

PARCS/Subchanflow – First step: Nodal level steady state internal coupling

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Agenda

- Motivation
- Subchanflow (SCF)
 - Short introduction
 - Previous work done at KIT
- PARCS v3.2 /Subchanflow v2.6 Internal Coupling
 - Coupling Steps
 - Coupling Description
 - Current Status
- Testing and Results
 - 3x3 minicore
 - OECD PWR MOX UO₂ benchmark (Part II)
- Summary and Outlook

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Motivation

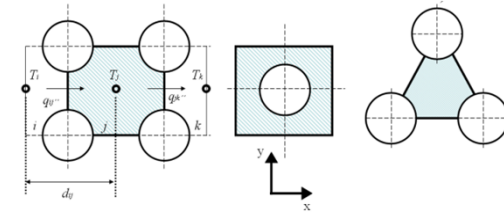
- Current codes are not able to predict local (pin-based) safety parameters directly.
- Better Neutronics/Thermal hydraulics description is wanted by the industry.
 - A 3D pin-wise transient solution is one of the current goals.
- Further advancement in the TH coupled with PARCS requires a more sophisticated TH tool than the current internal TH, e.g. a sub-channel code.
- The implementation of a pin level N/TH solution will give us a tool to analyze the physics behavior in a better manner than it is done nowadays in fast running system codes.

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Subchanflow Features

- Fast running, stable and flexible subchannel TH code for the description of the single and two-phase flow.
 - Water, air, helium, lead, lead-bismuth and sodium
 - Sub-channel or subassembly discretization of the reactor core
 - DNBR calculation, boron transport, unstructured mesh.
- Developed by INR/KIT since 2010 (Uwe Imke)
- Programmed in Fortran 95 in a modular manner, platform independent, with error handling.
- SCF is coupled with
 - MC codes: SERPENT, MCNP5
 - Diffusion codes: COBAYA3, DYN3D Diff (In EU NURESIM Simulation Platform)
 - SP3 codes: DYN3D-SP3 (DYNSUB)
- Availability: Signature of a “SUBCHANFLOW User Agreement” with KIT for research or commercial use



Previous work done at KIT on coupling with SCF

- **MCNP/SCF** – A. Ivanov, V. Sanchez and U. Imke, "Development of a Coupling Scheme Between MCNP5 and SUBCHANFLOW for the pin- and fuel assembly-wise simulation of LWR and Innovative Reactors," in *M&C 2011*, Rio de Janeiro, 2011.

- **Serpent/SCF** – M. Daeubler, J. Jimenez and V. Sanchez, "Development of a High-Fidelity Monte Carlo Thermal Hydraulics coupled code system SERPENT/SUBCHANFLOW - First Results," in *Physor 2014*, Kyoto, Japan, 2014.

- **DYN3D/SCF** – A. Gomez, V. Sanchez and U. Imke, "Pin Level Neutronic - Thermalhydraulic two-way-coupling using DYN3D-SP3 and SUBCHANFLOW," in *M&C 2011*, Rio de Janeiro, Brazil, 2011.

- **COBAYA/SCF** – M. Calleja, J. Jimenez, U. Imke and V. Sanchez, "Validation of the Coupling between COBAYA3 and SUBCHANFLOW for the Simulation of Boron Dilution Transients," in *Annual Meeting of the Spanish Nuclear Society 2012*.

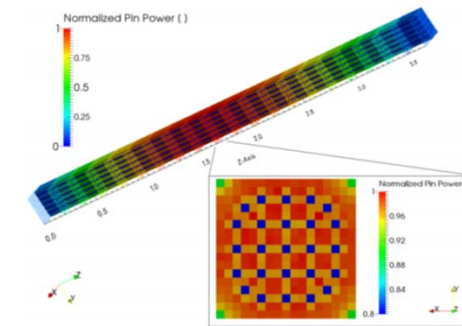
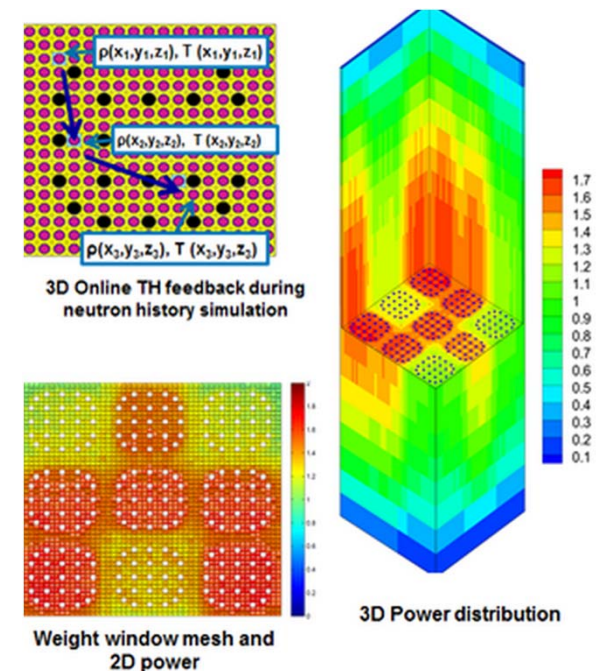


Figure 5. Normalized pin powers predicted by Serpent/SUBCHANFLOW

Serpent-SCF . M. Daeubler



MCNP-SCF . A. Ivanov

Example: COBAYA3/SCF Boron Dilution Problem

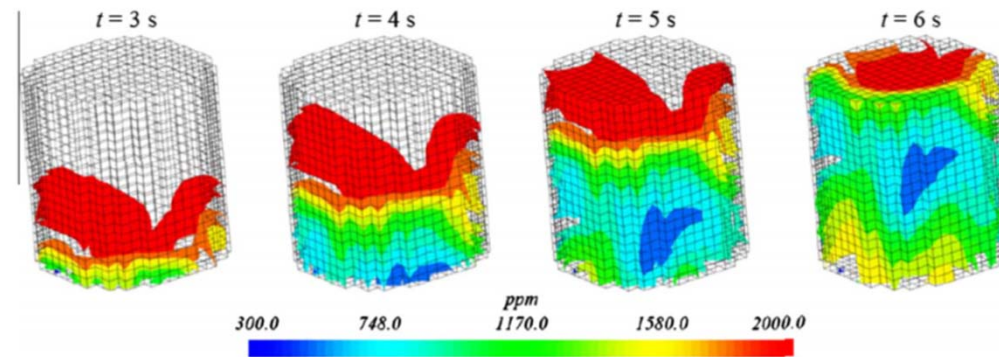


Fig. 13. Evolution of the boron concentration during the transient for the slug size 1 ($t = 3$ – 6 s).

