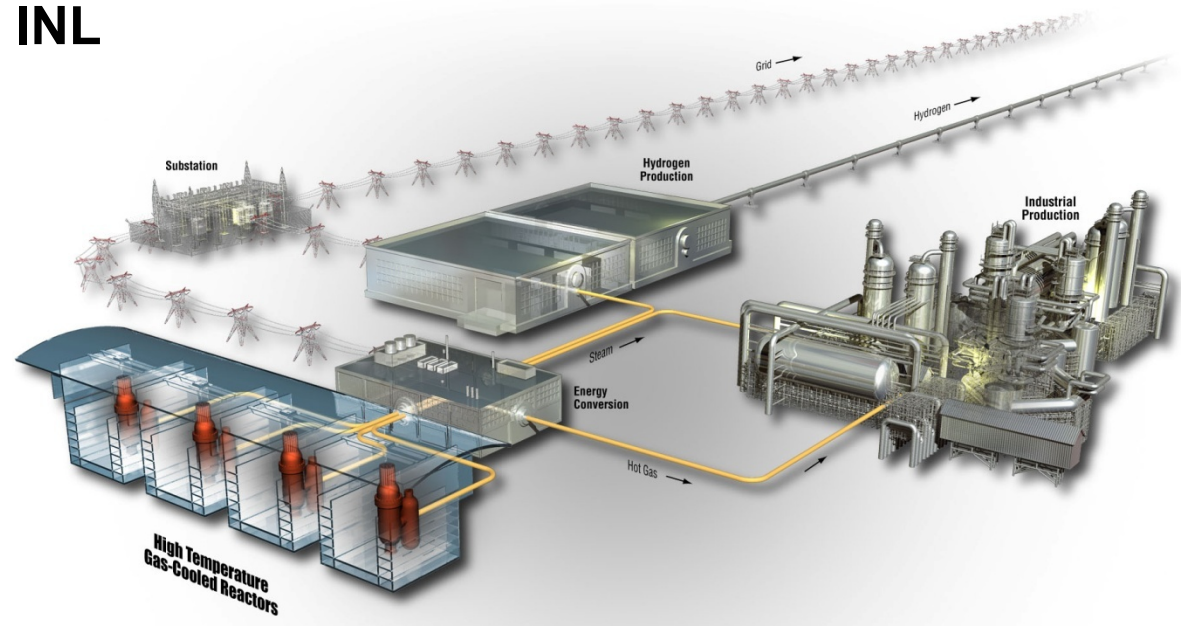


# Status of the PHISICS/ RELAP5-3D Coupling and Application to Phase I of the OECD/NEA MHTGR-350 MW Benchmark

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## ***Presentation Overview***

- PHISICS/RELAP5-3D Code Suite Overview
- OECD/NEA MHTGR-350 MW Benchmark Description
- Results for Phase I: Exercise 1
- Results for Phase I: Exercise 2
- Results for Phase I: Exercise 3
- Future PHISICS/RELAP5-3D Development

# PHISICS-RELAP5 Code Overview (1)

- PHISICS (**P**arallel and **H**ighly Innovative **S**imulation for **I**NL **C**ode **S**ystem) code suite was developed at INL during 2010-2013 (*reference list on final slide*)
- Aaron Epiney (now back at PSI) reported on the development at IRUG 2012
- The coupling is available to users on a separate license agreement (C. Rabiti) Presentation by Andrea Alfonsi (tomorrow) will give more detail on the development activities performed since IRUG 2012 as well as licensing details
- It consists of three modules/kernels providing general reactor physics simulation capabilities:
  - **Neutronics:** INSTANT (**I**ntelligent **N**odal and **S**emi-structured **T**reatment for **A**dvanced **N**eutron **T**ransport)
    - ✓ solves time dependent 2D/3D problems in hexagonal, triangular, Cartesian, and unstructured geometry,
    - ✓ direct and adjoint fundamental modes up to PN33 in parallel computing environments

## **PHISICS-RELAP5 Code Overview (2)**

- **Depletion:** MRTAU (**M**ulti-**R**eactor **T**ransmutation **A**nalysis **U**tility)
  - ✓ Bateman solver with either CRAM or Taylor evaluation of the exponential
  - ✓ Tracks time dependent isotopic concentration and accounts for both activation and decay reactions
  - ✓ Controlled via a separate .xml input file; can be used stand-alone or as part of coupled depletion-neutronics-TH sequence in PHISICS/RELAP5-3D
- **Thermal Fluids:** RELAP5-3D provide primary and secondary system thermal fluid simulation capability
  - ✓ The INSTANT kinetics solver option was integrated directly into RELAP5-3D source as a module, instead of the usual PVM (Parallel Virtual Machine) coupling methodology
  - ✓ Compatibility is retained with past input decks. Uses “instant” keyword on RELAP5-3D kinetics card 30000000 input



## ***OECD/NEA MHTGR-350 MW Benchmark: Status and Objectives***

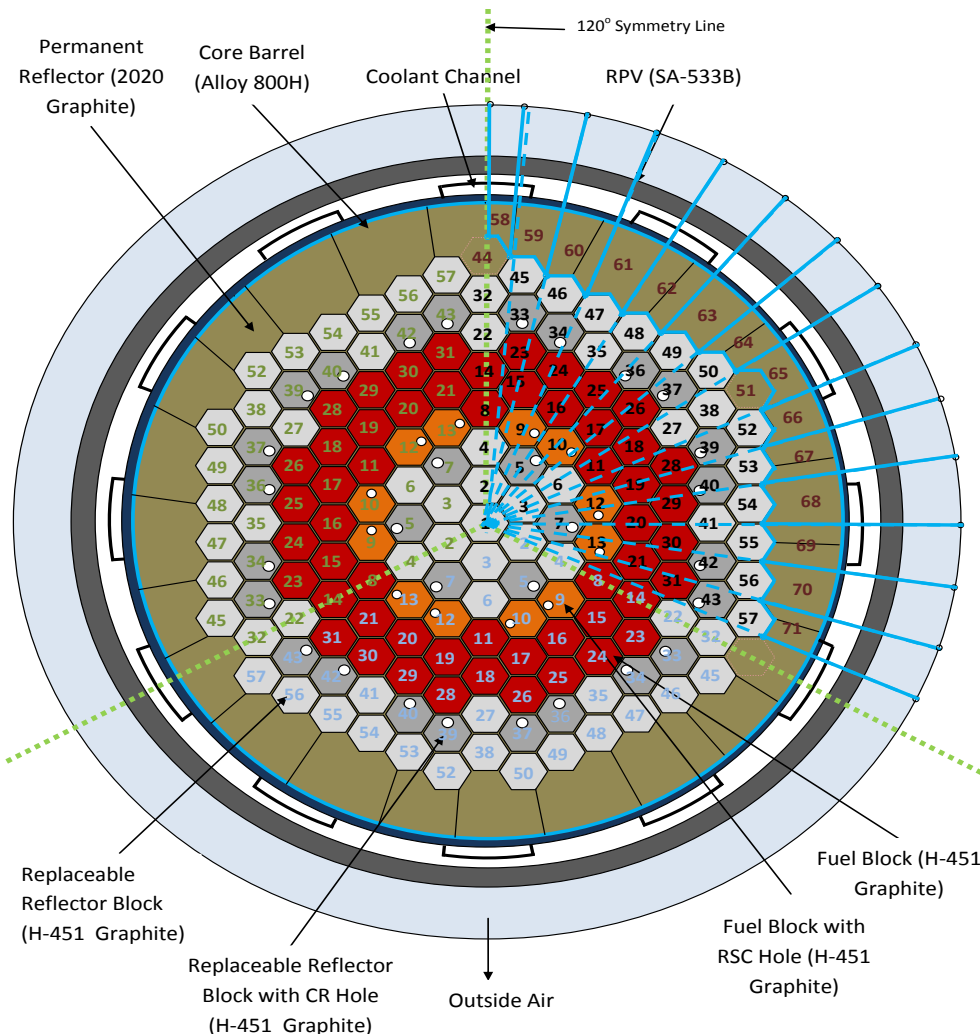
- In cooperation with General Atomics (GA), the VHTR Methods group at INL developed a benchmark specification in 2011, based on the Modular High Temperature Gas Reactor (MHTGR) 350 MW design
- The benchmark was opened for international participation in March 2012 after formal approval was received from the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD)
- The objectives for Phases I and II are:
  - to establish a well-defined core simulation problem for prismatic HTGRs, based on a common cross-section (XS) and thermo-physical (TP) data set,
  - and to compare HTGR methods and tools for both neutronic and thermal fluids steady state and transient modeling

