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

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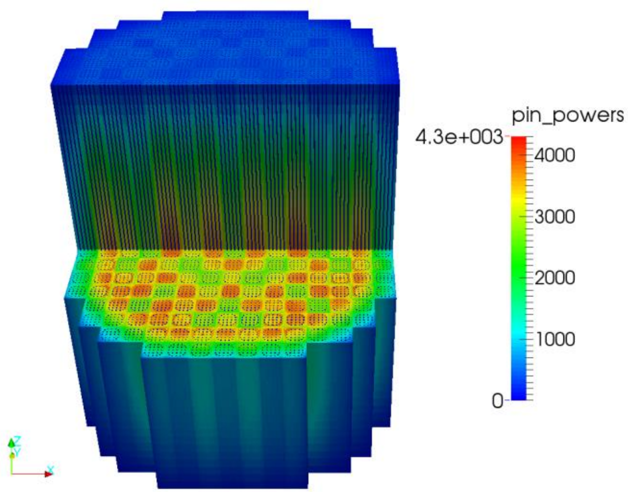


Thermal-hydraulic feedback modeling in Serpent

- ‚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

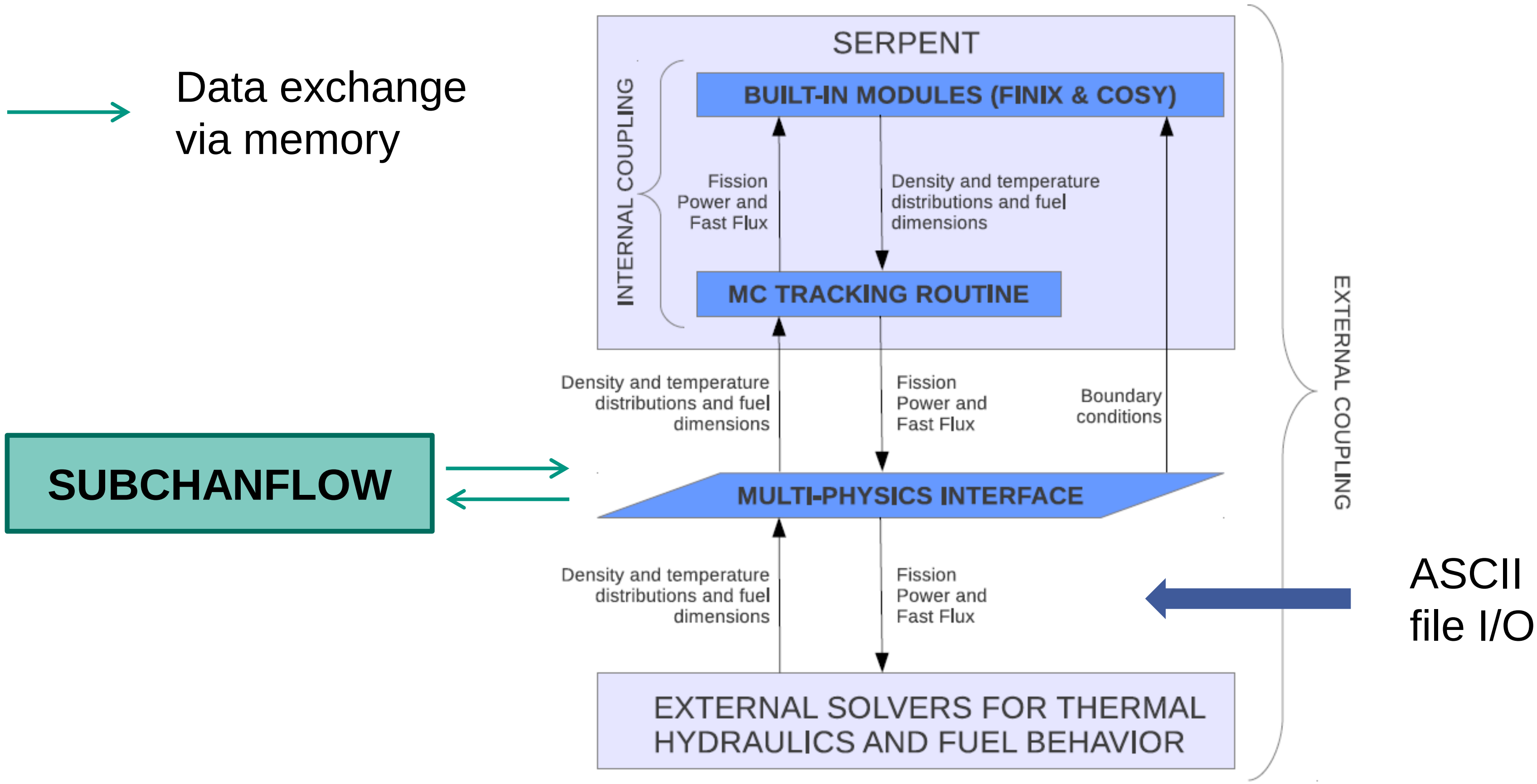
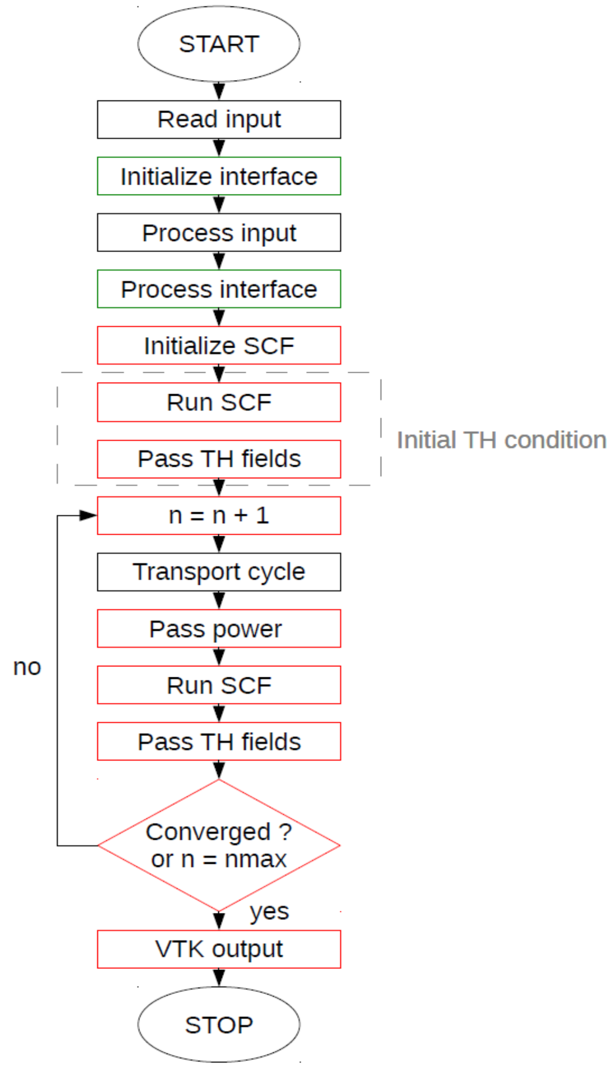
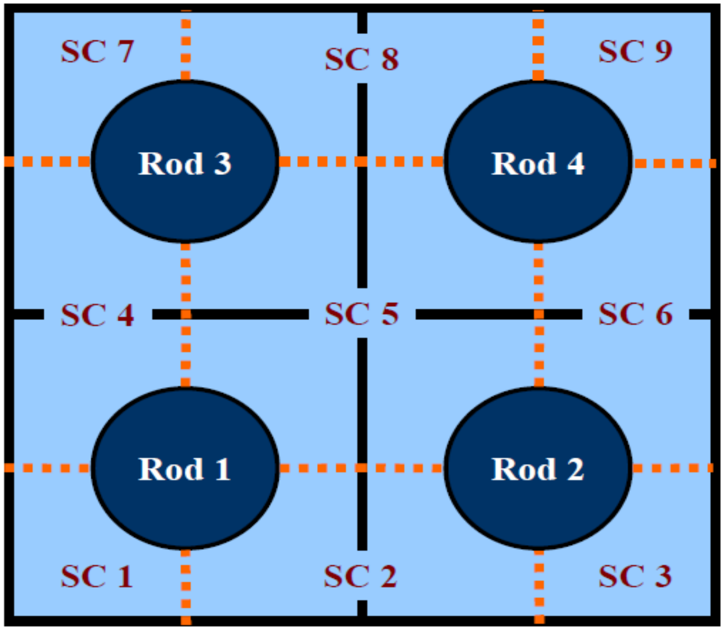


