Inspiring Change.
Impacting Tomorrow.

Applications of Serpent's Fission Matrix Capability

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Penn State University
Ken and Mary Alice Lindquist Dept. of Nuclear Engineering

Presented at the Serpent User's Group Meeting
Atlanta, GA
10/17/2019

The Fission Matrix method is in theory fairly simple

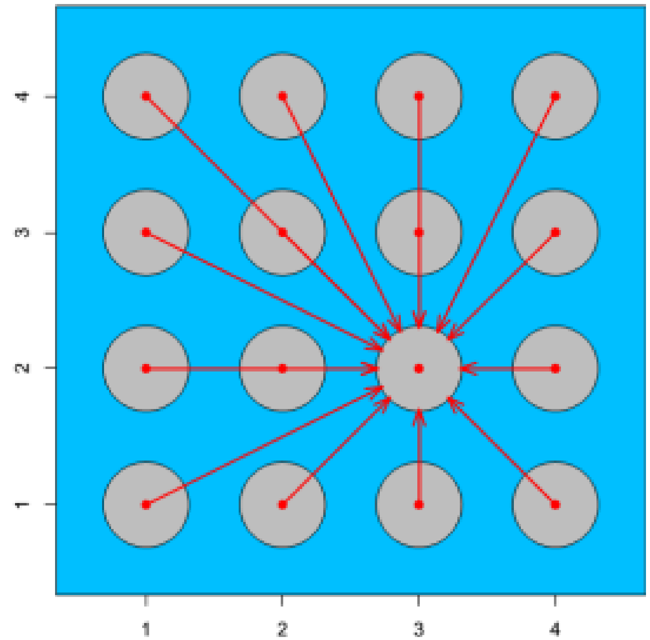
$$F_i = \frac{1}{k}\sum_{j=1}^{N} a_{i,j}F_j$$

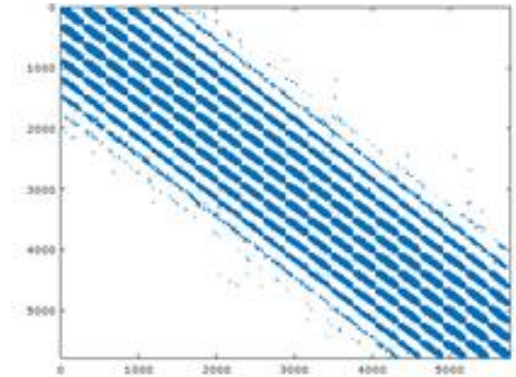
F_i = fission neutrons in cell i

$a_{i,j}$ =number of neutrons created in cell i due to a neutron born in cell j

$$\vec{F} = \frac{1}{k}A\vec{F}$$

- Calculate $a_{i,j}$ using Monte Carlo
- Solve linear system for $\vec{F}$, k





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Fission matrices have been used for several purposes

- Criticality convergence acceleration / checking
- Higher-order modes / importance
- Two-step hybrid calculation
  - Pre-calculate fission matrices for “representative” problems
  - Use pre-calculated data to estimate fission matrix for particular problem

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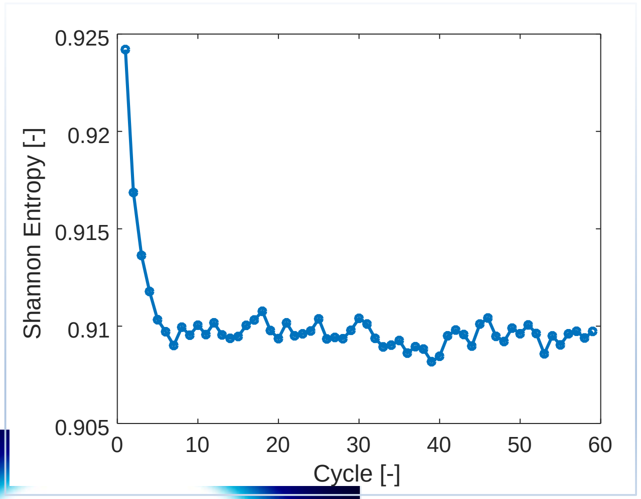
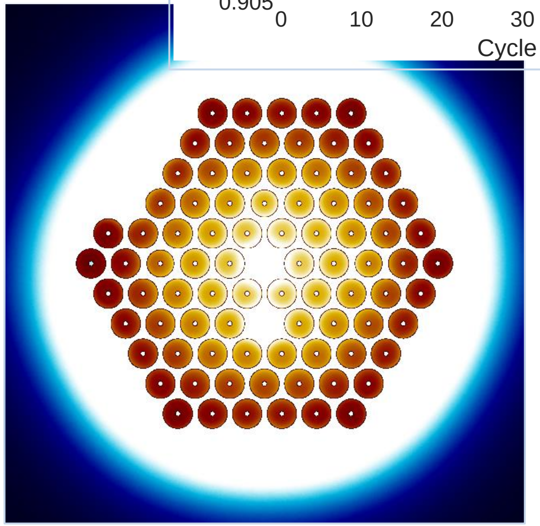
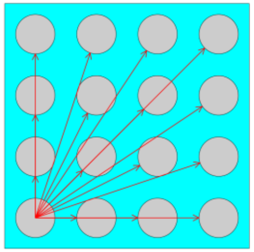
Serpent can tally fission matrices in a set of fixed-source or a criticality calculation

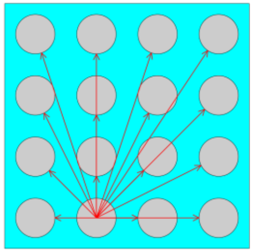
Criticality



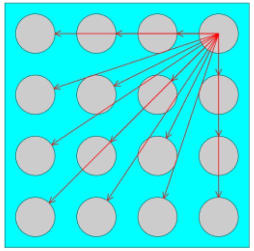


Fixed Source

Source 1  $\rightarrow \begin{bmatrix} a_{1,1} \\ a_{2,1} \\ \cdots \\ a_{N,1} \end{bmatrix}$

Source 2  $\rightarrow \begin{bmatrix} a_{1,2} \\ a_{2,2} \\ \cdots \\ a_{N,2} \end{bmatrix}$

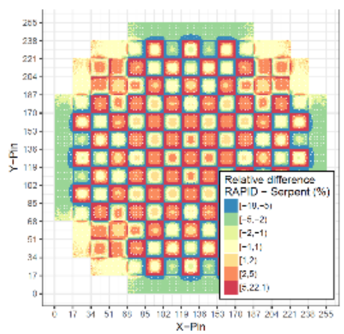
$\vdots$

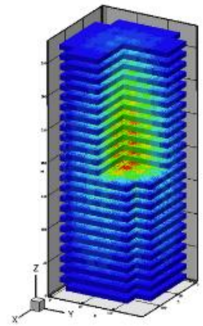
Source N  $\rightarrow \begin{bmatrix} a_{1,N} \\ a_{2,N} \\ \cdots \\ a_{N,N} \end{bmatrix}$

$\boldsymbol{A}$

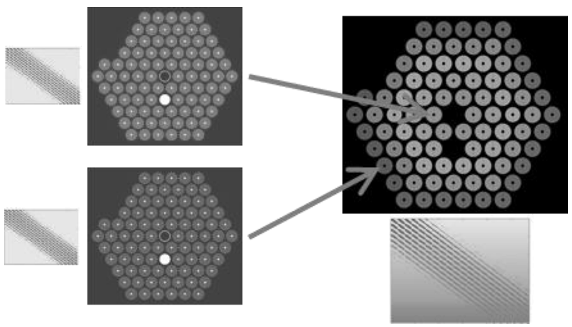
Presentation Outline

RAPID Matl. Correction Ratios (Donghao He)

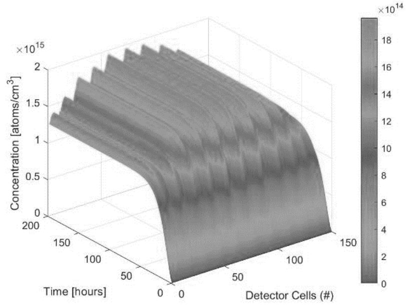




Temperature/Control Methods for TRIGA and NTP (Adam Rau)



Fission-Matrix-Based Xenon Transients (Jake Eichenlaub)



$$\vec{F} = \frac{1}{k} A\vec{F}$$

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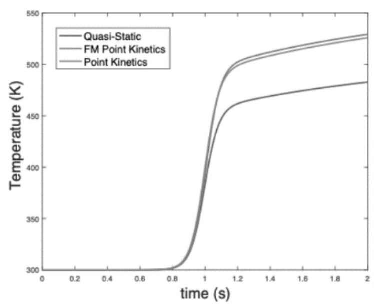
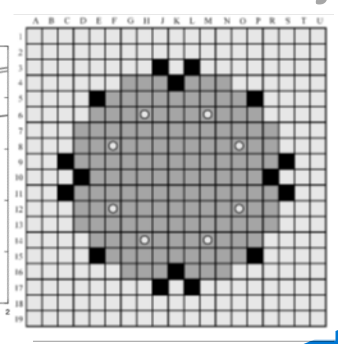
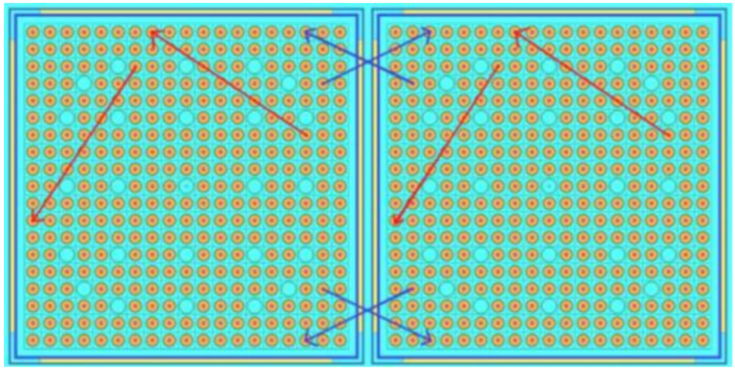
Transient Fission Matrix in TREAT Reactor (Alvaro Pizarro-Vallejos)

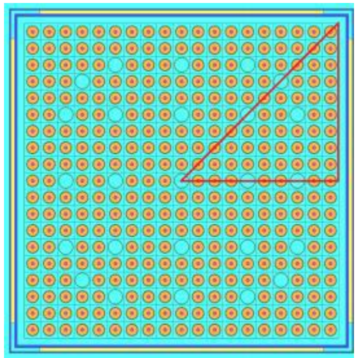




RAPID uses fission matrix methods for fast calculations

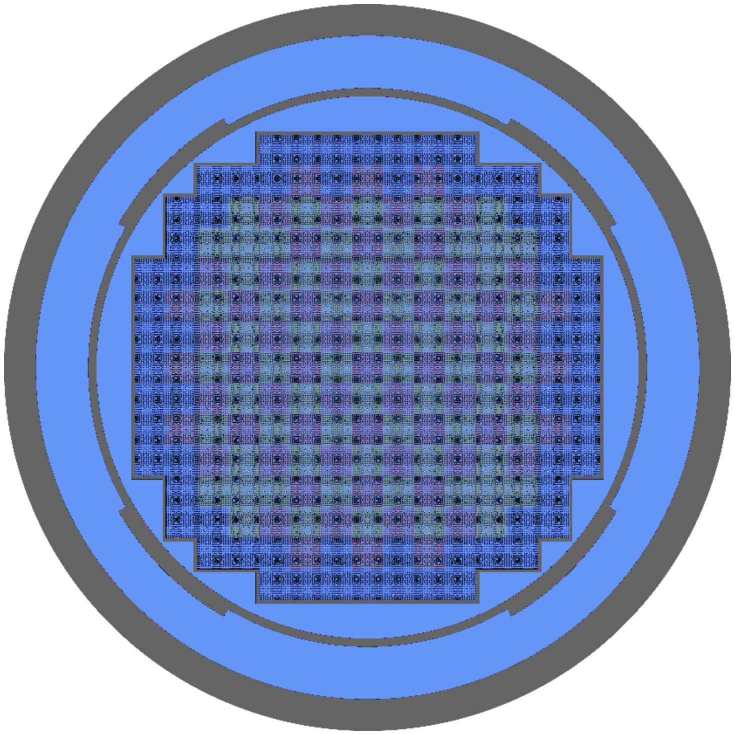
- Pre-calculate assembly-level fission matrices using *fixed-source* calculations
- Combine using geometric symmetry and similarity to simulate different loading patterns

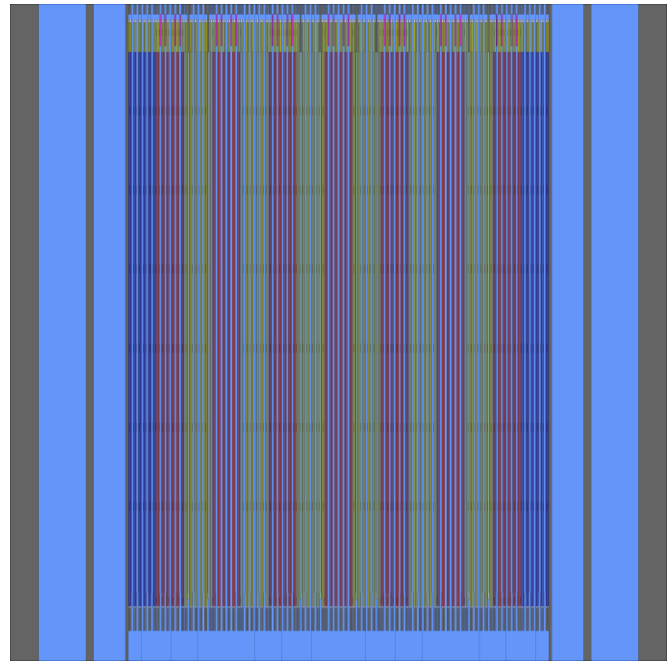




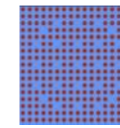
Walters et al., 2014

RAPID has been applied to the BEAVRS benchmark

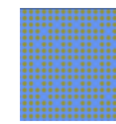




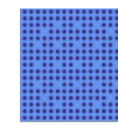
- Red: 1.6%



- Yellow: 2.4%



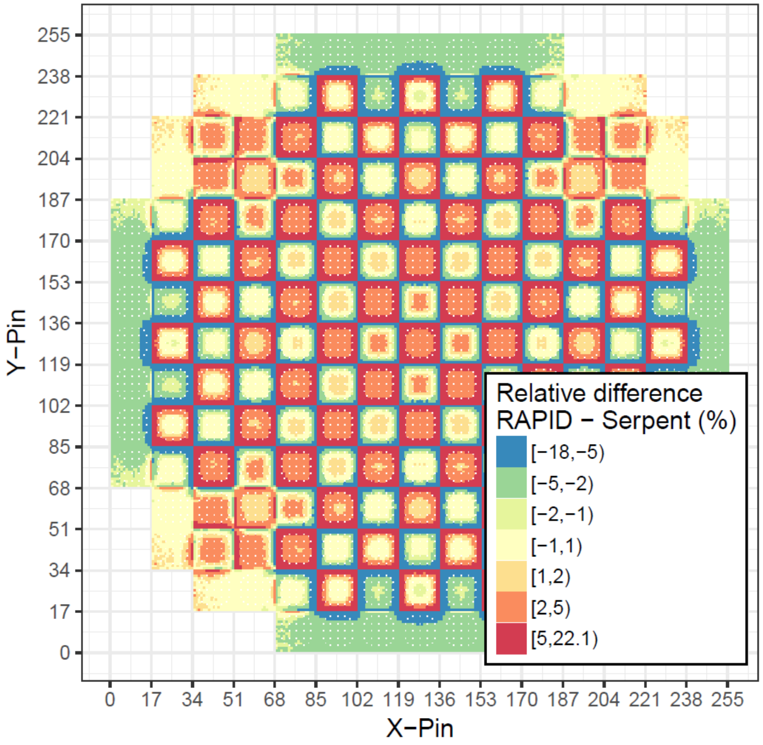
- Blue: 3.1%



193 fuel assemblies

Each assembly has 264 fuel pins and 25 guide tubes in a 17 × 17 lattice

Adjacent fuel assemblies with different enrichments may induce errors in RAPID



Code was originally designed for spent-fuel pools, where heterogeneity problems did not occur due to strong absorbers between fuel assemblies

