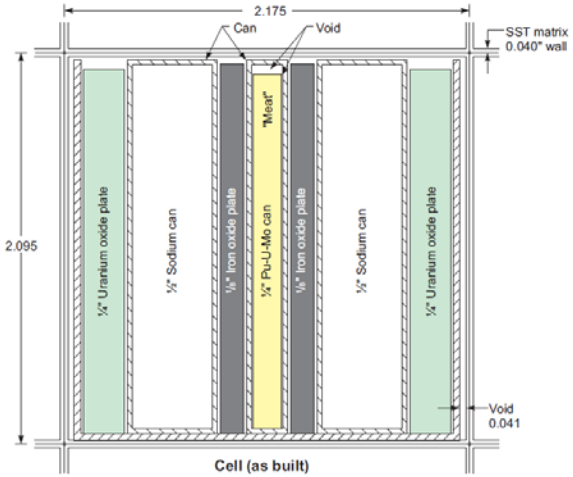
ZPR-6 Assembly 7 Critical Experiments

- Loadings 104, 106, 120, and 132 of high Pu-240 reactor physics benchmark
  - Control rod worth measurements
  - Sodium channel and BeO ring at the core center









ZPR6 Assembly 7 Critical Experiments (cont'd)

- MC^2-3/SN2ND analyses
  - 70 energy groups, 1M spatial meshes, 72 angular directions, P_3 scattering order

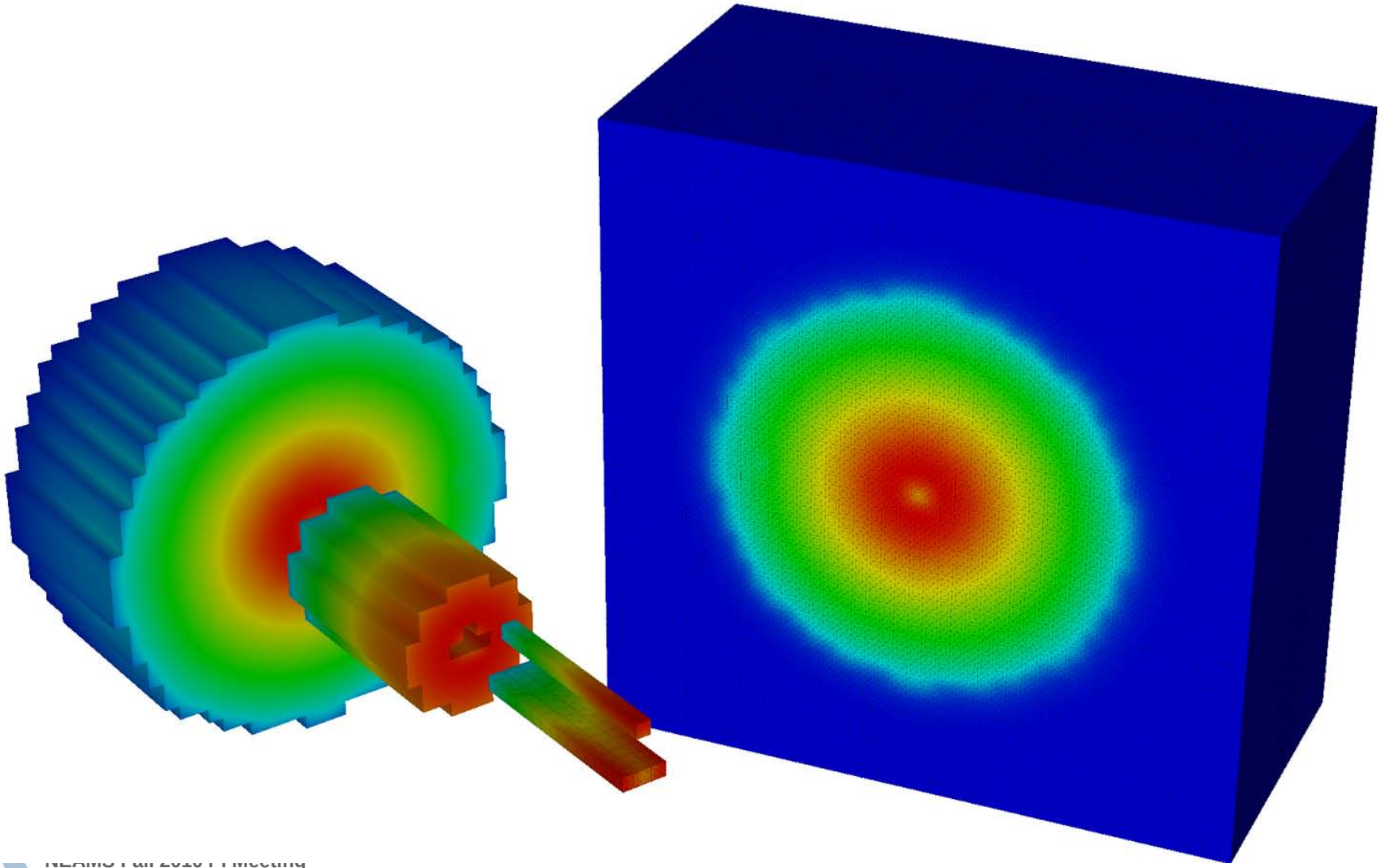
	Loading 104	Loading 106	Loading 120	Loading 132
MC^2-3/UNIC	1.00147	1.00134	1.00127	1.00016
	0.075%	0.043%	0.028%	-0.024%
MCNP5 (as-built model)	1.00016 ±0.00007	1.00049 ±0.00007	0.99967 ±0.00007	1.00040 ±0.00007
	-0.056%	-0.042%	-0.132%	0.000%
Measurement	1.00072 ±0.00002	1.00091 ±0.00003	1.00099 ±0.00003	1.00040 ±0.00002

* Measurement uncertainty only

* Combined uncertainty due to geometry and composition uncertainties estimated for the Loading 99 is ~0.080%