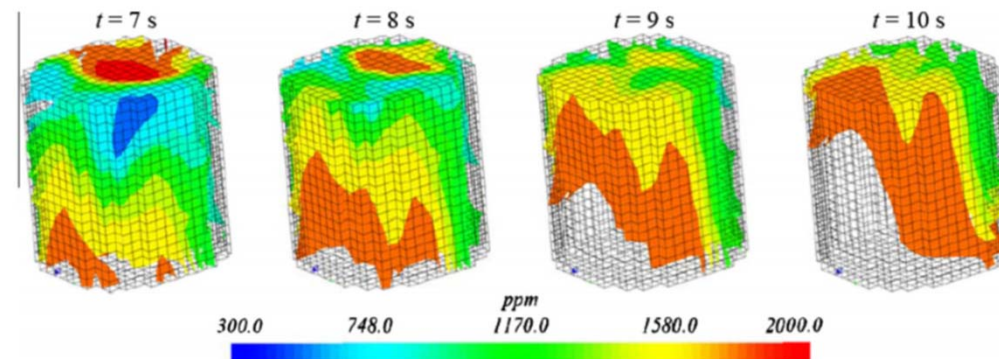


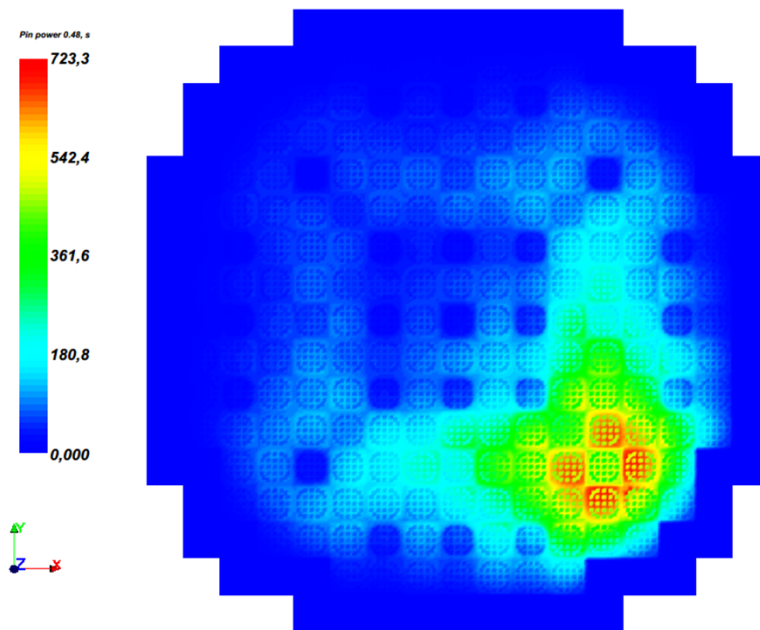
Fig. 14. Evolution of the boron concentration during the transient for slug size 1 ($t = 7$ – 10 s).

- Calleja, J. Jimenez, V. Sanchez, U. Imke, R. Stieglitz and R. Macian, "Investigations of boron transport in a PWR core with COBAYA3/SUBCHANFLOW inside the NURESIM platform," *Annals of Nuclear Energy*, pp. 74-84, 2014.

Full Core Pin-by-Pin Simulations of a PWR Core

High Fidelity DYN3D-SP3 / SUBCHANFLOW Coupling

SP3 Transport /Subchannel

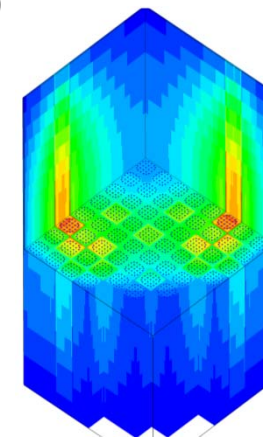


***DYNSUB**: 3D Avg. Pin Power
Density [W/cm³]; PWR MOX core

* M. Daeubler et al. – “Static and Transient Pin-by-Pin Simulations of a Full PWR Core with the Extended Coupled Code System DYNSUB” - accepted ANE

High Fidelity Monte Carlo / SUBCHANFLOW Coupling

- Whole core MC-simulations with TH feedback and use of HPC
- MC-Based depletion with TH-feedback
- Advance time-dependent MC for safety evaluations (industry applications)

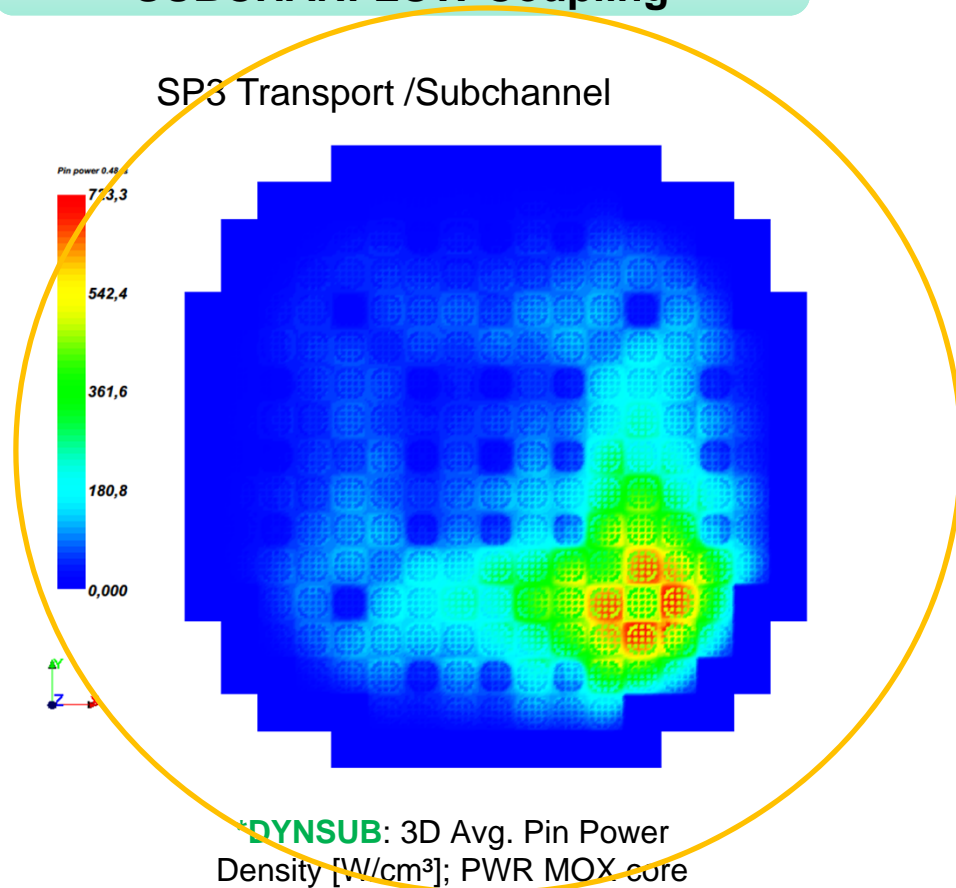


EU High Performance
Monte Carlo Core
Analysis Project



Full Core Pin-by-Pin Simulations of a PWR Core

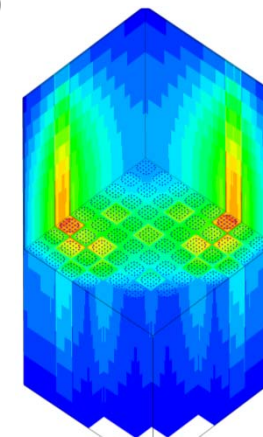
High Fidelity DYN3D-SP3 / SUBCHANFLOW Coupling



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EU High Performance Monte Carlo Core Analysis Project



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Coupling Approach

■ Codes

- PARCS v3.2
- Subchanflow v2.6

■ Type of Coupling

- Internal coupling
- Merge SCF into PARCS (one executable)

■ 3 Steps Coupling Plan

- 1st Step: Nodal level coupling
- 2nd Step: Pin level coupling without pin level TH feedback
- 3rd Step: Pin level coupling with pin level XS feedback