# MHTGR-350 MW Reference Design Specifications

Core Parameter	Value	Unit
Installed Capacity	350 / 165	MW(t) / MW(e)
# Fuel Elements STD / RSC	540 / 120	
# Control Rods Inner /Outer Reflector	6 / 24	
Oxy-carbide UCO Fuel (U-235 enrichment)	15.5	wt%
Primary Pressure	6.4	MPa
Inlet / Outlet Temperatures	259 / 687	°C
Mass flow rate	157	kg /s
Core Inner/Outer Radii	0.83 / 1.75	m
Core Fuel Height	7.93	m

# MHTGR-350 MW Radial Core Layout

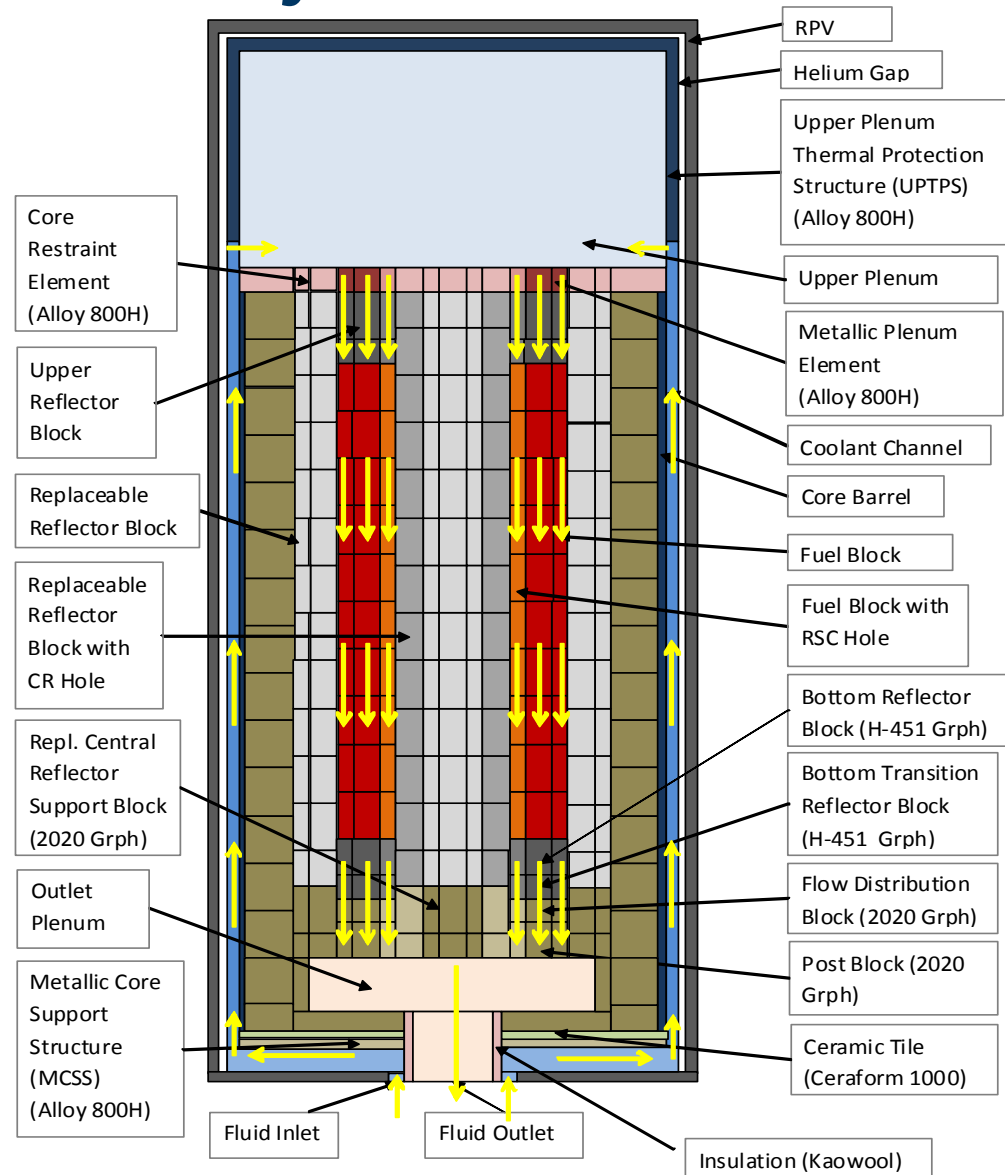
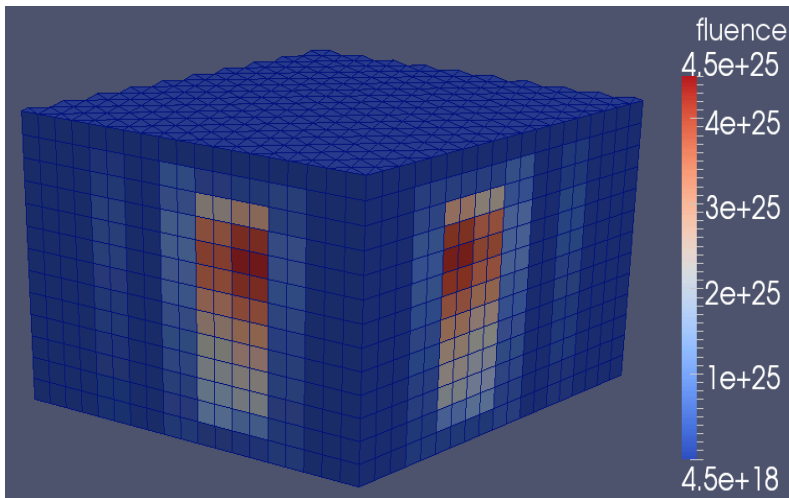
- 3D core with 1/3 symmetry
- Utilized GA End of Equilibrium Cycle (EOEC) number densities
- DRAGON-4 cross section data (based on ENDF/B-VII.r0) supplied in 26 FZ-Julich group structure
  - Cross section sets provided for 220 active core regions, 11 reflector regions and 1 CR region as functions of:
    - Four fuel temperatures
    - Seven moderator temperatures
    - Three Xe concentrations
    - Four H concentrations





# MHTGR-350 MW Axial Core Layout

- Inlet is placed at radial centre of bottom reflector
- Helium flows into upper plenum, then downwards into fuel coolant channels
- Variable thermo-physical properties specified (conductivity, specific heat)
- Spatially dependent decay heat distribution (peak moves upwards during sub-critical phase)