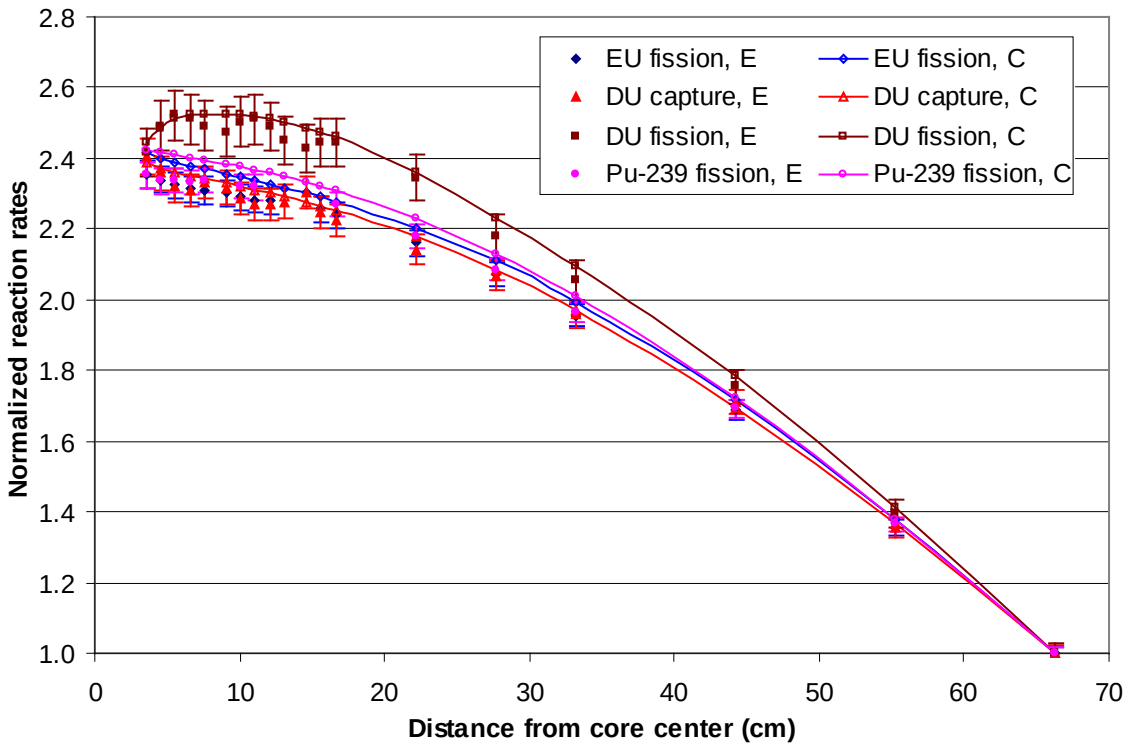
ZPR6 Assembly 7 Critical Experiments (cont'd)

- Distribution of neutron flux from 10 MeV to 14.2 MeV for Loading 106



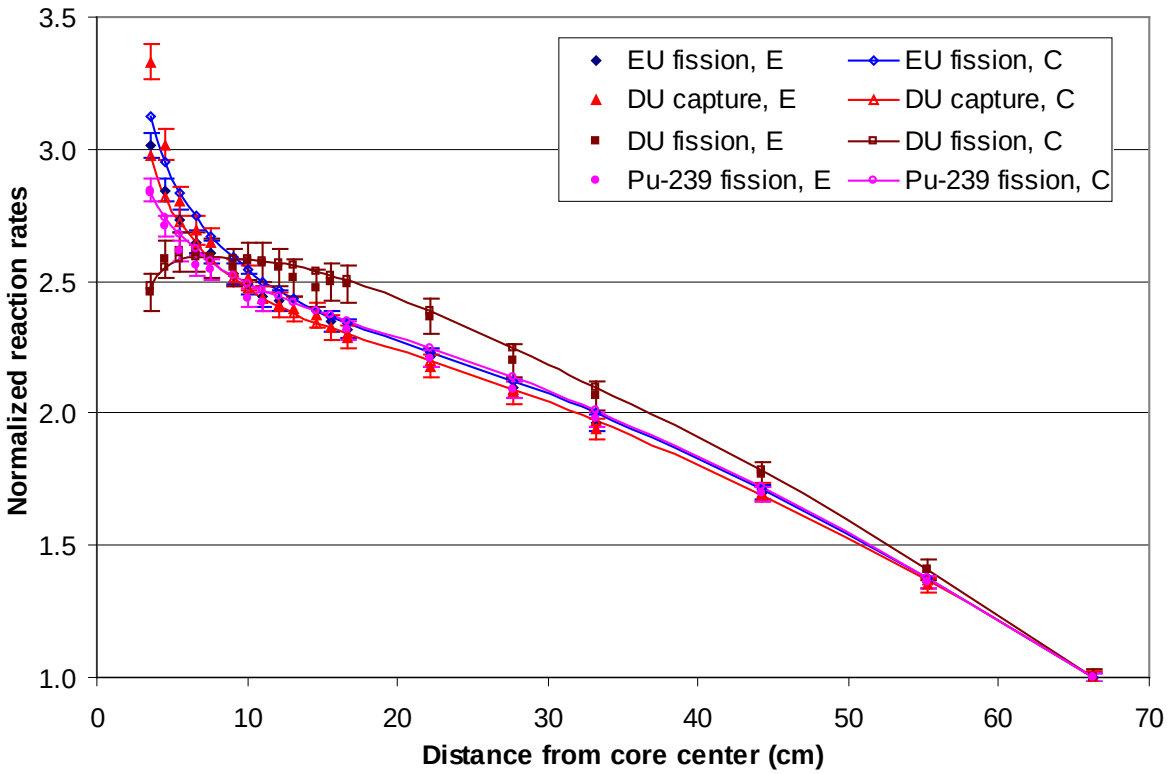
ZPR6-7 Foil Measurement Comparisons

- 69 foil activation measurements were analyzed for each of four loadings
- Calculated reaction rates agreed very with the measurements except for a couple of depleted uranium capture rates near the BeO plates (in loadings 106 and 132)
  - Enhanced self-shielding of low energy resonances of U-238 (below 1 keV)
- Additional studies are ongoing to account for surface sources in MC^2-3 calculations



ZPR6-7 Foil Measurement Comparisons

- Foil reaction rates in the loading 106 with BeO plates around the central sodium drawer