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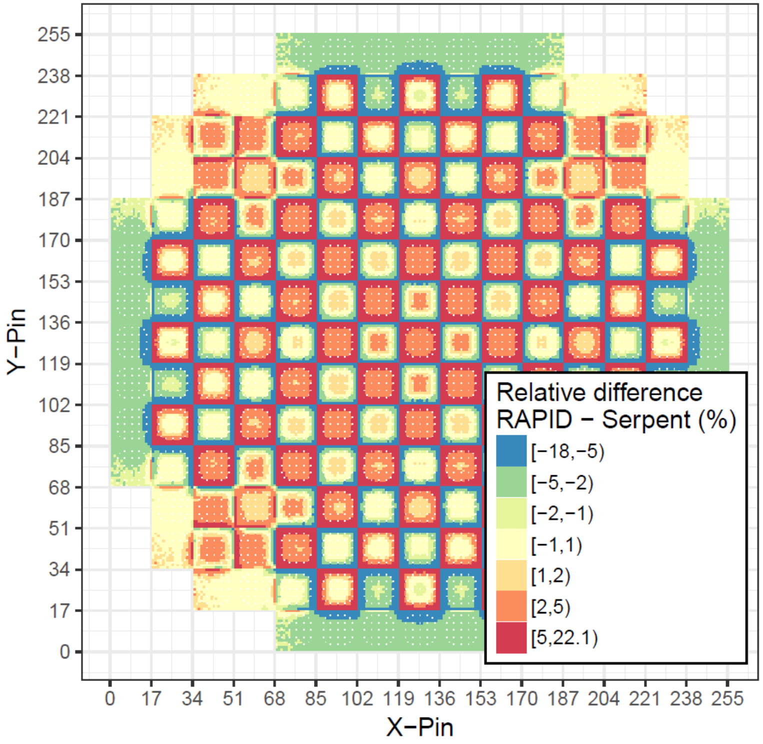
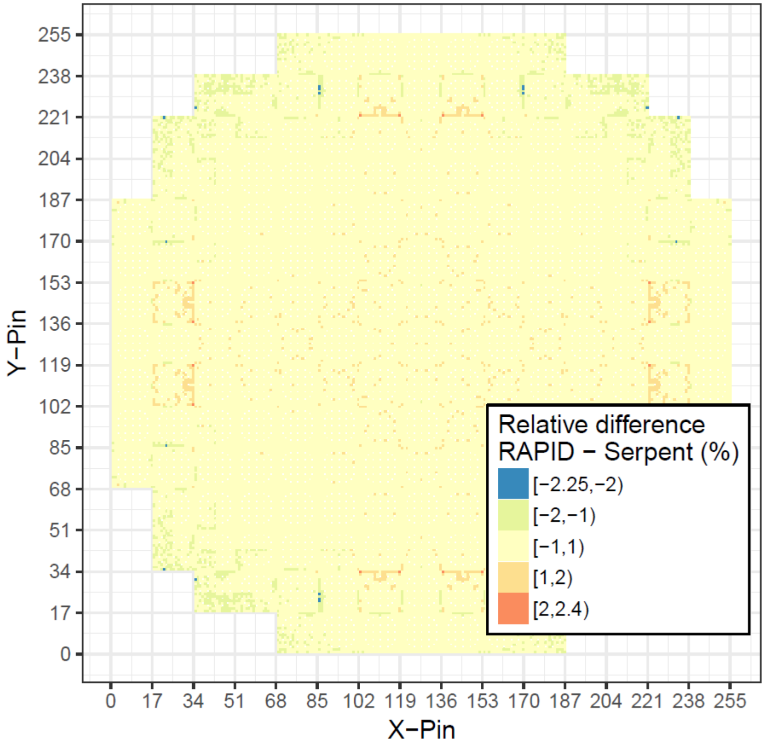
Methods were added to RAPID to correct enrichment-heterogeneity-induced errors

Without correction



Corrected



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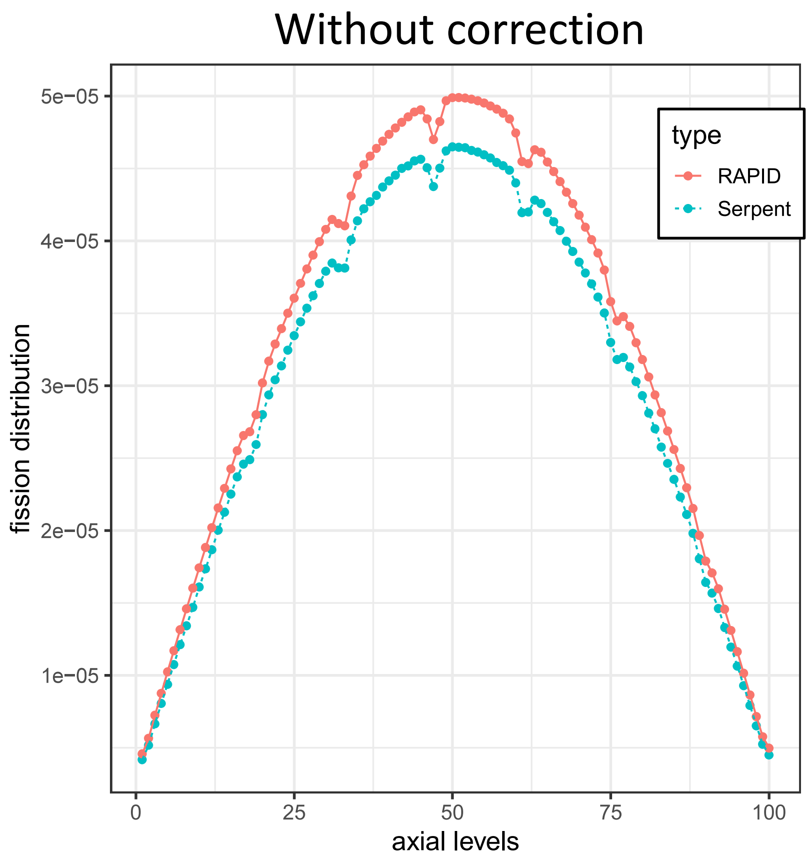

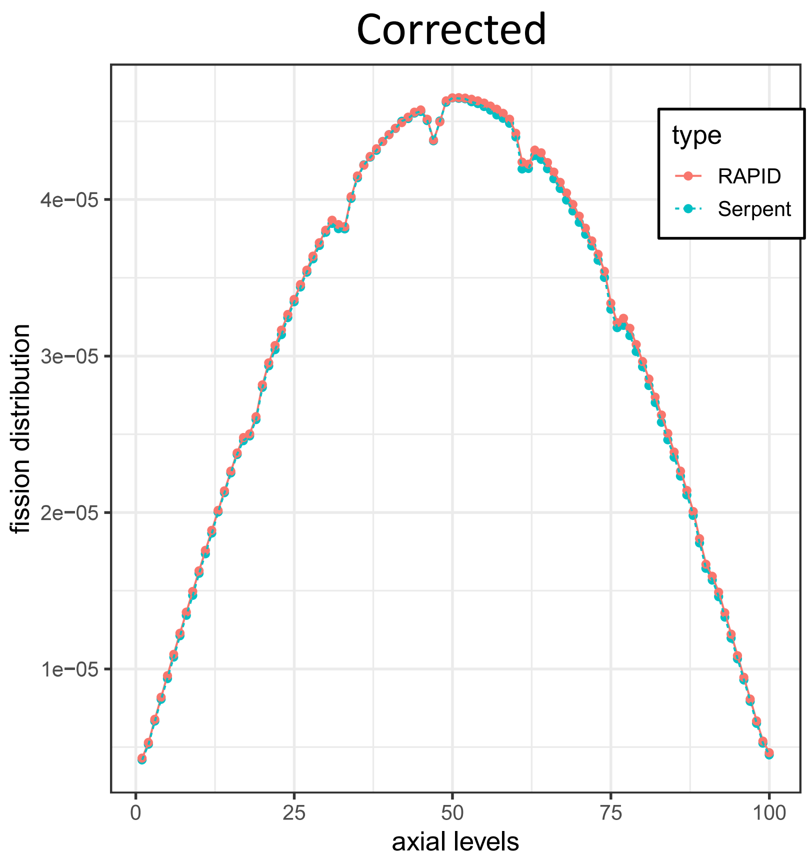

New methods incur only a small up-front computational cost

Calculation	Model Description: Geometry	Model Description: Source	Number of Variations	Time (CPU-hr) per Var.	Time (CPU-hr) Total
$\tilde{a}_{i,j}$ FM	1) Inf. assemblies	Single pin	7×39	0.45	121.9
Refl. correction	2) Standard core	Criticality	1	3.8	156.2
	3) Inf. core	Fixed from (2)	1	50.5	
	4) Inf. radial core	Fixed from (2)	1	50.7	
	5) Inf. axial core	Fixed from (2)	1	51.2	
Enrich. correction	6) Four-assembly	Uniform	3×3 (exact)	3.3	29.7
Total (exact R)					337.5

New method

Total

Correction method requires 9 fixed source calculations on four-assembly geometry

Accuracy of k_{eff} and 3D fission source estimation is improved

		Uncertainty (Serpent) and relative error (RAPID)					Wall-clock
			2D pin-wise		3D (100 axial levels)		Time
Method	k_{eff}	k_{eff}	RMS	MAX	RMS	MAX	(20 cores)
Serpent	1.00402	0.5 pcm	0.18%	0.43%	1.86%	11.35%	80 hr
RAPID (old)	1.00245	-156 pcm	6.26%	22.27%	6.63%	57.53%	2.4 min
RAPID (exact)	1.00427	25 pcm	0.54%	2.39%	2.26%	54.29%	2.4 min

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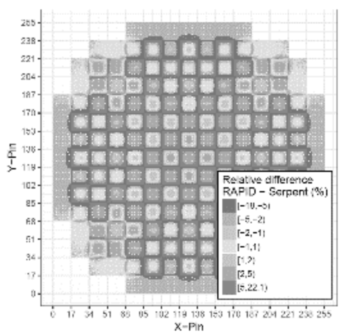

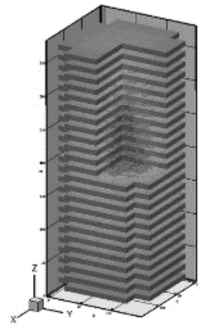

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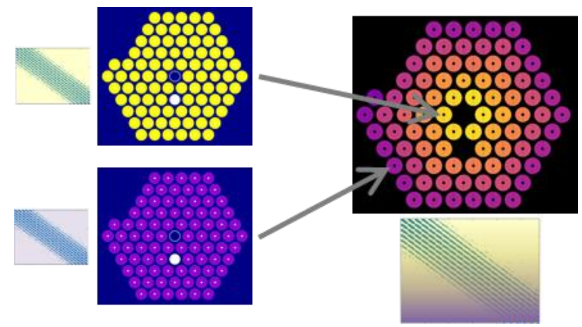

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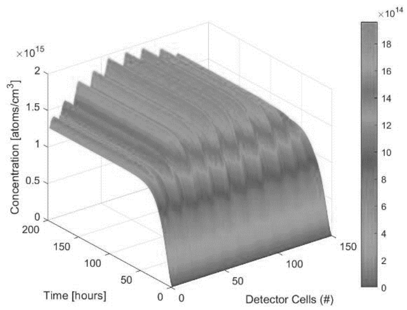

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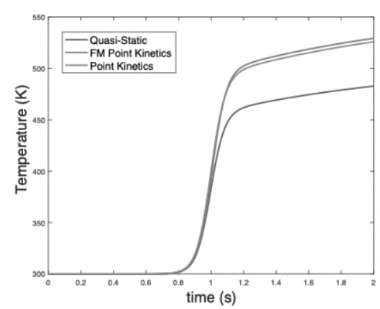
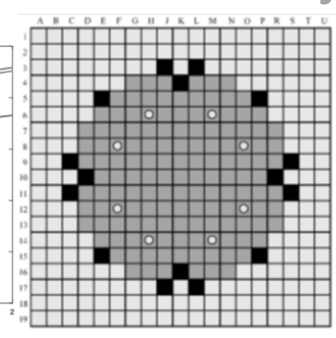
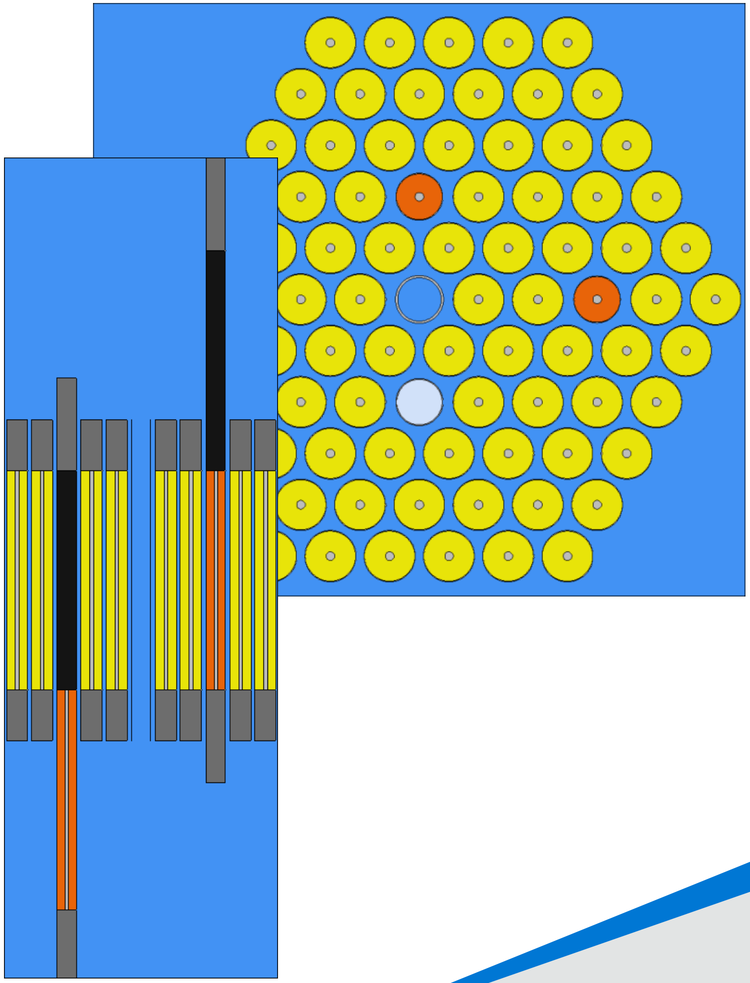




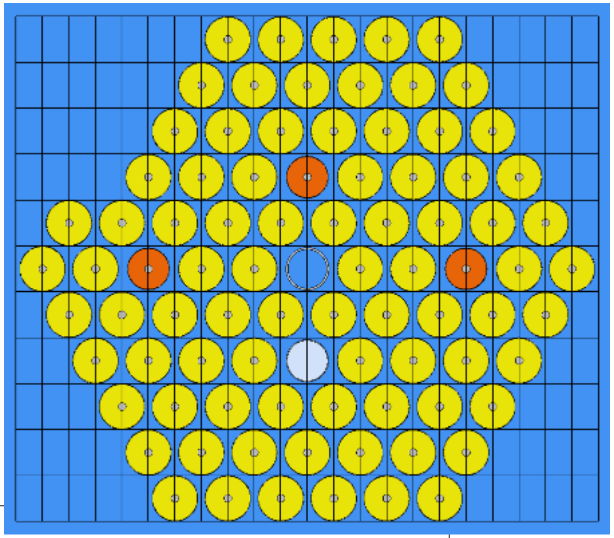
We have also developed fission matrix methods for the Penn State TRIGA reactor

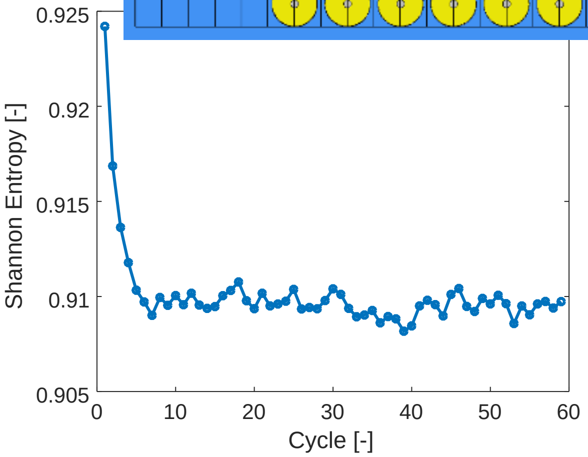
- TRIGA pool-type reactor
- $UZrH_x$ fuel ("cell effect" feedback)
- Four control rods
  - Three fuel-followed
  - One air-followed (pneumatically-actuated "transient" rod)
- Small core – 47 x 41 x 38 cm (approx.)
- Natural circulation cooling
- 1 MW nominal steady-state power



Several Serpent options simplify this work

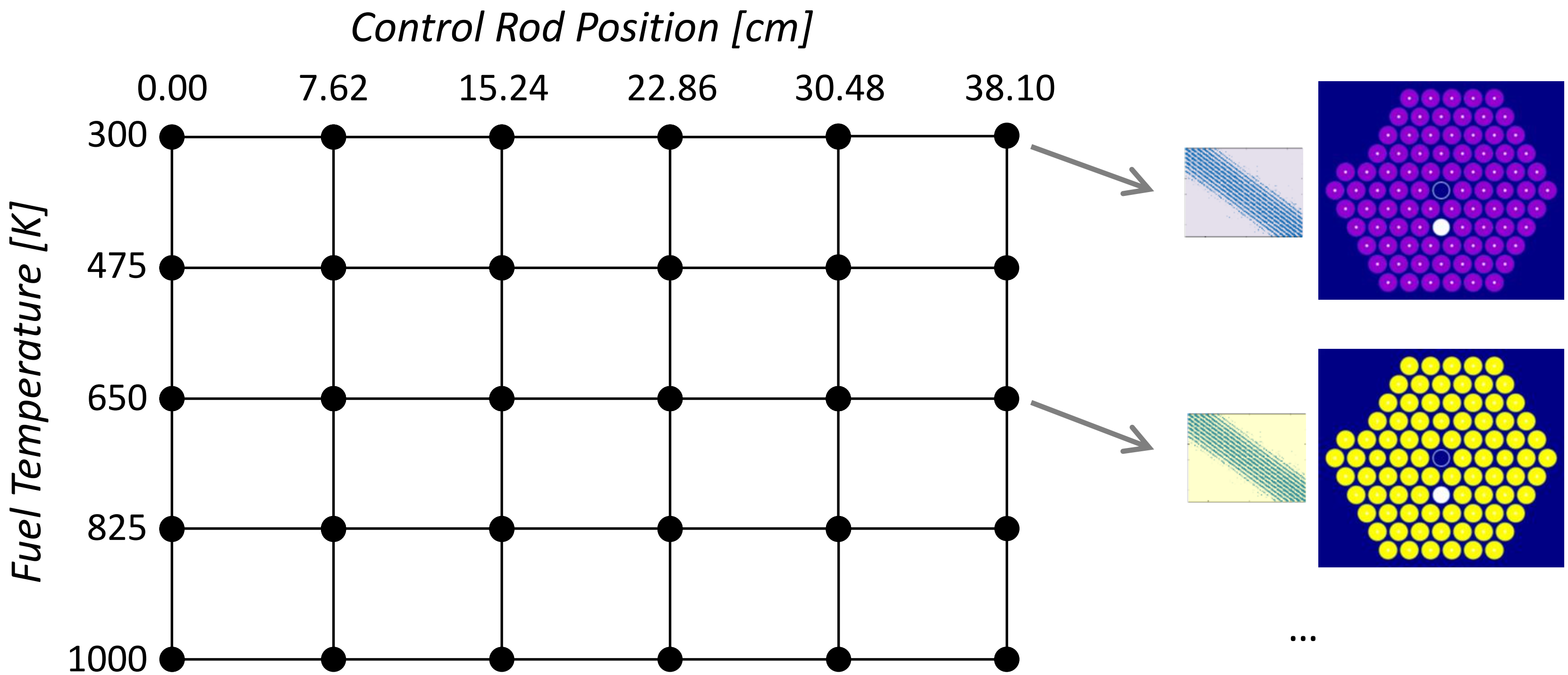
- **"set fmtx"** option for calculating fission matrix in criticality simulation
  - Easy to perform criticality calculations on small core
  - Cartesian grid compatible with regular hexagonal mesh
- Fuel temperature profiles simulated with **multiphysics interface**
  - Use same options even when temperature profile is uniform (since goal is code-to-code verification)