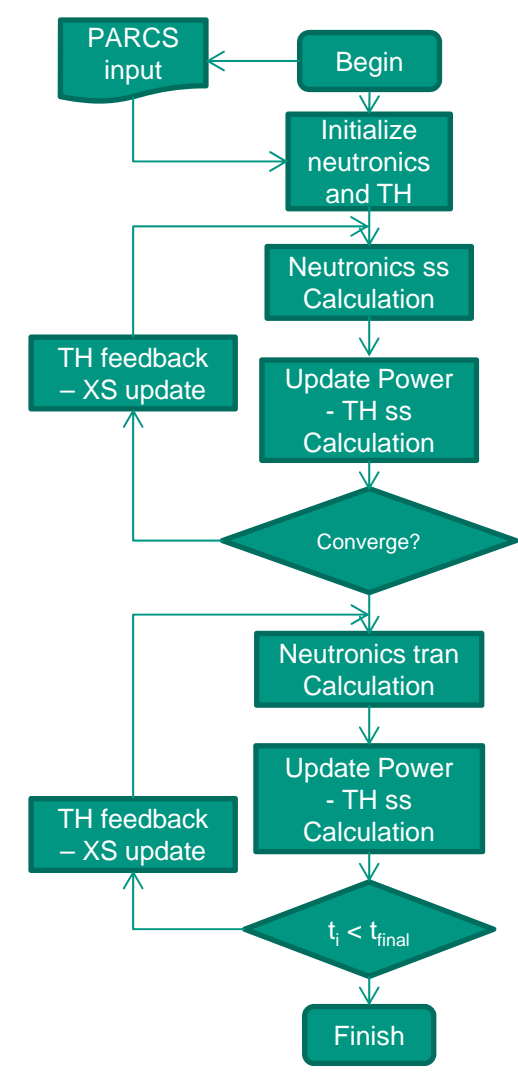
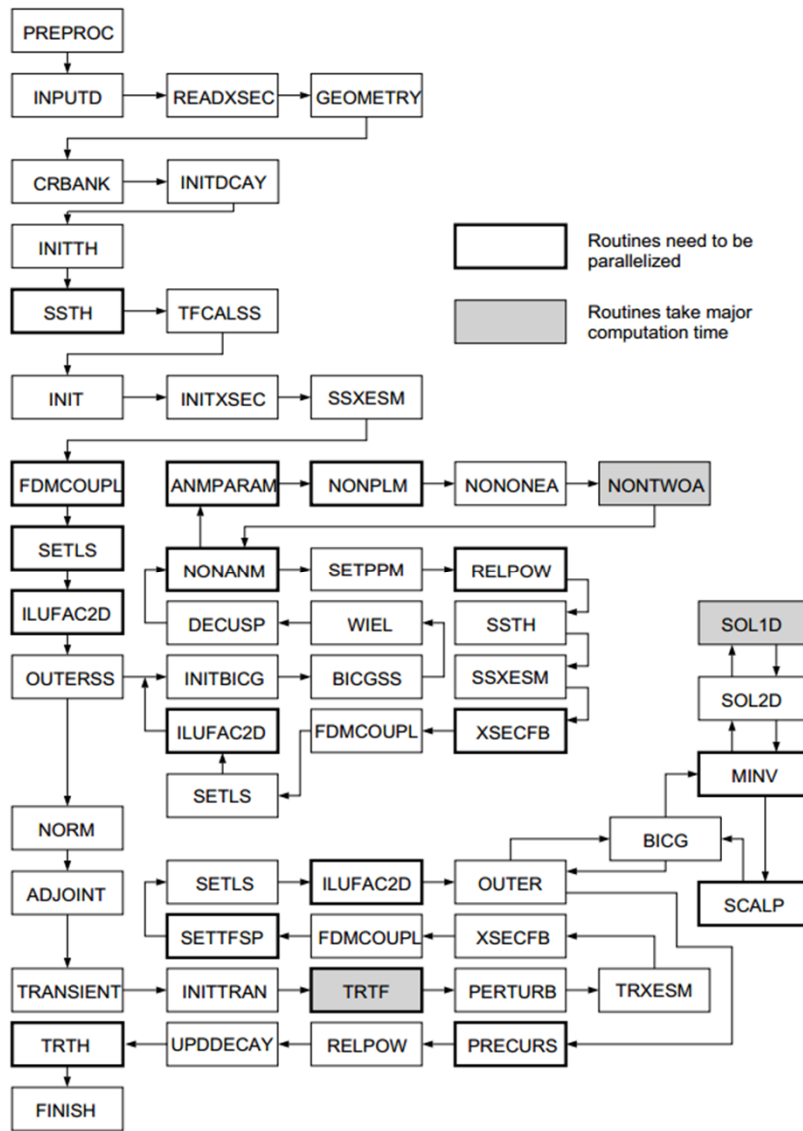
3 Steps Coupling

- 1st Step: Nodal level coupling
 - Simplest and natural way to start.
 - One to one node mapping between N and TH.
 - Implementation similar to current internal TH module.
 - Testing against PARCS with internal TH solution.

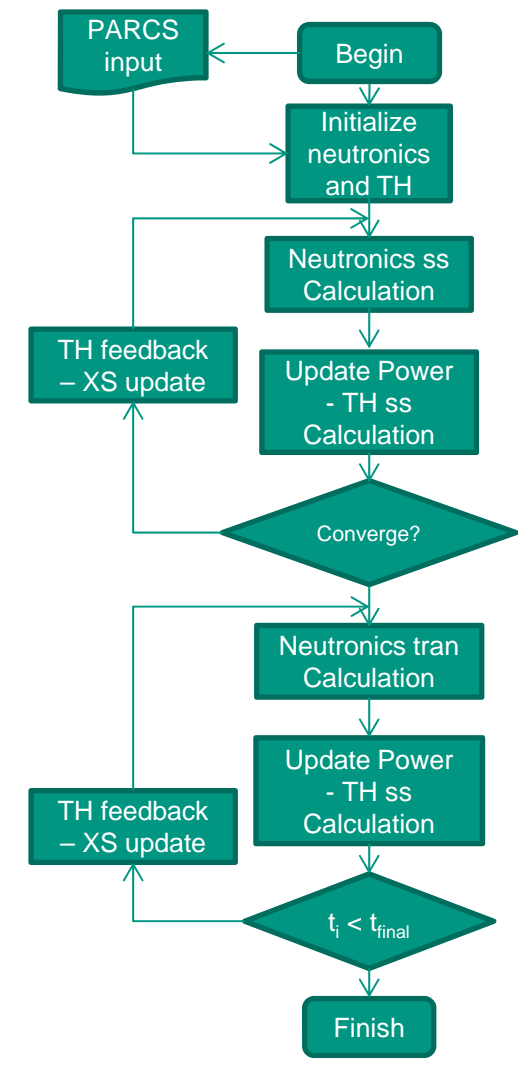
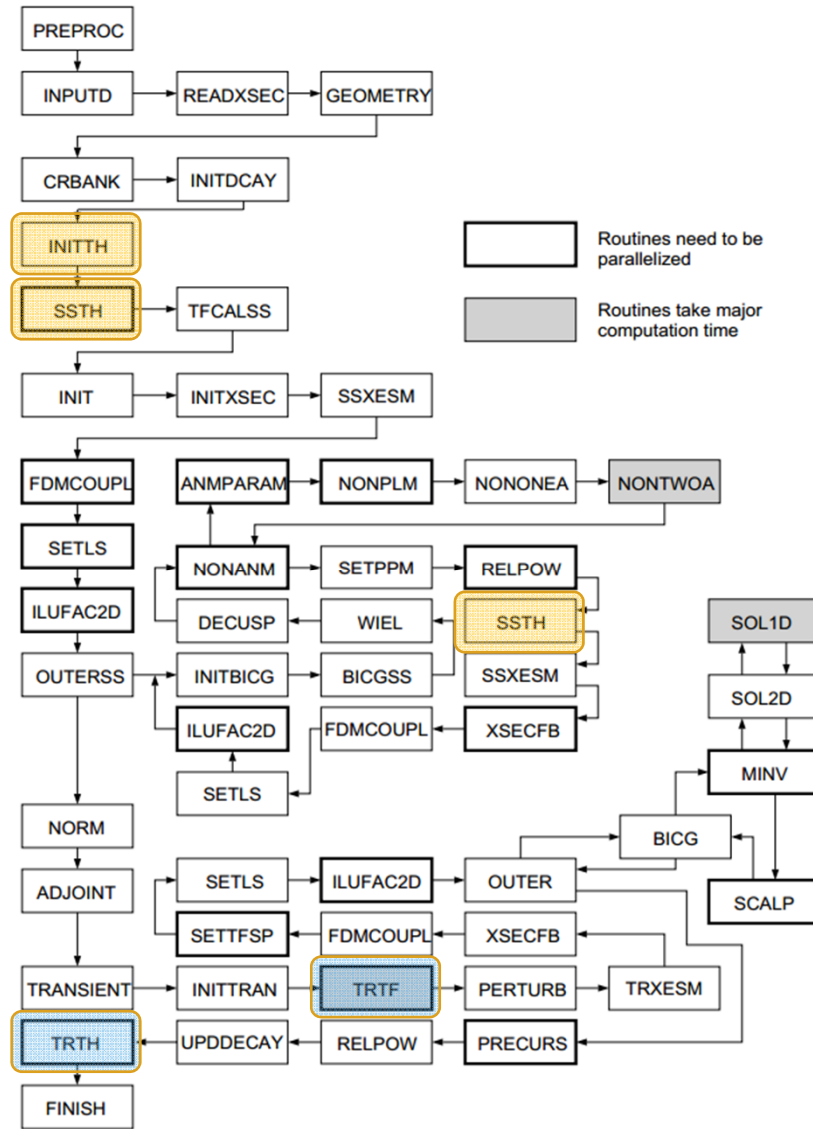
- 2nd Step: Pin level coupling without pin level TH feedback
 - Pin level calculation in PARCS, sub-channel calculation in SCF.
 - TH parameters averaged to node level to XS feedback.
 - Comparison against previous results obtained at KIT with other Coupled codes.

