Demonstration of Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulations Using Serpent 2/ SUBCHANFLOW

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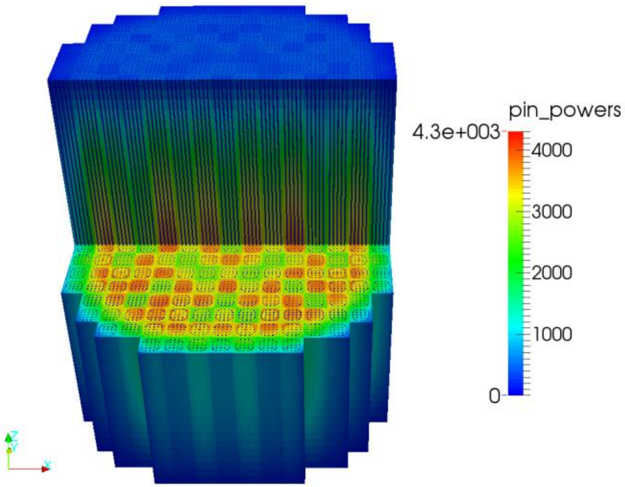


Outline

1. Internal coupling between Serpent 2 and SUBCHANFLOW
2. Stochastic mixing fall back for TMS method
3. Channel and sub-channel TH solution verification
4. Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation

Thermal-hydraulic feedback modeling in Serpent

- ‚Half-internal' universal multi-physics interface

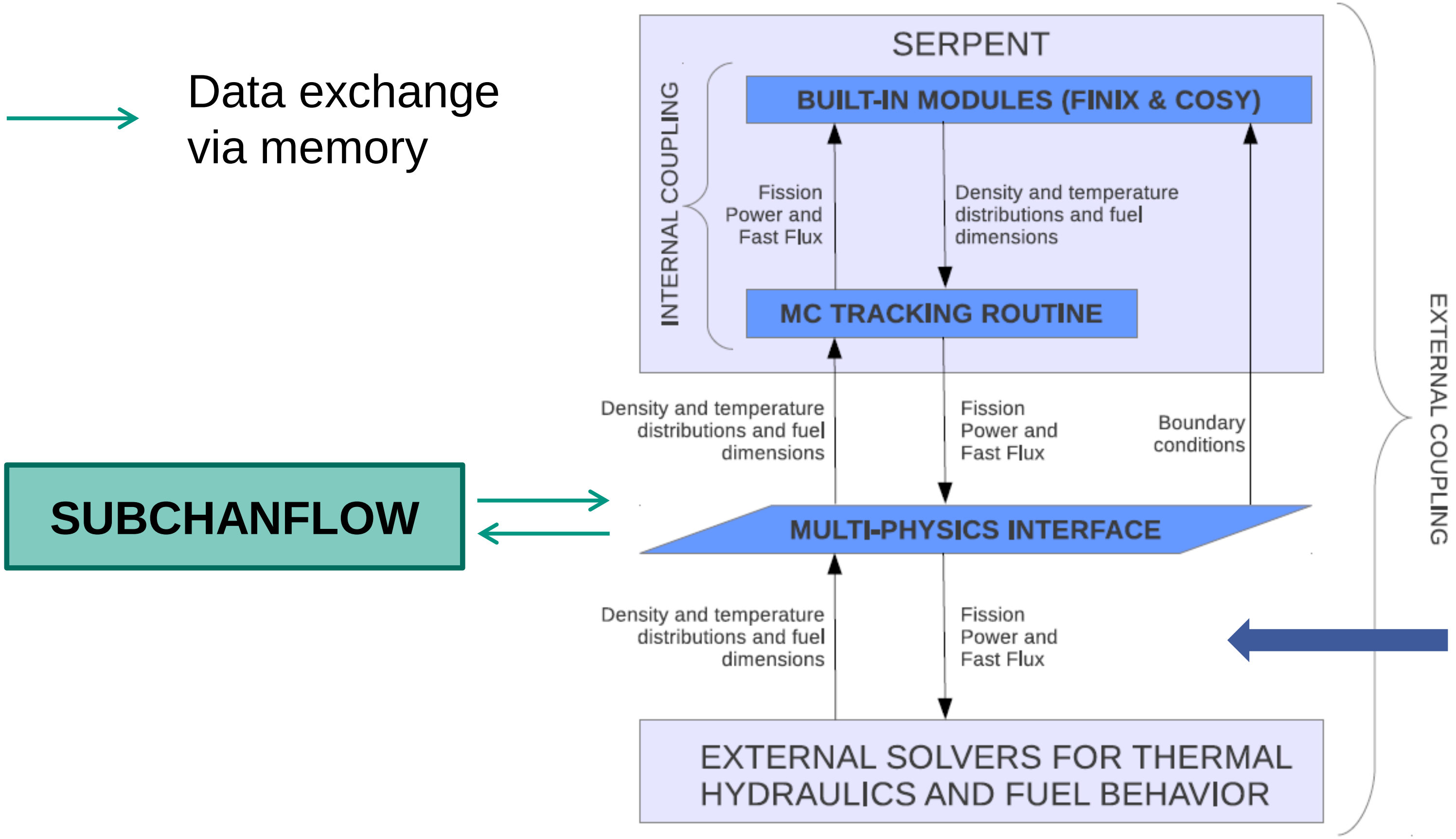
- Four types of interface:
  - piecewise constant distributions on regular meshes (type 1),
  - weighted averages of point-wise values (type 2),
  - a user-defined functional dependence (type 3)
  - unstructured three-dimensional meshes (type 4)

Used for Serpent/SCF

- Enabling the interface implies using the target motion sampling (TMS) method

- TMS is not compatible with thermal bound scattering and unresolved resonance treatment