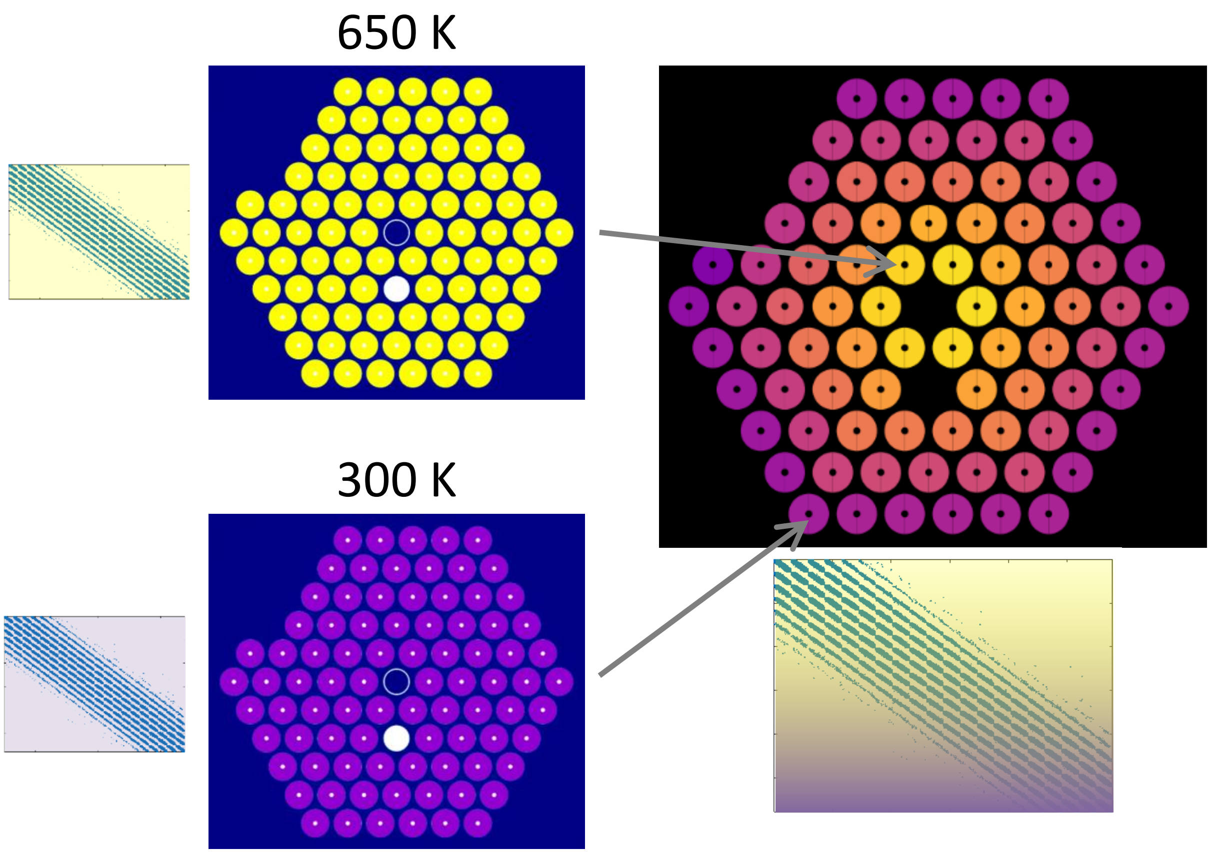
Set fmtx: https://ttuki.vtt.fi/serpent/viewtopic.php?f=24&t=2098&p=5370&hilit=fmtx#p5370
Multiphysics Interface: http://serpent.vtt.fi/mediawiki/index.php/Multi-physics_interface

We pre-calculate fission matrices at different uniform temperatures and control positions



(5 uniform fuel temperatures) ·
(6 control rod positions) =
30 calculations

Pre-calculated fission matrices can be combined to simulate any temperature profile

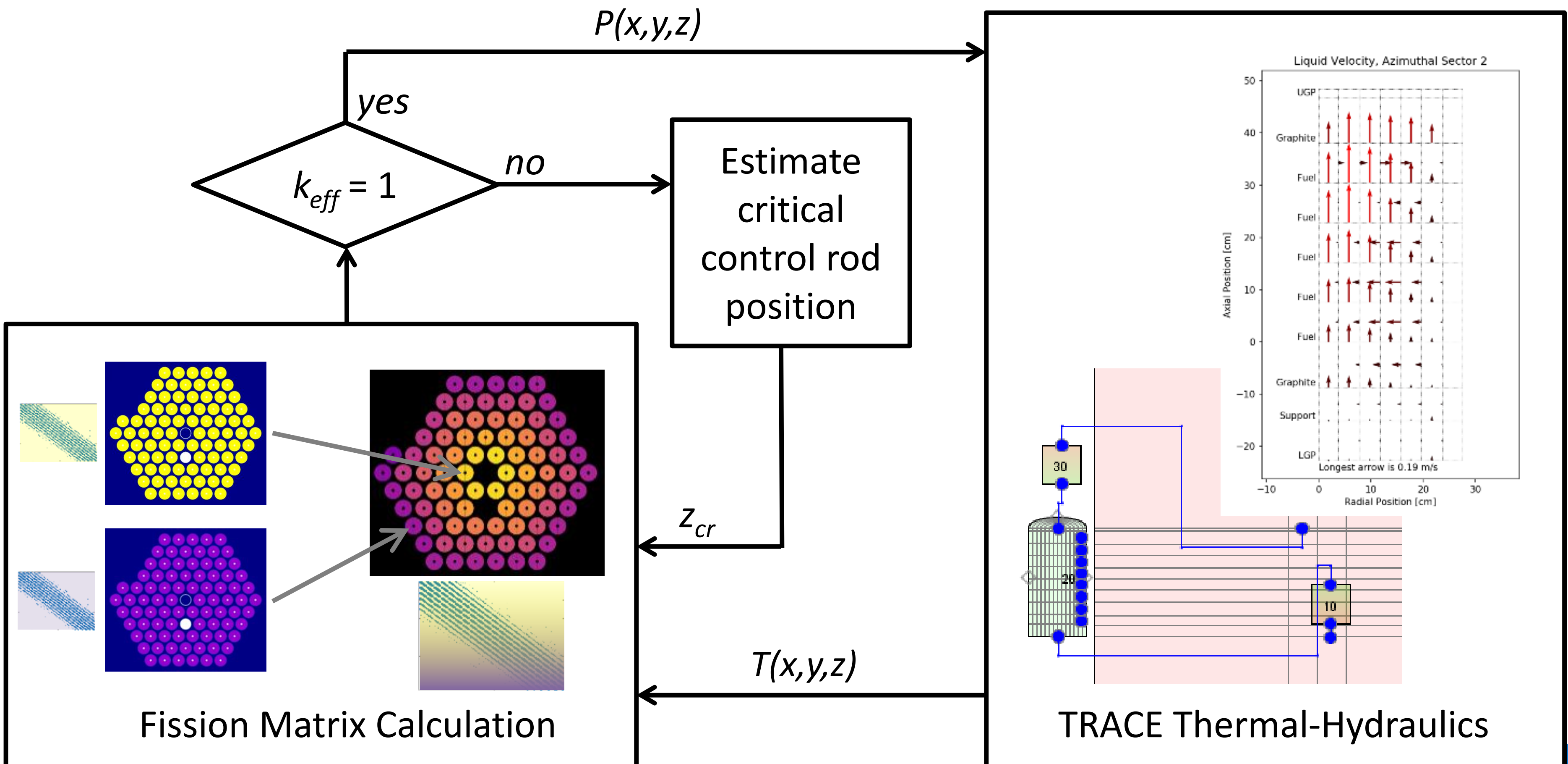


Fit 2D polynomial to each fission matrix element

$$a_{ij} = f_{ij}(T_{f,i}, z)$$

Assume element is function of destination temperature

Steady-state temperatures and rod positions were found by Picard iteration with TRACE



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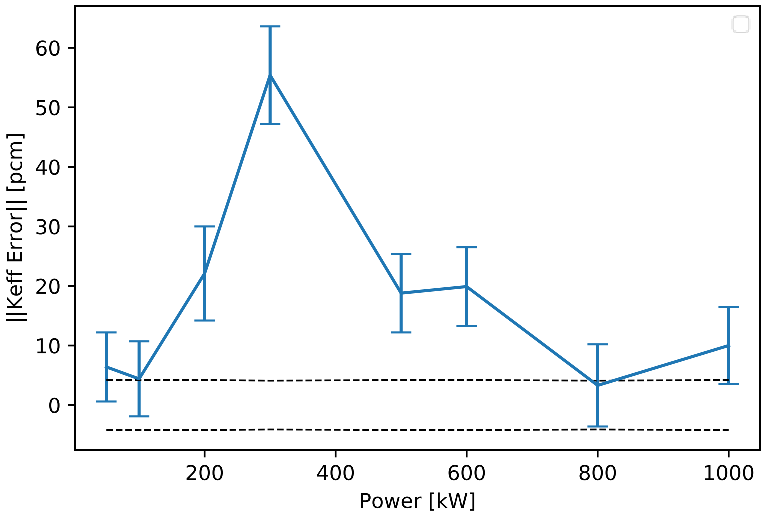
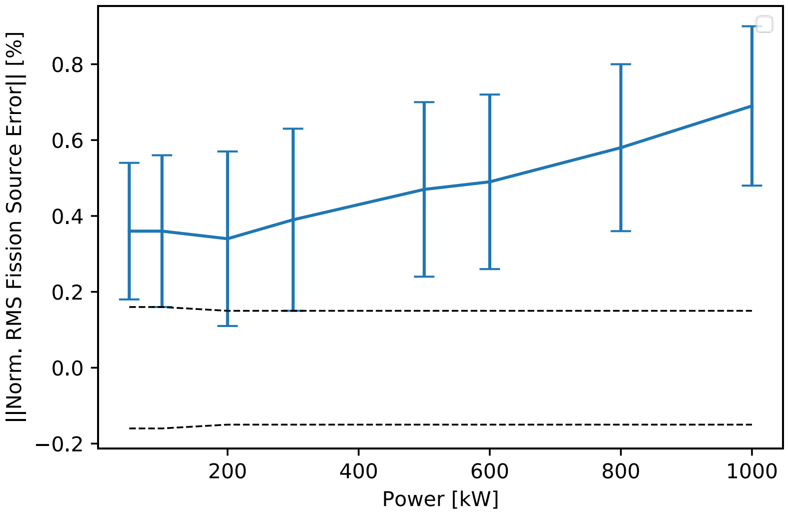
Code-to-code verification is performed with Serpent

k_{eff} Error



3D RMS Fission Source



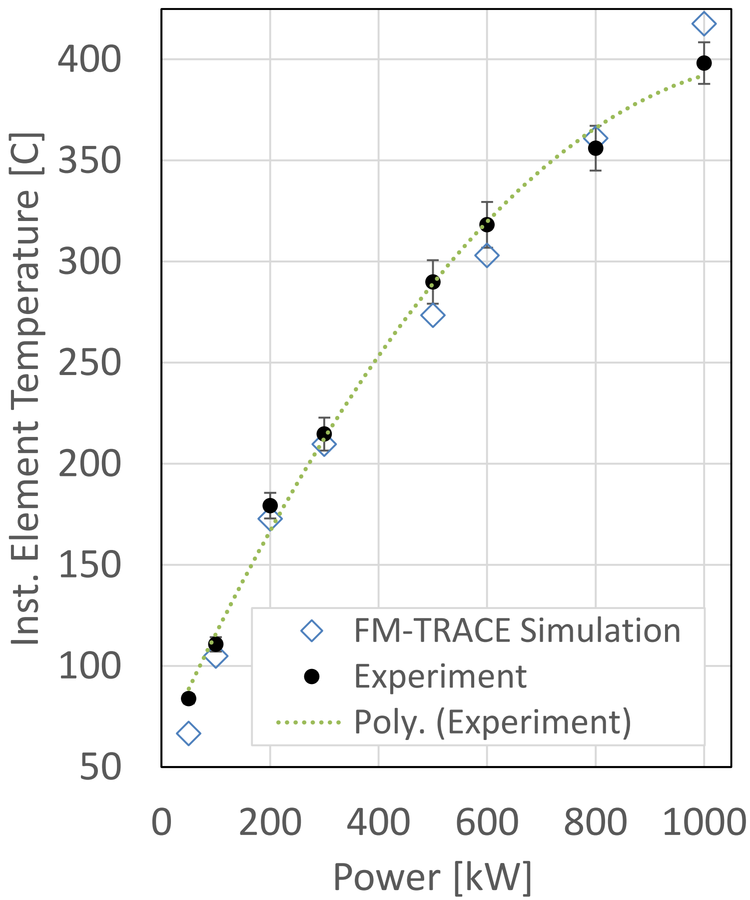
- Critical temperatures / rod positions from 50 kW to 1 MW
- k_{eff} within 60 pcm
- 3D RMS Source Error within 1%
- 3D Max. Source Error within 3%

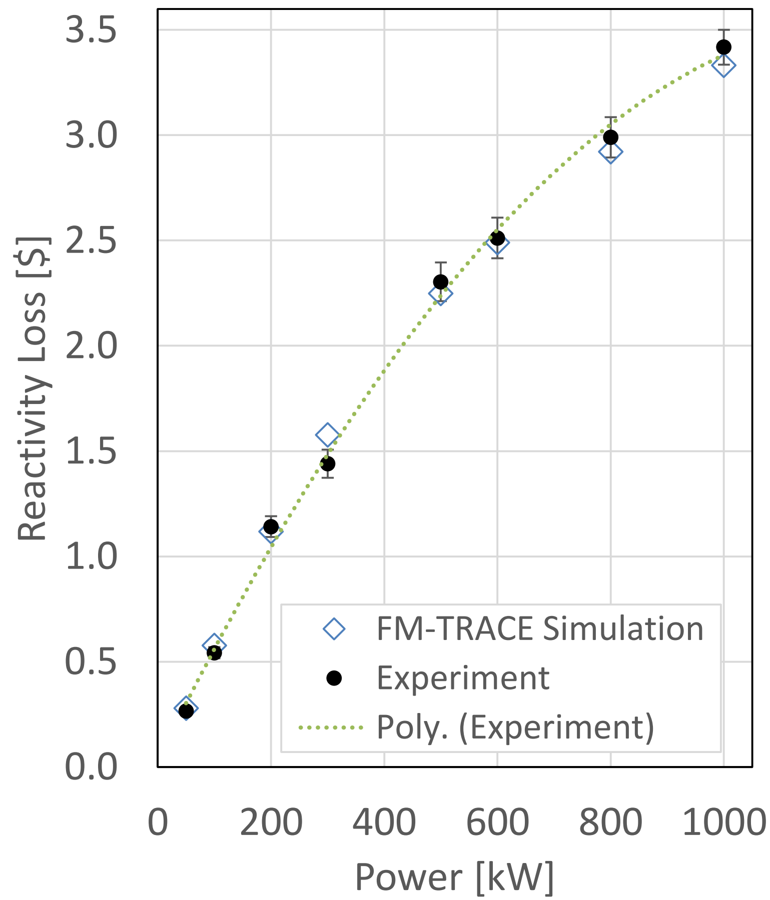
After pre-calculation, fission matrix solutions are completed in seconds

<u>For Database:</u>
40,000 neutrons/cycle
12,000 active cycles
10 inactive cycles

Fission Matrix Database Calculation (one calc.)	80 CPU-hrs
Fission Matrix Database Calculation (total)	2400 CPU-hrs
Fission Matrix Assembly / Solution (one calc.)	1.6 CPU-sec