# Benchmark Phase I – Steady State Exercises

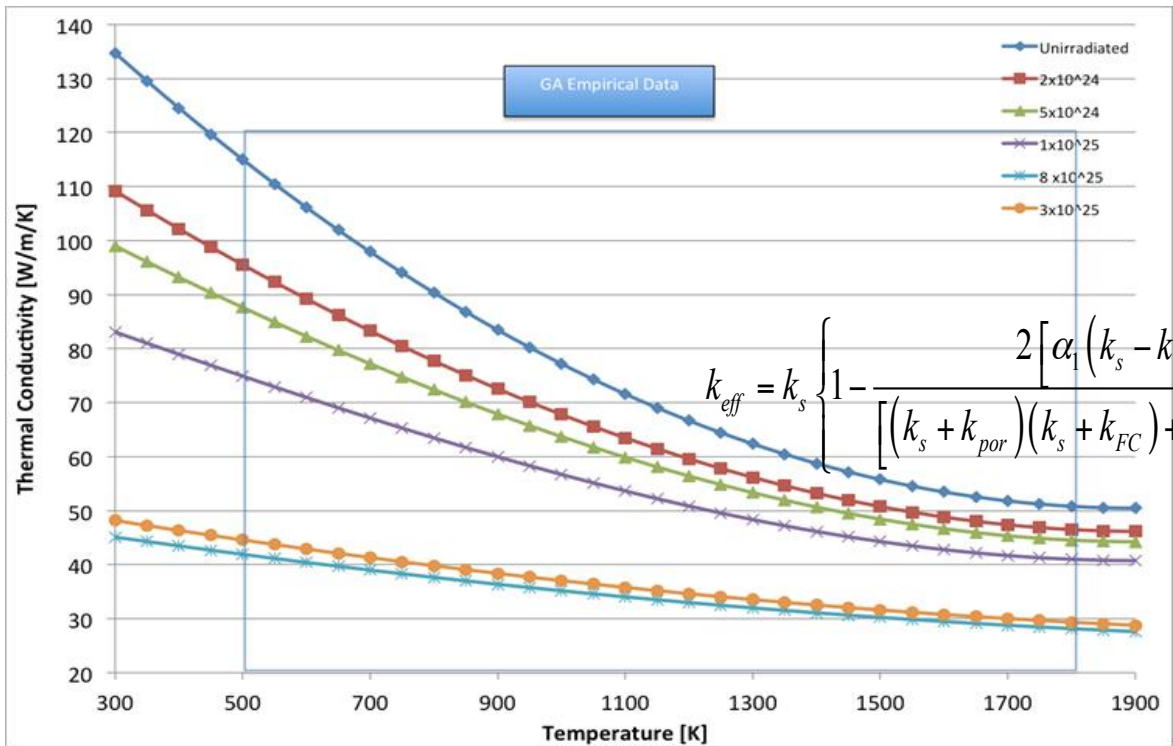
1. Neutronics stand-alone: fixed cross sections, no coupling with thermal fluids (*not the focus today*)
2. Thermal fluids stand-alone: fixed power distribution
  - Exercise 2a: Fixed thermophysical properties, no bypass flow
  - Exercise 2b: Fixed thermophysical properties, bypass flow type 1
  - Exercise 2c: Variable thermophysical properties, bypass flow type 1
  - Exercise 2d: Variable thermophysical properties, bypass flow type 2
3. Coupled neutronics – thermal fluids:
  - Temperature dependent cross sections and Xenon equilibrium contribution included
  - Variable thermo-physical properties
  - Bypass flow effect:
    - Exercise 3a: bypass flow type 1
    - Exercise 3b: bypass flow type 2



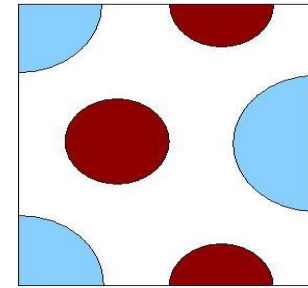
Component	%
In-core	1.50
Inner Reflector	0.50
Inner Control Rod Cooling	1.20
Outer Control Rod Cooling	1.80
Outer Reflector (First Ring)	1.38
Outer Reflector (Second Ring)	1.62
Permanent Side Reflector	3.00
Total	11.00

# Example: Thermo-physical Properties

- Graphite thermal conductivity: GA correlations dependent on temperature and fast neutron fluence (H-451 shown below)
- The effective thermal conductivity model of the thermal unit cell is based on Maxwell's theory of the conductivity of composite materials, that was extended to three materials by AMEC

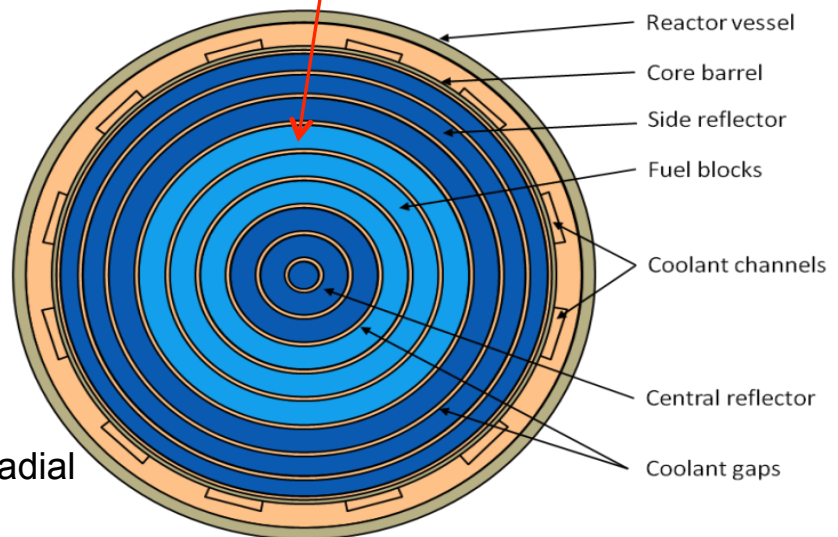
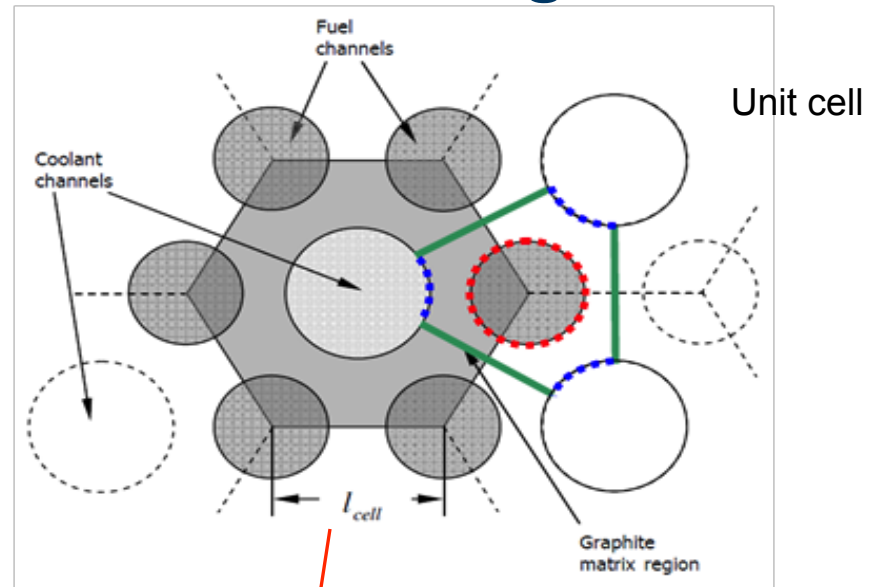
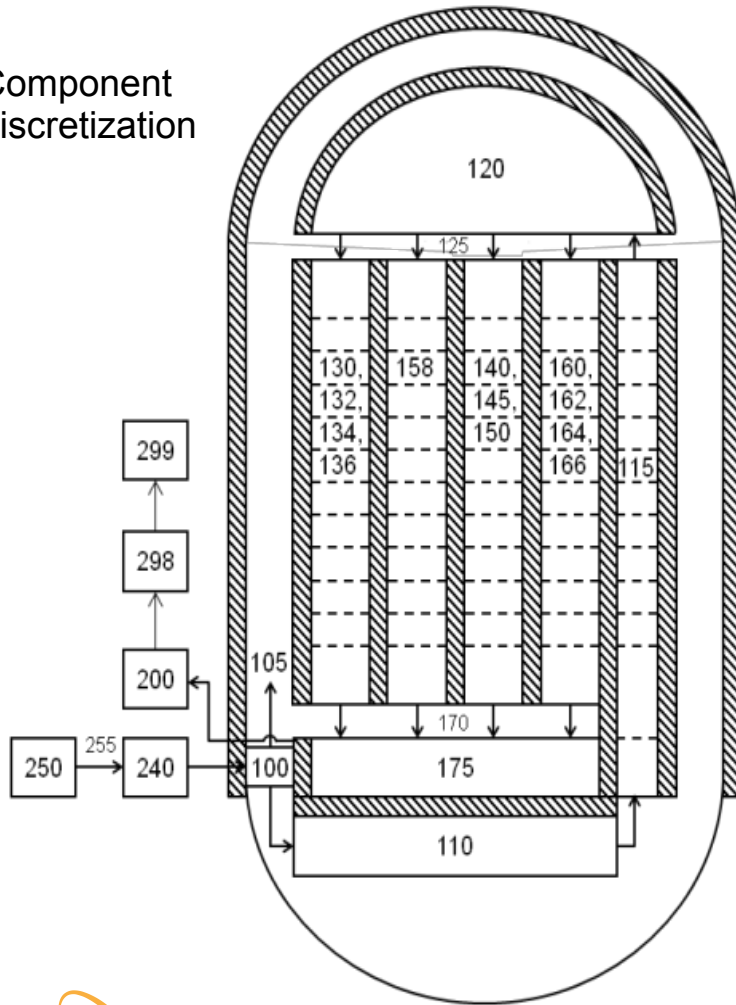