- 3rd Step: Pin level coupling
 - Pin wise dependent XS.

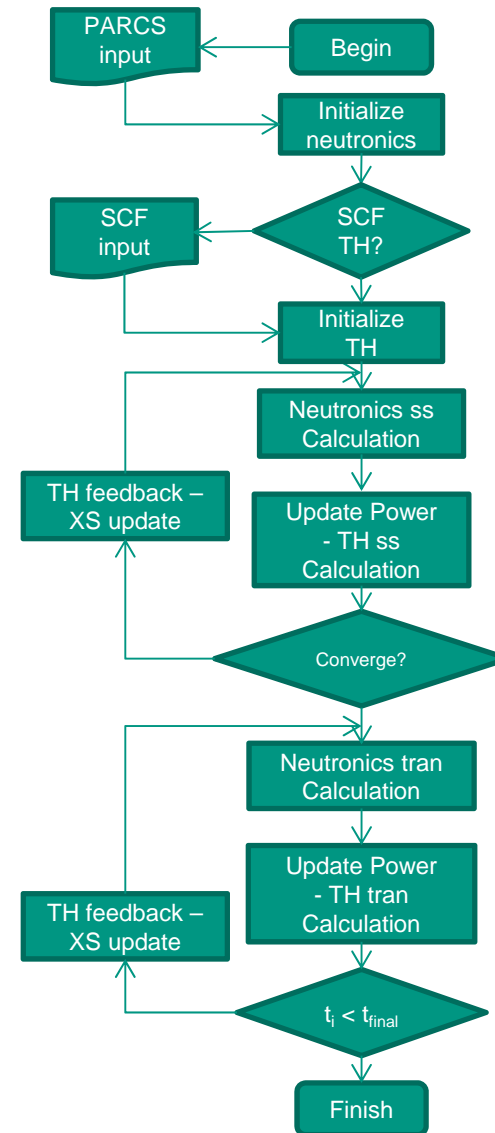
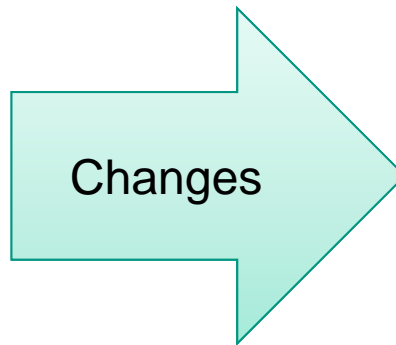
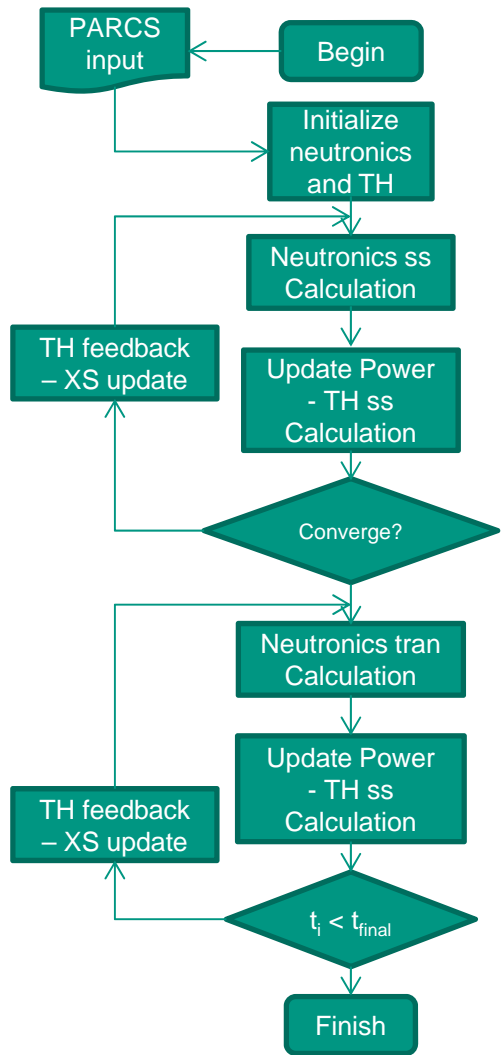
Calling Sequence of Major Routines in PARCS