Internal Serpent/SUBCHANFLOW coupling



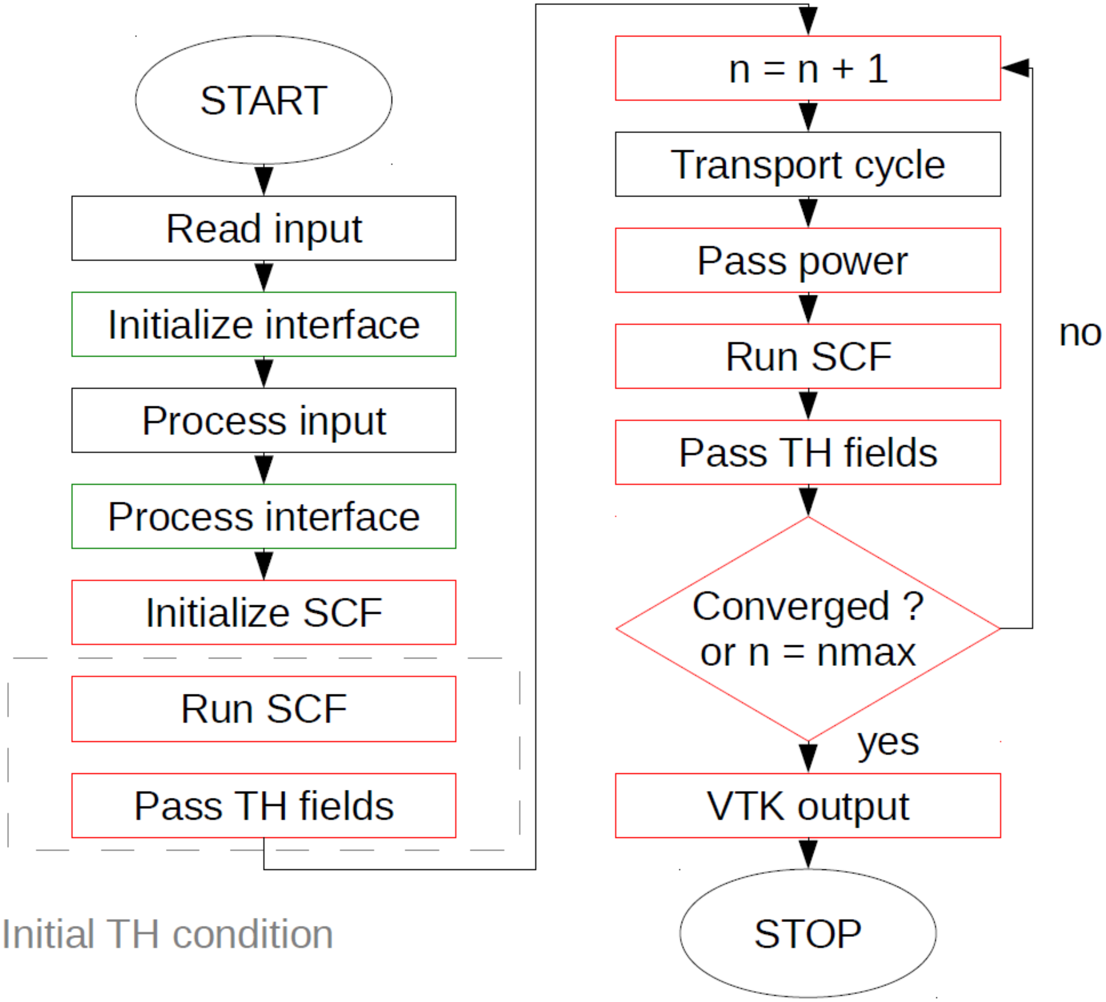
Data exchange via memory

SUBCHANFLOW

ASCII file I/O

Figure: Multi-physics coupling scheme in Serpent 2

Serpent/SCF coupled iteration algorithm



START

Read input

Initialize interface

Process input

Process interface

Initialize SCF

Run SCF

Pass TH fields

Initial TH condition

n = n + 1

Transport cycle

Pass power

Run SCF

Pass TH fields

Converged ?
or n = nmax

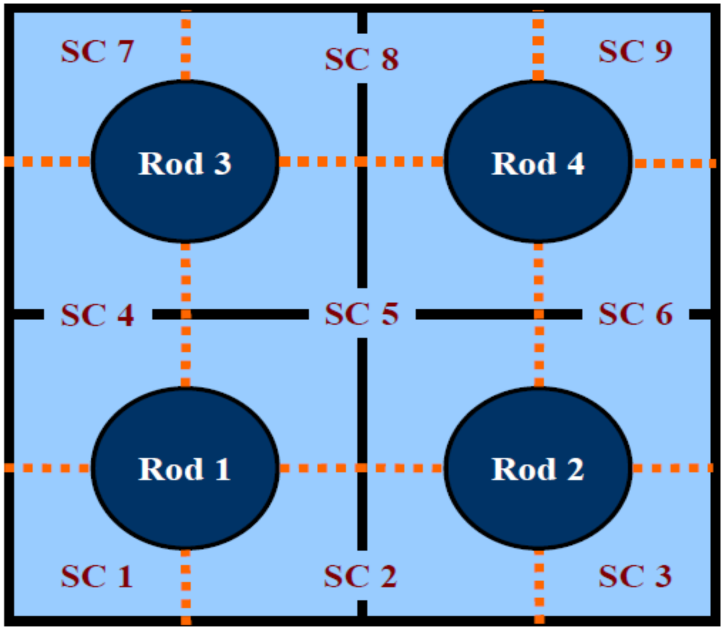
no

yes

VTK output

STOP

Spatial mapping between Serpent and SCF



$$T_{dopp} = (1-\alpha)\, T_{f,c} + \alpha\, T_{f,s}$$

Channel and sub-channel level TH models possible

Relaxation scheme and convergence criteria

- Relaxation scheme developed by J. Dufek et al.

$$\phi^n = \frac{1}{n} \sum_{i=1}^{n} \tilde{\phi}^i$$

$$\phi^n = \left(1 - \frac{1}{n}\right) \phi^{n-1} + \frac{1}{n} \tilde{\phi}^n$$

- Convergence checking based on l2 norm

$$\frac{\Delta X}{X} = \frac{\left\| X^n - X^{n-1} \right\|_{l^2}}{\left\| X^n \right\|_{l^2}} \leq \epsilon_X$$

Assuring a converged solution

- Coupled convergence is limited by maximum statistical uncertainty of Monte Carlo power tally

  → **Global variance reduction**, i.e. The Uniform Fission Site method (UFS)

- Testing convergence of fission source: Shannon entropy evaluated on a superimposed mesh

- Statistical uncertainty of all coupled fields only available by replica runs

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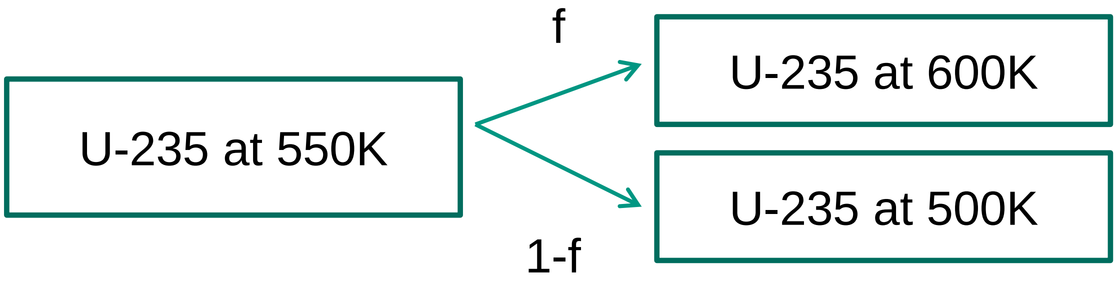
How to overcome shortcomings of TMS method?

- TMS method is limited to cases without
  - Thermal bound scattering
  - Need for treatment of unresolved resonance range

- Most coupled Monte Carlo thermal-hydraulic tools utilize stochastic mixing to realize changing cross sections with temperature



U-235 at 550K

f

U-235 at 600K

1-f

U-235 at 500K

Let Serpent automatically fall back to stochastic mixing where TMS is not applicable

Role of majorant cross section with varying material density and temperature (1/2)

Method only discussed for 0K basis CE cross sections

1. Sample neutron path length from

$$l = -\frac{\log(\xi)}{\Sigma_{maj}}$$

ξ is a uniformly distributed random variable

2. Accept or reject collision point candidate based on

$$g(\vec{r}) = {}^{\rho(\vec{r})}/_{\rho_{max}}$$

3. Sample collision nuclide based on nulide-wise majorants

$$p_n = {}^{\Sigma_{maj,n}(E)}/_{\Sigma_{maj}(E)}$$

4. Sample velocity and direction of target from Maxwellian distribution, switch into target-at-rest frame

Role of majorant cross section with varying material density and temperature (2/2)