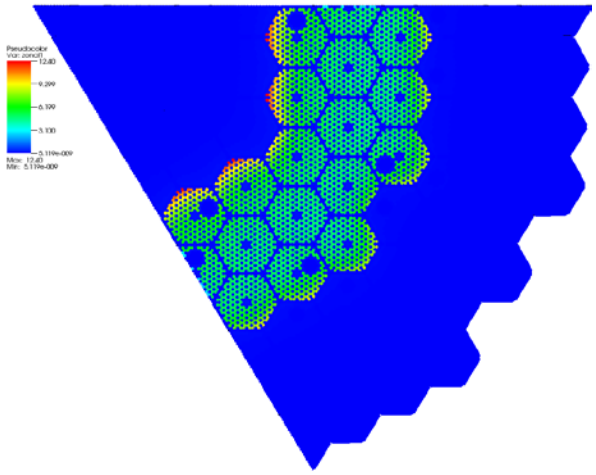


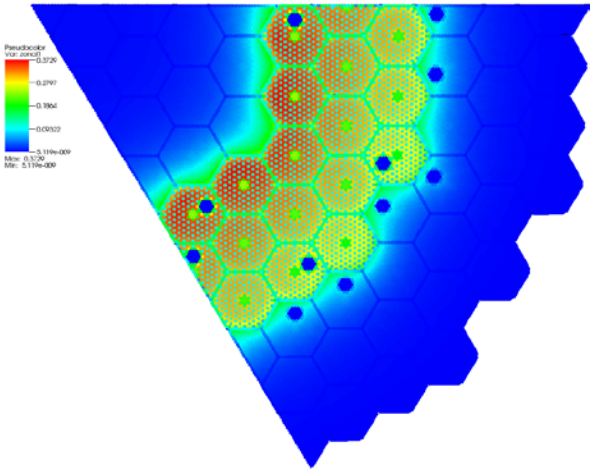
Progress in VHTR Simulation

- Implementation of angular domain decomposition scheme in DeCART
- Generation of gamma production and interaction cross section libraries
  - Neutron induced gamma production matrices for 261 isotopes in 238 neutron and 48 gamma groups
  - Gamma interaction cross sections for 100 elements in 48 gamma groups
- Implementation of coupled neutron and gamma heating calculation capability
- Verification and validation tests of DeCART
  - HTTR and VHTRC benchmark problems
- Validation study of CFD models using the core bypass flow experiments performed at Seoul National University
- Refined CFD modeling to enable variable thermo-physical properties and evaluate effects of buoyancy driven flow and turbulence contributions
- Mesh sensitivity analyses for coupled DeCART/STAR-CD simulations

Gamma Library and Transport Capabilities

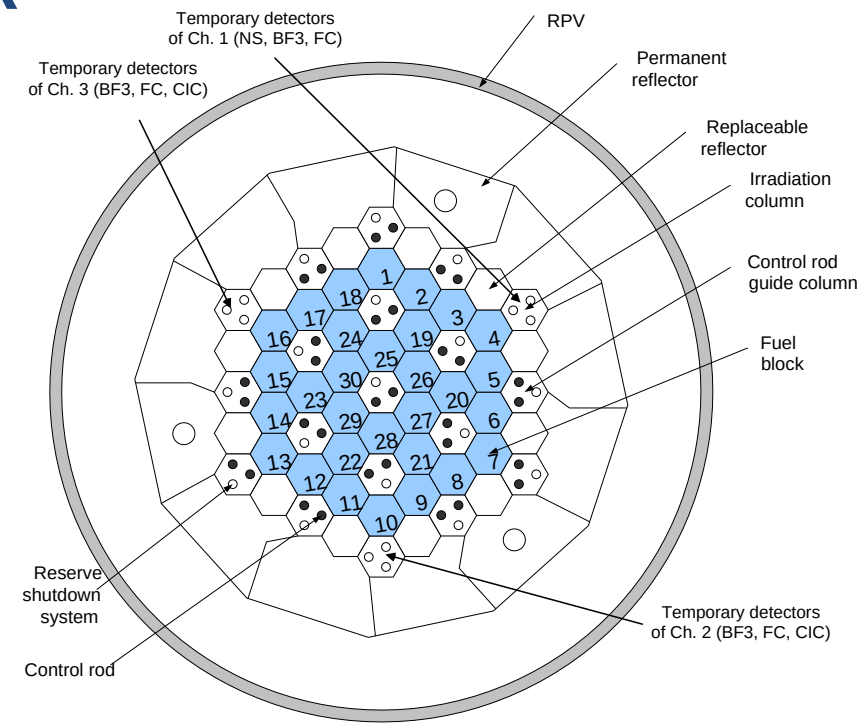
- Gamma production and interaction libraries were generated using NJOY with ENDF/B-VII data
  - Gamma production and neutron heating factors for 250 isotopes
  - Gamma interaction and heating factors for 70 elements
  - Delayed gamma data: Th-232, U-233, U-235, U-238, Pu-239, Pu-241
- Gamma transport calculation capability
  - Coupled neutron and gamma heating calculation
  - Preliminary calculation for 2D 1/6 core of VHTR with 48 neutron and 18 gamma groups
    - Gamma contribution to the total power is ~9.4% (7.6 % from fuel blocks, 0.7% from inner reflector graphite blocks, and 1.1% from outer reflector graphite blocks)