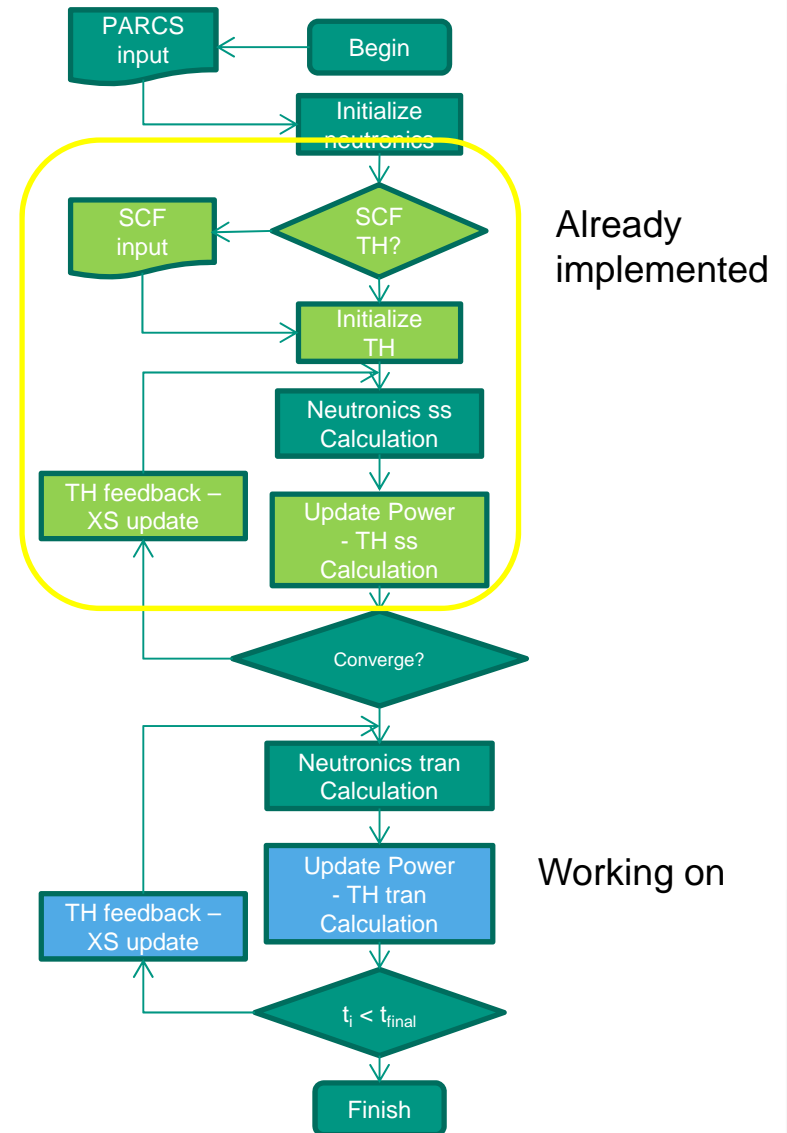
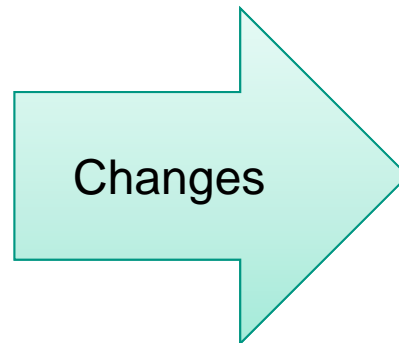
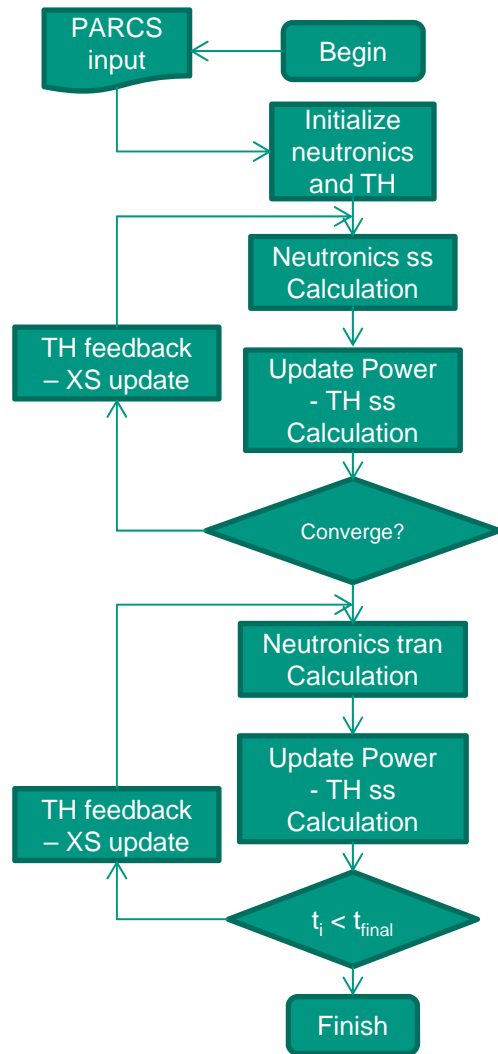
Subroutines to be modified in the PARCS/SCF coupling implementation



Flowchart change



Flowchart change



Global Convergence Criteria

- TH Magnitudes are calculated by SCF but **global convergence** still managed in the same way as before by PARCS.

ψ_n = Flux at n^{th} iteration

$T_{D,t+1}^m$ = Doppler temperature

Convergence checks:

$$\delta_{L2} = \frac{\|\psi_{n+1} - \psi_n\|_2}{\langle \psi_{n+1}, \psi_n \rangle^2}$$

$$\delta_k = |k_{eff}^{n+1} - k_{eff}^n|$$

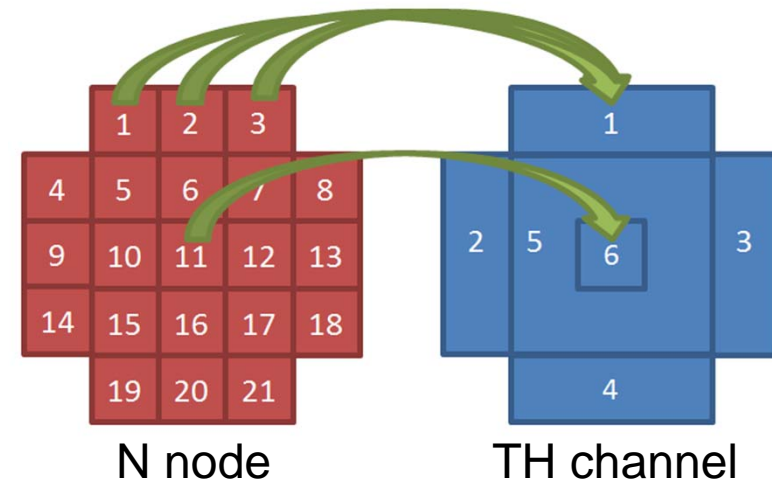
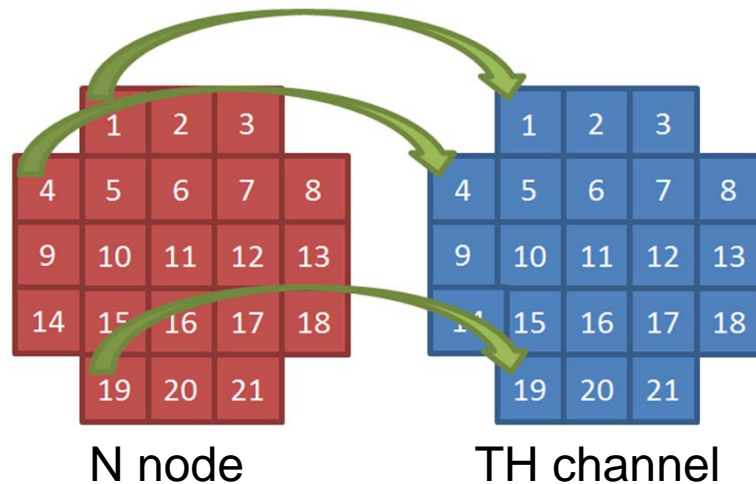
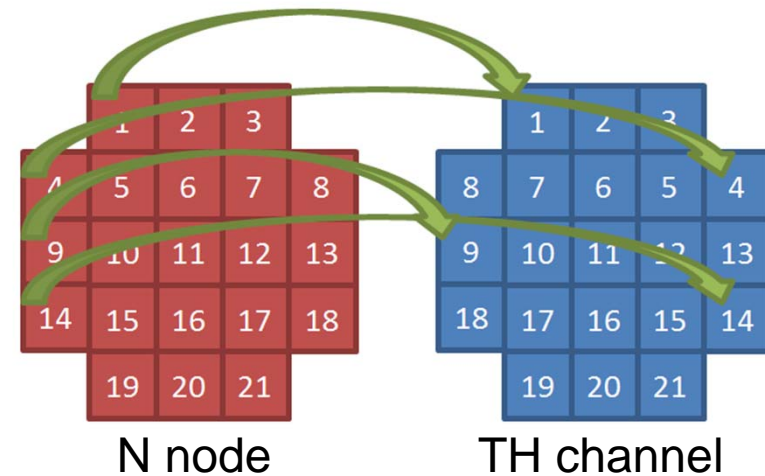
$$\delta_{L\infty} = \max \left| \frac{\psi_{n+1}^m - \psi_n^m}{\psi_{n+1}^m} \right|$$