5. Accept or reject collision point candidate based on

$$\xi < \Sigma_{tot,n}{}^{0K}\,(\vec{r},E') \Big/ \Sigma_{maj,n}(E)$$

6. Sample reaction type based on nuclide microscopic cross sections

Bound atoms do not have a Maxwellian velocity distribution

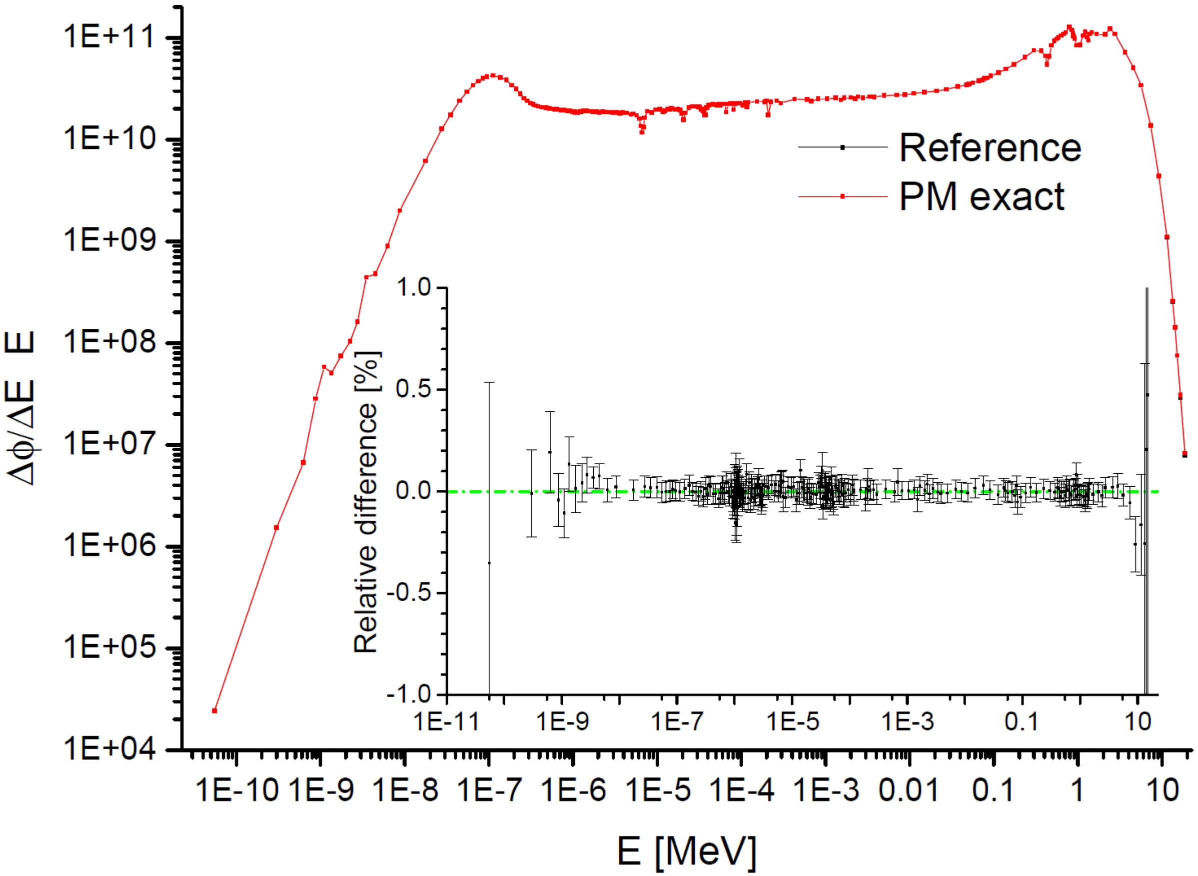
Stochastic mixing fall back for TMS

4. *If collision nuclide has no thermal scattering data associated with it*
   Sample velocity and direction of target from Maxwellian distribution, switch into target-at-rest frame

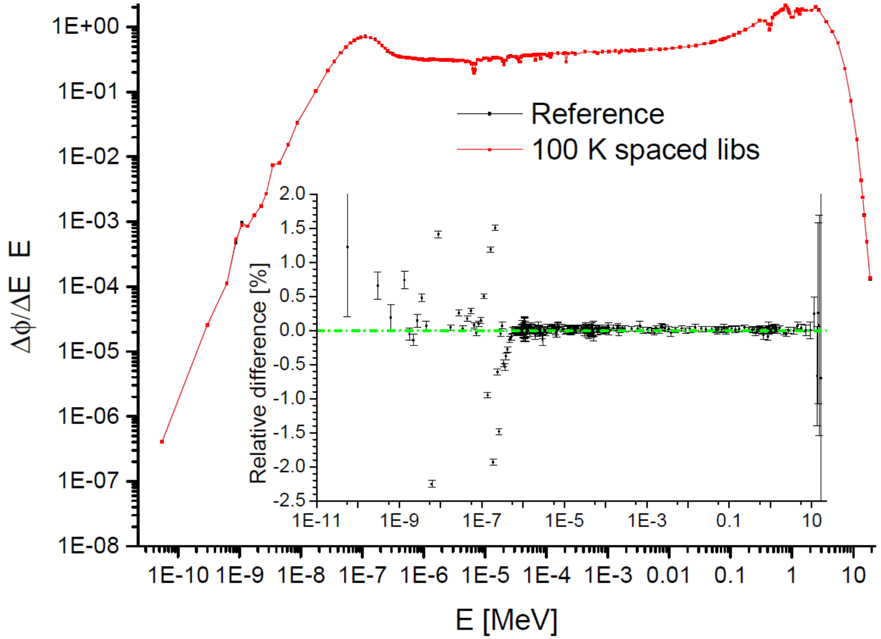
   else
   identify two scattering nuclides with temperatures enclosing the local temperature, compute the mixing fraction and use it to sample which scattering nuclide to use, do NOT transform into target-at-rest frame

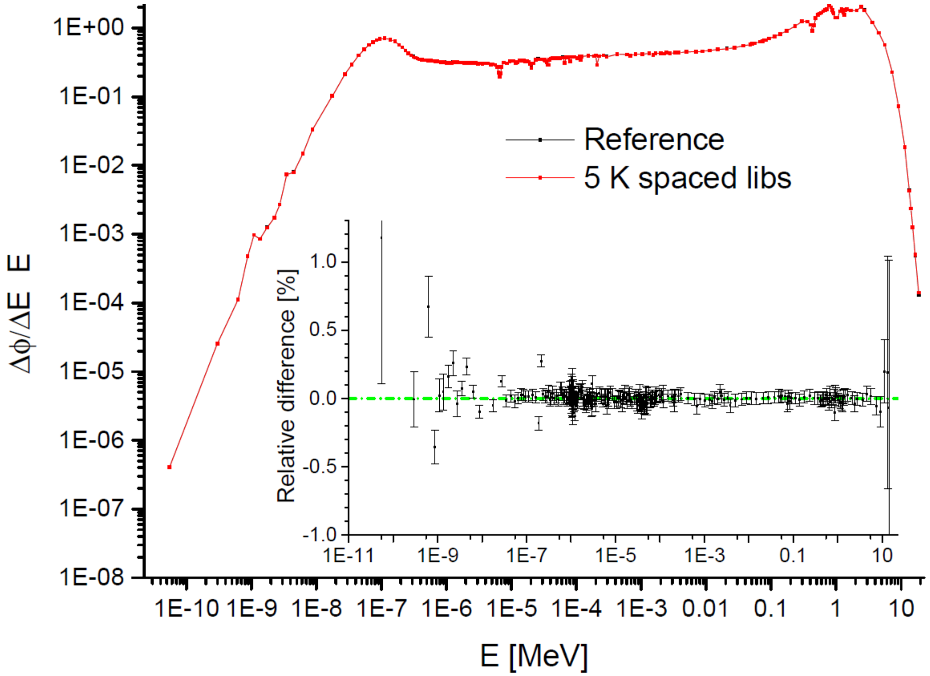
Code verification for stochastic mixing fall back

- Infinite lattice of 3.65755m high fresh UOX 4.2wt% fuel pins
- Two axial water zones: 500K and 600K
- Fuel temperature 900K and structures at 600K



Necessary temperature spacing of S(α,β)





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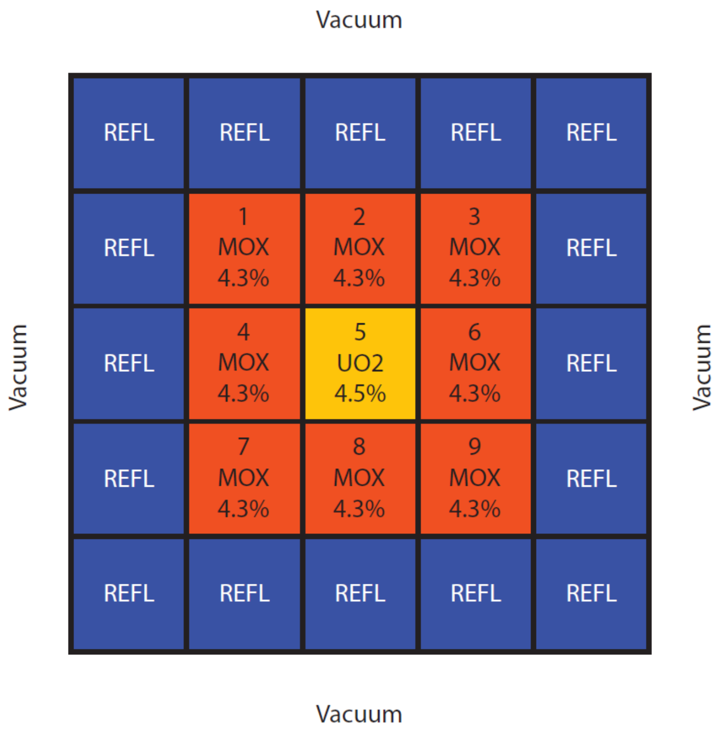
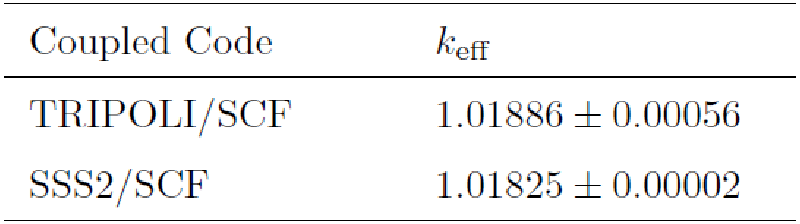
Channel TH solution verification case (1/3)