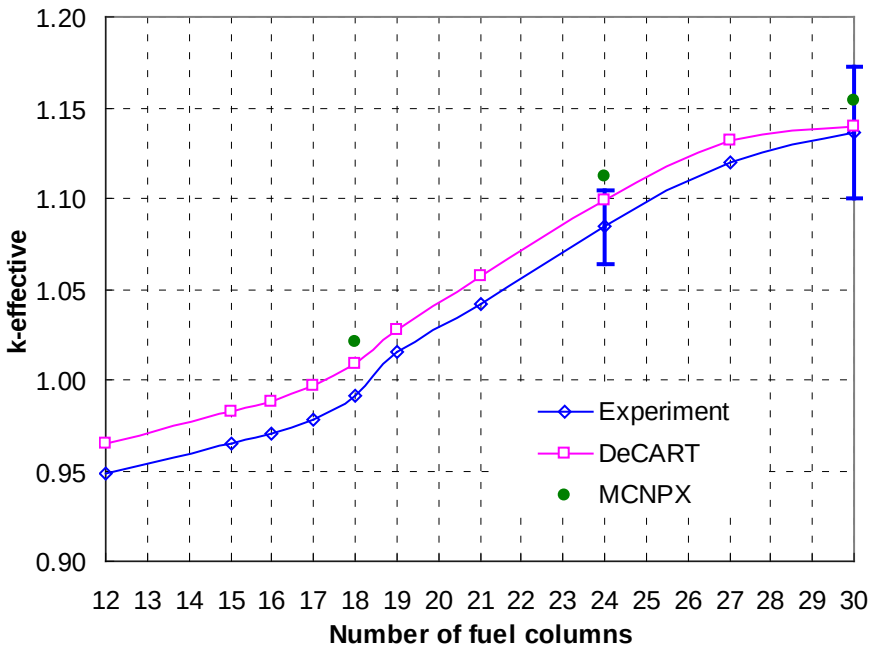


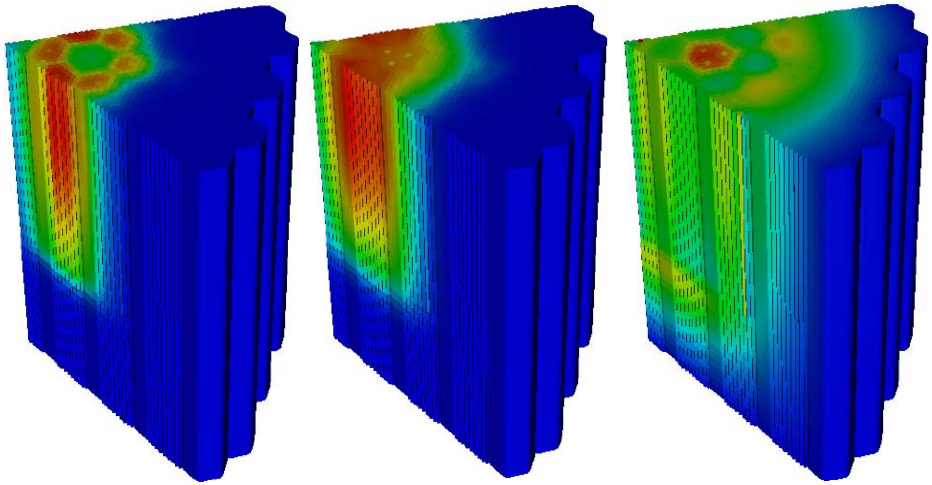


First Criticality Tests of HTTR

- IAEA benchmark for 30 MWt HTTR
  - First criticality tests conducted in 1998
  - Large measurement uncertainties reported (2.0% for 24 column, and 3.6% for 30 column case)
  - Specified born impurity (0.37 ppm) in reflector blocks is considered too low.



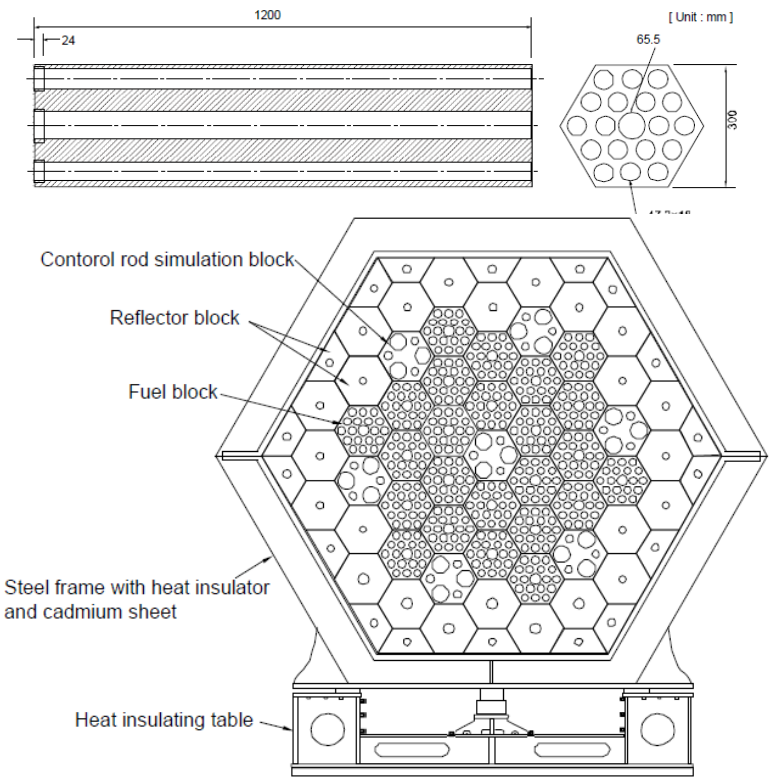




E > 20 keV 1.8 eV < E ≤ 20 keV E ≤ 1.8 eV

Temperature Coefficients of VHTRC

- IAEA benchmark for isothermal temperature coefficient measurements of VHTRC
  - A graphite moderated critical assembly which has a core loaded with pin-in-block fuel of low enriched uranium and a graphite reflector.
  - In the experiments, the assembly was first brought a critical state at room temperature, and then it was heated stepwise up to about 200 °C by using electric heaters.
  - In the benchmark, the actual core boundary was truncated (e.g., cadmium sheets and heat insulator were neglected).

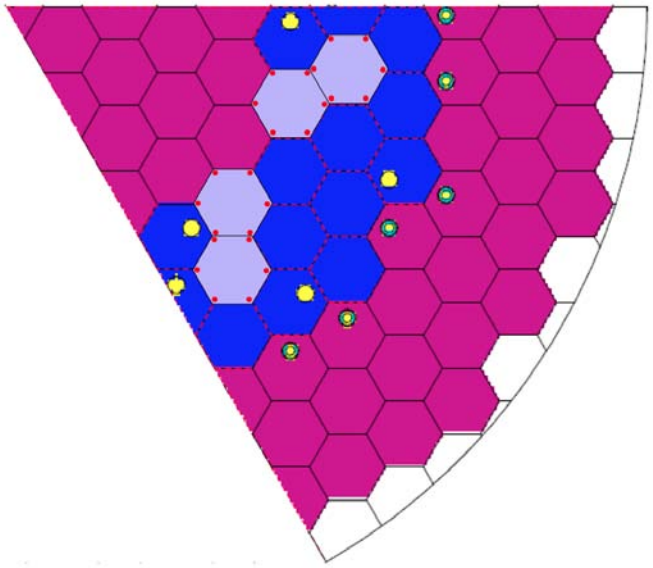


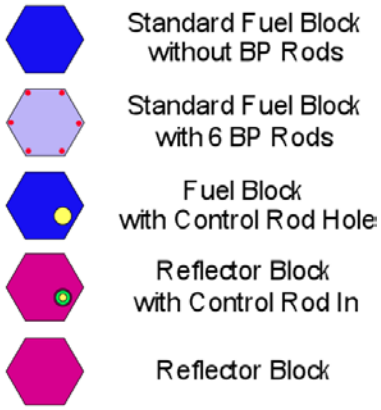
Isothermal Temperature Coefficient (pcm/°C)

Temp (°C)	Experiment	DeCART
25.5 – 71.2	-15.6 ± 0.4	-19.1
71.2 – 100.9	-17.9 ± 1.1	-17.6
100.9 – 150.5	-18.1 ± 0.9	-16.2
150.5 – 199.6	-17.7 ± 1.3	-14.7
25.5 – 199.6	-17.3 ± 0.3	-16.8