Figure: Multi-physics coupling scheme in Serpent 2

Serpent/SCF coupled iteration algorithm



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

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

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

- 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

Internal coupling to SUBCHANFLOW is an option

```
% ------ UFS methods
set ufs 1 1 17 -182.07 182.07 17 -182.07 182.07 22 0.0 407.555

% ----- Internal Coupling to SCF
set scf core 1 20 1 -160.65 160.65 -160.65 160.65 20.90 386.655
        2 0.7 7.5517538e-02
        coolant water
        fuel u_4.2_0.15 u_4.2_17.5 u_4.2_22.5 u_4.2_32.5 u_4.2_35.0 u_4.2_37.5 u_4.5_0.15 u_4.5_17.5 u_4.5_20.0 u_4.5_32.5 u_4.5_37.5 mox_1_0.15
mox_2_0.15 mox_3_0.15 mox_1_22.5 mox_2_22.5 mox_3_22.5 mox_1_37.5 mox_2_37.5 mox_3_37.5 mox_43_1_0.15 mox_43_2_0.15 mox_43_3_0.15 mox_43_1_17.5 m
ox_43_2_17.5 mox_43_3_17.5 mox_43_1_35.0 mox_43_2_35.0 mox_43_3_35.0 ifba_0.15 ifba_17.5 ifba_22.5 ifba_32.5 ifba_35.0 ifba_37.5 ifba45_0.15 ifba
45_17.5 ifba45_20.0 ifba45_32.5 ifba45_37.5
        gap gap1
        clad clad1

set coupl_conv 3 0.00005 0.005 0.005

% ------ GEOMETRY

include "pins.inp"
include "fa.inp"

% ----- global unit

surf z03 pz 0.0
surf z04 pz 407.555
```

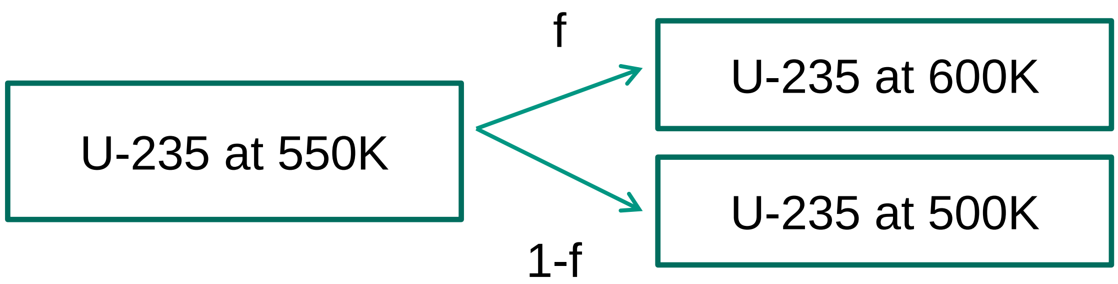
+

Main input of SUBCHANFLOW defining TH problem
(without geometry description)