- Code-to-code benchmark with TRIPOLI/SUBCHANFLOW
- 3x3 minicore from NURISP boron dilution benchmark
- JEFF 3.1.1 CE nuclear data
- Coupled convergence <1% for TH fields

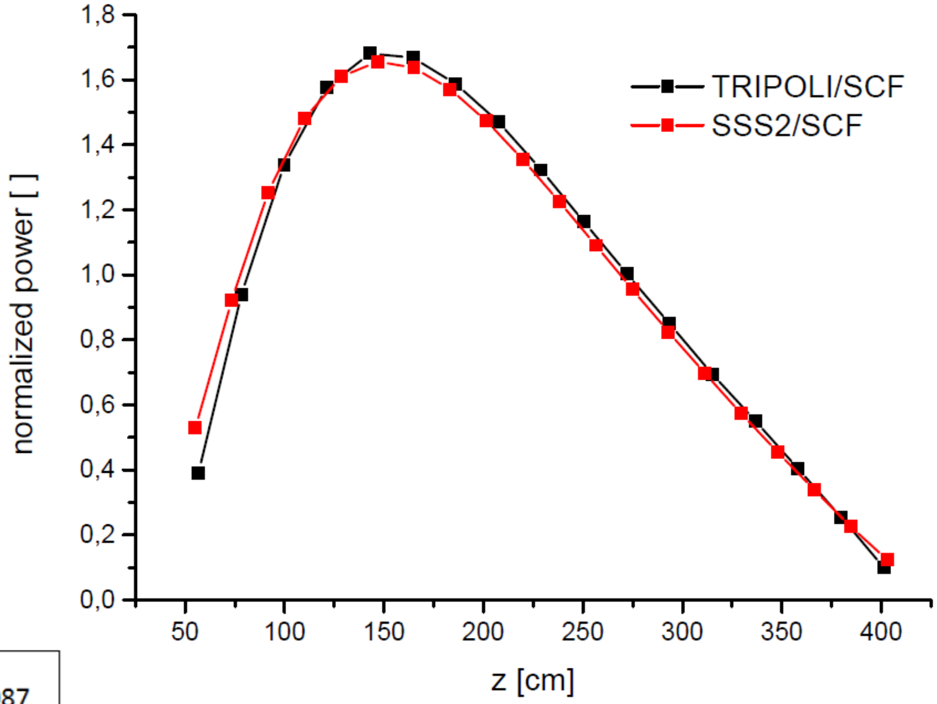


Quantity	Value
Power	100 MW
Core mass flow rate	739.08 $^{\mathrm{kg}}/_{\mathrm{s}}$
Outlet pressure	15.4 MPa
Coolant inlet temperature	560 K
Boron concentration	200 ppm

Channel TH solution verification case (2/3)

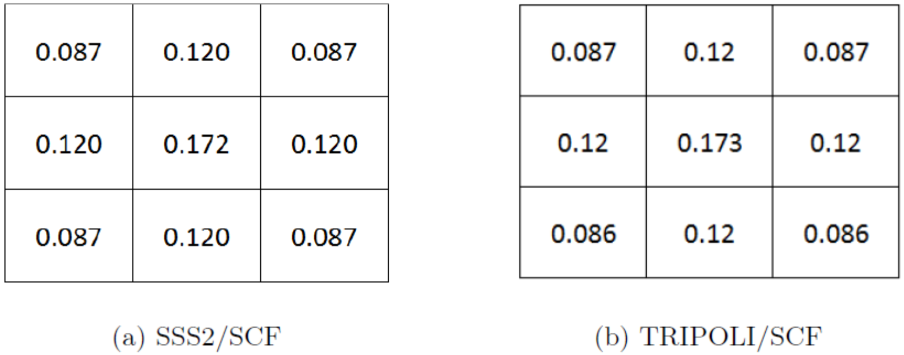


Coupled Code	k_{eff}
TRIPOLI/SCF	1.01886 ± 0.00056
SSS2/SCF	1.01825 ± 0.00002



Axial power profile in central assembly

Radial power profiles



0.087	0.120	0.087
0.120	0.172	0.120
0.087	0.120	0.087

(a) SSS2/SCF

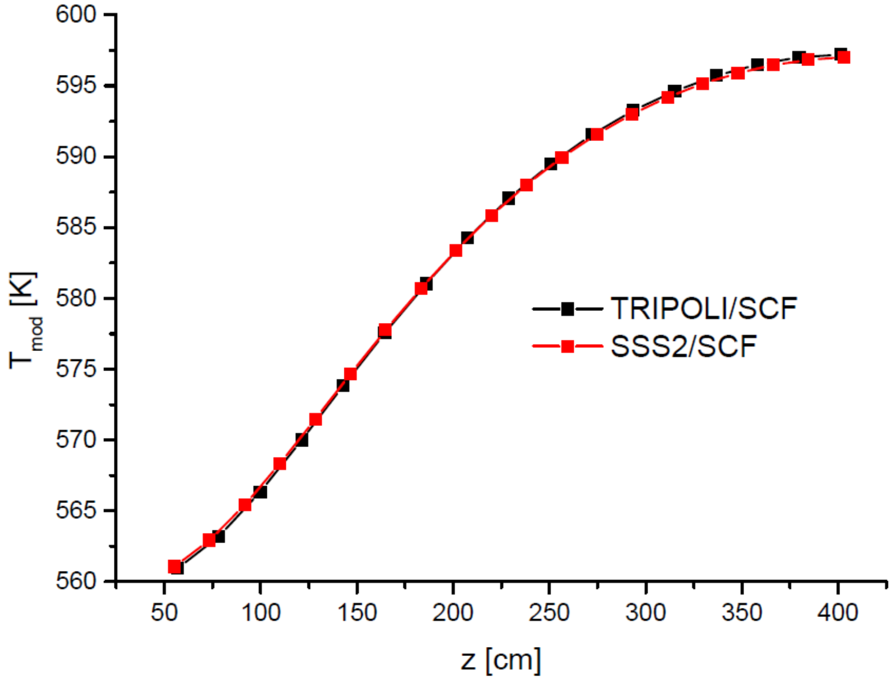
0.087	0.12	0.087
0.12	0.173	0.12
0.086	0.12	0.086

(b) TRIPOLI/SCF

SSS2/SCF: 11 CPU-months

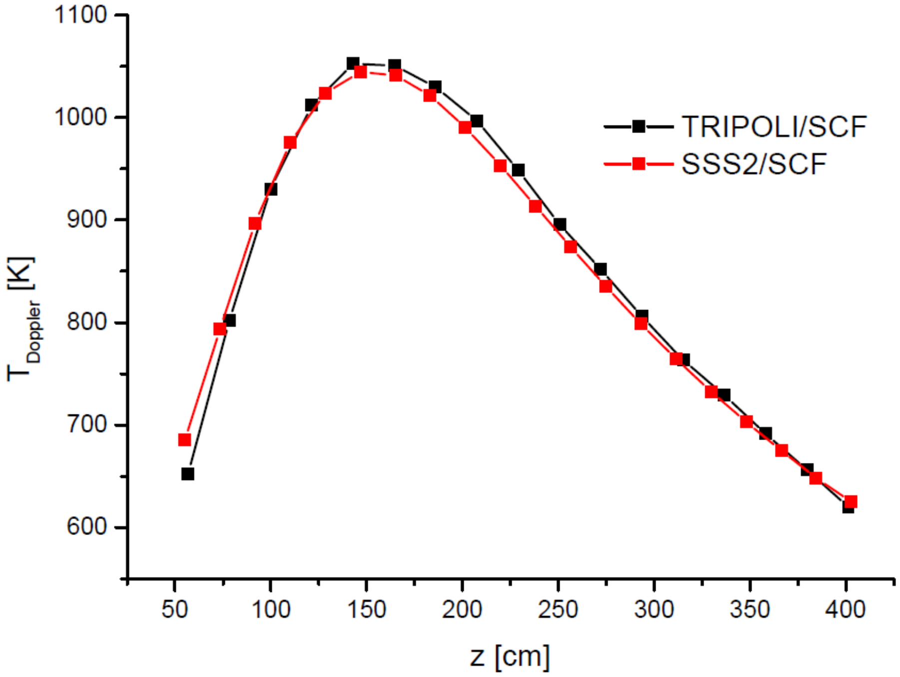
on Intel Xeon E5-2670, InfiniBand

Channel TH solution verification case (3/3)