Coupled DeCART/STAR-CD Simulation

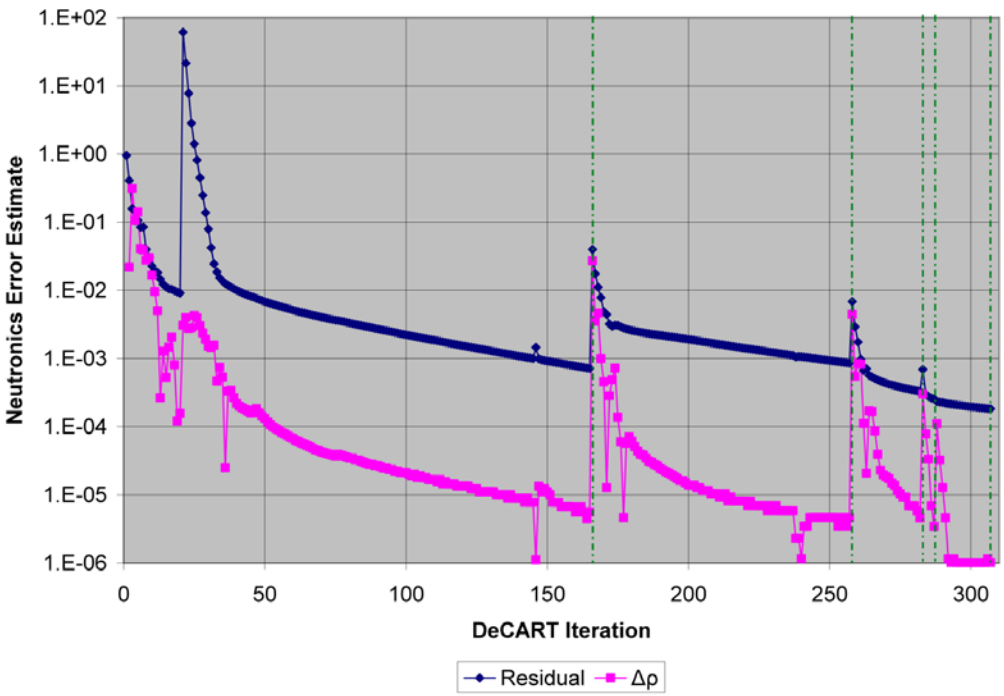
- DeCART Model
  - Axial discretization (in fuel)
    - 30 MOC planes, 26.4 cm thick
    - 2 CMFD subplanes, 13.2 cm thick
    - 2nd order nodal diffusion (LPEN)
  - Radial: 260k MOC regions/plane
  - 8 azimuthal & 2 polar angles/octant
  - 72 group VHTR library from ORNL
- STAR-CD Model
  - 44M hexahedral cells total
    - Axial layers 13.2 cm thick
  - Previous standalone initialization
  - Realizable k-e with law-of-the-wall
  - SIMPLE solver algorithm
  - Rhie-Chow interpolation for pressure-velocity coupling

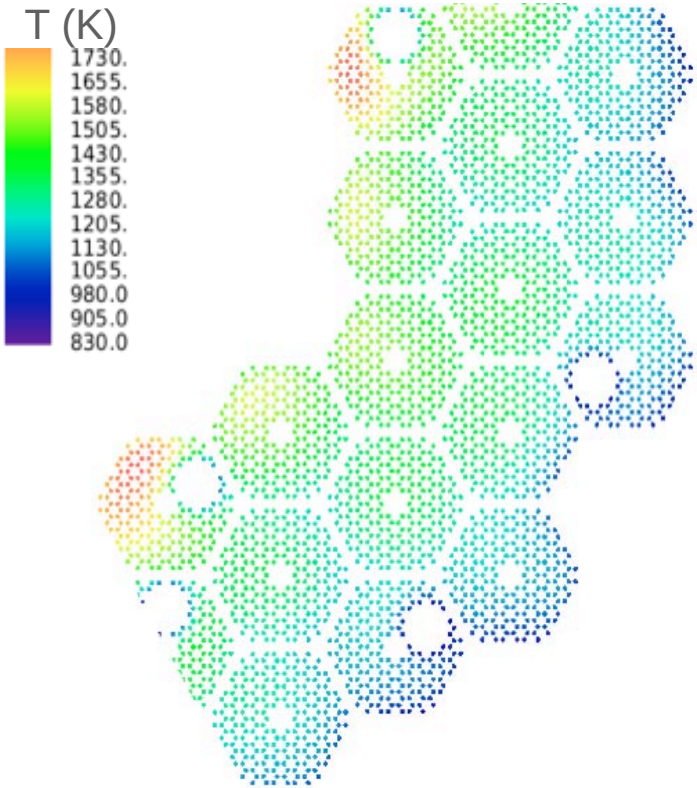




Coupled Neutronics and CFD Simulation

- Global balance residual (blue) and change in k-eff (pink)
  - Cross section update following STAR-CD temperature update (green lines) upsets global residual
  - Number of iterations between STAR-CD is reduced progressively