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



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

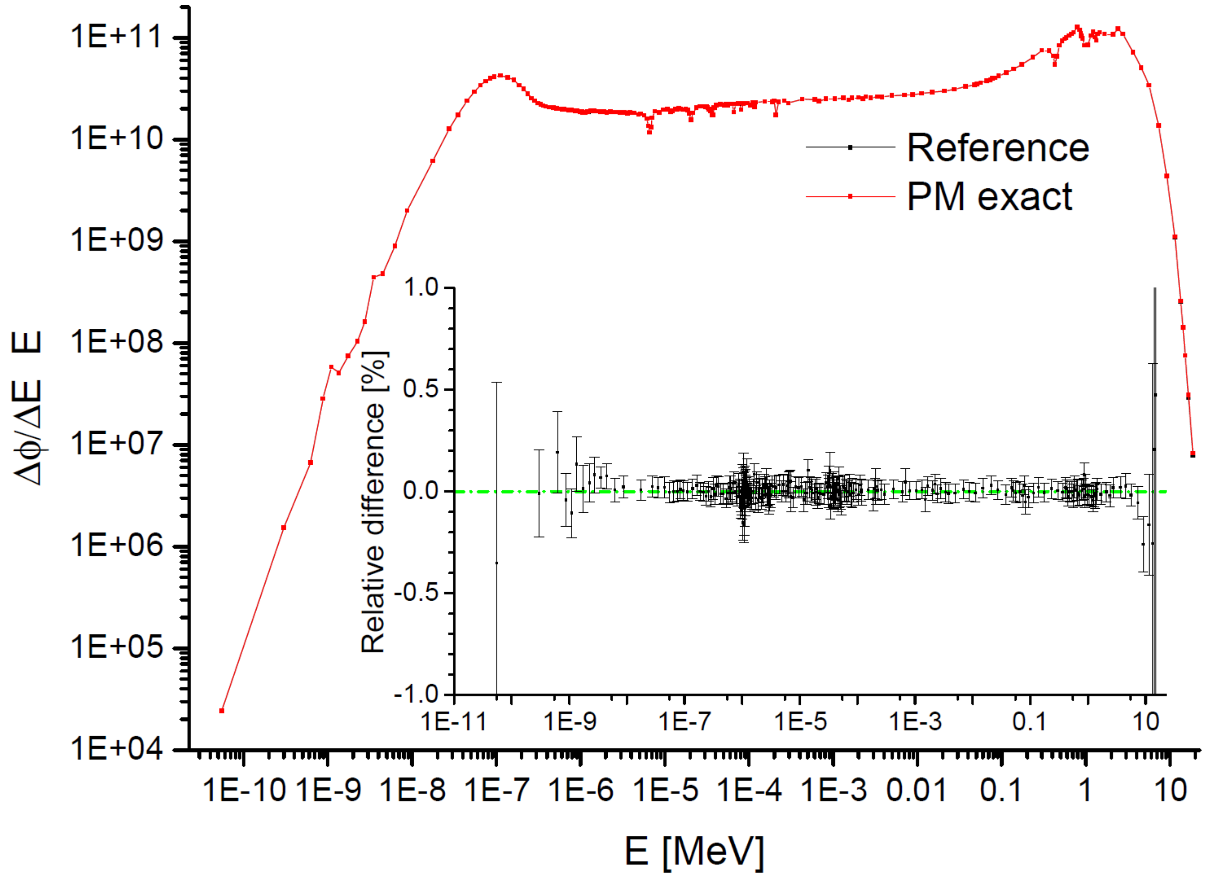
Stochastic mixing fall back for TMS

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

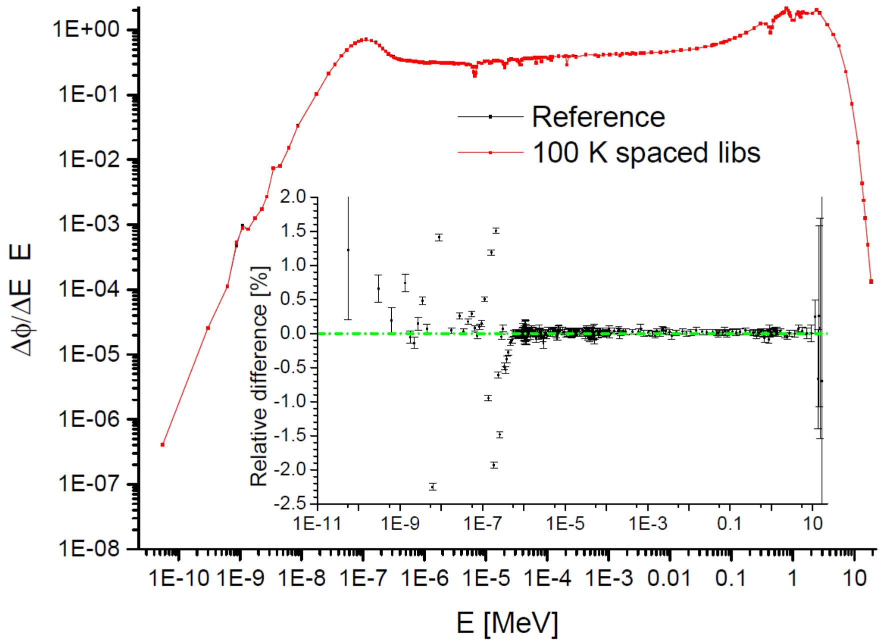
   else
   identify two scattering nuclides with temperatures enclosing the local temperature, compute the mixing fraction and use it to sample which scattering nuclide to use, do NOT transform into target-at-rest frame

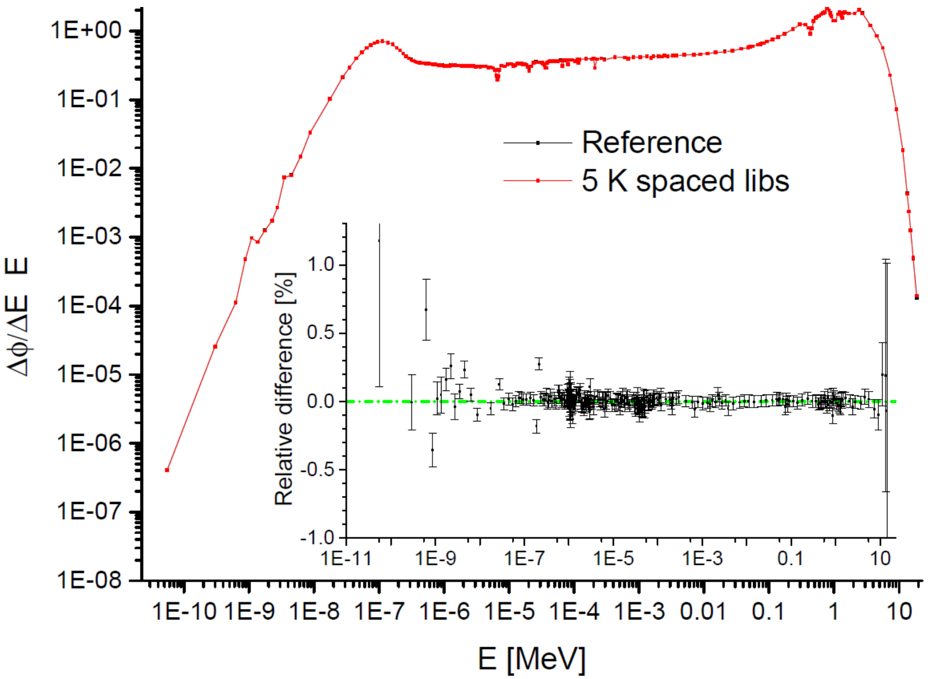
Code verification for stochastic mixing fall back