$$k_{eff} = k_s \left\{ 1 - \frac{2 \left[ \alpha_1 (k_s - k_{por}) (k_s + k_{FC}) + \alpha_2 (k_s - k_{FC}) (k_s + k_{por}) \right]}{\left[ (k_s + k_{por}) (k_s + k_{FC}) + \alpha_1 (k_s - k_{por}) (k_s + k_{por}) + \alpha_2 (k_s - k_{FC}) (k_s + k_{por}) \right]} \right\}$$



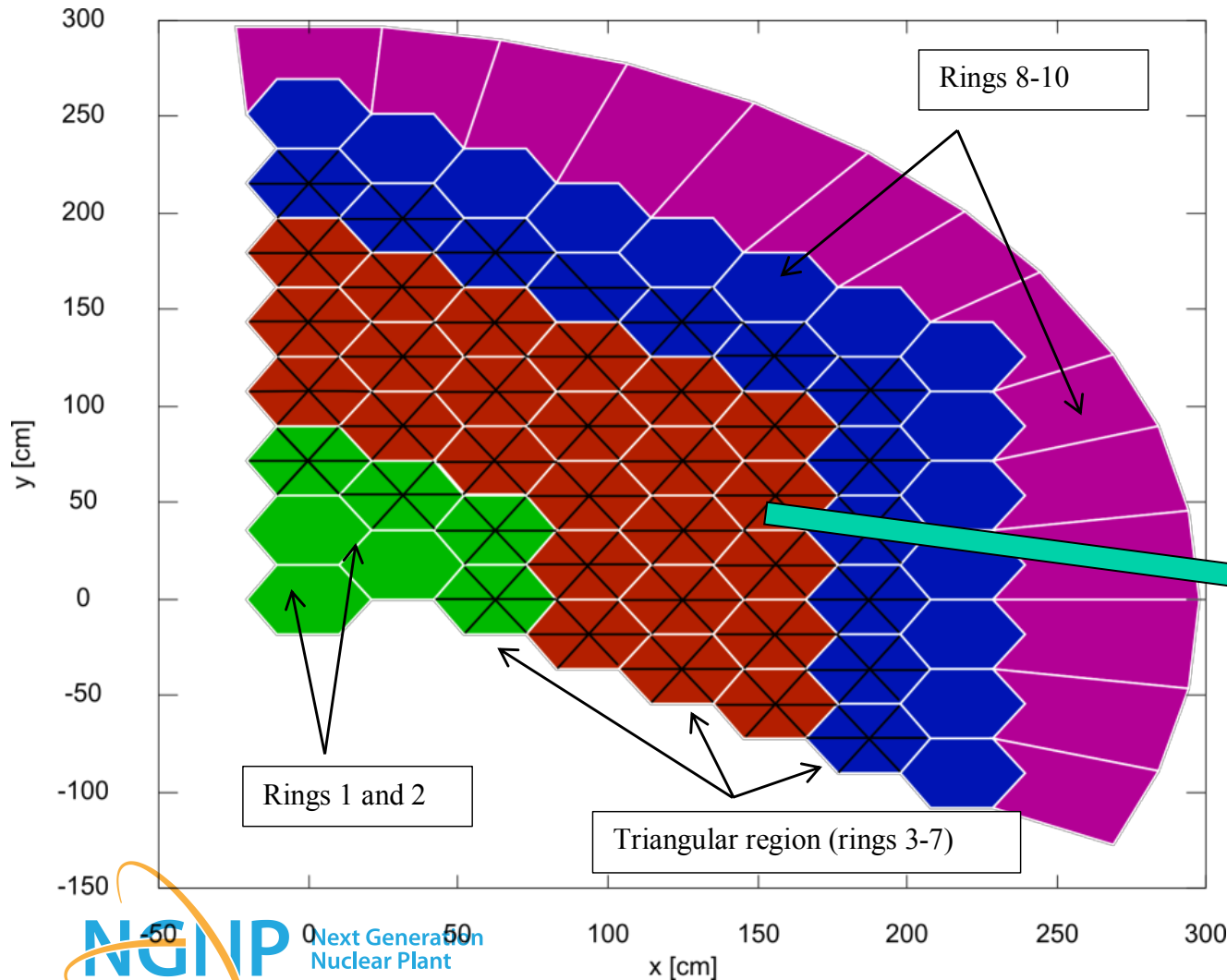
# Exercise 2: Traditional RELAP-5 "Ring" Model

Component discretization

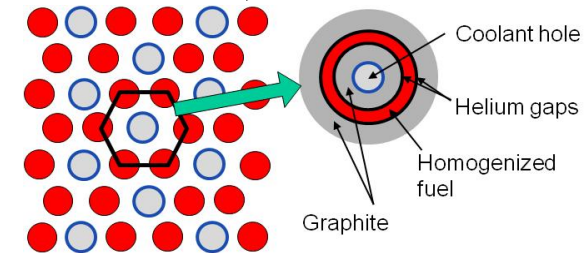


Core model radial discretization

# But what if we do this instead?

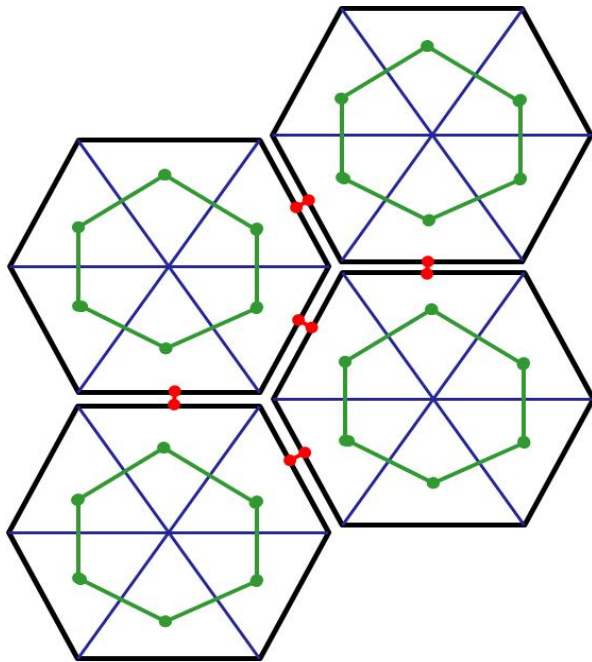


- One unit cell (heat structure) **per triangle**
- One bypass pipe **per triangle face**
- Kinetics feedback on fuel and moderator temperatures **per block, on each axial layer**