$$\delta_{Dop\infty} = \max \left| \frac{T_{D,t+1}^m - T_{D,t}^m}{T_{D,t+1}^m} \right|$$

Mapping between Neutronics and TH

Different ways of mapping the nodes can be thought:

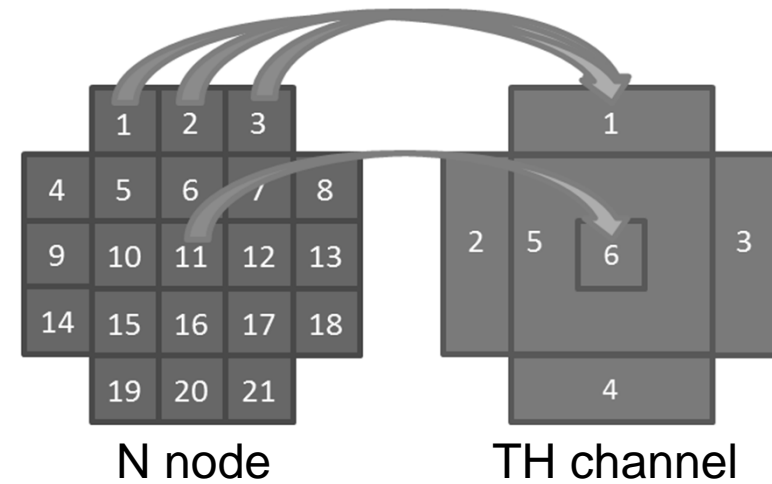
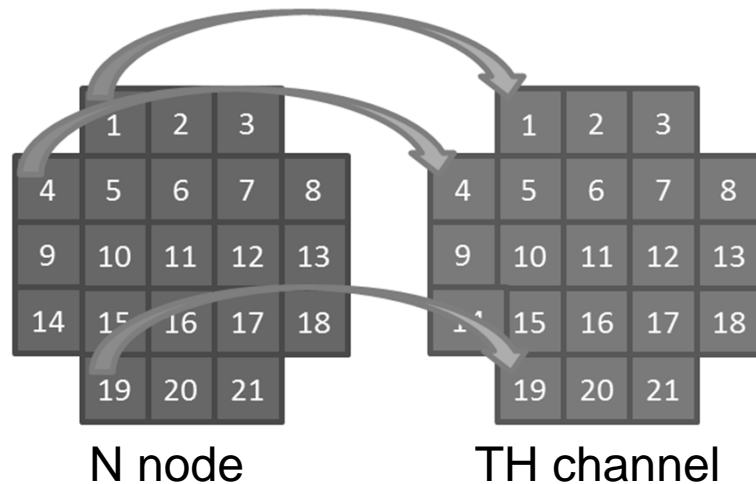
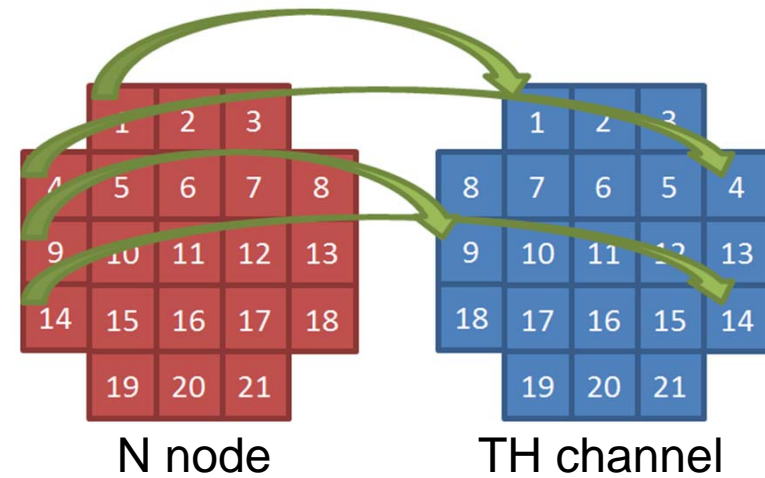
- One to one mapping. Same nodalization and numbering of N nodes and TH channels.
- Same nodalization different numbering.
- Different nodalization and numbering.