- 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(a,b)





Stochastic mixing fall back for TMS

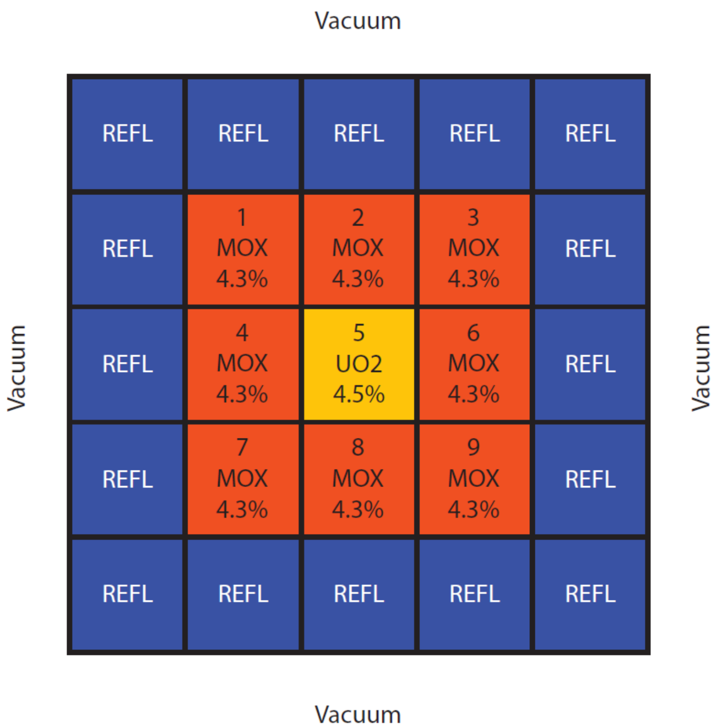
- The stochastic mixing fall back algorithm is automatically enabled in the internal coupling with SUBCHANFLOW

- It may be enabled by the user for any other application using TMS by

```
mat water1 sum moder lwtr1 1001
1001.03c 5.02932E-02
5010.03c 8.33778E-06
5011.03c 3.35608E-05
8016.03c 2.51573E-02

therm lwtr1 lwMD.09t

% ------- Boundary condition

set bc 2 2 1

% ------ Multiphysics interface

ifc water.ifc

% ------ Stochastic mixing fall back

set pm 1

% ------ Record shannon entropy

set his 1

% ------ Record power distribution

set cpd 1
```

Selected solution verification case (1/6)

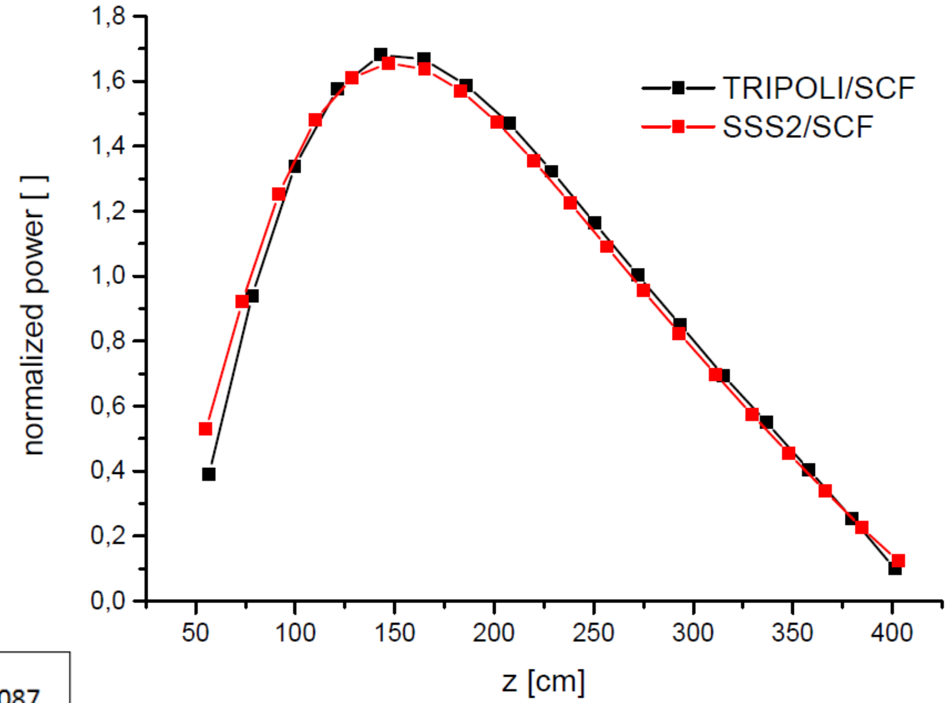
- Code-to-code benchmark with TRIPOLI/SUBCHANFLOW
- 3x3 minicore from NURISP boron dilution benchmark



Quantity	Value
Power	100 MW
Core mass flow rate	739.08 kg/s
Outlet pressure	15.4 MPa
Coolant inlet temperature	560 K
Boron concentration	200 ppm

Selected solution verification case (2/6)