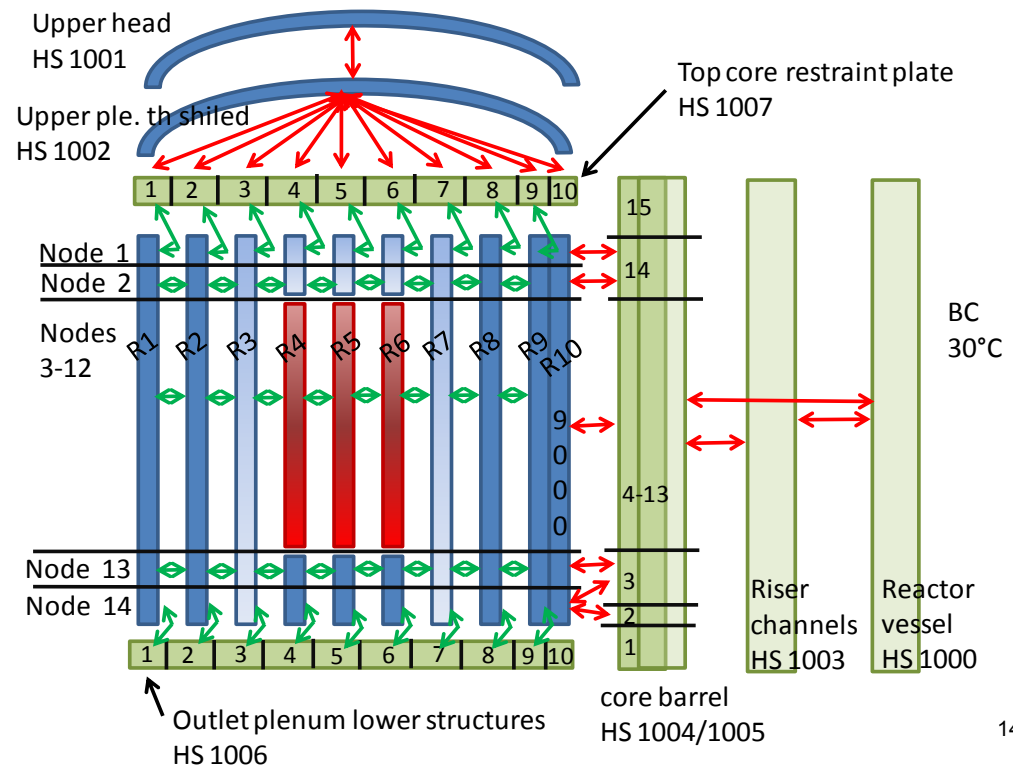


# RELAP-5 Radiation and Conduction Models

- Conduction enclosures defined between 6 triangles within each block
- Radiation enclosures between block faces over 2 mm gaps
- Creates much higher resolution than ring model (6 triangles x 22 blocks = 132 elements vs. 3 rings...)



- Conduction enclosures defined between top and bottom graphite and metal structures
- Radiation between metal components and radial rings



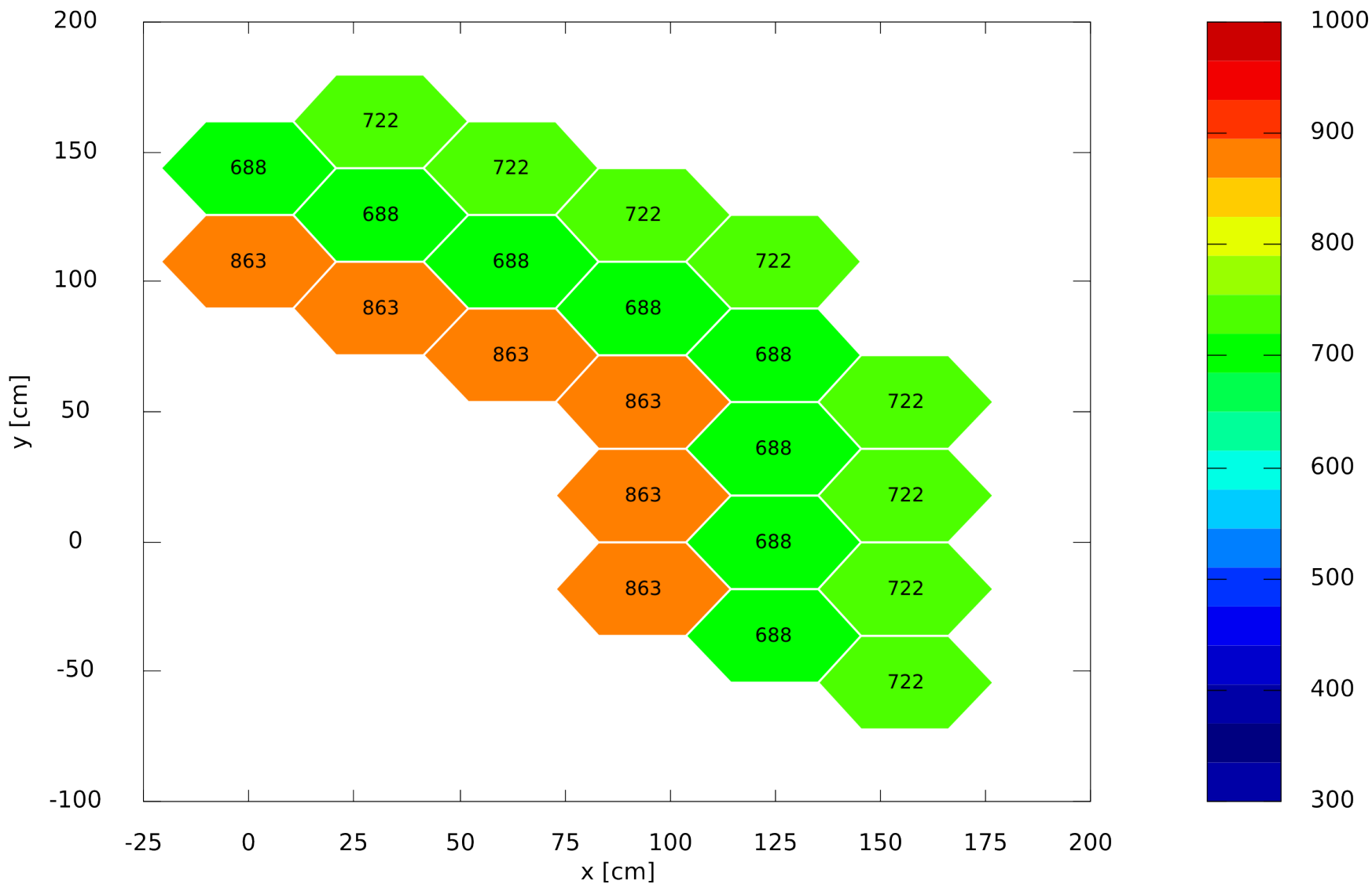
# RELAP-5 Ring and Block Model Comparison

Description	Ring model	Block model
Hydrodynamic components	~20	251
Heat structures	20	~1,100
Materials	9 (constant properties)	~100 (temperature and fluence dependent)
Kinetic feedback zones	170	~4,700
Radiation and conduction enclosures	17 enclosures with 350 surfaces	88 enclosures with >7,000 surfaces
Decay heat treatment	1 table (global core power vs. time)	220 tables (individual core block power vs. time)
Input file size (number of lines)	29,000	88,000
Real time required for converged steady state (hours)	Ex. 2 (RELAP5-3D only): 0.1 Ex. 3 (PHISICS/RELAP5-3D): 11	Ex. 2 (RELAP5-3D only): 5 Ex. 3 (PHISICS/RELAP5-3D): 20