Method is validated against historic clean-core experimental data



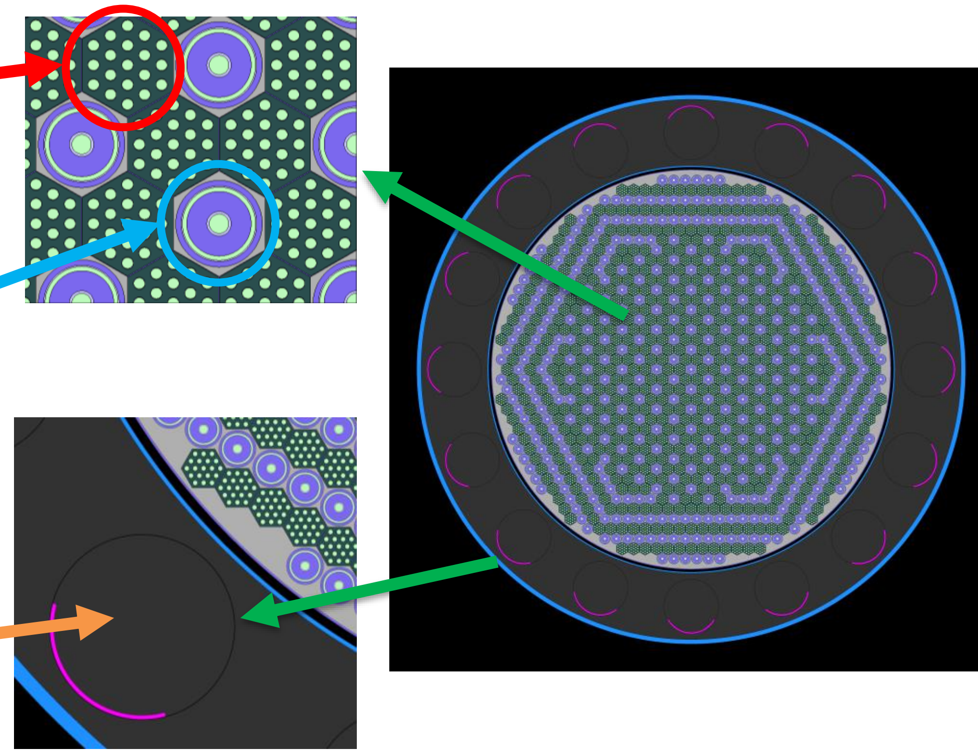


The same methods have been applied to a Nuclear Thermal Propulsion type reactor

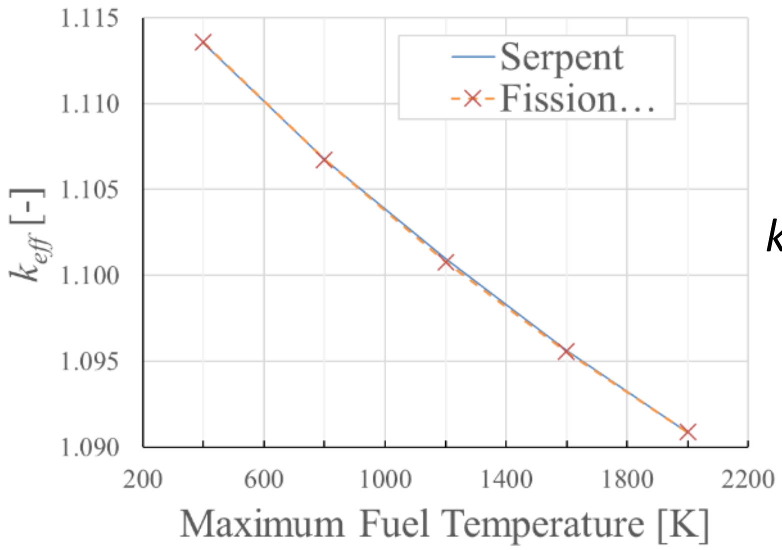
(U,Zr)C composite fuel

$ZrH_{1.7}$ moderator
Separated from fuel

Rotating control drums
instead of fuel-followed
rods

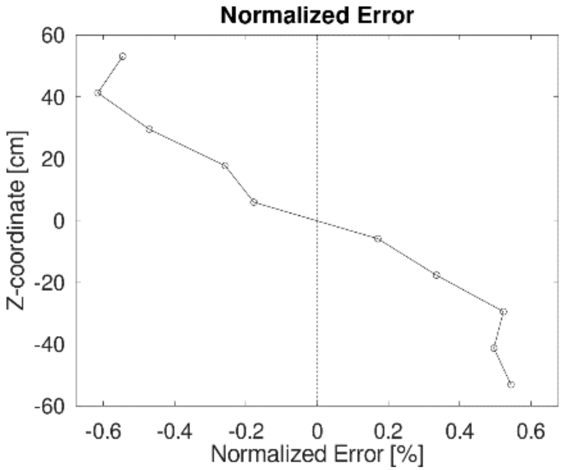


Despite different application, method has similar accuracy on NTP and TRIGA

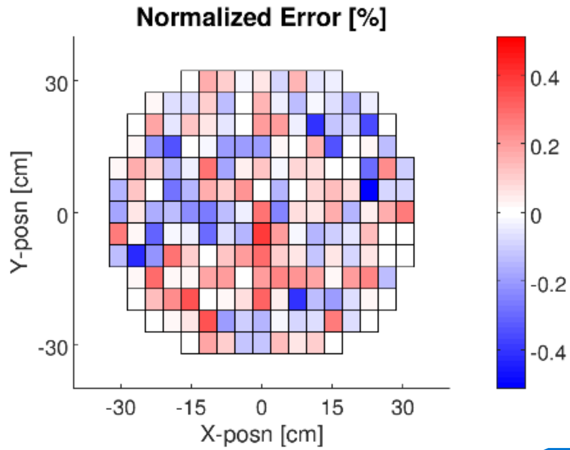


k_{eff}

Axial Fission Source



x-y Fission Source



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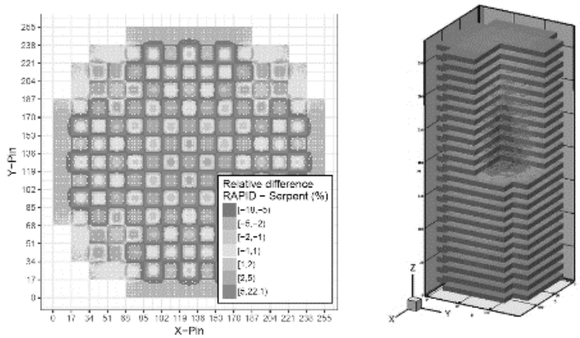

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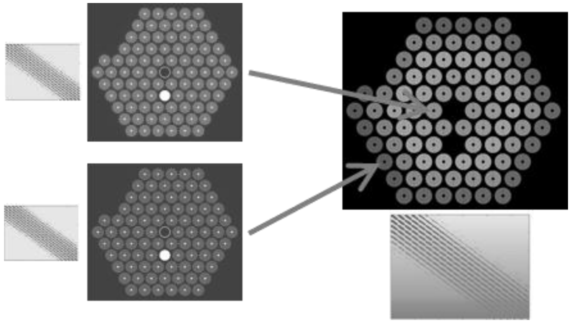

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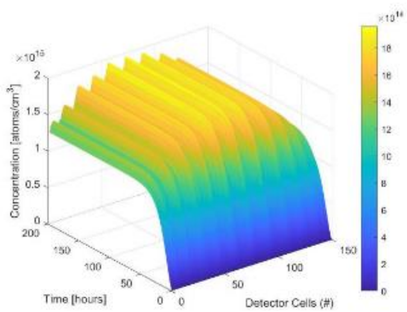

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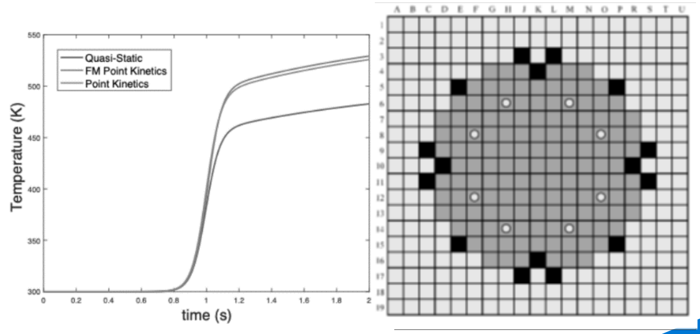
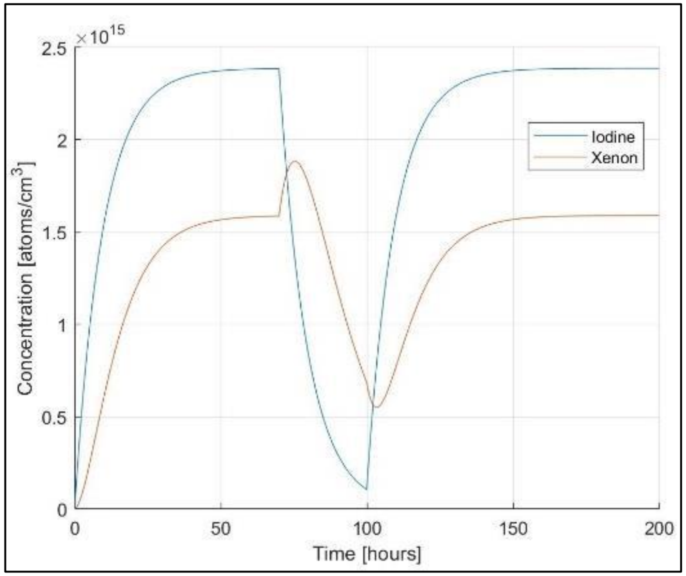
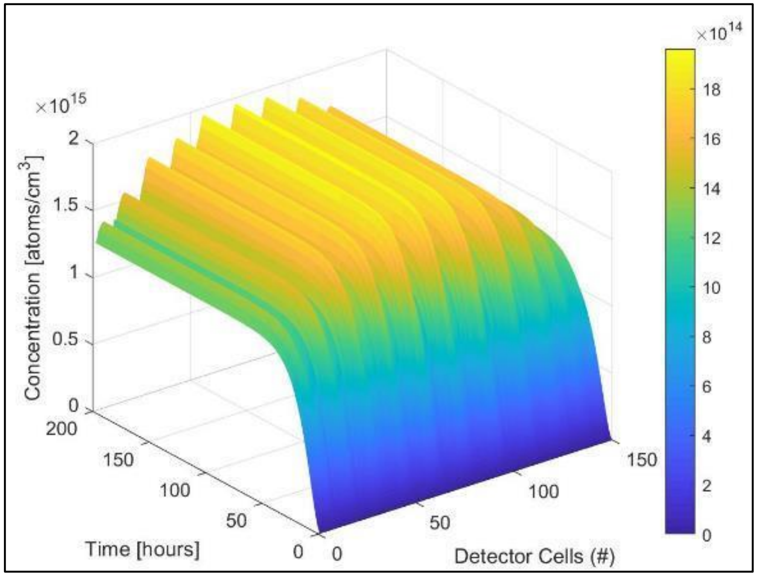


Short operation times require calculation of xenon dynamics





$$\frac{\partial I}{\partial t} = \gamma_I \Sigma_f \phi(r,t) - \lambda_I I(r,t)$$

$$\frac{\partial X}{\partial t} = \gamma_X \Sigma_f \phi(r,t) + \lambda_I I(r,t) - \lambda_X X(r,t) - \sigma_a^X \phi(r,t) X(r,t)$$

$$\vec{F} = \frac{1}{k} A \vec{F}, \qquad \boxed{\vec{F} \propto \gamma_X \Sigma_f \phi(r,t)}$$

Xenon production assumed proportional to fission source

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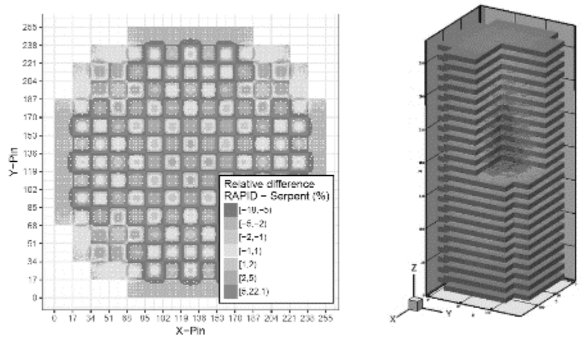

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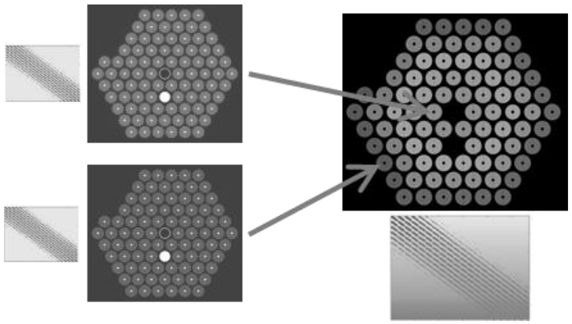

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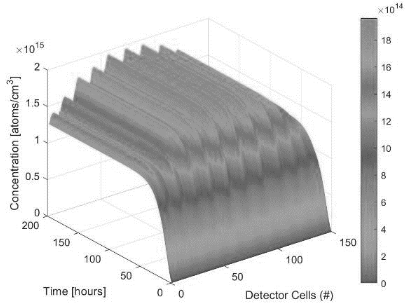
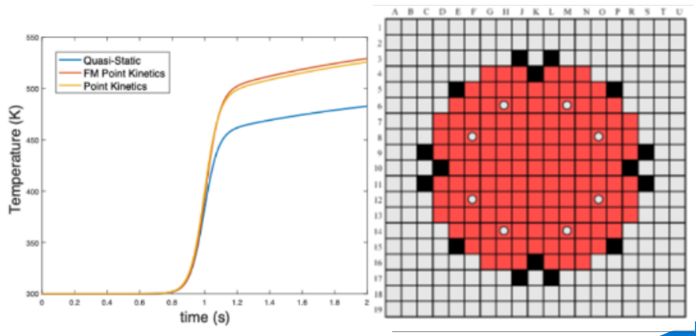
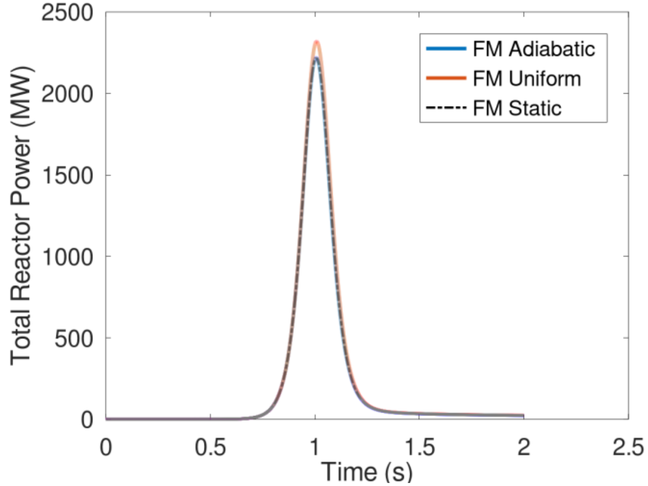


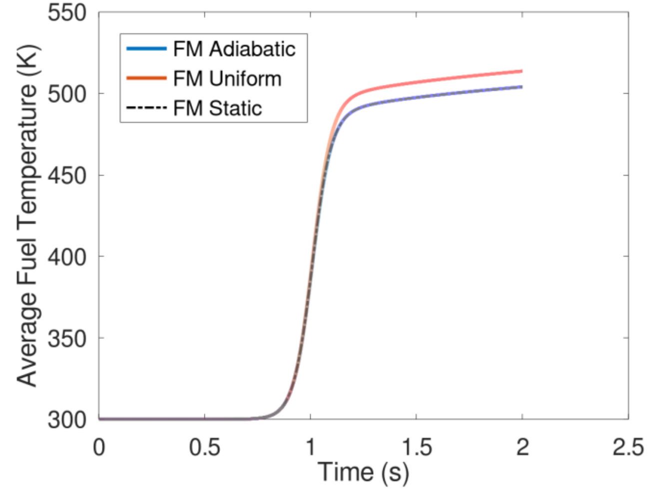
$$\vec{F} = \frac{1}{k} A \vec{F}$$
$$\vec{F} \propto \gamma_X \Sigma_f \phi(r,t)$$

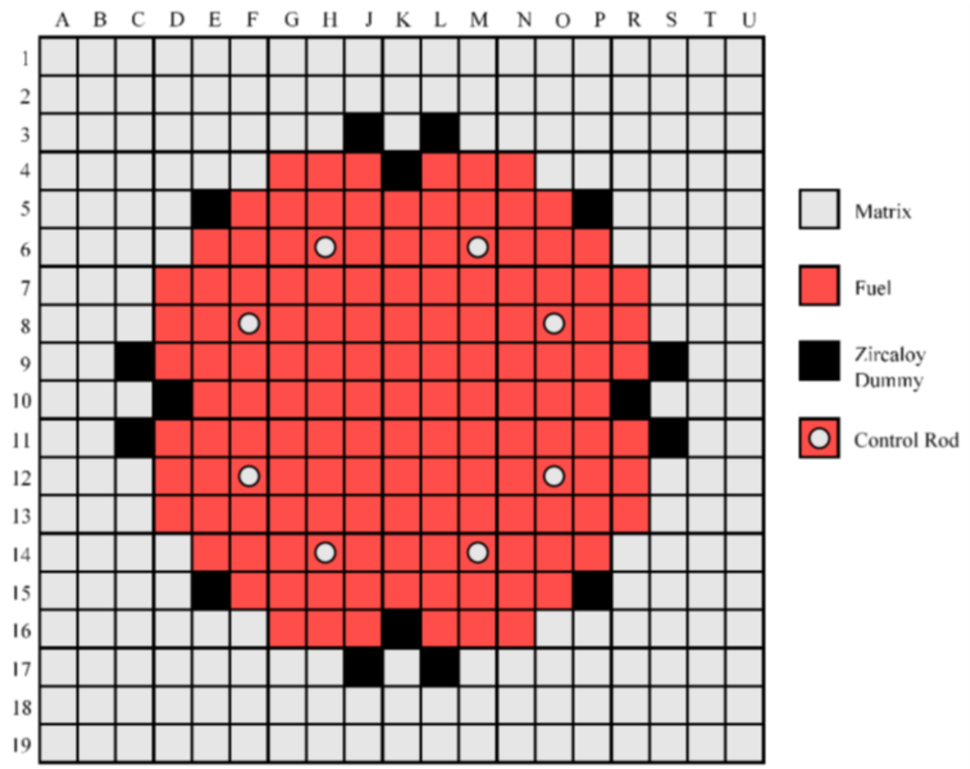
Transient Fission Matrix in TREAT Reactor (Alvaro Pizarro-Vallejos)



Transient fission matrix methods have been investigated for the TREAT reactor





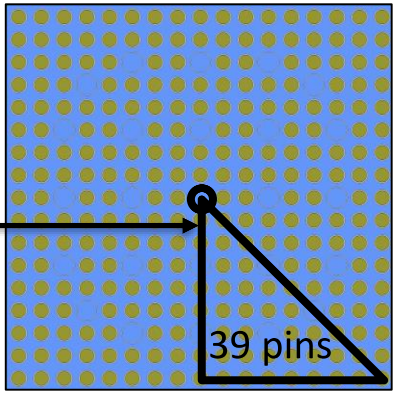


Thank you!
Questions?