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

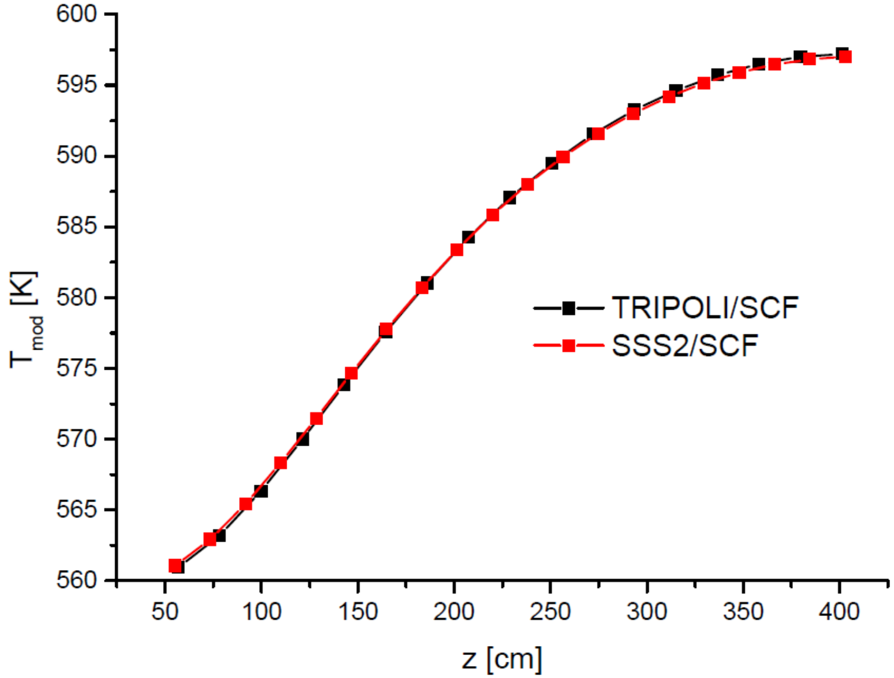
0.087	0.120	0.087
0.120	0.172	0.120
0.087	0.120	0.087

(a) SSS2/SCF

0.087	0.12	0.087
0.12	0.173	0.12
0.086	0.12	0.086

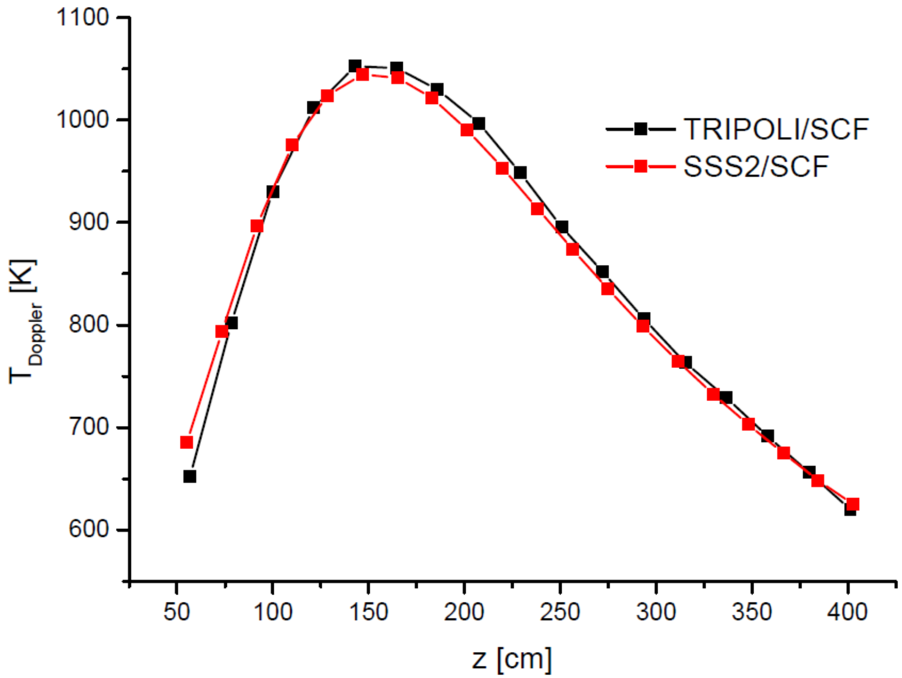
(b) TRIPOLI/SCF

Selected solution verification case (3/6)



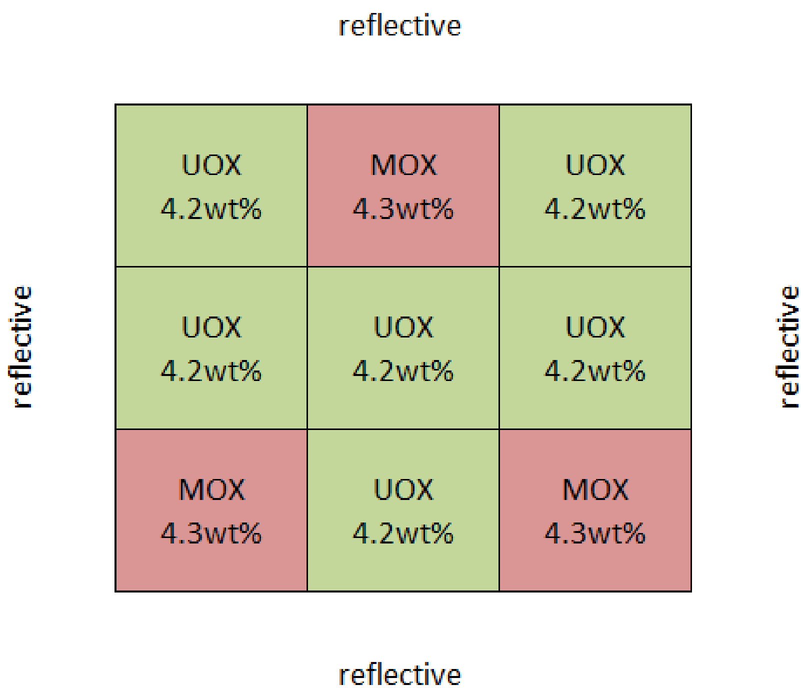
Axial moderator temperature profile in central assembly

Axial Doppler temperature profile in central assembly



Selected solution verification case (4/6)