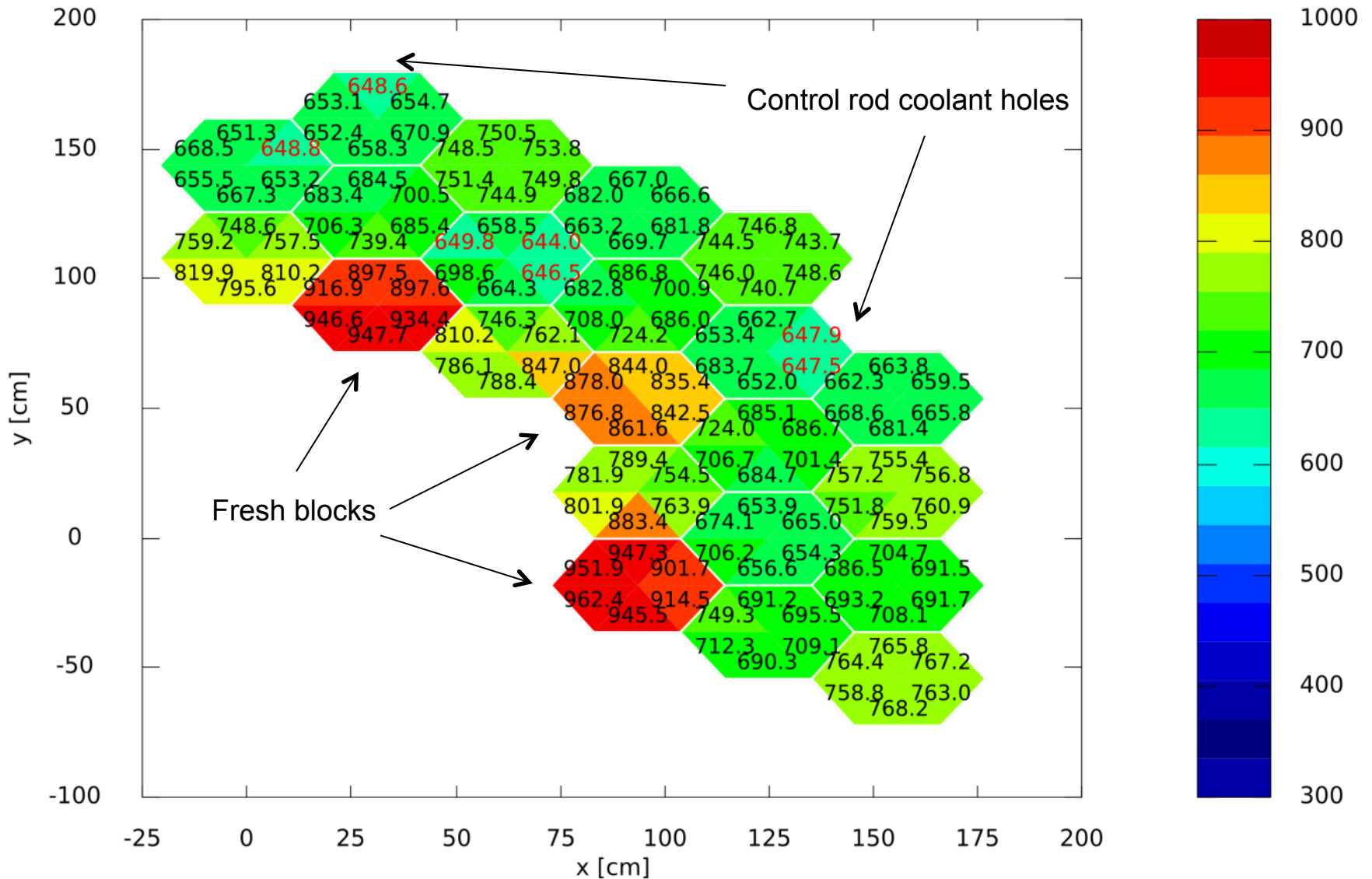
*Is it worth it?*

# Exercise 2a: Ring Fuel Temperatures (°C)





# Exercise 2a: Block Fuel Temperatures (°C)



# Steady State Exercise 2a: Fuel Temperatures (K)

Comparison of ring and block model axially averaged results:

- Ring average fuel temperatures (K) compare well
- Block model predicts almost 90K higher fuel temperatures than “smeared-out” ring model
- Variance between triangular elements for this case: 37K to 114K

Block model

Ring model

z (from top of core) (cm)	Core ring 1
119	722
198	826
278	903
357	958
436	1000
515	1030
595	1061
674	1089
753	1113
833	1132
ring average	984
ring maximum	1132

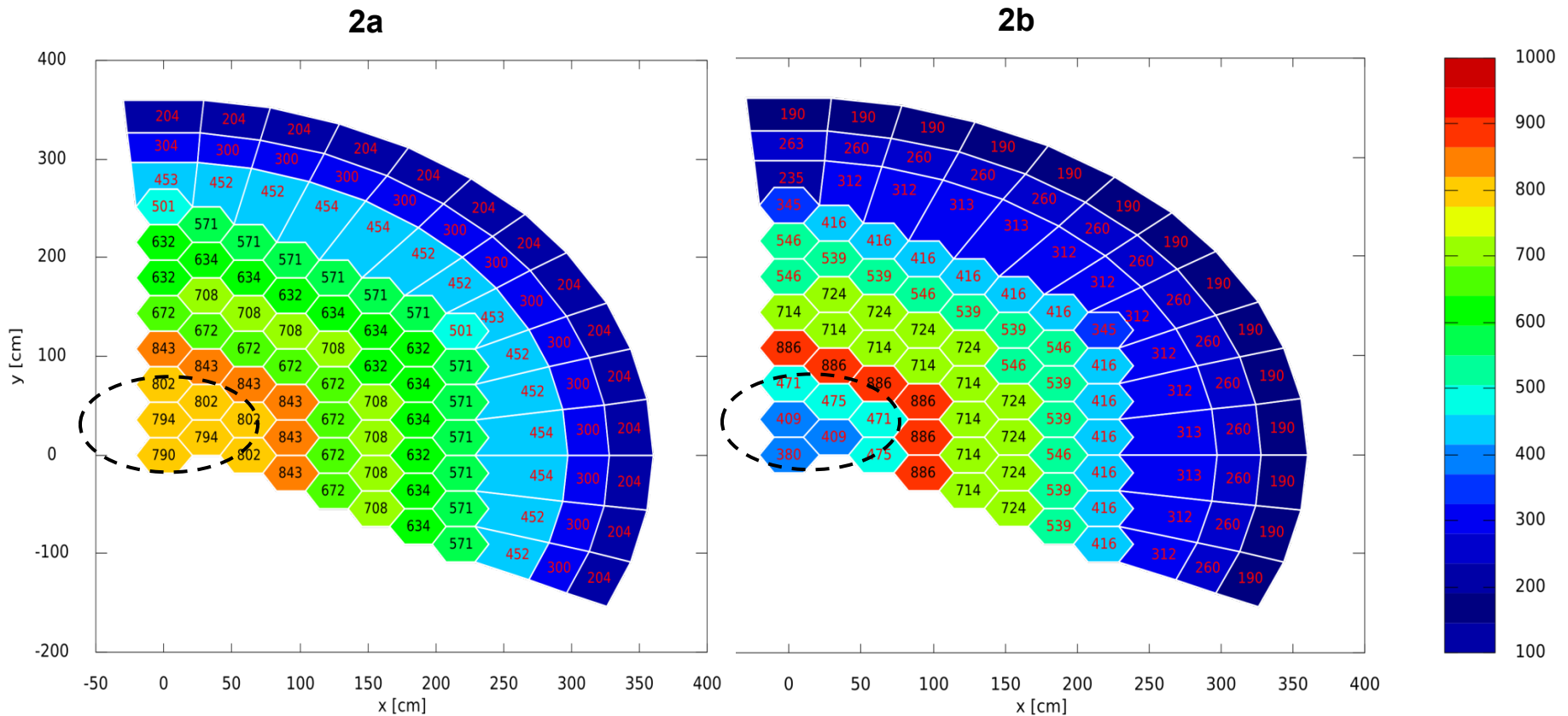
Block #	Triangle #	Triangle		Block		Ring	
		avg	max	avg	max	avg	max
8	1	934	1066	928	1090		
	2	950	1090				
	3	916	1037				
	4	912	1027				
	5	915	1036				
	6	943	1082				
9	1	1048	1210	1039	1210		
	2	1046	1209				
	3	1032	1187				
	4	1021	1170				
	5	1023	1170				
	6	1063	1199				
10	1	938	1060	943	1115		
	2	935	1055				
	3	952	1081				
	4	916	1025				
	5	925	1040				
	6	989	1115				
11	1	983	1135	980	1148		
	2	989	1146				
	3	992	1148				
	4	973	1120				
	5	969	1112				
	6	972	1119				
12	1	1010	1147	945	1147		
	2	944	1071				
	3	933	1054				
	4	938	1065				
	5	919	1033				
	6	925	1041				
13	1	1068	1210	1047	1224		
	2	1057	1224				
	3	1049	1213				
	4	1050	1213				
	5	1025	1174				
	6	1033	1186				