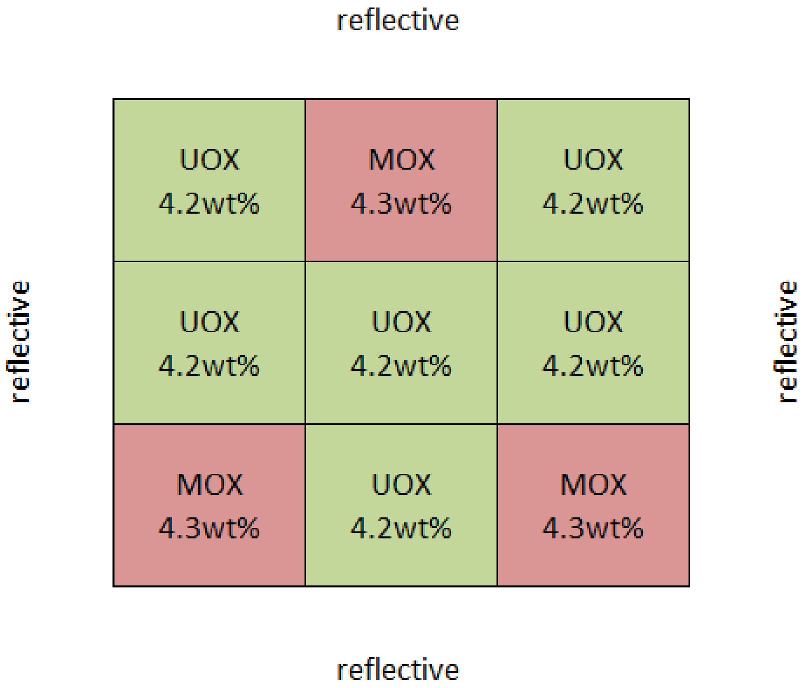
Axial moderator temperature profile in central assembly

Axial Doppler temperature profile in central assembly



Sub-channel TH solution verification case (1/3)

- Code-to-code benchmark with MCNP5/SUBCHANFLOW
- 3x3 minicore from HPMC project, sub-channel
- JEFF 3.1.1 CE nuclear data
- Coupled convergence <0.05% for TH fields



UOX 4.2wt%	MOX 4.3wt%	UOX 4.2wt%
UOX 4.2wt%	UOX 4.2wt%	UOX 4.2wt%
MOX 4.3wt%	UOX 4.2wt%	MOX 4.3wt%

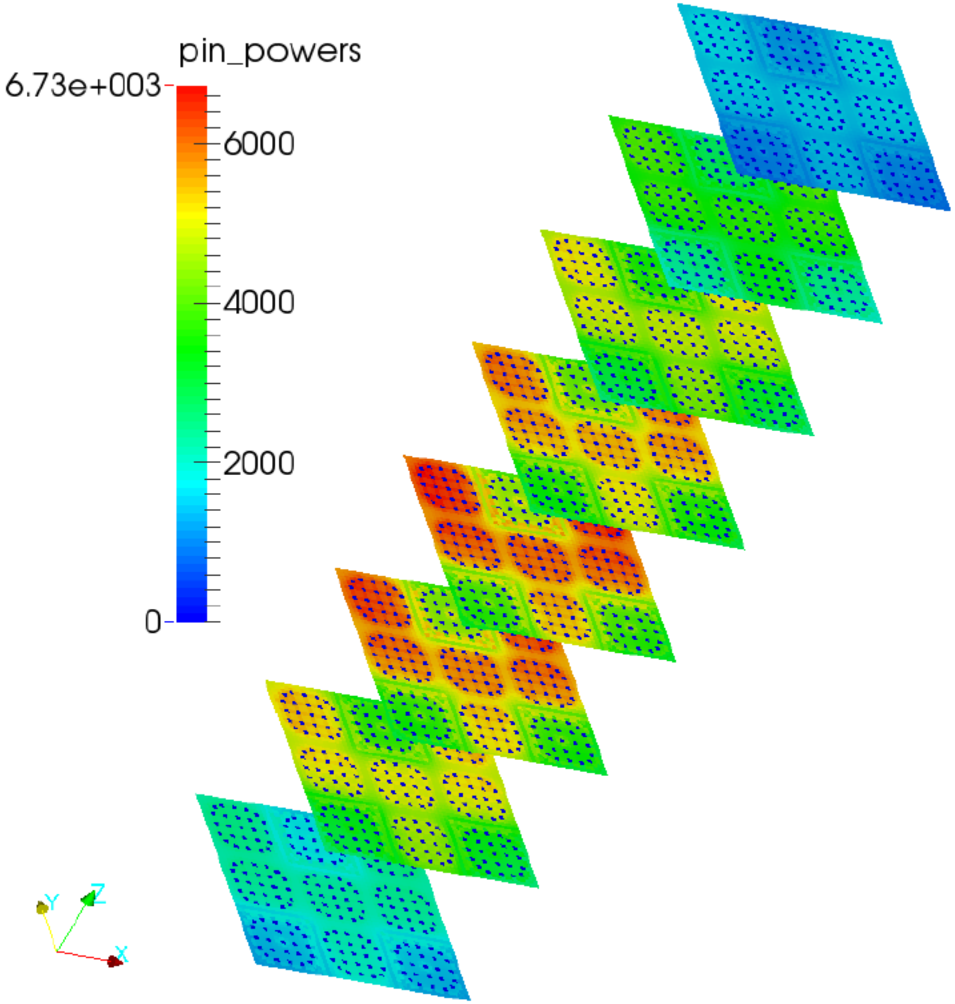
Quantity	Value
Power	166.24 MW
Core mass flow rate	739.09 $^{\mathrm{kg}}/_{\mathrm{s}}$
Outlet pressure	15.45 MPa
Coolant inlet temperature	560 K
Boron concentration	1200 ppm

Sub-channel TH solution verification case (2/3)