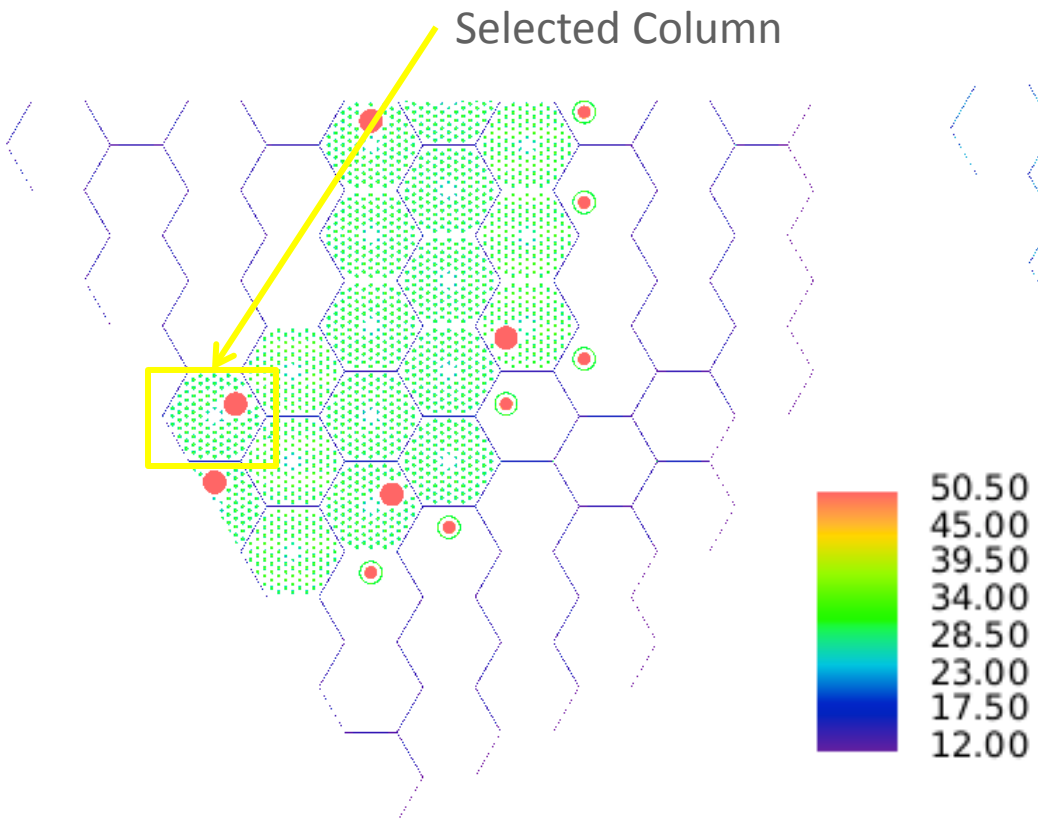


Fuel Temperature Profile Near Core Outlet

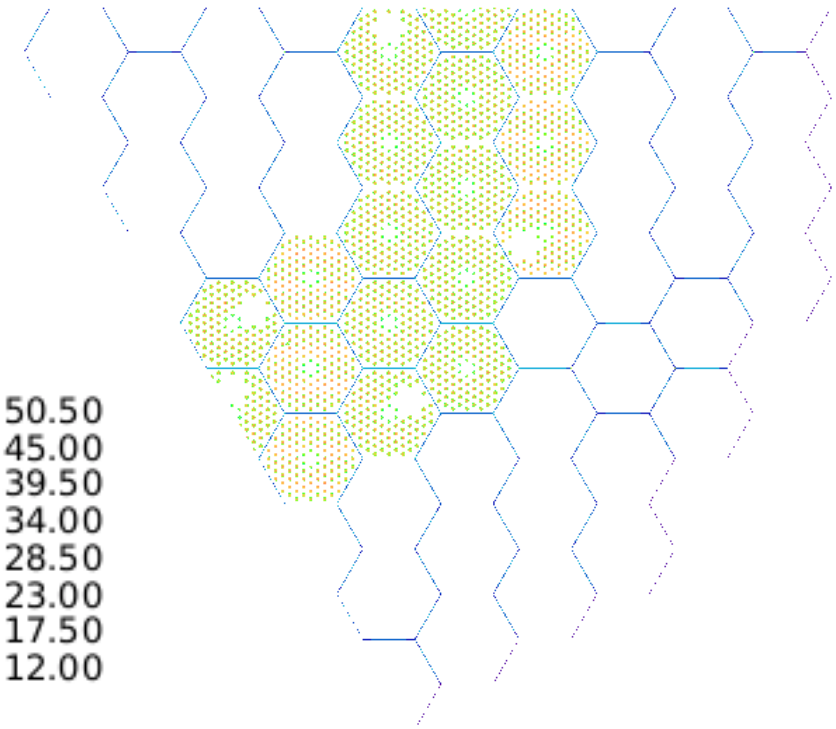
Sensitivity Study of Control Rod Hole Models

- Reflector blocks at the inlet and outlet of the core have complex flow networks
  - Lower reflector blocks partially block flow in control rod channels
  - Actual design data is not available
- Simplify: straight channels
- Previous case: CR holes completely open
  - Exaggeratedly high bypass flow rate
  - Correspondingly high fuel temperature
- New case: CR holes completely blocked
  - Opposite extreme for bypass flow rate
  - Filled with solid with the same thermal conductivity as helium
- Coupled DeCART/STAR-CD simulations
  - Only modest differences in power distribution
  - Substantial difference in fuel temperature profile, 180K difference in peak temperature

STAR-CD Predictions of Velocity Distribution

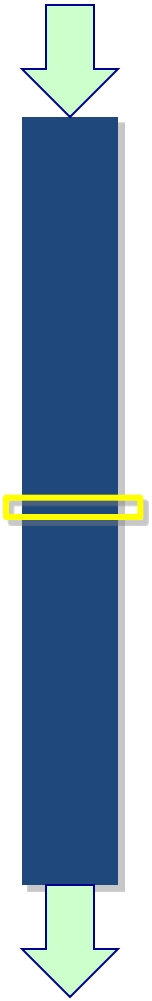


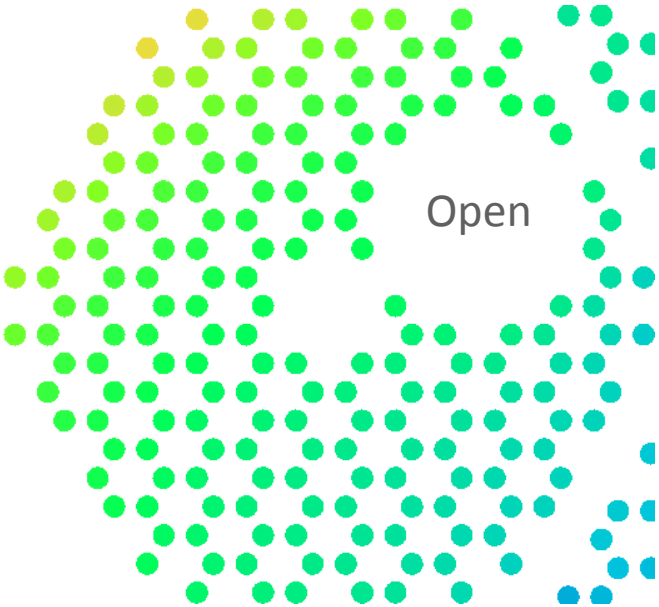
Fully Open Control Rod Holes
(Peak Velocity in CR Hole ~ 80m/s)