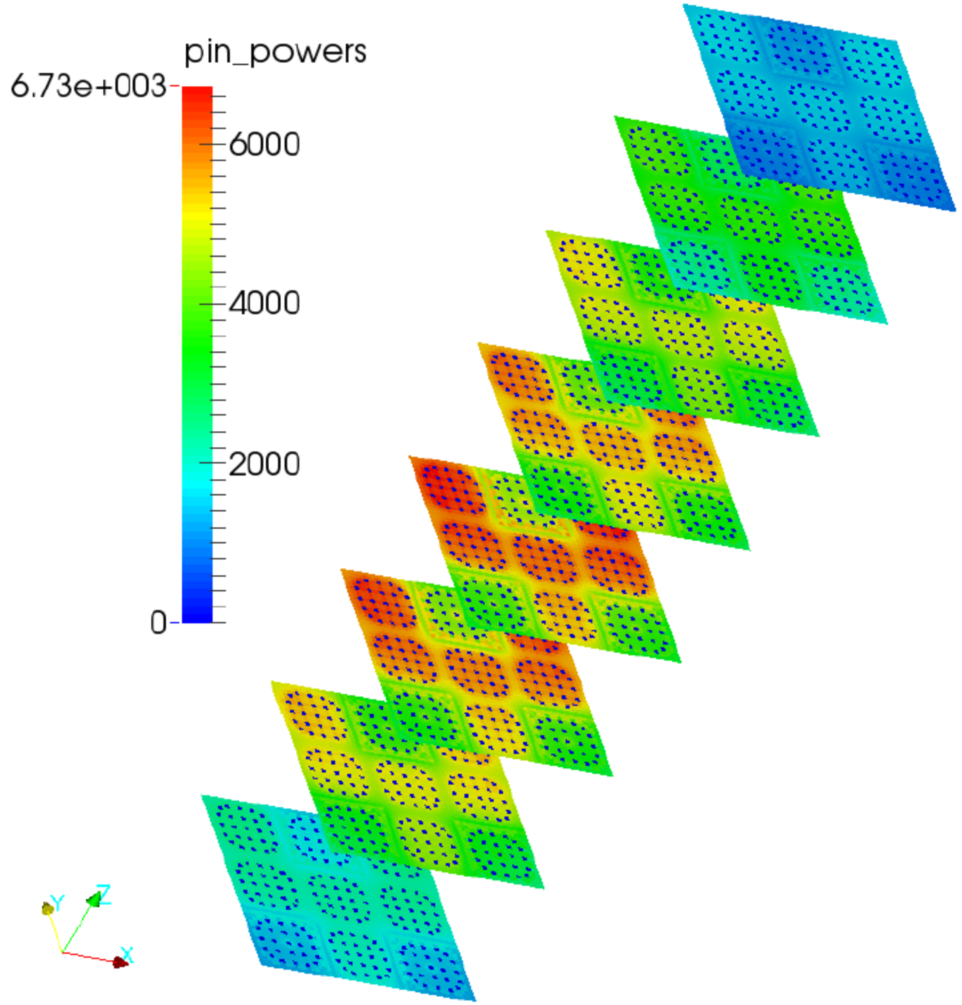
- Code-to-code benchmark with MCNP5/SUBCHANFLOW
- 3x3 minicore from HPMC project, sub-channel



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

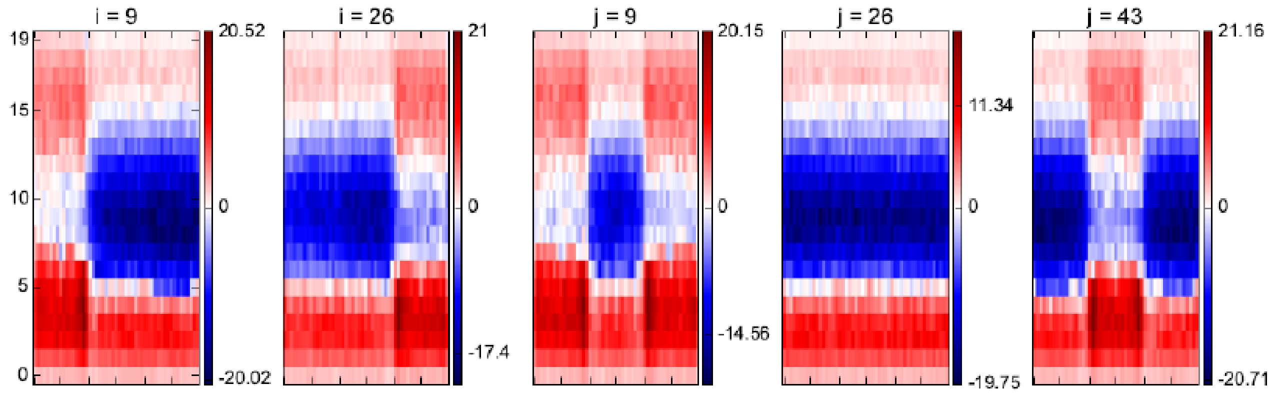
Selected solution verification case (5/6)

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

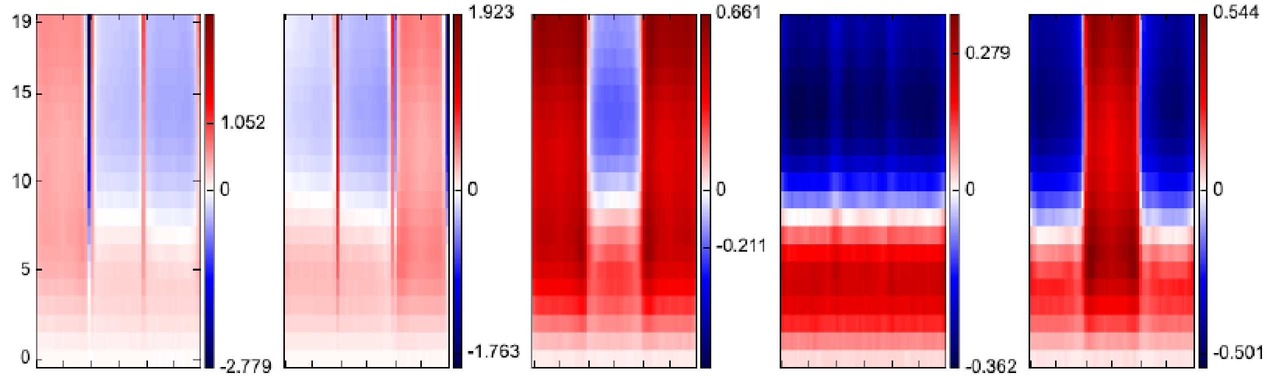


Selected solution verification case (6/6)