Coupled Code	k_{eff}
MCNP5/SCF	1.22298 ± 0.00004
SSS2/SCF	1.22192 ± 0.00001

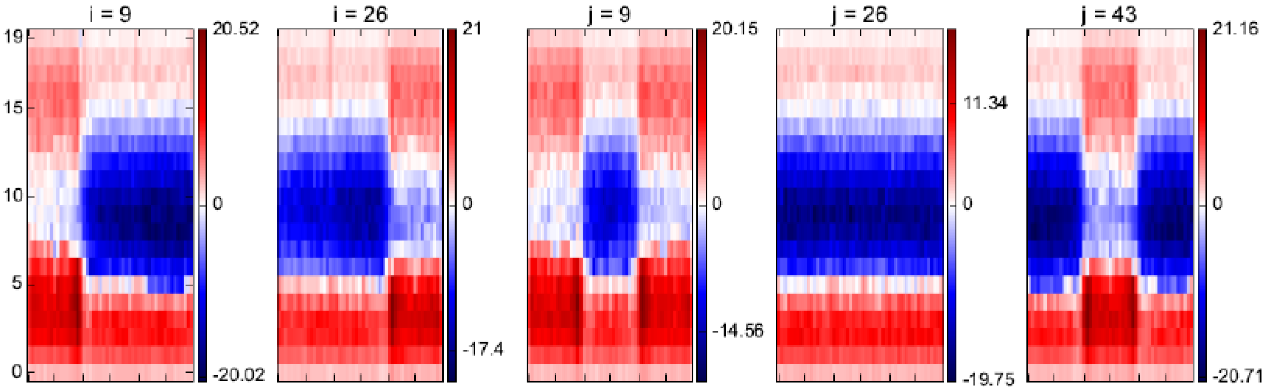
SSS2/SCF: 11.2 CPU-months

on Intel Xeon E5-2670, InfiniBand

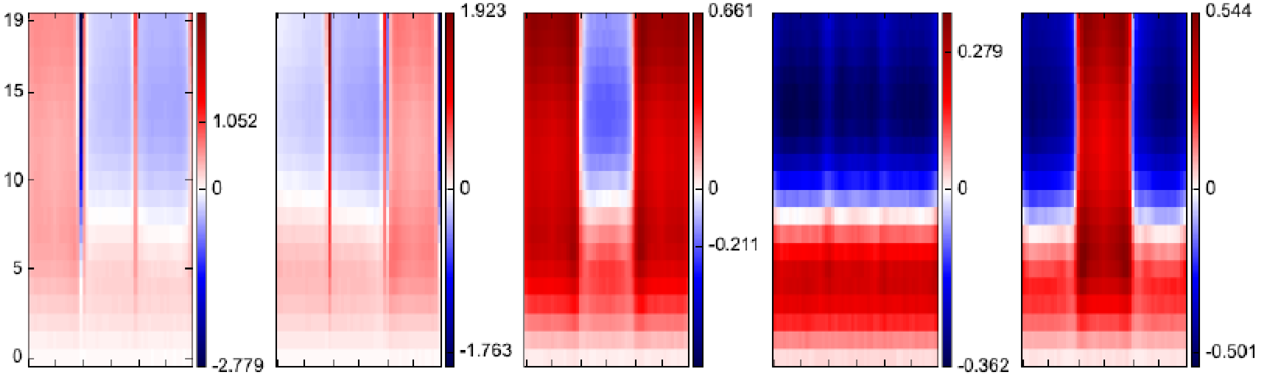


Sub-channel TH solution verification case (3/3)

- Absolute differences in Kelvin for five vertical cuts through minicore



(a) Effective Doppler temperature



(b) Moderator temperature

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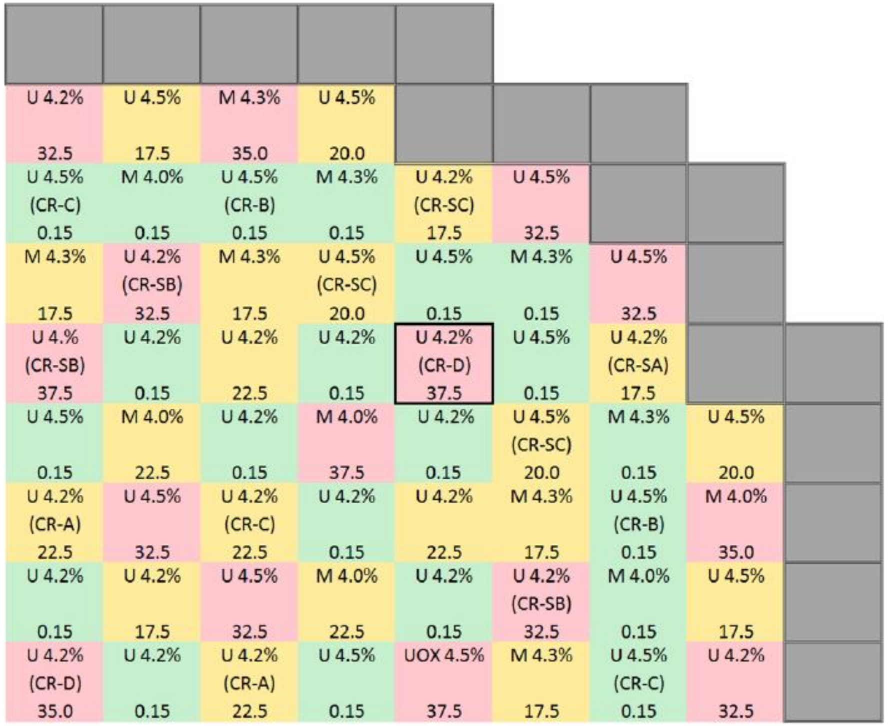
Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (1/6)

- Channel and sub-channel TH model of OECD NEA and U.S. NRC PWR MOX/UO2 core transient benchmark

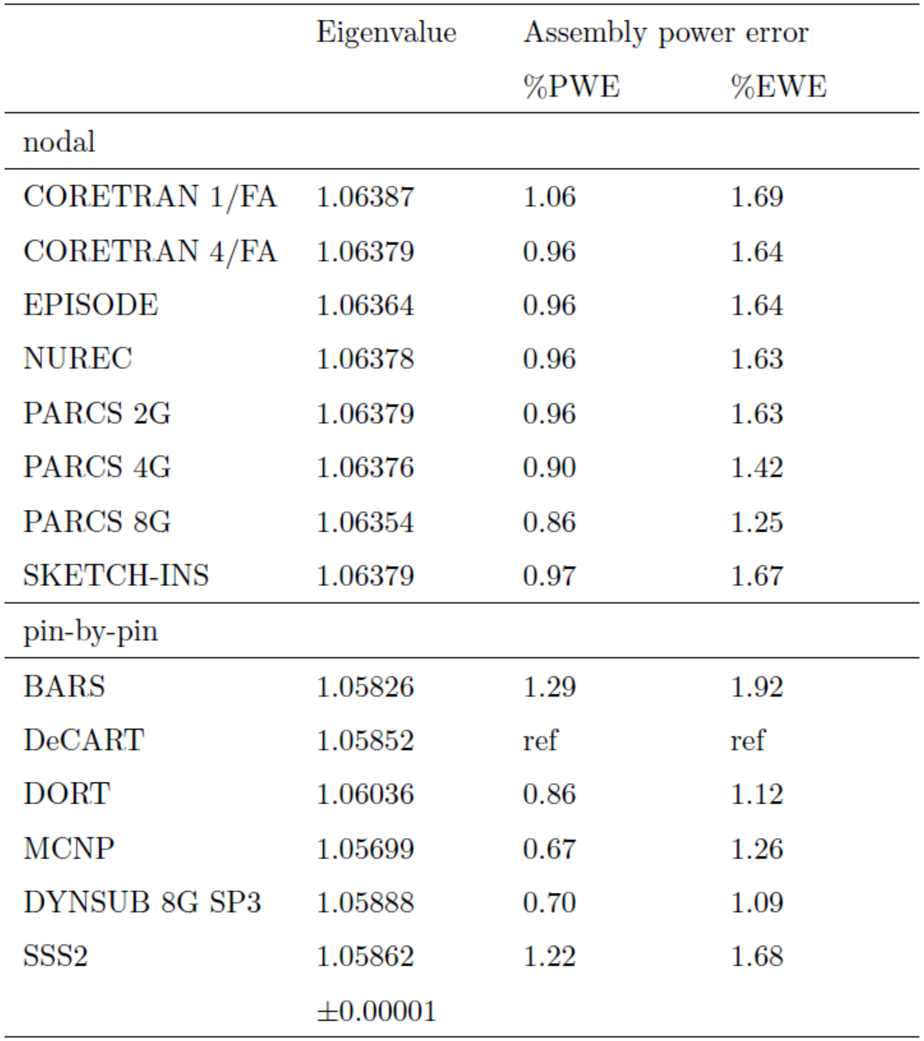


U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0					
U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SC) 17.5	U 4.5% 32.5			
M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5		
U 4.% (CR-SB) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5		
U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0	
U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.0% 35.0	
U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5	
U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	UOX 4.5% 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5	

Quantity	Value
Power	3565 MW
Core mass flow rate	15849.4 $\mathrm{kg/s}$
Inlet pressure	15.5 MPa
Coolant inlet temperature	560 K

Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (2/6)