Mapping between Neutronics and TH

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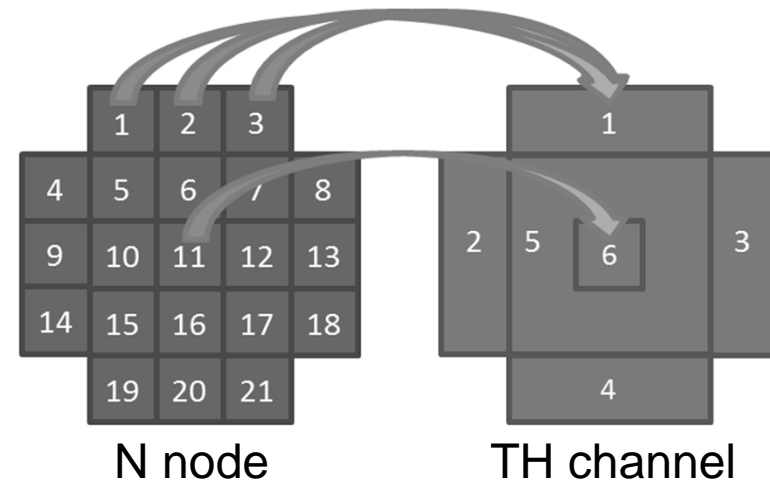
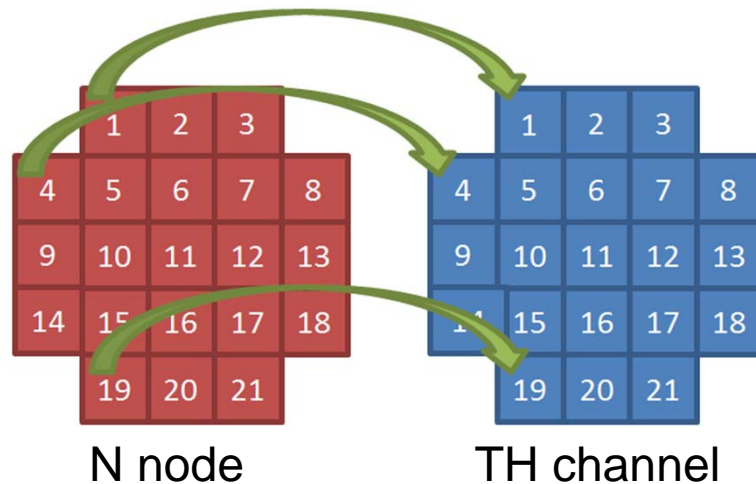
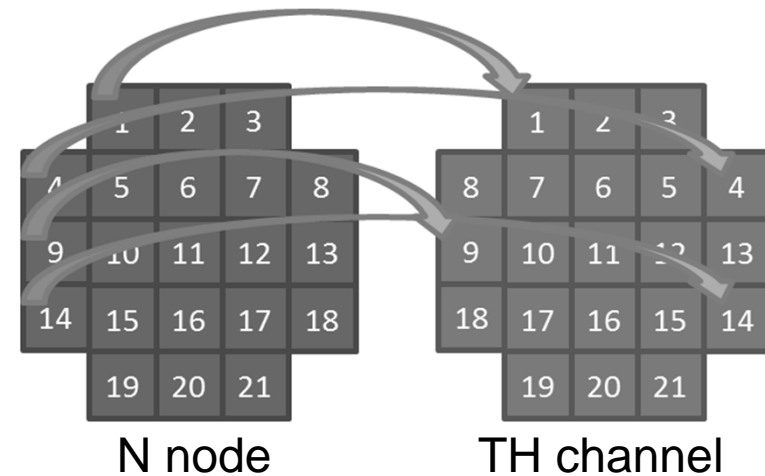
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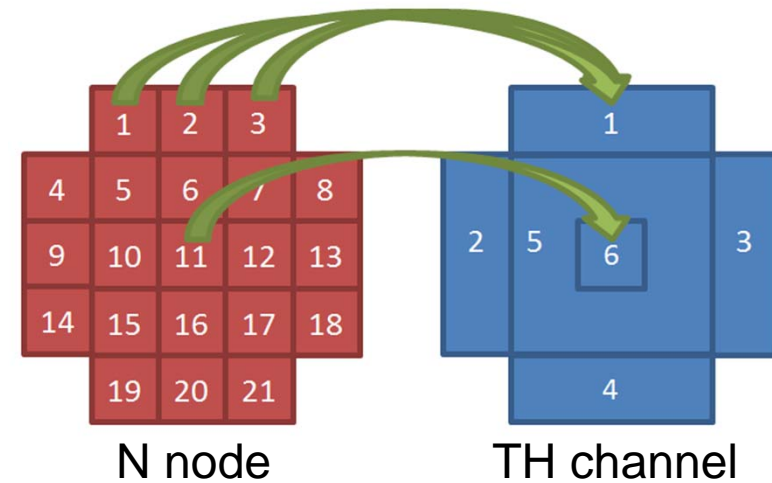
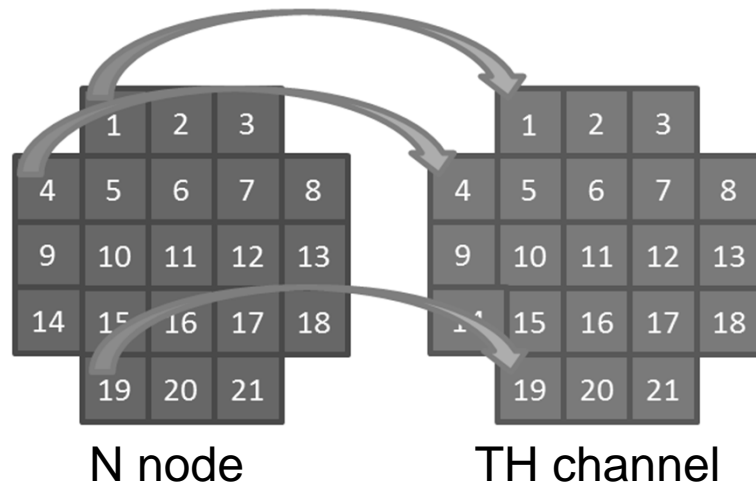
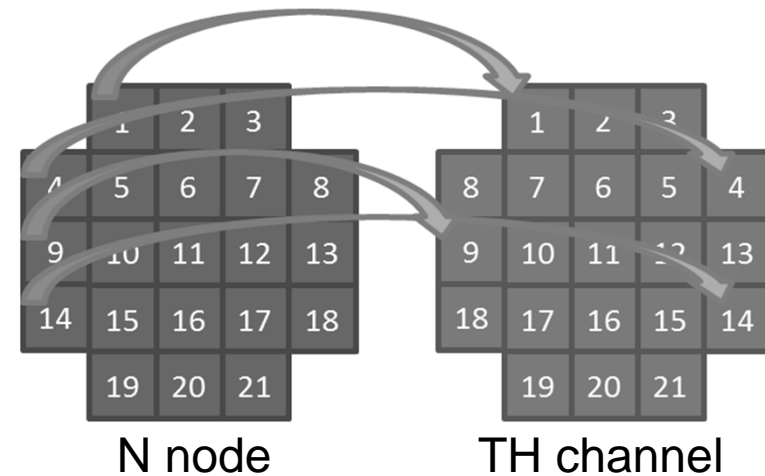
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Mapping between Neutronics and TH

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- Same nodalization different numbering.
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Programming Features

■ Internal coupling

- Merge SCF into PARCS as modules
 - SCF will be a new internal TH module of PARCS (like PATHS)
- Adapt SCF to be compatible with PARCS modular structure
- Input parameters cross checking e.g. FA-power, meshing, etc.

■ Programming practices

- Keep documentation of all new implemented variables and changes.
- Control common variable names.
- Modification of PARCS and SCF only when utterly necessary.
 - Making easier the implementation of future versions.
- New subroutines and variables are declared in new 'coupling' modules
- Preprocessor directives to compile PARCS optionally with or without SCF coupling
- Use of SVN.

1st Step: Steady State Nodal Coupling Implementations in the code

- Implemented in MVS 2010 with Intel Compiler
- Original PARCS has 6 projects: *parcsexec*, *parcs*, *paths*, *pvm*, *TPRLib*, *xdr*
- Scf project added to the Solution
 - The original SCF code is fully added with small modifications.
- New coupling Modules are added to the *parcsexec* project
 - Added folder containing all new modules
- New modules added:
 - ***scf_init***: part of the original subchanflow main program to initialize SCF
 - ***scf_ss***: part of the original subchanflow main program to that runs the steady state
 - ***scf2parcs***: contains subroutines to pass variables from neutronics to TH
 - ***parcs2scf***: contains subroutines to pass variables from TH to neutronics
 - ***exchangeScfM***: variables and subroutines related to renaming SCF variables
 - ***scfcouplingM***: variables and subroutines necessaries for the coupling
- Some other small changes in PARCS and SCF modules

1st Step: Steady State Nodal Coupling – New cards in PARCS Input deck

- SCF_TH (TRUE/FALSE) card added to PARCS
 - FALSE is default
 - If .TRUE. → check, and sets:
 - fdbk=.TRUE.
 - pathsflag = .FALSE.
 - extth = .FALSE.
 - Warnings are given in case any of these variables are changed.

- SCFCHAEQ (opt [chan_list / file])card added to PARCS
 - opt: 0 (default)
 - opt: 1 → chan_list must be given
 - Nchan ordered numbers (1,...*i*,..., nchan) given the equivalent SCF channel number to the *i* PARCS channel number.
 - opt: 2 → file with mapping description must be given (not implemented yet)

- Remark: If the SCF input is prepared in a consistent way. The SCF_TH set to true is enough to use SCF TH.