- Absolute differences in Kelvin for five vertical cuts through minicore



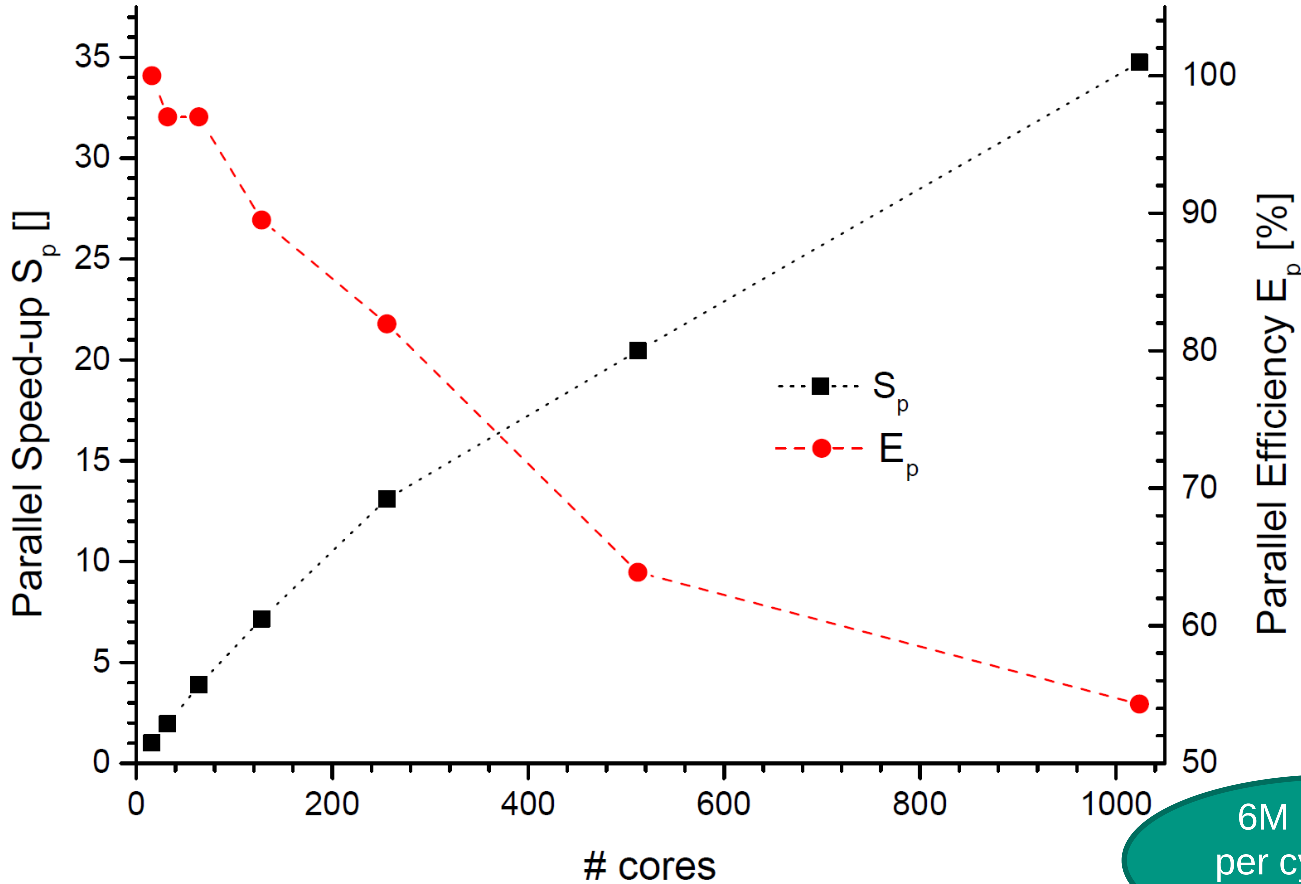
(a) Effective Doppler temperature



(b) Moderator temperature

Numerical performance of SSS2/SCF

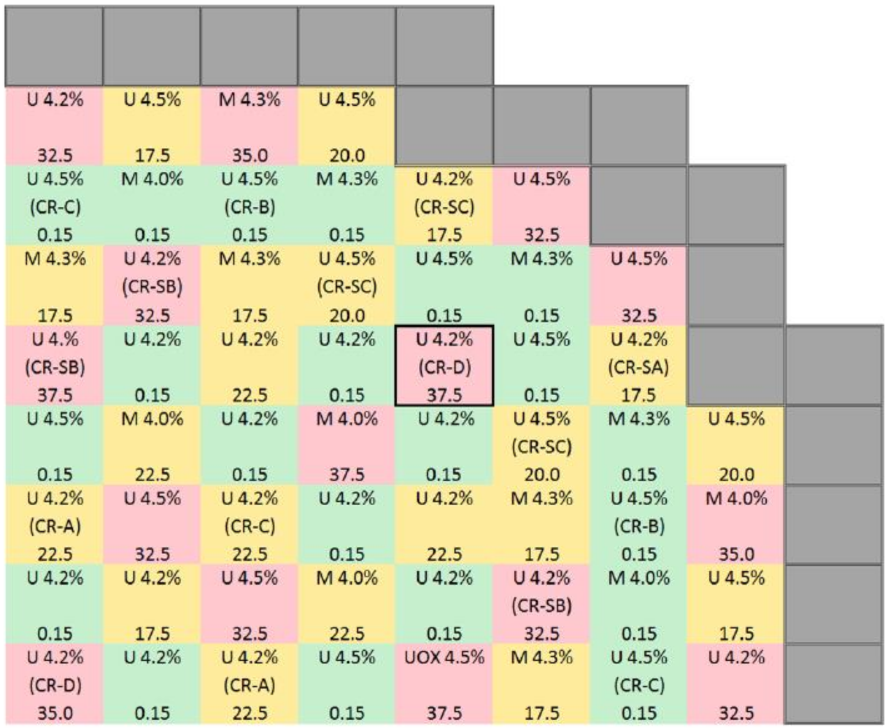
- 3x3 reflected fuel assembly cluster with subchannel TH model
- Speed-up relative to execution on 16 cores