980

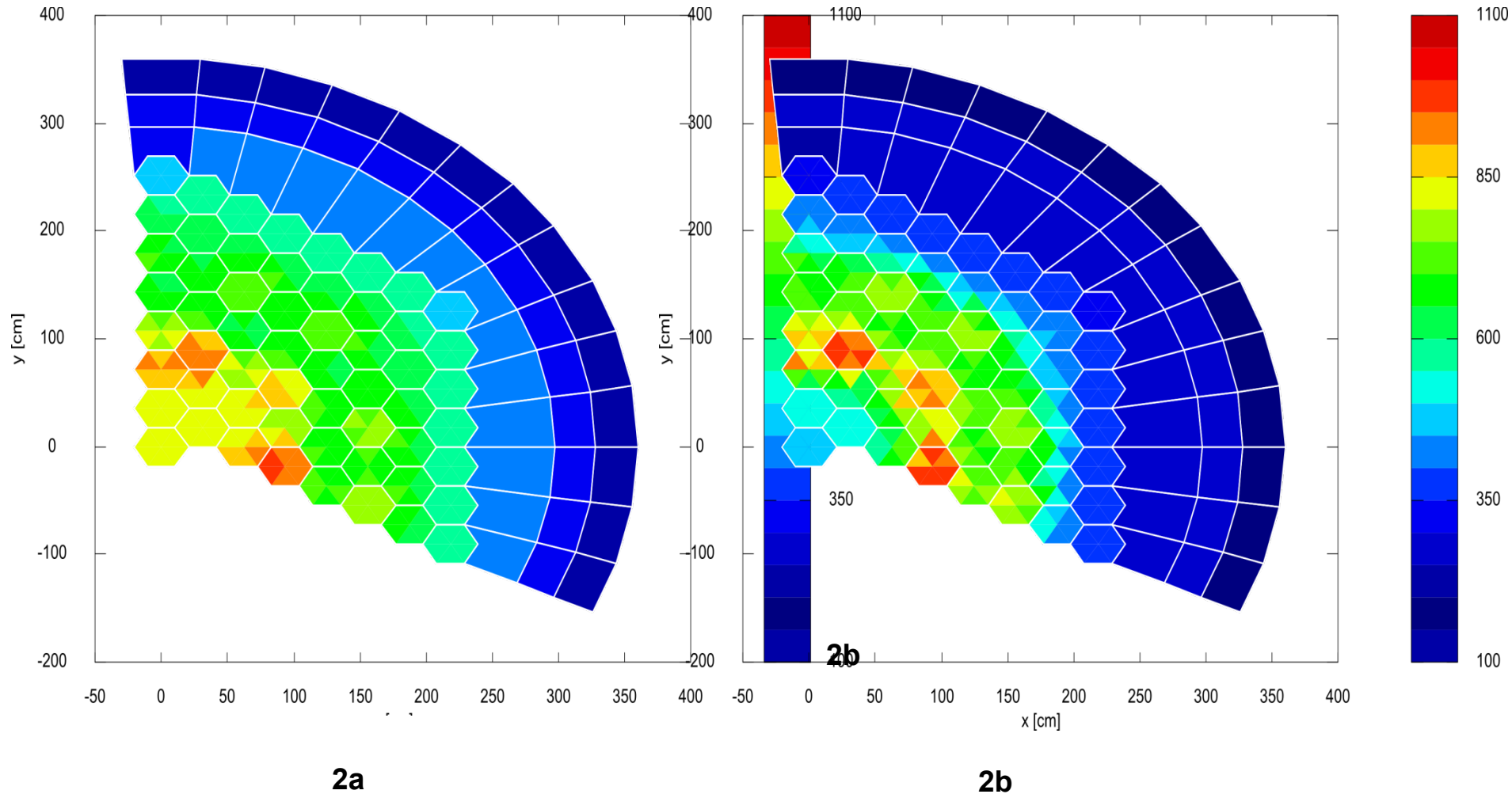
1224

# Exercise 2a vs. 2b Ring Model Temperatures

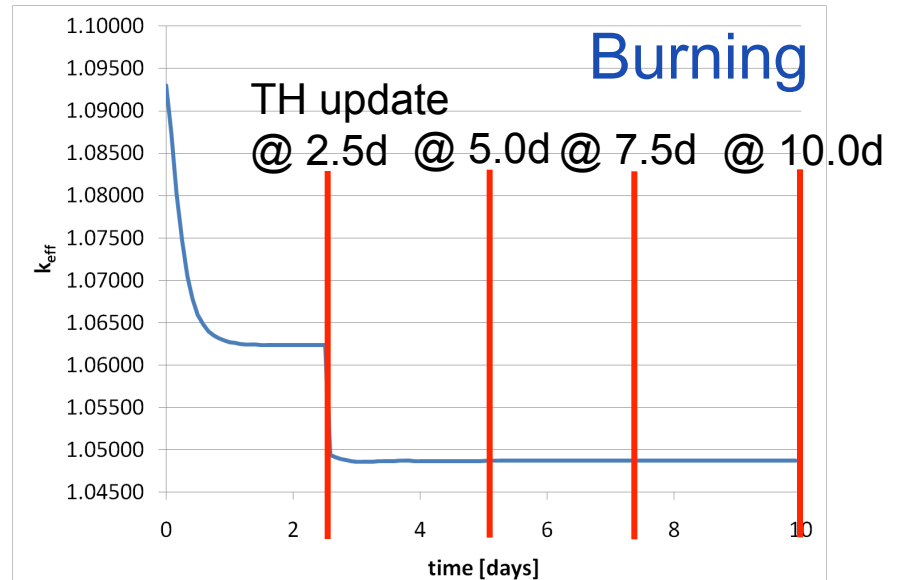
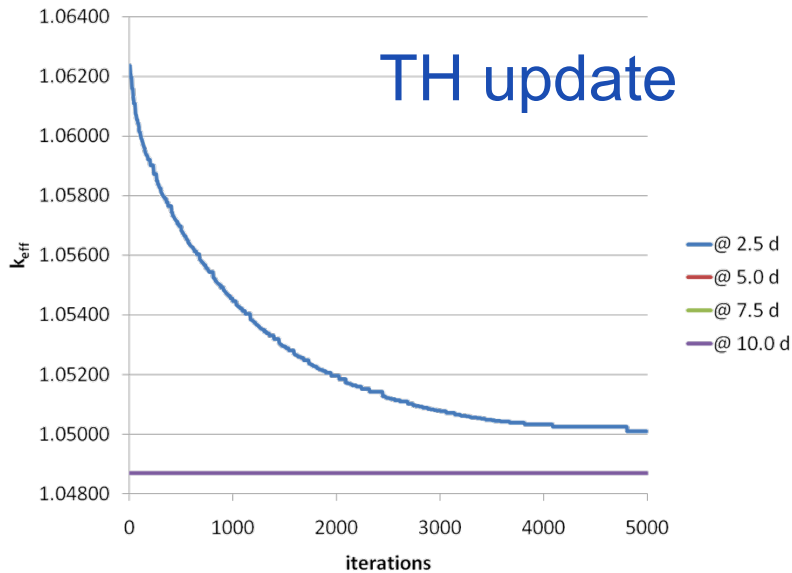
- Ex. 2a (constant properties, no bypass): lowest fuel temperatures, **very hot** inner reflector (no cooling outside core)
- Ex. 2b (constant properties, bypass Type I): inner reflector **much colder**, but small effect on fuel temperature (< 50 K)