Backup Slides

The time of the RAPID database calculation is summar

Calculation	Model Description: Geometry	Model Description: Source	Number of Variations	Time (CPU-hr) per Var.	Time (CPU-hr) Total
$\tilde{a}_{i,j}$ FM	1) Inf. assemblies	Single pin	7×$\boxed{39}$	0.45	121.9
Refl. correction	2) Standard core	Criticality	1	3.8	156.2
	3) Inf. core	Fixed from (2)	1	50.5	
	4) Inf. radial core	Fixed from (2)	1	50.7	
	5) Inf. axial core	Fixed from (2)	1	51.2	
Enrich. correction	6) Four-assembly	Uniform	2 (interp)	3.3	6.6
	7) Four-assembly	Uniform	3×3 (exact)	3.3	29.7
BA correction	8) Four-assembly	Uniform	4×16	3.3	52.8
Local correction	9) Four-assembly	Criticality	17	50	850
Total (exact R)					337.5
Total (interp. R)					314.4
Total (local. R)					1128



RAPID result is compared to the Serpent 2 reference calculation

Method	k_{eff}	Uncertainty (Serpent) and relative error (RAPID)					Wall-clock Time (20 cores)
			2D pin-wise		3D (100 axial levels)		
		k_{eff}	RMS	MAX	RMS	MAX	
Serpent	1.00402	0.5 pcm	0.18%	0.43%	1.86%	11.35%	80 hr
RAPID (old)	1.00245	-156 pcm	6.26%	22.27%	6.63%	57.53%	2.4 min
RAPID (interp.)	1.00428	26 pcm	0.75%	2.88%	2.30%	54.96%	2.4 min
RAPID (exact)	1.00427	25 pcm	0.54%	2.39%	2.26%	54.29%	2.4 min
RAPID (local)	1.00411	9 pcm	0.60%	2.11%	2.28%	54.51%	2.4 min

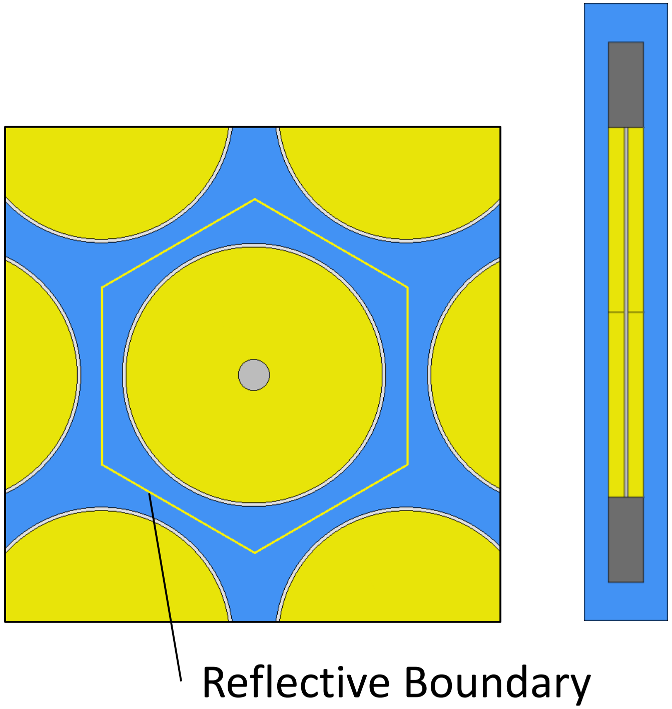
Note: $1\ pcm = 10^{-5}\ k_{eff}$

Pre-calculation time:

- Exact : 16.8 hours
- Interpolated: 15.7 hours
- Localized: 56.4 hours

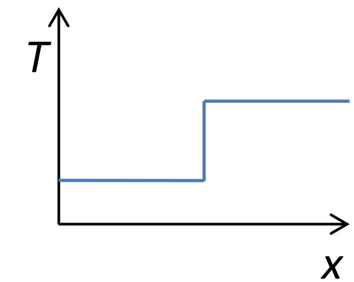
Test Problems: Problem Geometry

- Used Serpent 2.1.30 for Monte Carlo
- Single fuel pin
  - Graphite reflector at ends
  - Fresh 8.5% U-$ZrH_{1.6}$ fuel
- Boundary conditions:
  - Reflective in X-Y
  - Vacuum in Z
- Vary axial fuel temperature
- Tally fission source in 128 axial bins

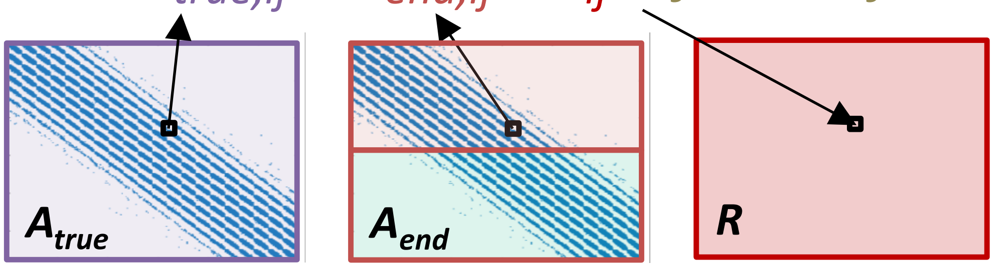


Method: Ratio-Correction in Present Work

- Pre-calculation:
  - Simulate one additional, non-uniform case
  - Obtain true fission matrix $\boldsymbol{A_{true}}$ from (Monte Carlo) criticality calculation
  - Construct $\boldsymbol{A_{end}}$
  - Calculate matrix $\boldsymbol{R}$

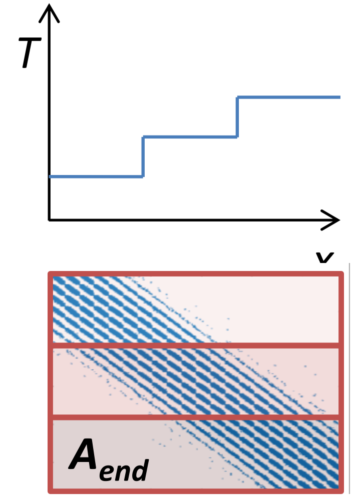


$a_{true,ij}$ / $a_{end,ij}$ = r_{ij} *for all i,j*



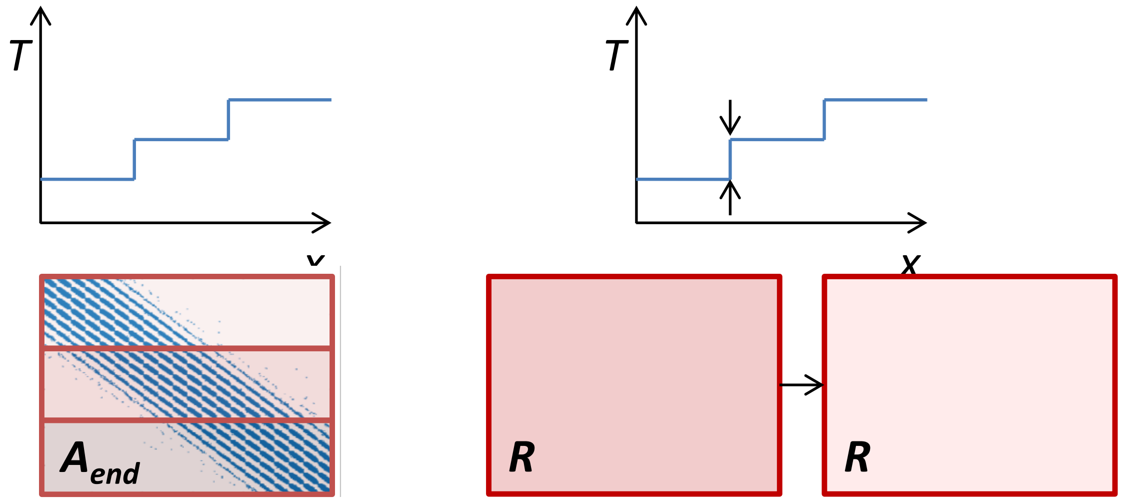
Method: Ratio-Correction in Present Work

- Apply to arbitrary temperature distribution:
  - Superimpose correction matrix ***R*** for each temperature change in arbitrary profile
- Application assumes:
  - Geometric similarity (***R*** independent of position)
  - ***R*** scales linearly with temperature



Method: Ratio-Correction in Present Work

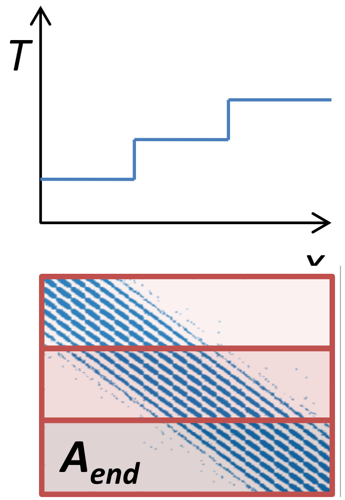
- 1. Scale ***R*** by temperature

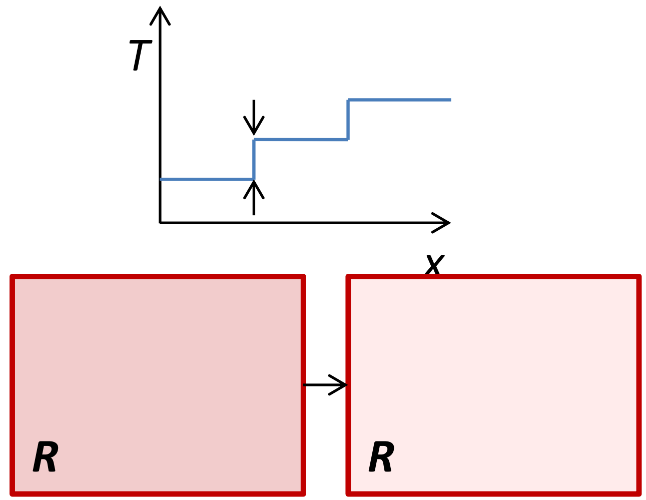


Scale ***R*** for temperature

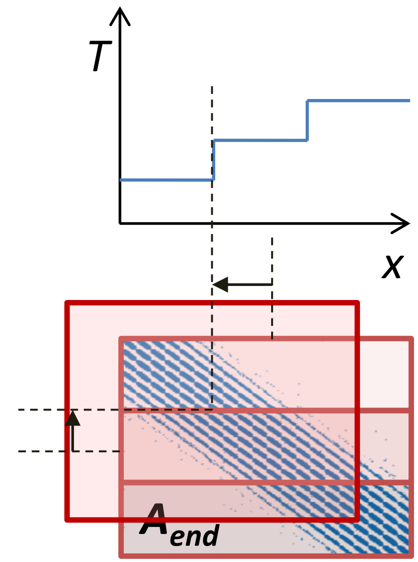
Method: Ratio-Correction in Present Work

- 2. Translate ***R*** and multiply





Scale ***R*** for temperature



Translate ***R*** and multiply

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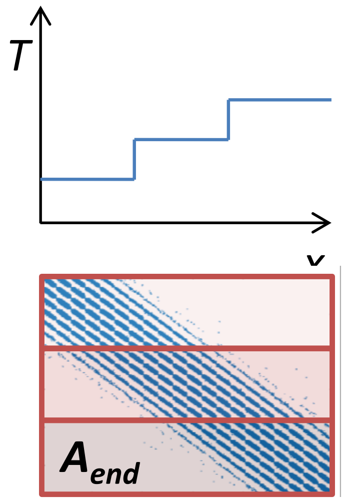
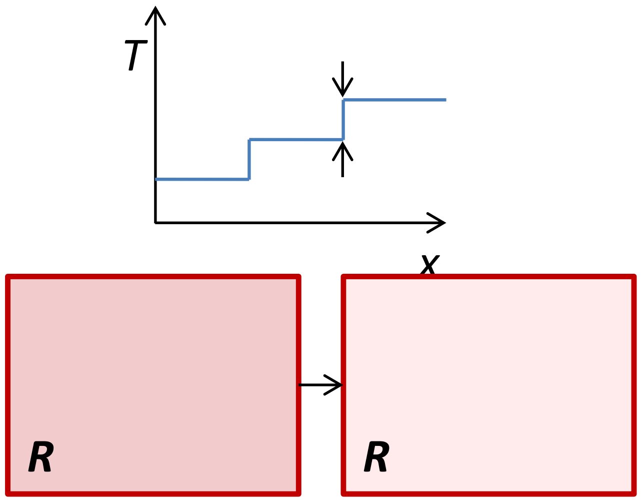
PennState College of Engineering

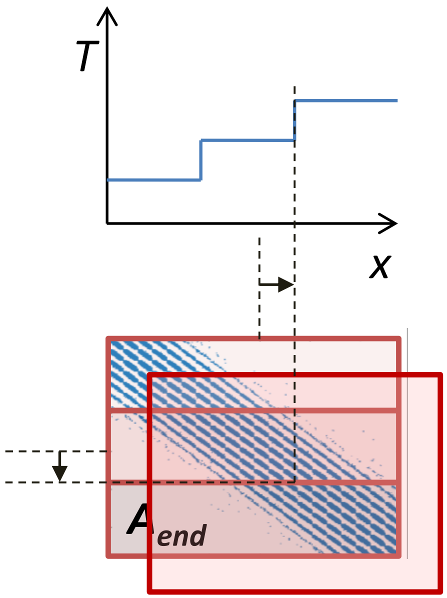
Method: Ratio-Correction in Present Work

- 3. Repeat for all temperature changes





Scale ***R*** for temperature



Translate ***R*** and multiply

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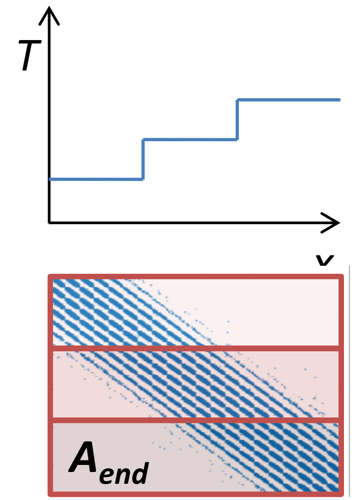
Method: Ratio-Correction in Present Work

- Apply to arbitrary temperature distribution:
  - Superimpose correction matrix ***R*** for each temperature change in arbitrary profile
- Application assumes:
  - Geometric similarity (***R*** independent of position)
  - ***R*** scales linearly with temperature