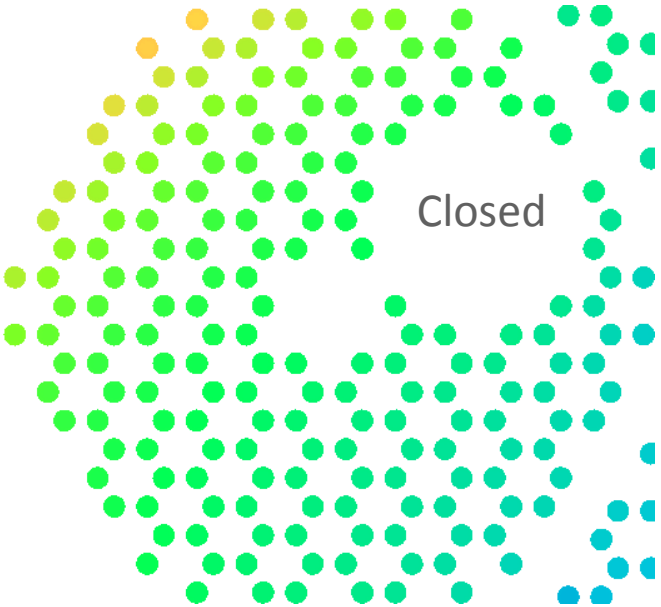
Fully Closed Control Rod Holes

DeCART/STAR-CD Predictions of Fuel Power Density in Selected Column

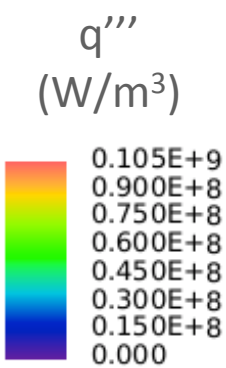




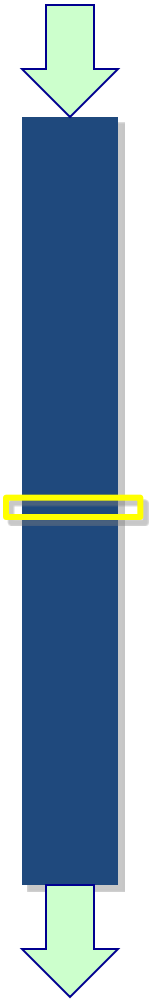
Fully Open Control Rod Holes

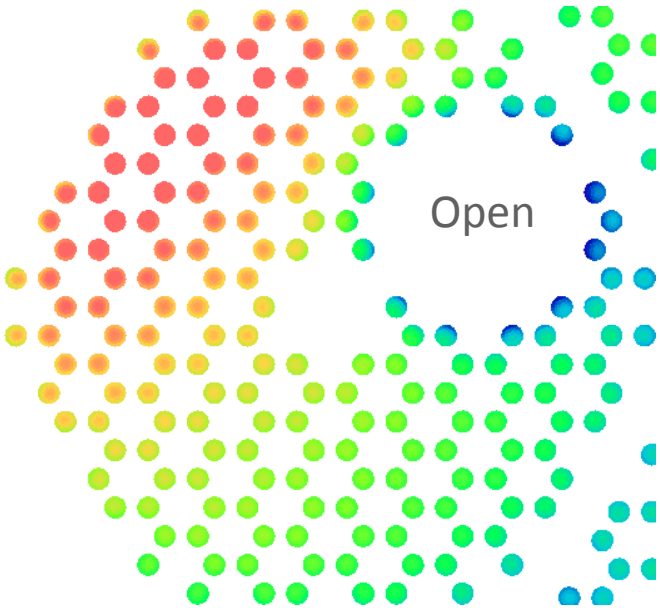


Fully Closed Control Rod Holes

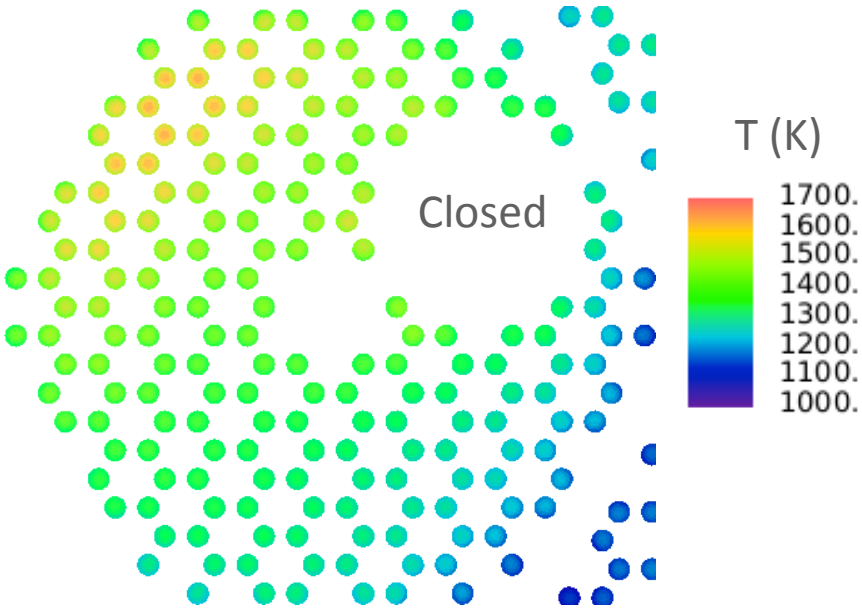


DeCART/STAR-CD Predictions of Fuel Temperature in Selected Column





Fully Open Control Rod Holes
(Global Peak 1880K)



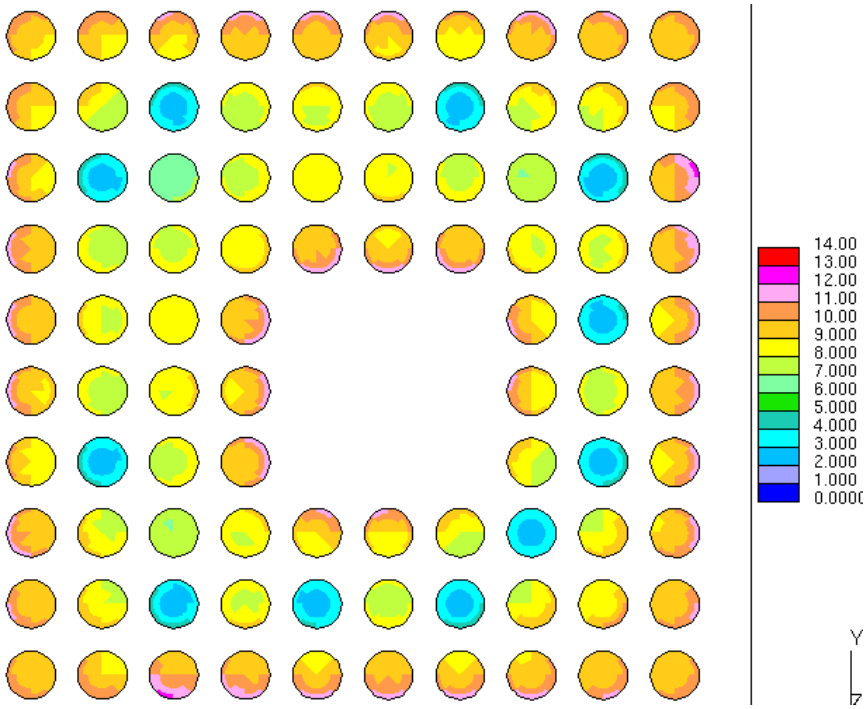
Fully Closed Control Rod Holes
(Global Peak 1700K)