6M neutrons per cycle, 2000 active cycles

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



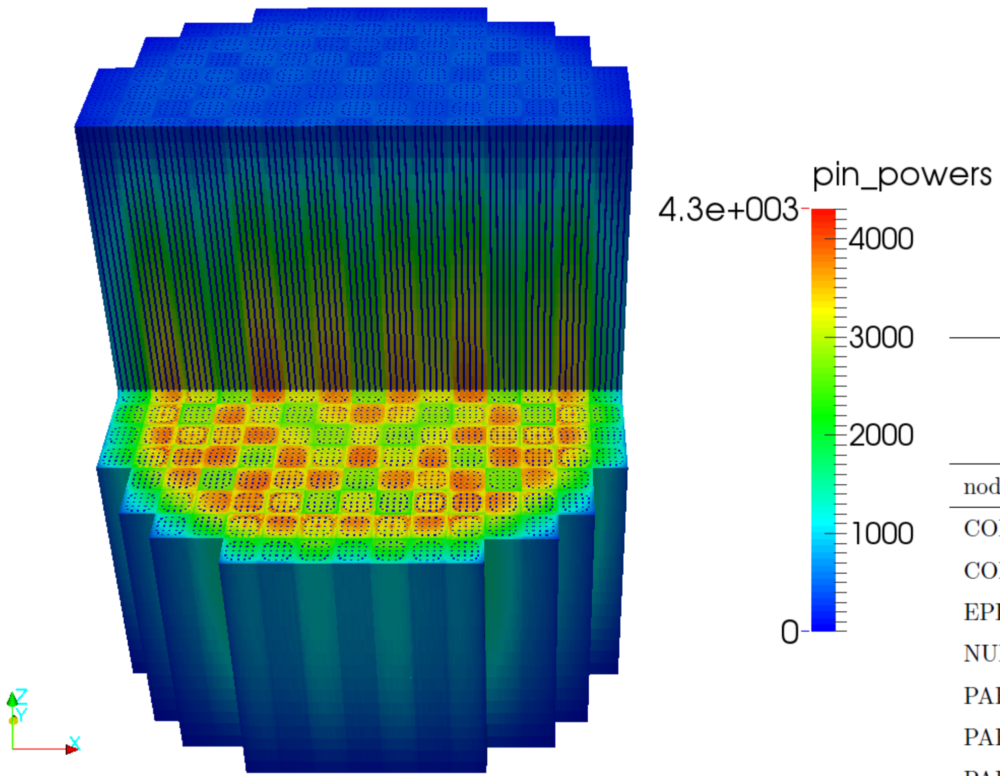
Quantity	Value
Power	3565 MW
Core mass flow rate	15849.4 kg/s
Inlet pressure	15.5 MPa
Coolant inlet temperature	560 K

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

	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		

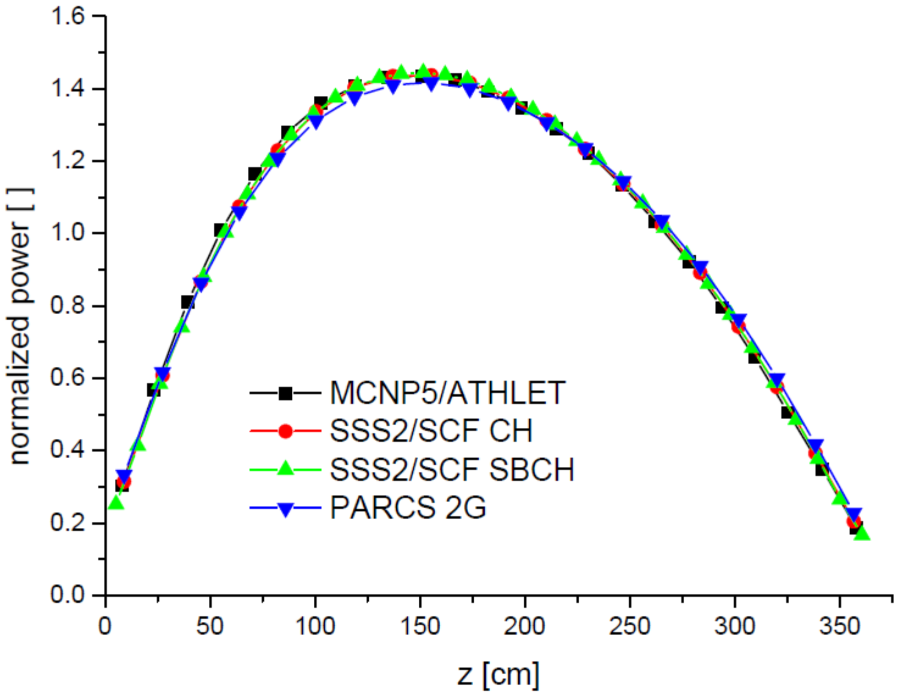
Full PWR Core Coupled Monte Carlo Neutron Transport and Thermal-Hydraulic Simulation (3/6)



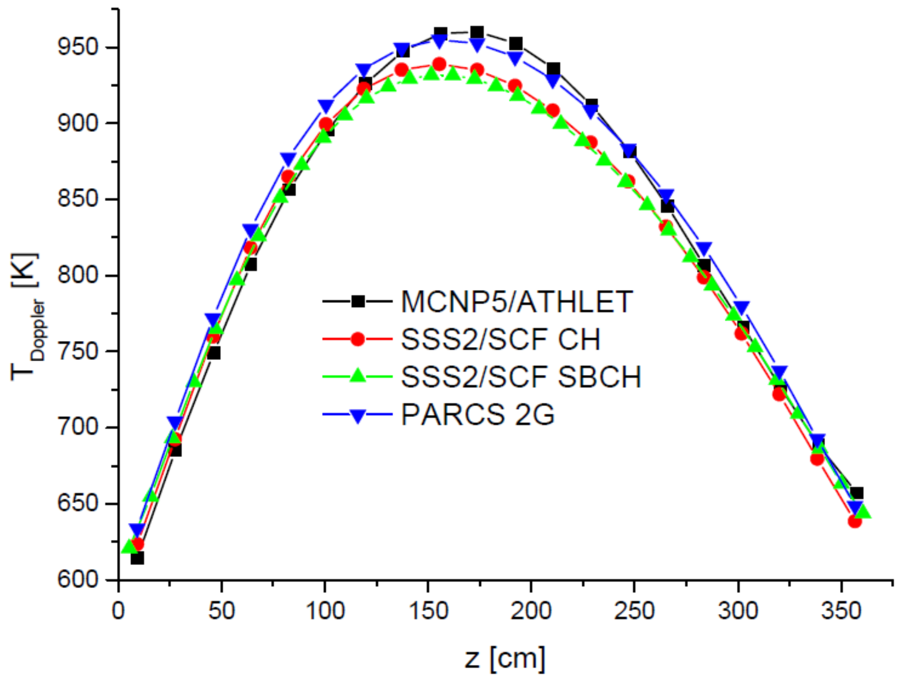
5M neutrons per cycle, 2000 active cycles per iteration

	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

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)

Karlsruher Institut für Technologie

	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
- 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)