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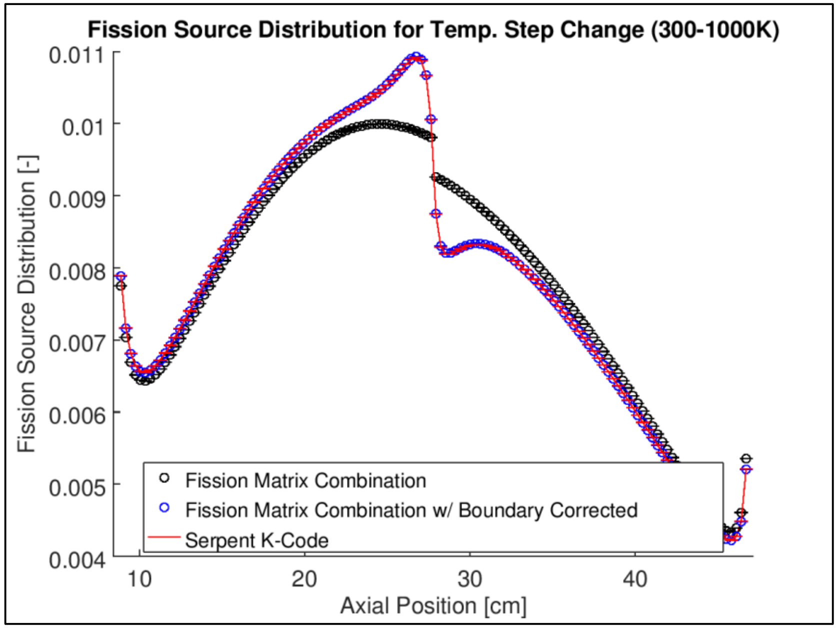
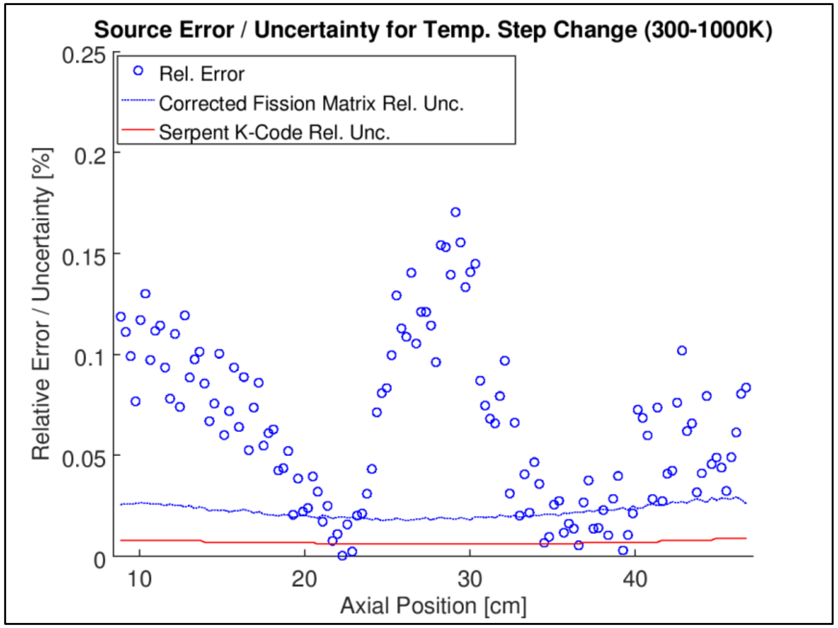
Results: Step Temperature Profile





Results: Sine Temperature Profile

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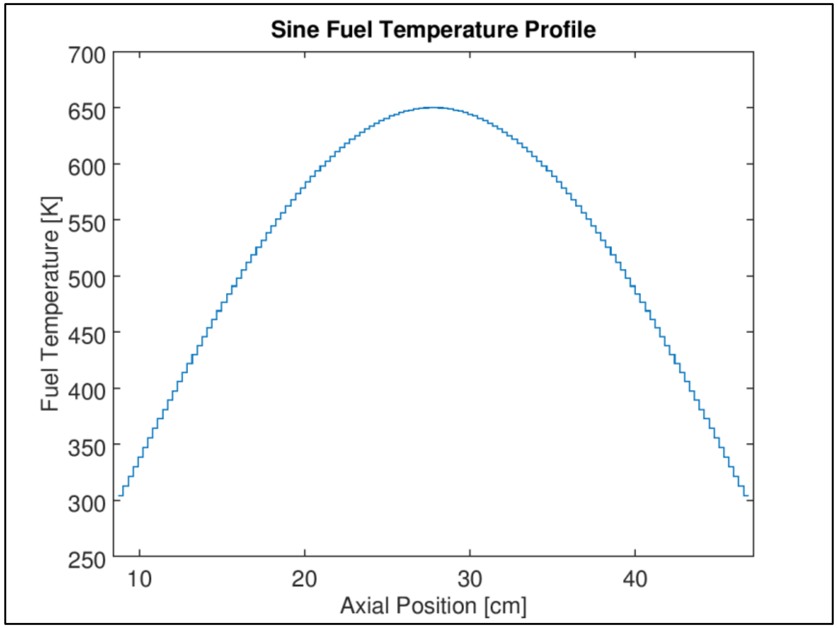
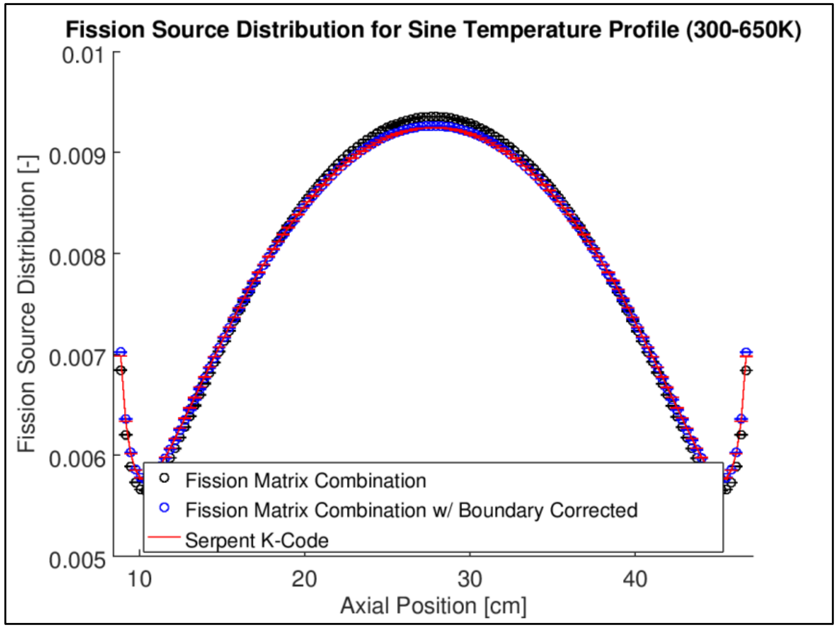
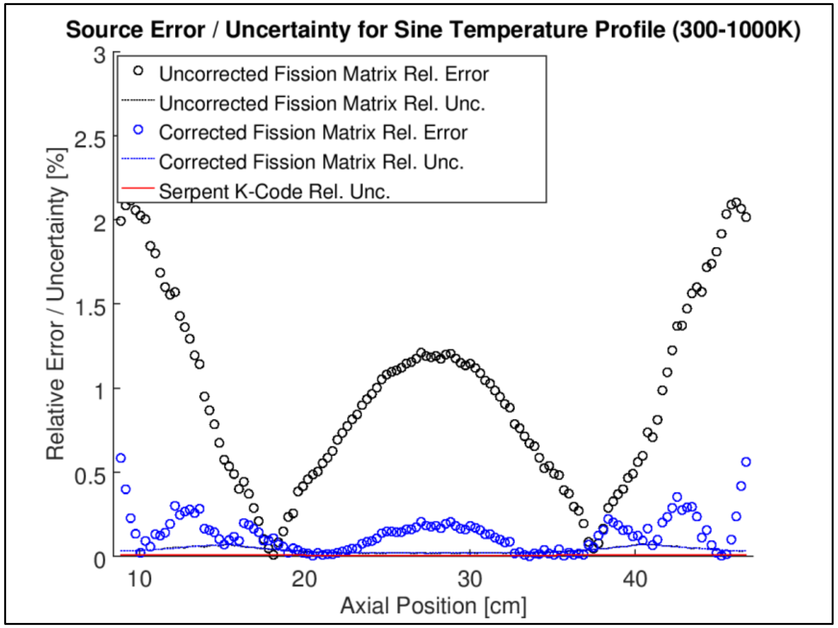


Results: Sine Temperature Profile

32





Results: Sine Temperature Profile

- End method produces reasonable estimate of k_{eff}
- Correction reduces source RMS error by factor of 5
- Calculation takes ~4 seconds on personal laptop

	K_{eff} Relative Error [pcm]	Source RMS Rel. Error [%]	Source Max. Rel. Error [%]
End Method	-41	1.1	-2.11
Corrected End Method	-39.6	0.17	0.58

Results: Sine Temperature Profile

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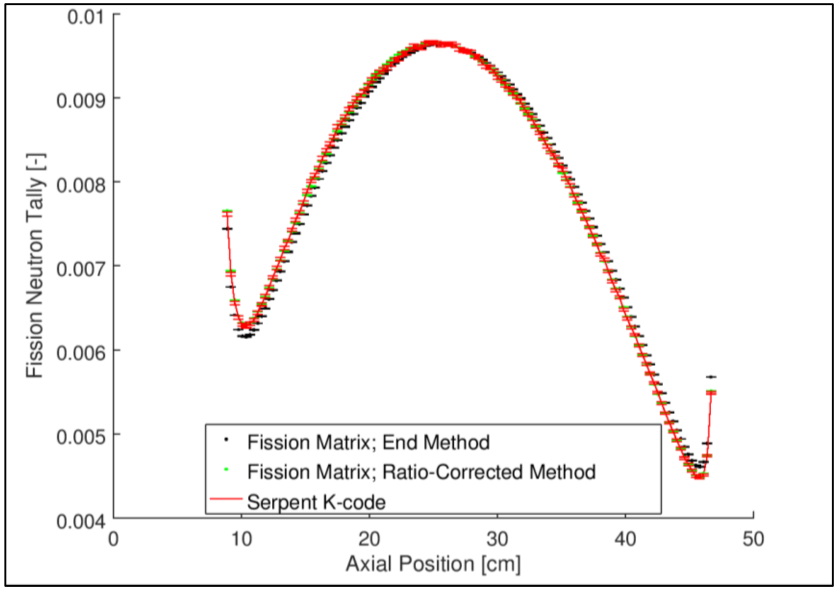
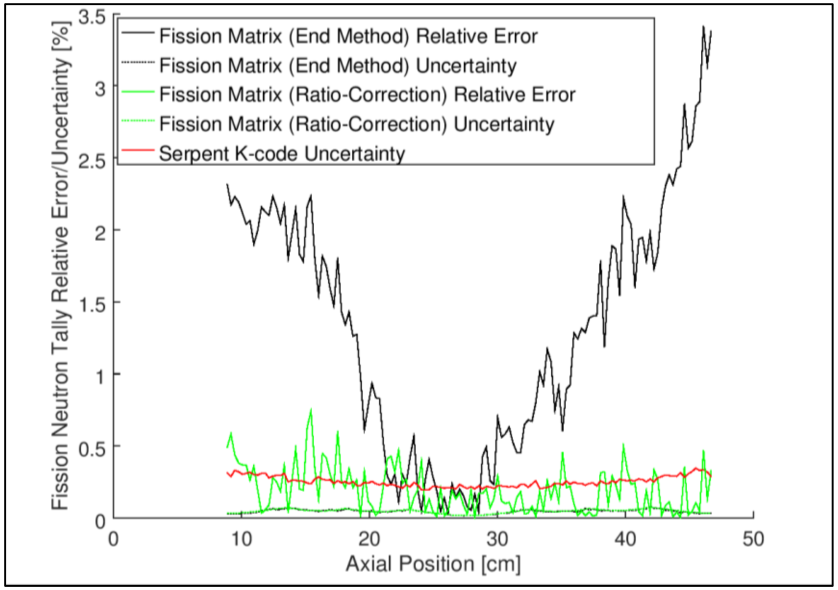
Temp. Range [K]	k_{eff} RE [pcm]	Src. RMS RE [%]	Src. Max. RE [%]
End Method			
300-1000	-6.4	2.41	-4.9
300-650	-41	1.10	-2.11
300-475	-53.1	0.47	-0.9
650-1000	20.5	1.21	-2.82
Corrected End Method			
300-1000	7.4	0.40	-1.01
300-650	-39.6	0.17	0.58
300-475	-53.8	0.14	0.47
650-1000	23.2	0.17	-0.47

Linear Temperature Profile

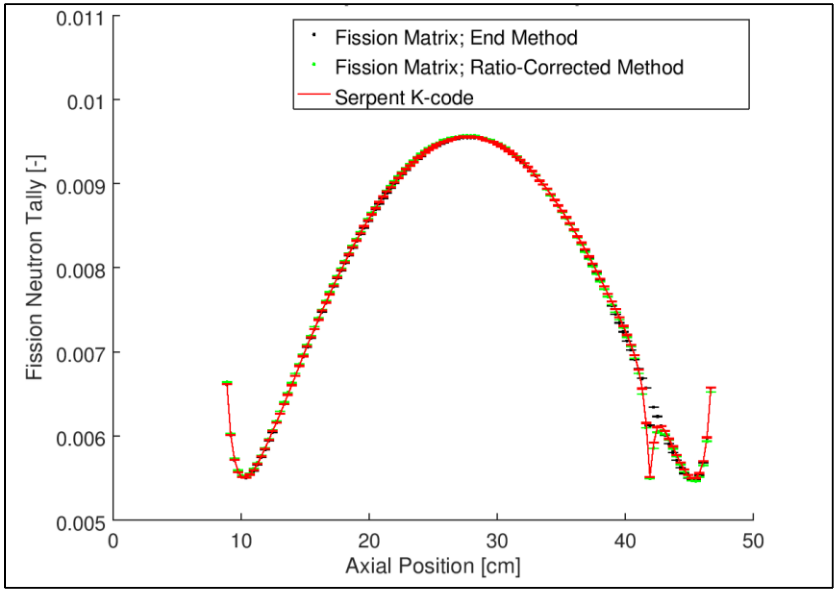
Linearly increasing 300K to 1000K from bottom to top

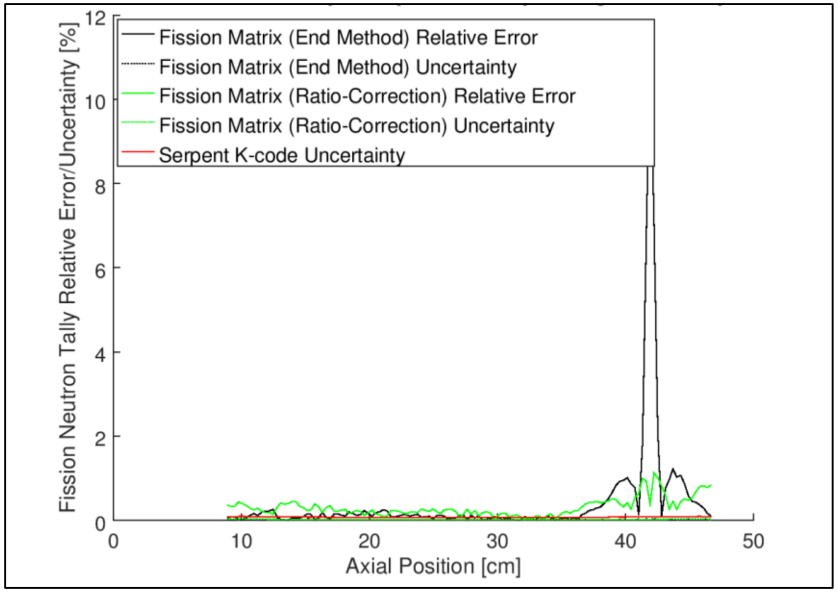




“Dirac” Temperature Profile

Uniform 300K with one “cell” elevated to 1000K



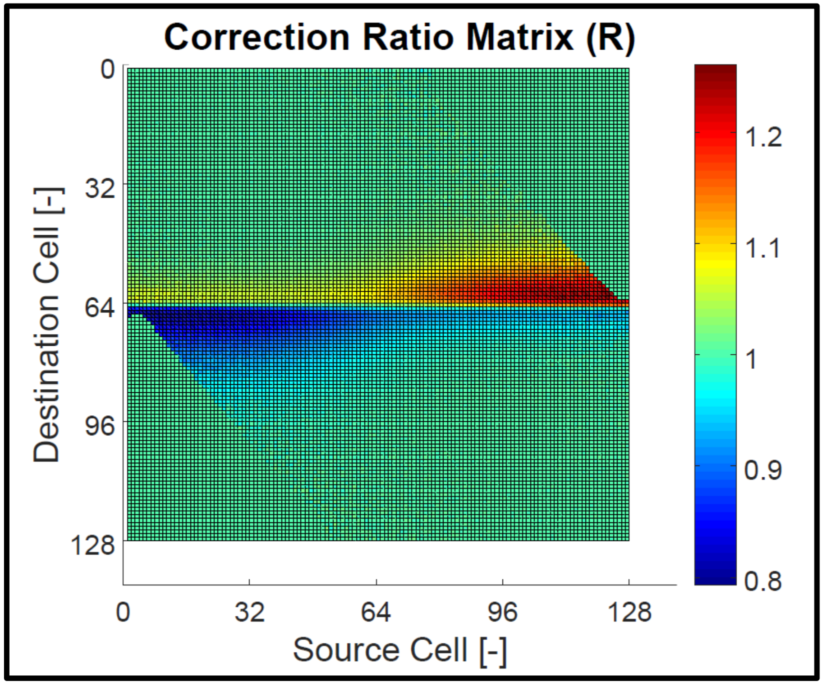


Additional Temperature Profiles

Profile - Method [-]	k_{eff} RE [pcm]	Src. RMS RE [%]	Src. Max. RE [%]
Linear - End	-88.9	1.58	3.41
Linear - Corrected	-68.4	0.25	-0.74
Dirac - End	8.4	1.38	11.09
Dirac - Corrected	-26.4	0.37	-1.13