Plans for FY2011

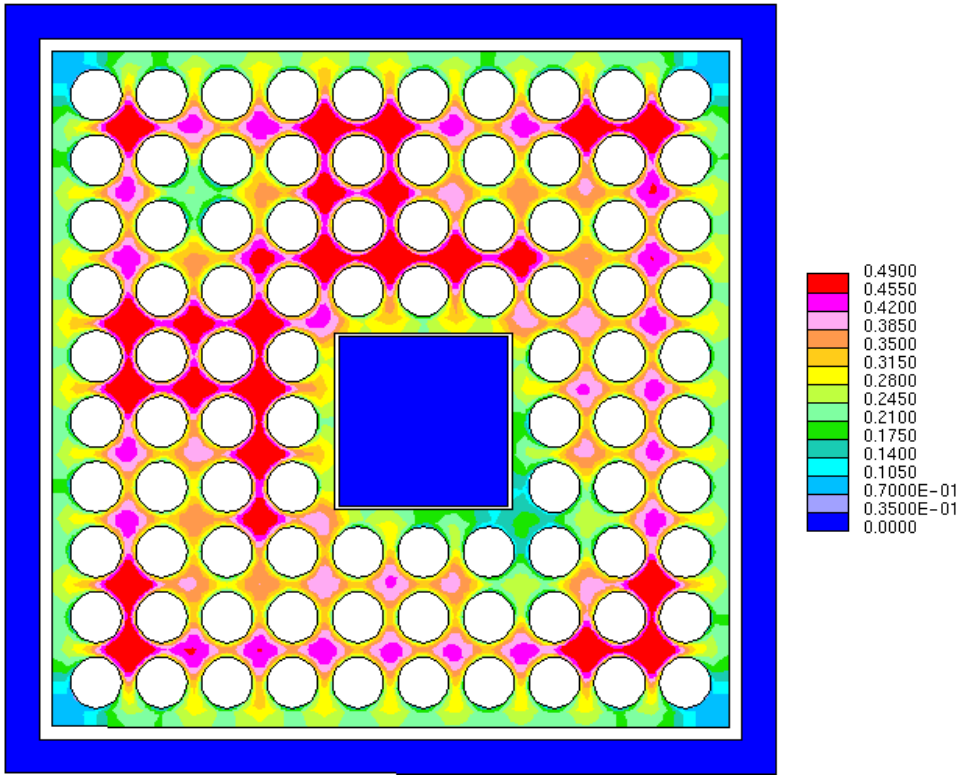
- Advanced Reactor Concepts
  - Incorporate the kinetics codes DIF3D-K and VARIANT-K into SHARP
    - Modernize DIF3D-K and VARIANT-K to be compatible with SHARP
    - Support the coupled system and neutronics analysis for the challenge problem #1
  - Deliver a production version of the multigroup cross section generation code MC2-3 with ENDF/B-VII libraries
    - Meet continual industry request (TerraPower, Westinghouse, and GE)
- Small Modular Reactor
  - Improve the performances of the high-fidelity SN2ND and MOC solvers of UNIC and implement a kinetics capability in SN2ND
    - Will eventually provide high-fidelity analysis capabilities for SMR
  - Develop “intermediate” fidelity methods for routine design calculations (< 1000 processors) by fully integrating the DeCART functionalities into UNIC
    - For SMR designs with conventional PWR or BWR fuel assemblies, the NNR (Numerical Nuclear Reactor) system can readily be applied

BWR Fuel Assembly Calculations with NNR

Pin Power Density (MW/cc)

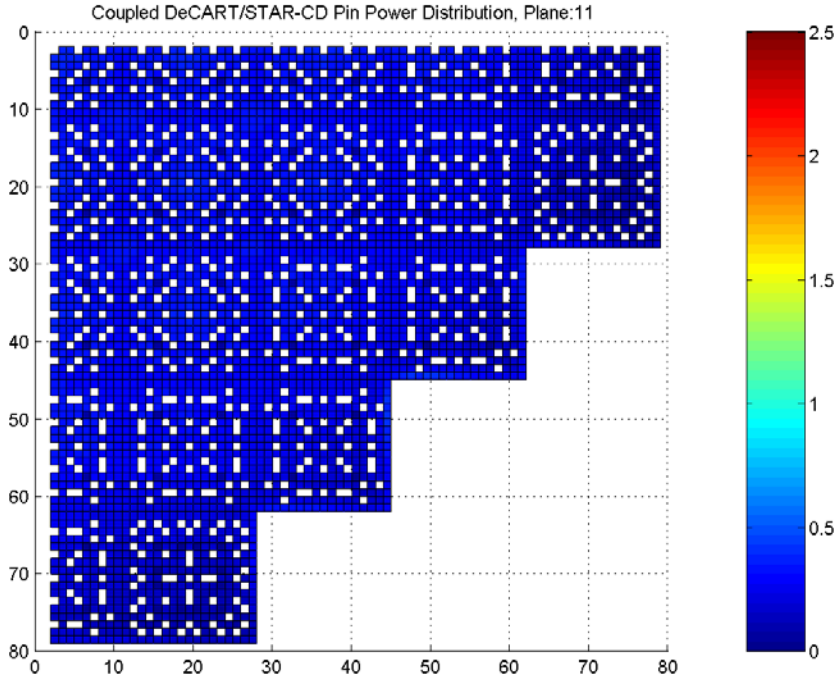
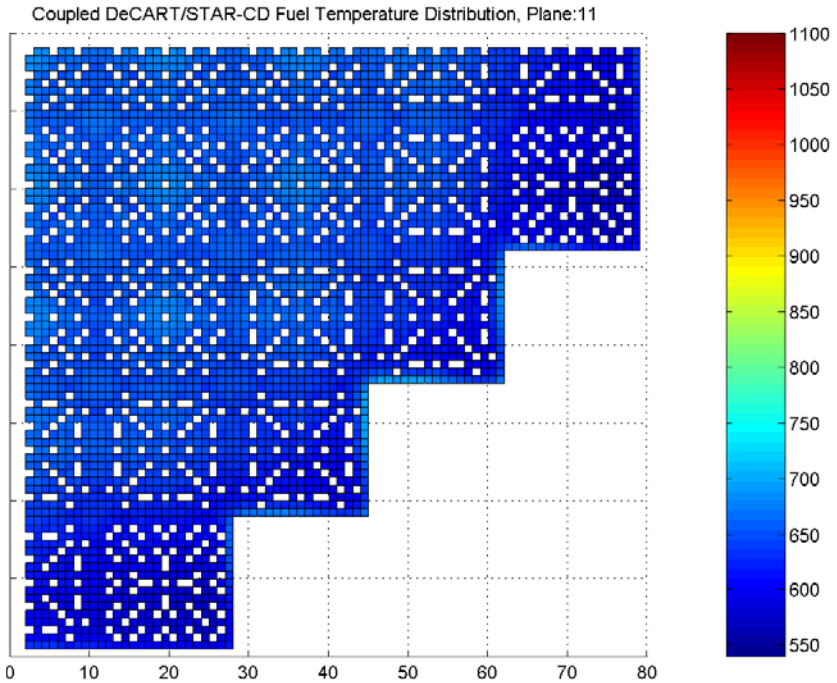


Void Fraction



PWR Whole-Core Calculations with NNR

Pin Power



Avg. Fuel Temperature