# Exercise 2a vs. 2b Block Model Temperatures



# Phase I: Exercise 3 (coupled TH/neutronics)

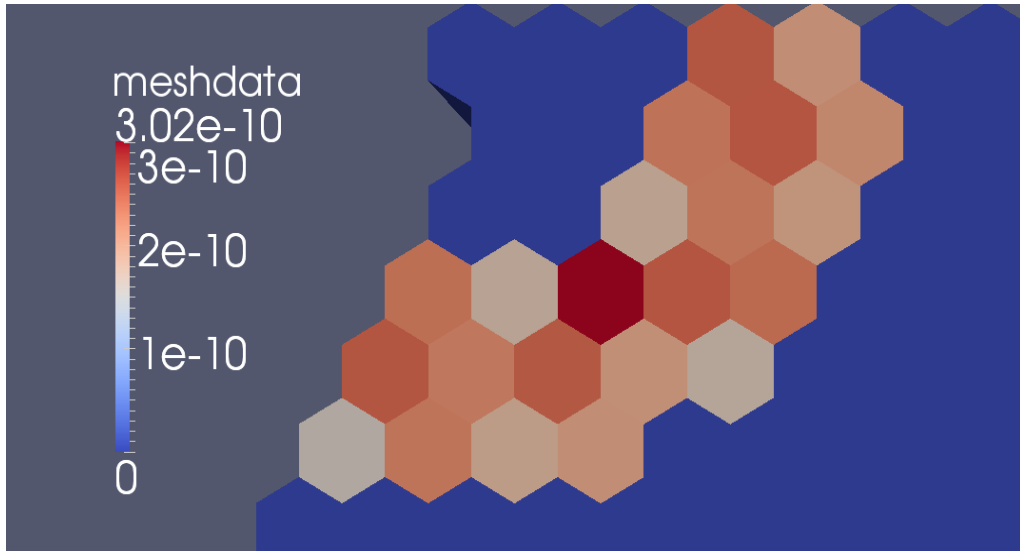


	ring model				
	CR at nominal	CR fully inserted	CR worth (delta rho)	peak fuel temp (K)	bypass flow (% of total)
<b>3a</b>	1.05163	1.04248	835	1148	10.9
<b>3b</b>	1.05102	1.04172	849	1169	14.2
	detail block model				
<b>3a</b>	1.04940	-		1269	10.9
<b>3b</b>	1.04940	-		1267	12.0

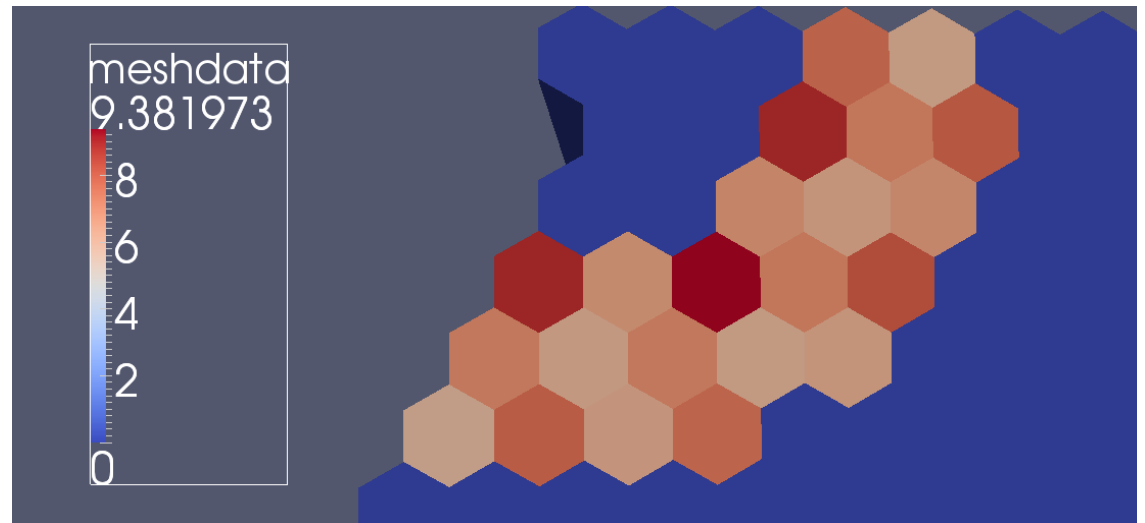
162 pcm

2.2%

# Steady State Exercise 3: Results



← xenon concentration



power density



## *Future Developments (1)*

- Complete Phase II of the OECD/NEA MHTGR-350 Benchmark. This would require coupled modeling of LOCAs, water ingress and 100-80-100 load follow transients. Results to be reported at IRUG 2015.
- INL NGNP group also participates in IAEA Coordinated Research Program (CRP) on HTGR uncertainties. This project requires quantification of uncertainties and sensitivities from the cell/lattice level through to coupled transients. PHISICS/RELAP5 will be used on the MHTGR-350 design for the core simulation phases
- However, NGNP funding for further development declined significantly in FY13 and FY 14. **If** sufficient funds are available, **uncertainty** and **sensitivity** quantification is first on the wish list...

## Future Developments (2)

- The challenge is to account for all uncertainties in a systematic manner (material correlations, neutronics, TH, solver & geometry factors, etc.)
- *Neutronics*: 44 group co-variance data now available for ENDF-VII. Cross section uncertainties can be propagated from cell to lattice to full core (e.g. SCALE 6.2 beta release now includes new SAMPLER sequence in addition to Generalized Perturbation Theory (GPT) based TSUNAMI).
- *TH*: Not so easy to obtain uncertainty distributions for parameters like conductivity (fluence and temperature dependent), bypass flows (non-linear), non-local heat distribution in reflectors, etc.
- At least two routes are possible at INL NGNP:
  - PHYSICS and RELAP5 standalone wrappers; either using in-house coding, or external products like SUS3D, DAKOTA or SUSAN.
  - Integrated methodology (possibly through RAVEN) within coupled PHYSICS/RELAP5 code (GPT-free approach, Monte Carlo or mixture of both)



## References

- **PHISICS**: C. Rabiti, et al., “PHISICS: a New Reactor Physics Analysis Toolkit”, Transactions of the American Nuclear Society, Vol. 104, Hollywood, USA, INL/CON-11-21116 (2011).
- **PHISICS/RELAP5-3D**: A. Epiney, et al., “New Multi-group Transport Neutronics (PHISICS) capabilities for RELAP5-3D and its Application to Phase I of the OECD/NEA MHTGR-350 MW Benchmark”, Proceedings of HTR2012, Tokyo, Japan (2012).
- **MHTGR-350 benchmark**: J. Ortensi, et al., “Prismatic Core Coupled Transient Benchmark”, INL/CON-11-20811.
- **AMEC study**: “Investigation of Local Heat Transfer Phenomena in a Prismatic Modular Reactor Core” NR001/RP/001 R1, AMEC NSS Limited. March 2009.

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