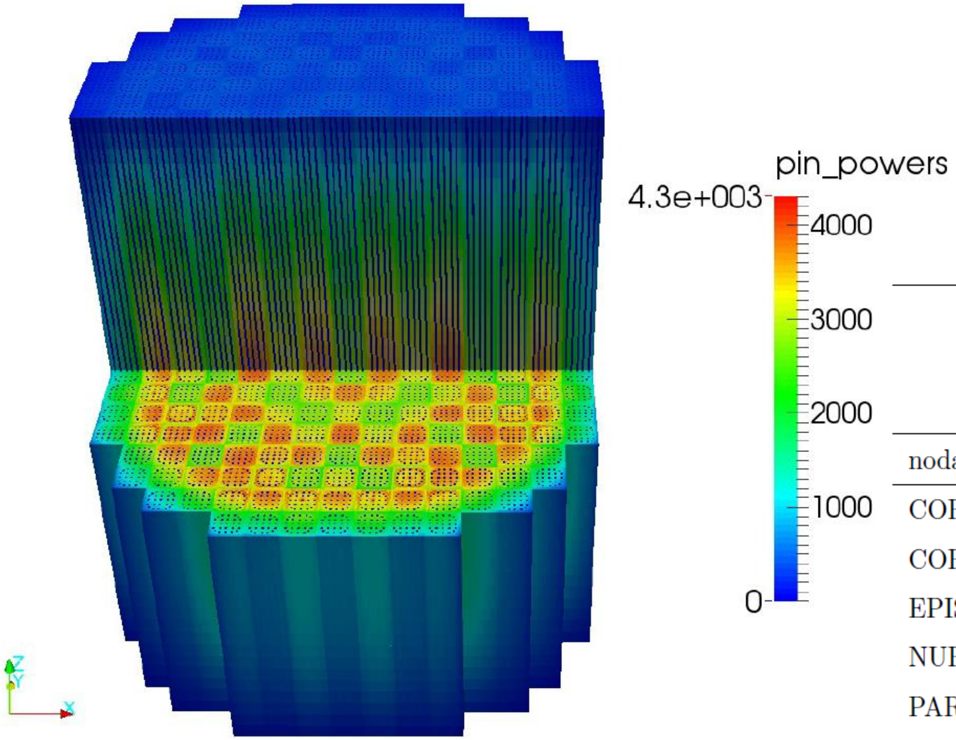
- Neutron transport model test with 2D HZP conditions
- Benchmark based on ENDF/B VI
- SSS2 used ENDF/B VII.0
- Coupled convergence <0.5% TH fields



	Eigenvalue	Assembly power error	
		%PWE	%EWE
nodal			
CORETRAN 1/FA	1.06387	1.06	1.69
CORETRAN 4/FA	1.06379	0.96	1.64
EPISODE	1.06364	0.96	1.64
NUREC	1.06378	0.96	1.63
PARCS 2G	1.06379	0.96	1.63
PARCS 4G	1.06376	0.90	1.42
PARCS 8G	1.06354	0.86	1.25
SKETCH-INS	1.06379	0.97	1.67
pin-by-pin			
BARS	1.05826	1.29	1.92
DeCART	1.05852	ref	ref
DORT	1.06036	0.86	1.12
MCNP	1.05699	0.67	1.26
DYNSUB 8G SP3	1.05888	0.70	1.09
SSS2	1.05862	1.22	1.68
	±0.00001		

Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (3/6)

5M neutrons per cycle, 2000 active cycles per iteration

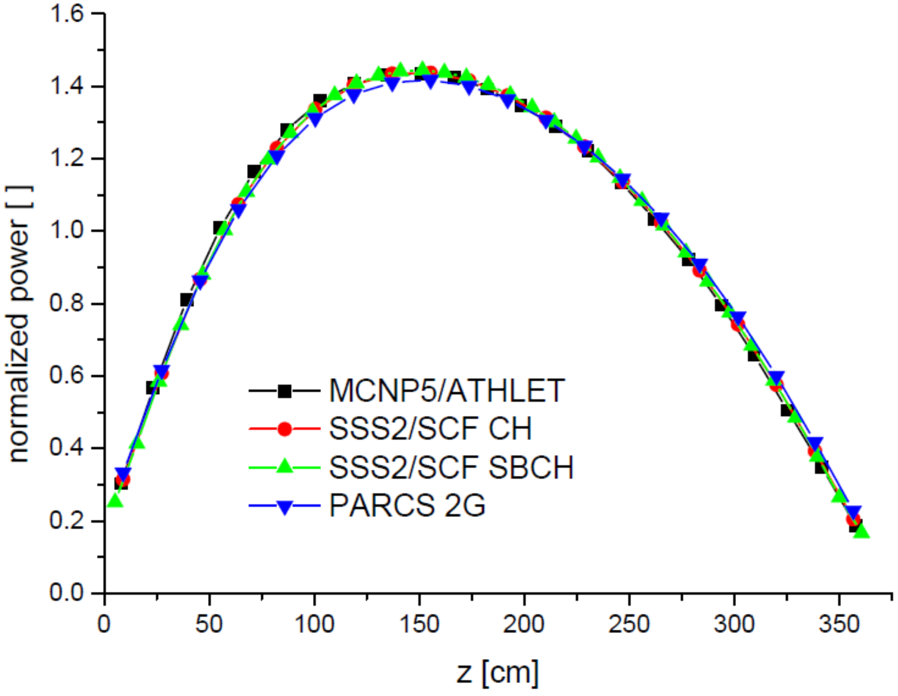


	Critical c_b [ppm]	Average T_{Dopp} [K]	Average ρ_M [kg/m3]	Average T_M [K]	Outlet ρ_M [kg/m^3]	Outlet T_M [K]
nodal						
CORETRAN 1/FA	1647	908.4	706.1	581.0	658.5	598.6
CORETRAN 4/FA	1645	908.4	706.1	581.0	658.5	598.6
EPISODE	1661	846.5	701.8	582.6	697.4	585.5
NUREC	1683	827.8	706.1	581.1	661.5	598.7
PARCS 2G	1679	836.0	706.1	581.3	662.1	598.8
PARCS 4G	1674	836.1	706.1	581.3	662.1	598.8
PARCS 8G	1672	836.2	706.1	581.3	662.1	598.8
SKETCH-INS	1675	836.6	705.5	580.9	659.6	598.9
pin-by-pin						
DYNSUB 8G SP3	1600	824.3	705.1	580.6	678.8	593.1
SSS2/SCF CH	1593	824.6	702.8	582.5	660.5	599.2
SSS2/SCF SBCH	1599	819.7	704.0	582.1	660.8	599.4

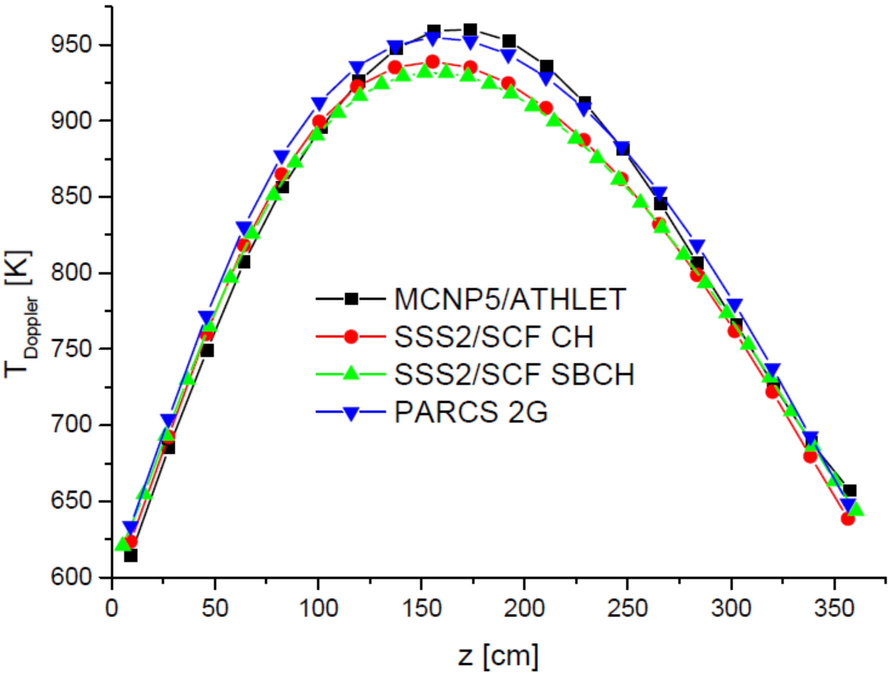
SSS2/SCF CH:	3.7 CPU-years
SSS2/SCF SBCH:	5.8 CPU-years