Results: Step Temperature Profile

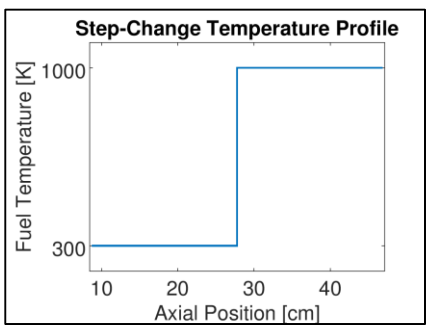
- Calculate ***R:***

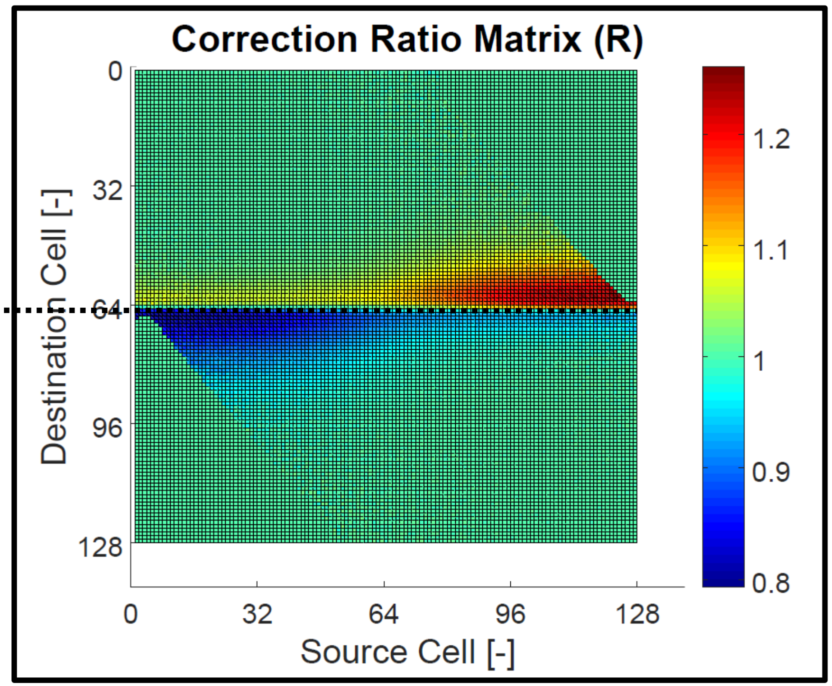


Results: Step Temperature Profile

- Calculate ***R:***

Temperature step change





Most entries near ~1

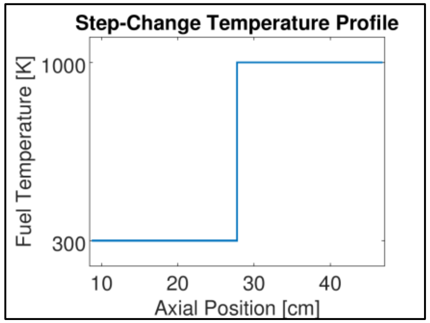
Entries with uncertainty >1% set to 1

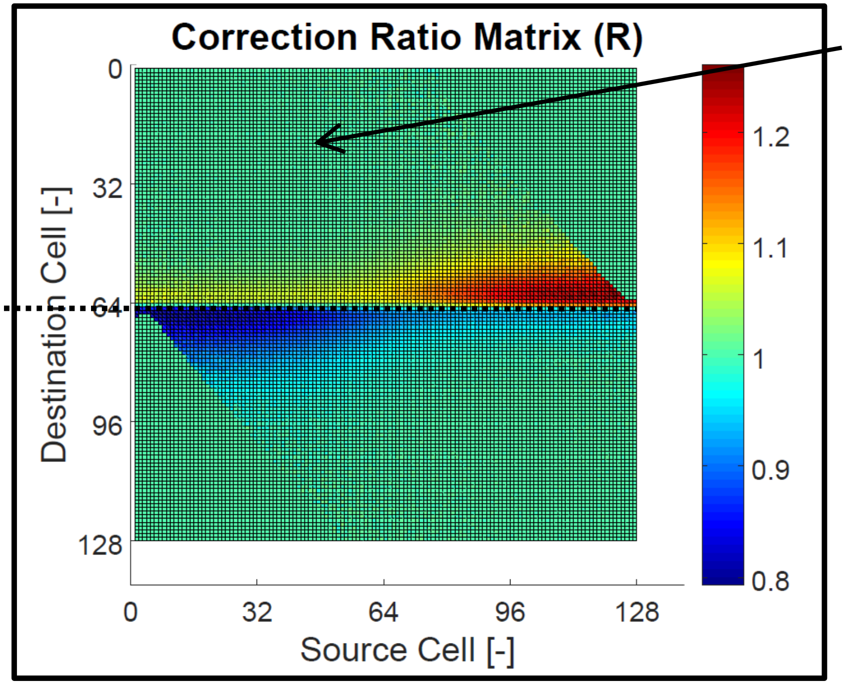
Contribution from high-temperature cells increases and vice versa

Results: Step Temperature Profile

- Calculate ***R:***

Temperature step change





Most entries near ~1

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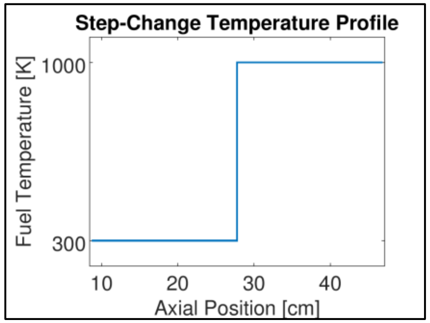
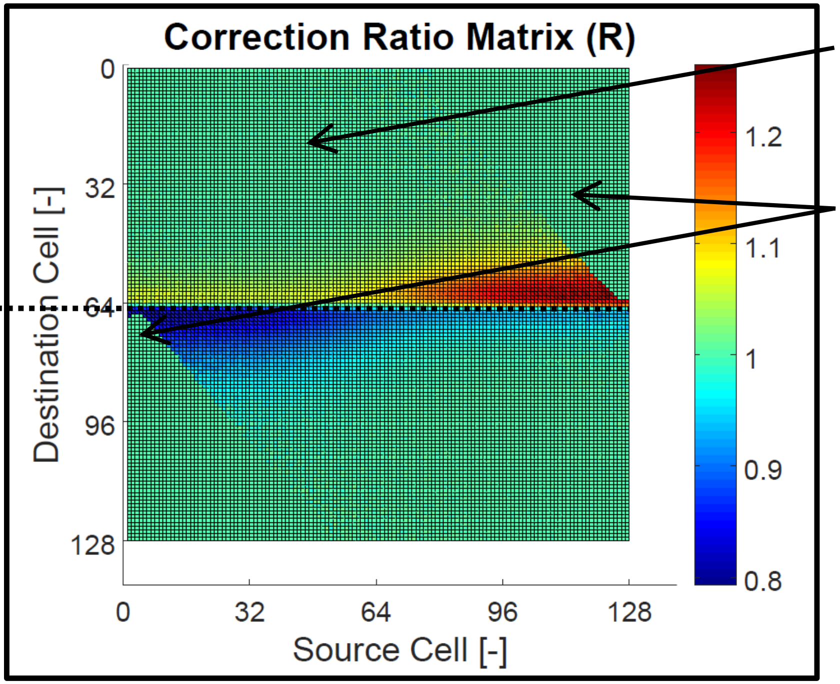
Contribution from high-temperature cells increases and vice versa

Results: Step Temperature Profile

- Calculate ***R:***

Temperature step change





Most entries near ~1

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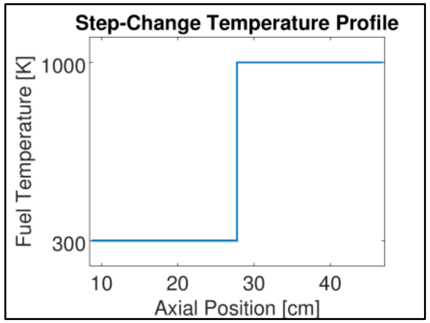
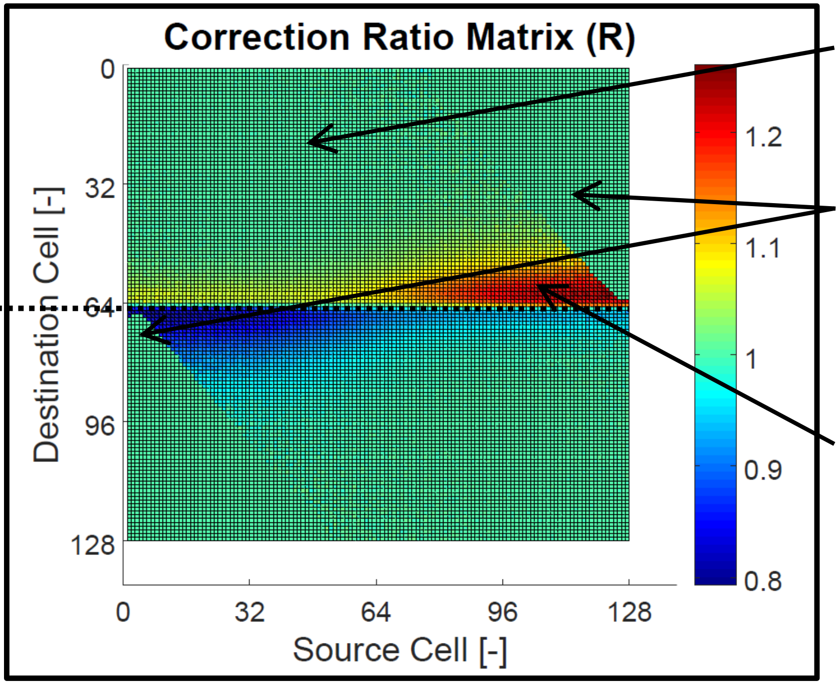
Results: Step Temperature Profile

- Calculate ***R:***

Temperature step change





Most entries near ~1

Entries with uncertainty >1% set to 1

Contribution from high-temperature cells increases and vice versa

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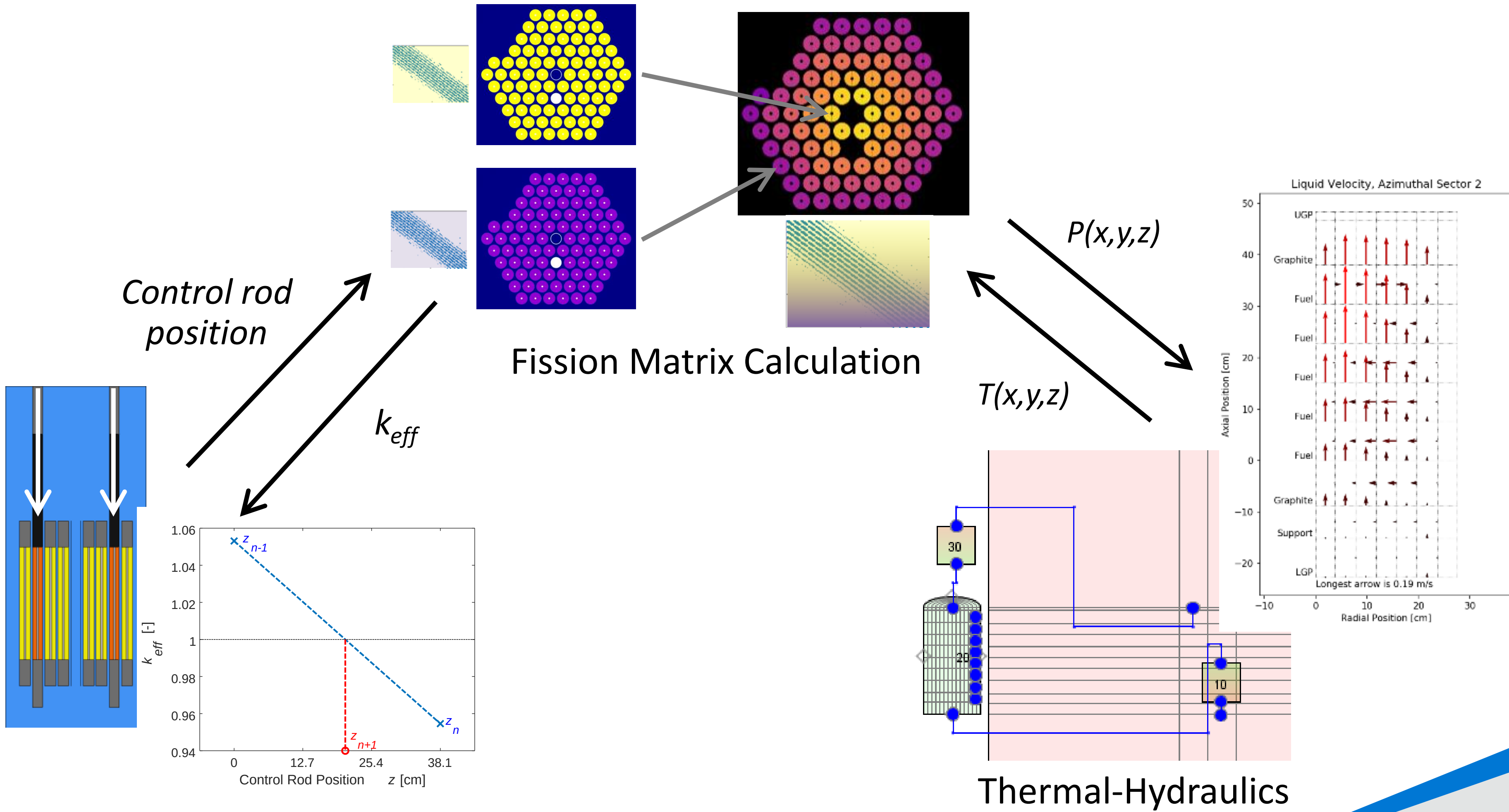
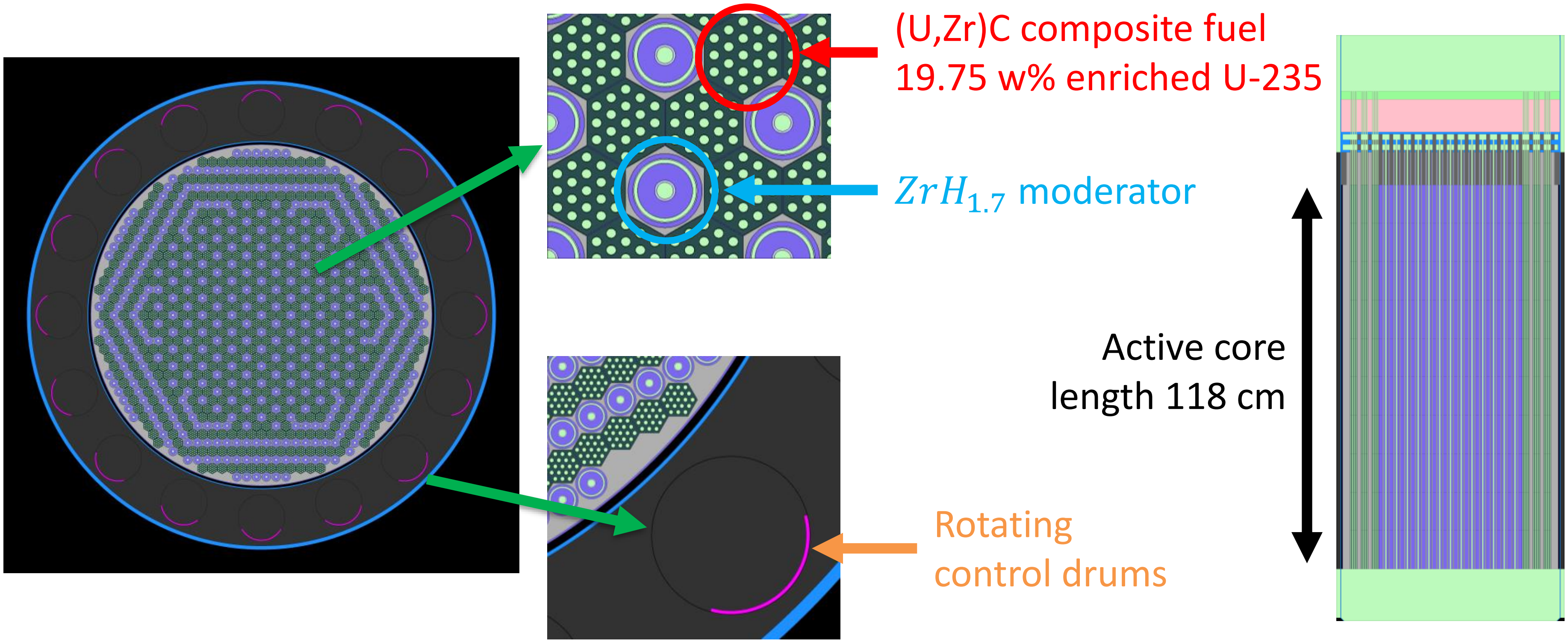
Steady-state temperatures / control rod positions were found by iterating with TRACE



After pre-calculation, calculations are completed in seconds/minutes

Fission Matrix Database Calculation (one calculation)	80 CPU-hrs
Fission Matrix Database Calculation (total)	2400 CPU-hrs
Fission Matrix Assembly and Solution (per fission matrix)	0.4 seconds
Uncertainty Calculation (per fission matrix)	6.2 seconds
Error Calculation / Printing / Plotting (per fission matrix)	5.4 seconds
Reading FM database and fitting polynomials (per batch)	41 seconds