on Intel Xeon E5-2670, InfiniBand

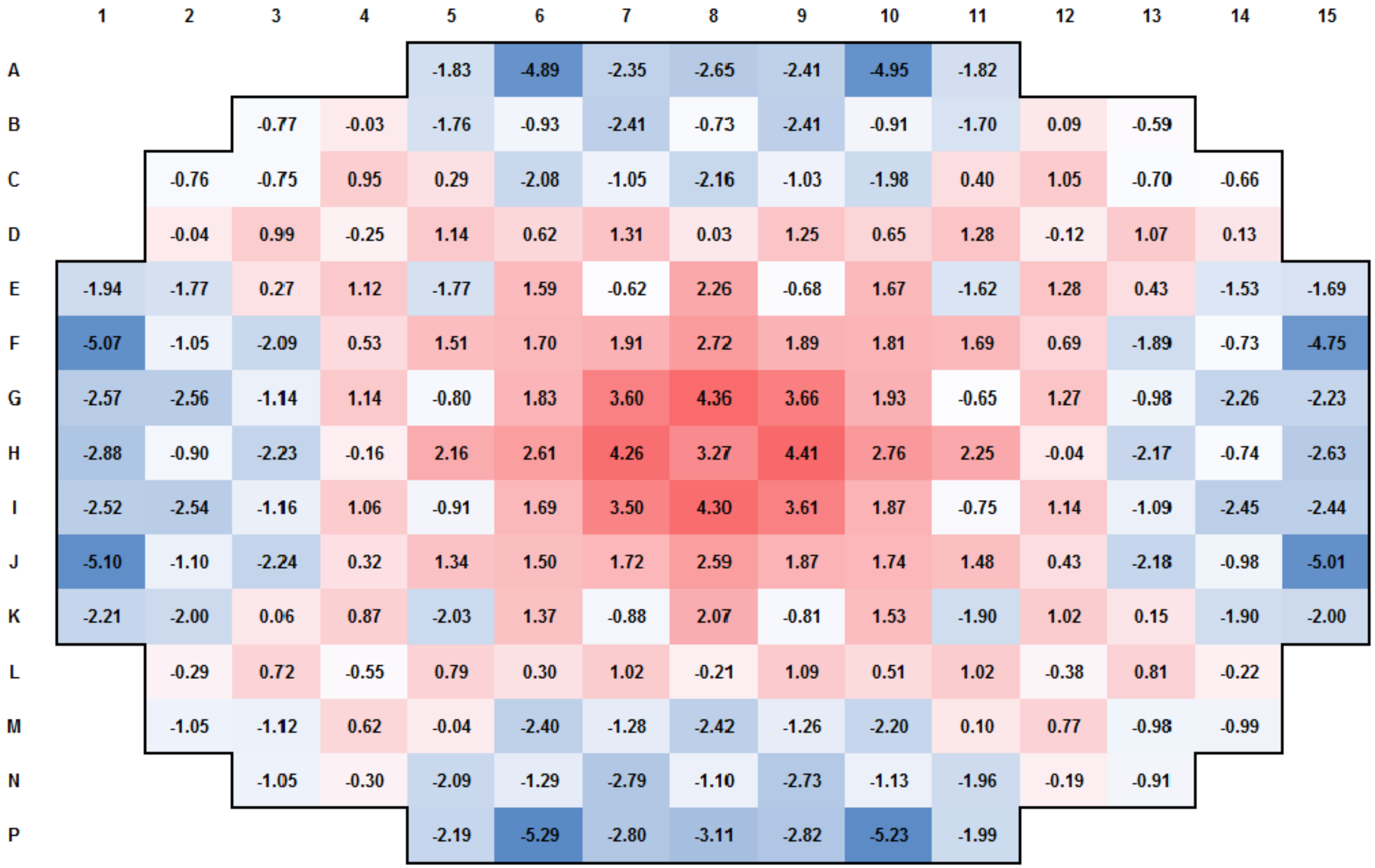
Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (4/6)



MCNP5/ATHLET solution: GRS at PHYSOR 2012



Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (5/6)



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
A					-1.83	-4.89	-2.35	-2.65	-2.41	-4.95	-1.82				
B			-0.77	-0.03	-1.76	-0.93	-2.41	-0.73	-2.41	-0.91	-1.70	0.09	-0.59		
C		-0.76	-0.75	0.95	0.29	-2.08	-1.05	-2.16	-1.03	-1.98	0.40	1.05	-0.70	-0.66	
D		-0.04	0.99	-0.25	1.14	0.62	1.31	0.03	1.25	0.65	1.28	-0.12	1.07	0.13	
E	-1.94	-1.77	0.27	1.12	-1.77	1.59	-0.62	2.26	-0.68	1.67	-1.62	1.28	0.43	-1.53	-1.69
F	-5.07	-1.05	-2.09	0.53	1.51	1.70	1.91	2.72	1.89	1.81	1.69	0.69	-1.89	-0.73	-4.75
G	-2.57	-2.56	-1.14	1.14	-0.80	1.83	3.60	4.36	3.66	1.93	-0.65	1.27	-0.98	-2.26	-2.23
H	-2.88	-0.90	-2.23	-0.16	2.16	2.61	4.26	3.27	4.41	2.76	2.25	-0.04	-2.17	-0.74	-2.63
I	-2.52	-2.54	-1.16	1.06	-0.91	1.69	3.50	4.30	3.61	1.87	-0.75	1.14	-1.09	-2.45	-2.44
J	-5.10	-1.10	-2.24	0.32	1.34	1.50	1.72	2.59	1.87	1.74	1.48	0.43	-2.18	-0.98	-5.01
K	-2.21	-2.00	0.06	0.87	-2.03	1.37	-0.88	2.07	-0.81	1.53	-1.90	1.02	0.15	-1.90	-2.00
L		-0.29	0.72	-0.55	0.79	0.30	1.02	-0.21	1.09	0.51	1.02	-0.38	0.81	-0.22	
M		-1.05	-1.12	0.62	-0.04	-2.40	-1.28	-2.42	-1.26	-2.20	0.10	0.77	-0.98	-0.99	
N			-1.05	-0.30	-2.09	-1.29	-2.79	-1.10	-2.73	-1.13	-1.96	-0.19	-0.91		
P					-2.19	-5.29	-2.80	-3.11	-2.82	-5.23	-1.99				

Difference in percent assembly power between SSS2/SCF CH and PARCS 2G

Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (6/6)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
A					0.21	0.17	0.15	0.23	0.15	0.17	0.21				
B			0.25	0.24	0.04	0.06	0.02	0.07	0.02	0.06	0.04	0.24	0.26		
C		0.26	0.08	0.11	0.20	0.12	0.29	0.09	0.29	0.12	0.21	0.11	0.09	0.26	
D		0.24	0.11	0.37	0.18	0.30	0.19	0.38	0.19	0.30	0.19	0.37	0.11	0.24	
E	0.21	0.04	0.21	0.18	0.33	0.23	0.27	0.24	0.27	0.23	0.33	0.19	0.21	0.04	0.21
F	0.17	0.06	0.12	0.30	0.23	0.32	0.38	0.38	0.38	0.33	0.23	0.30	0.12	0.07	0.17
G	0.15	0.01	0.29	0.18	0.26	0.38	0.39	0.38	0.39	0.38	0.27	0.19	0.29	0.02	0.16
H	0.23	0.06	0.09	0.37	0.23	0.37	0.37	0.53	0.38	0.38	0.24	0.37	0.09	0.07	0.23
I	0.15	0.01	0.29	0.18	0.26	0.37	0.38	0.37	0.39	0.38	0.26	0.18	0.29	0.01	0.15
J	0.16	0.05	0.11	0.28	0.21	0.31	0.37	0.37	0.38	0.32	0.22	0.29	0.11	0.06	0.17
K	0.21	0.03	0.20	0.17	0.31	0.21	0.25	0.23	0.26	0.22	0.32	0.18	0.20	0.03	0.21
L		0.23	0.10	0.36	0.17	0.28	0.18	0.36	0.18	0.29	0.18	0.37	0.11	0.24	
M		0.25	0.07	0.10	0.19	0.10	0.28	0.08	0.28	0.11	0.20	0.10	0.08	0.25	
N			0.25	0.23	0.03	0.04	0.00	0.05	0.00	0.05	0.03	0.24	0.25		
P					0.21	0.16	0.14	0.22	0.14	0.16	0.21				

Difference in percent moderator temperature between SSS2/SCF CH and PARCS 2G

Future work

- Improve numerical performance and scaling of SSS2/SCF
- Domain decomposition for thermal-hydraulics
- Validate using NPP measurement data
- Work on efficient method to achieve converged fission source
- Extend coupling algorithm to cover burn-up calculations
- Extend coupling to Serpent‘s dynamic mode (dynSerpent)