The same method can be applied to Nuclear Thermal Propulsion type reactors

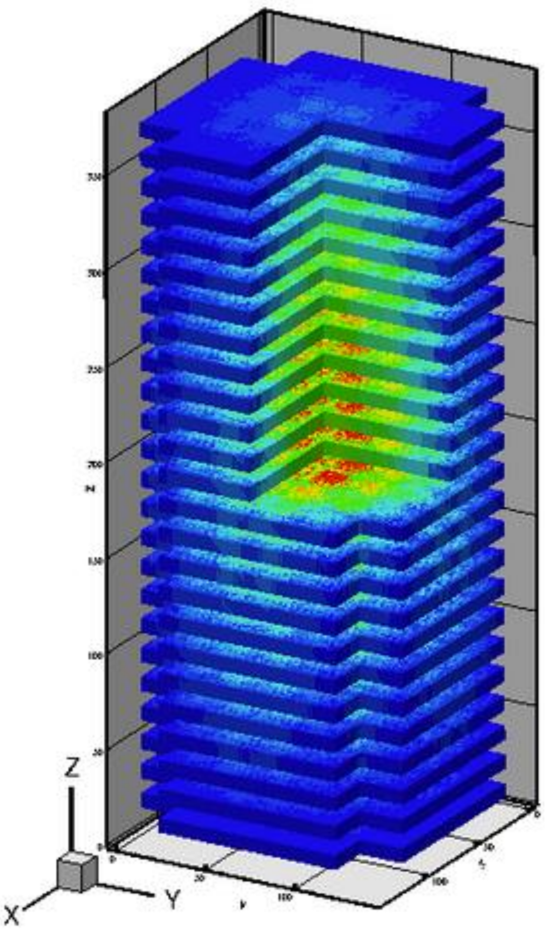


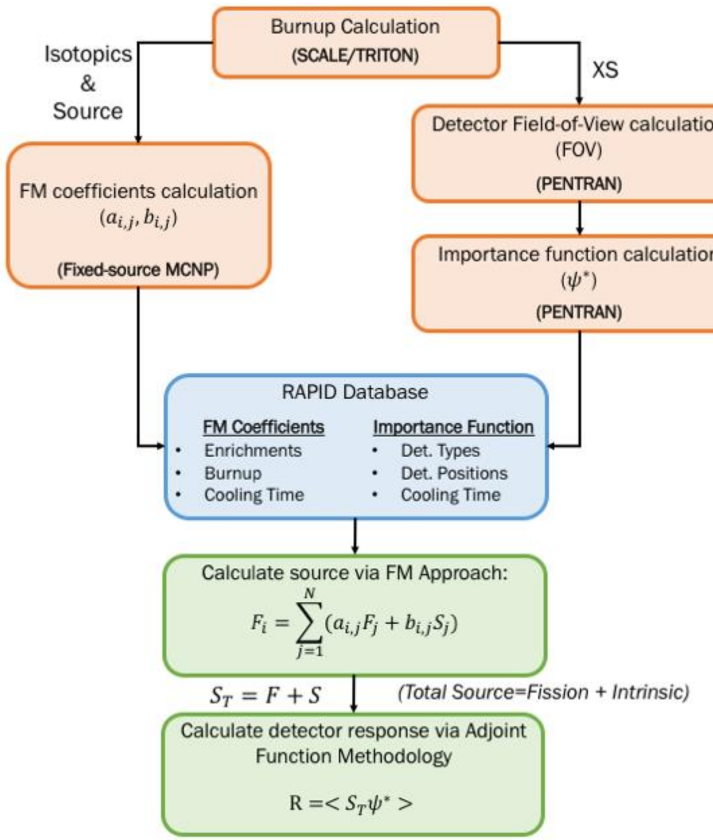
Both are small cores, hexagonal loading patterns
Control geometry is different (drums vs. fuel-followed rods)
Fuel/Moderator Heterogeneity and Feedback Mechanisms are different

Presentation Outline

- RAPID Material Correction Ratios (Donghao He)
- Temperature/Control Methods for TRIGA and NTP (Adam Rau)
- Xenon Transients in Penn State TRIGA Reactor
  (Jake Eichenlaub)
- Transient Fission Matrix Methods in TREAT Reactor (Alvaro Pizarro-Vallejos)

RAPID uses fission matrix methods for fast calculations





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Fission Matrix Method

2. Fit polynomial coefficients to fission matrix database

$$a_{ij}^{(n_T n_\theta)} = \sum_{k=0}^{K} \sum_{l=0}^{L} c_{ijkl} \left(T^{(n_T)}\right)^k \left(\cos\left(\theta^{(n_\theta)}\right)\right)^l$$

$$\boldsymbol{A_{ij}} = \boldsymbol{C_{ij}} \boldsymbol{V}$$

$$\boldsymbol{C_{ij}} = \boldsymbol{A_{ij}} \boldsymbol{V^T} \left(\boldsymbol{V} \boldsymbol{V^T}\right)^{-\mathbf{1}}$$

Control Drum Angle: Summary

Control Drum Angle [deg]	k_{eff} Error [pcm]	Norm. RMS Fiss. Src. Error [%]	Norm. Max. Fiss. Src. Error [%]
0	5.2	0.67	-2.29
8	9.7	0.60	-2.54
25	3.8	0.54	-2.17
38	-1.3	0.57	-1.87
53	0.1	0.58	2.01
68	17.3	0.68	-2.67
83	3.4	0.59	-2.22
98	12.4	0.63	-2.88
113	-7.0	0.65	-2.27
123	-22.0	0.71	-2.38
126	7.4	0.57	-2.35
128	3.1	0.65	-2.58
129	-6.8	0.55	-2.51
132	-5.8	0.65	-2.44
143	-10.6	0.53	-2.11
153	-11.8	0.68	-2.80
156	-7.4	0.66	-2.39
158	-19.5	0.53	-2.88
159	-14.6	0.62	-2.03
162	3.4	0.56	-2.03
173	-8.6	0.63	-2.20
180	-13.9	0.69	-2.59

Case: Temperature Profile

- Inlet:
  - Uniform 300K
- Outlet:
  - Proportional to lateral peaking factor at 300K
  - Max. temp. controlled as parameter
- Linearly increasing along axis

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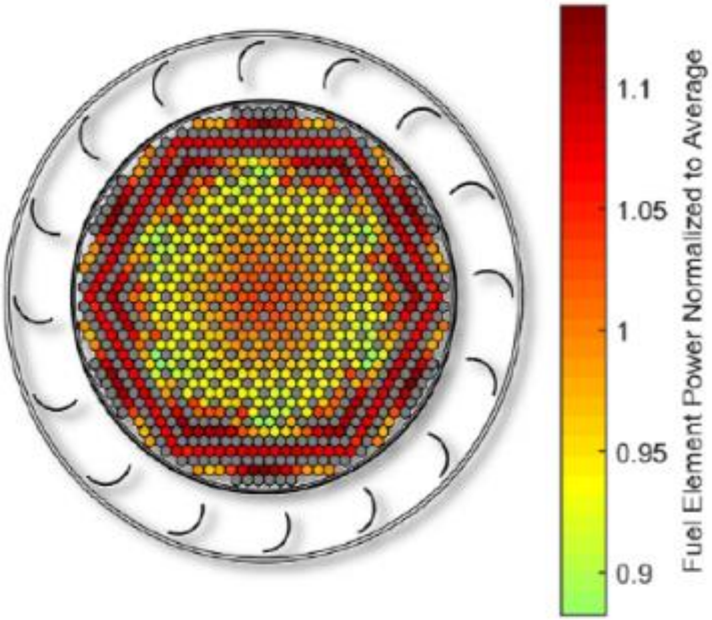
Case: SULEU Core

- Superb Use of Low-Enriched Uranium (SULEU) Core (Venneri et al., 2016)
- Based on heritage NERVA design
  - Demonstrate feasibility of LEU
  - Retains graphite-composite fuel elements and other peripherals
- Meets NASA DRA 5.0 requirements
  - Mass: 2,498 kg
  - Thrust: 35,000 lb_f
  - T_{max}: 2,850 K
  - Specific Impulse: 898 s



Venneri et al., 2016

Cases: Test Cases

- Fuel Temperature Cases:
  - Max. Fuel Temperature set to 400, 800, 1200, 1600, 2000 K
  - Control drums fully withdrawn
- Control Drum Cases:
  - Control drums set to 0, 8, 25, 38, 53, 68, 83, 98, 113,123, 126, 128, 129, 132, 143, 153, 156, 158, 159, 162, 173, 180 degrees
  - Max. Fuel Temperature fixed at 2000 K

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Cases: Test Cases

- Varied max. temperature and control drum angle separately (no case has uniform temperature)

Varied control drum angle

Max. Fuel Temp. [K]	Control Drum Angle [deg.]	Max. Fuel Temp. [K]	Control Drum Angle [deg.]
2000	0	2000	128
2000	8	2000	129
2000	25	2000	132
2000	38	2000	143
2000	53	2000	153
2000	68	2000	156
2000	83	2000	158
2000	98	2000	159
2000	113	2000	162
2000	123	2000	173
2000	126	2000	180

Varied temperature

Max. Fuel Temp. [K]	Control Drum Angle [deg.]
400	0
800	0
1200	0
1600	0
2000	0

Previous Work: Steady-State

- Rau and Walters 2018, Topham et al. 2019
  - Coupled TRACE/Fission Matrix simulation of TRIGA reactor
  - Fission matrix method used to investigate sensitivities in TRACE and validate on initial startup data

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Features of Fission Matrices

$$k_{eff}\vec{s} = \mathbf{A}\vec{s}$$

$\vec{s}$ is eigenvector of ***A***

k_{eff} is eigenvalue of ***A***

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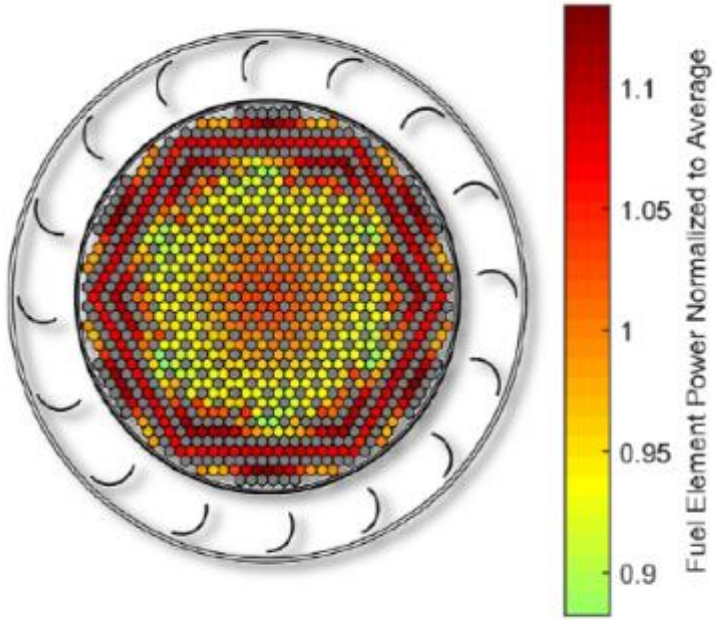
Case: SULEU Core (cont.)

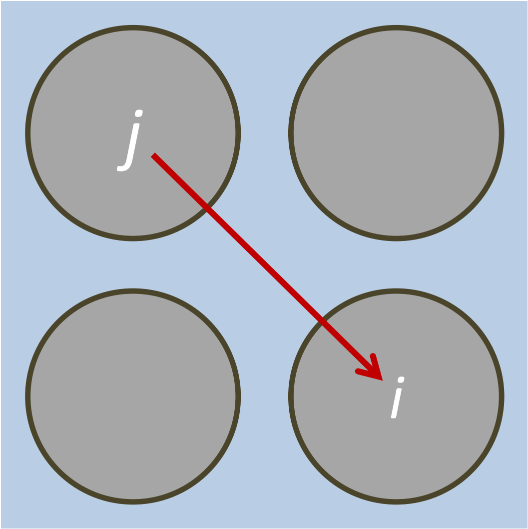
- (U,Zr)C composite fuel
- $ZrH_{1.7}$ moderator
- 66 cm core diameter (~26 in.)
- 16 rotating control drums on core periphery



Venneri et al., 2016

Features of Fission Matrices

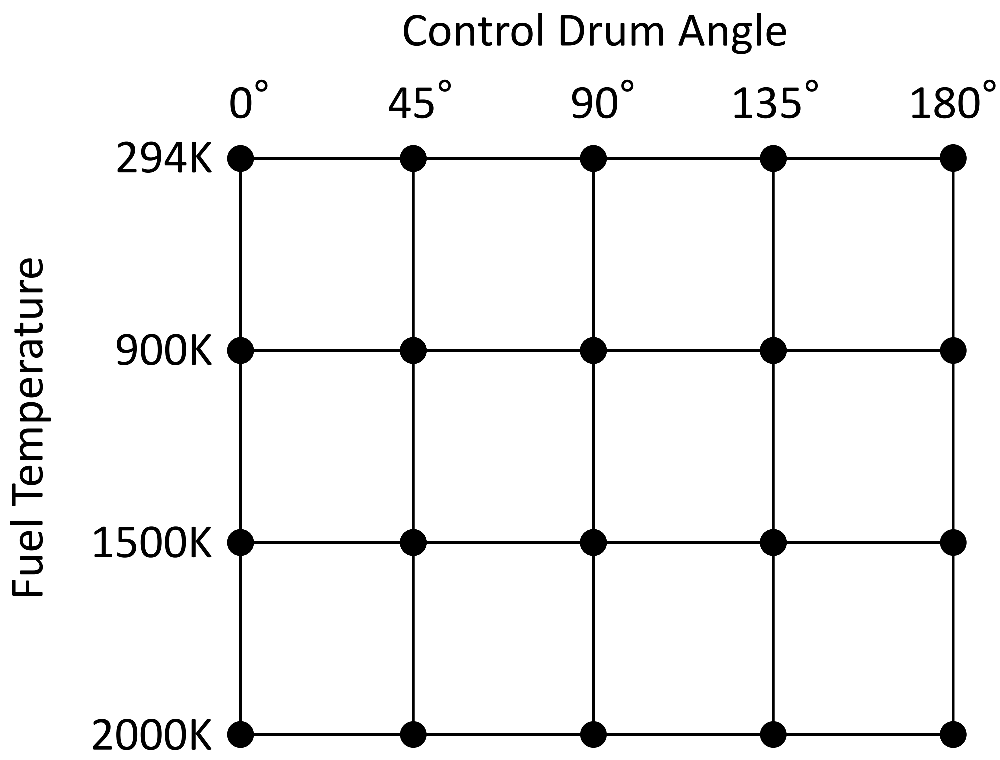
$$a_{ij} = f(\vec{r}_j \rightarrow \vec{r}_i)$$



Elements of $\boldsymbol{A}$ (a_{ij}): expected number of neutrons induced in cell i from a neutron born in cell j

Methodology: Preprocessing

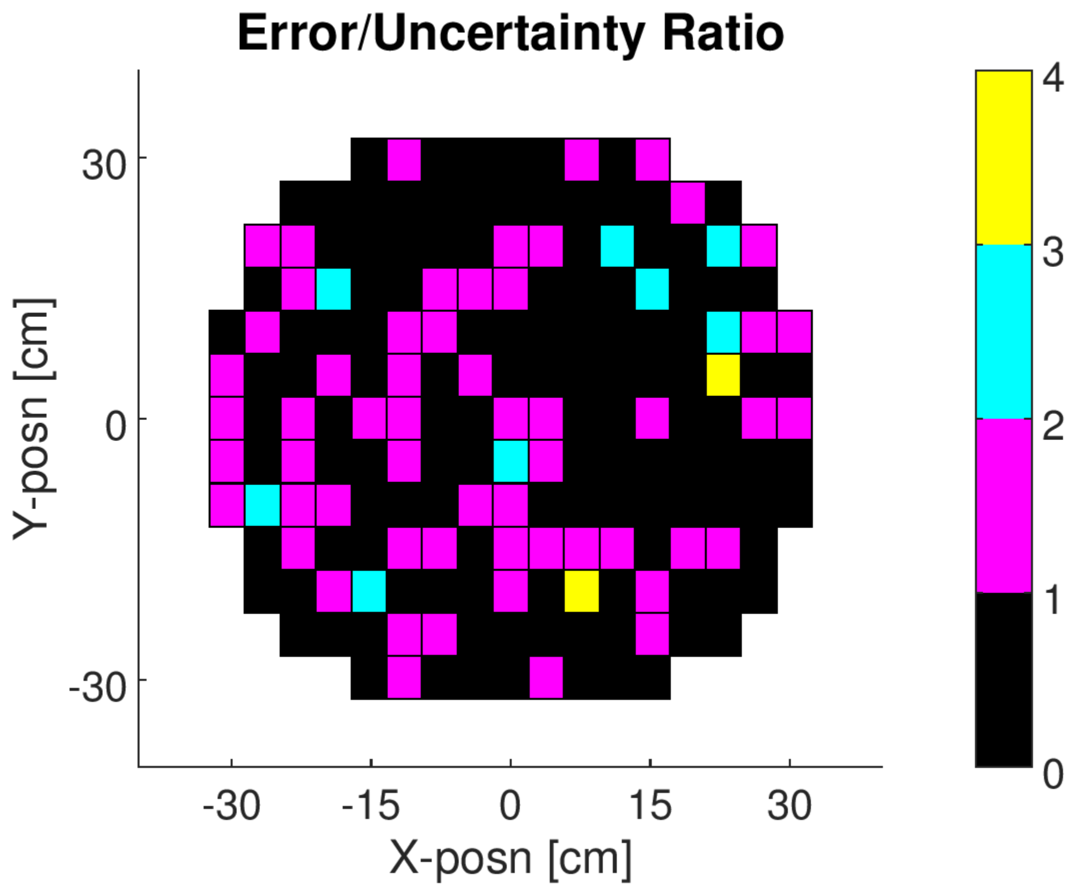
1. Serpent used to pre-calculate fission matrices at uniform fuel temperature and control drum angle



4 fuel temperatures
× 5 control drum angles

20 database calculations

Fuel Temperature: Error/Uncertainty



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Normalized Error

$$\hat{e_i} = \frac{f_{i,FM} - f_{i,serp}}{\left(\frac{1}{n}\right)\sum_i^n f_{i,serp}}$$

Margins