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 - Flowchart
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Testing PARCS/SCF Steady State Coupling

- Selected cases:
 - 3x3 PWR Minicore
 - PWR MOX UO2 Core
- Method: code-to-code comparison
 - PARCS/SCF versus PARCS+Internal TH solver
- Compared parameters:
 - Assembly-wise Power distribution
 - Axial distributions of Power, Temperature of the Coolant and the Fuel
- Considerations for comparison:
 - Core TH model:
 - SCF: parallel channels with cross flow – SCF input needed
 - PARCS internal TH module: parallel channels, TH defined in PARCS input
 - Core neutronic model:
 - **Same PARCS input:** only one card (SCF_TH card) changed: TRUE or FALSE

3x3 FA PWR Minicore Description

- Fast running: Good for testing initial implementation.
- XS from OECD UOX/UO₂ Benchmark
- Asymmetric problem chosen

Power [MW]	10
T_{in} [°C]	286
Boron [ppm]	566
Mass flow rate/FA [kg/seg]	18.121

ref	ref	ref	ref	ref
ref	UO ₂ + CR	UO ₂	UO ₂	ref
ref	UO ₂	MOX	UO ₂	ref
ref	UO ₂	UO ₂	UO ₂	ref
ref	ref	ref	ref	ref

Core configuration.

3x3 FA PWR Minicore Results

0.3378	1.0296	0.8167
1.0296	1.6112	1.2411
0.8167	1.2411	0.8764

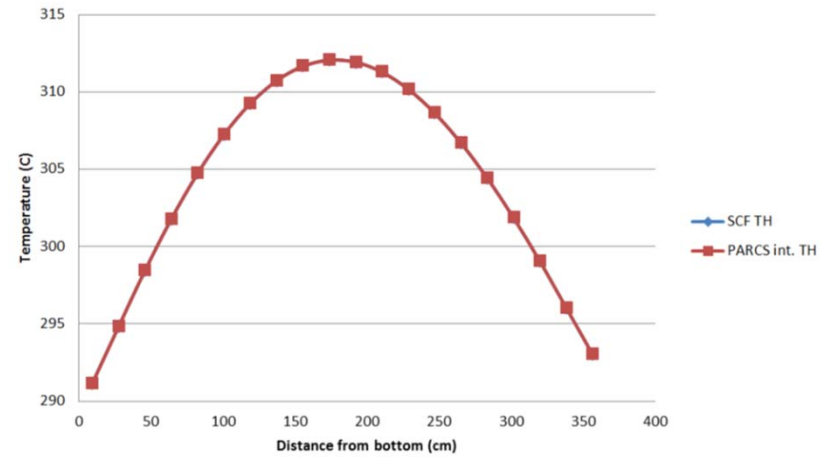
Assembly wise power distribution (AU)

Relative error (%)

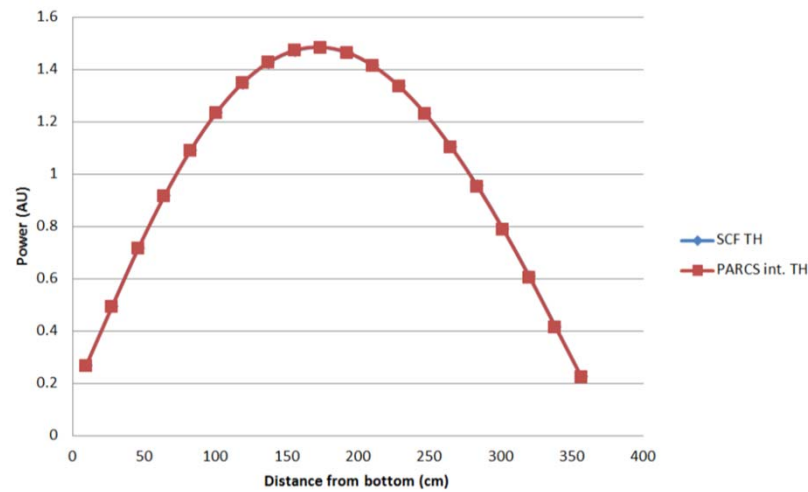
0.000	0.000	0.012
0.000	-0.019	0.008
0.012	0.008	0.011

$$100 \cdot \frac{TH_{SCF} - TH_{internal}}{TH_{internal}}$$

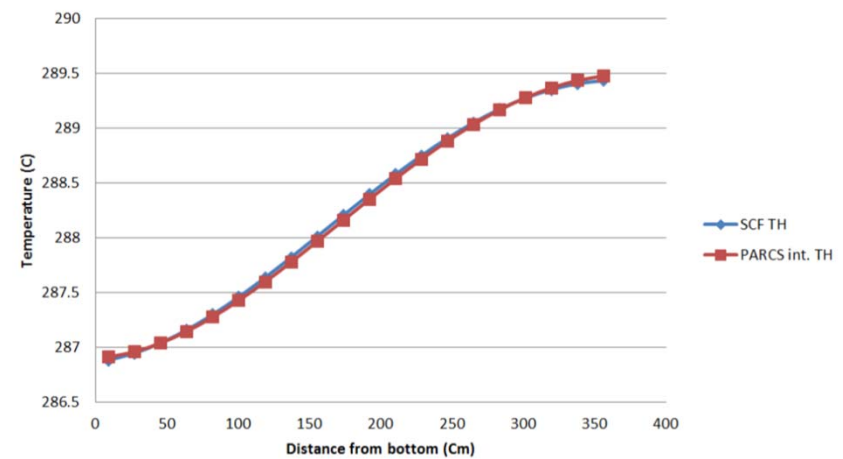
Axial Fuel Temperature Distribution



Axial Power Distribution



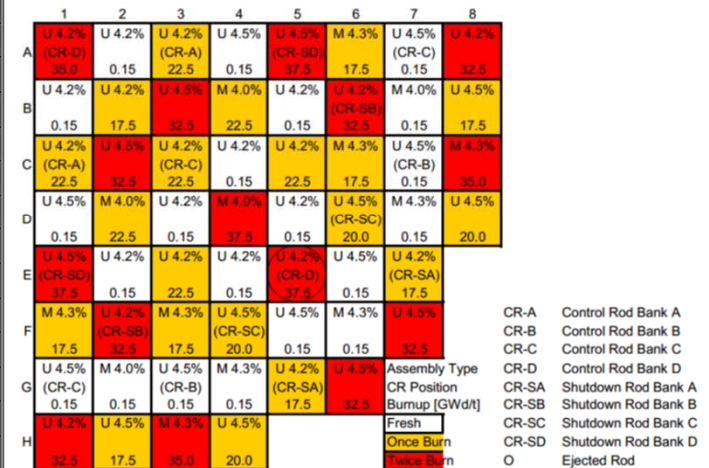
Axial Moderator Temperature Distribution



OECD/NEA AND U.S. NRC PWR MOX/UO2

Number of fuel assemblies	193
Power level (MW _{th})	3565
Core inlet pressure (MPa)	15.5
Hot full power (HFP) core average moderator temperature (K)	580.0
Hot zero power (HZIP) core average moderator temperature (K)	560.0
Hot full power (HFP) core average fuel temperature (K)	900.0
Fuel lattice, fuel rods per assembly	17x17, 264
Number of control rod guide tubes	24
Number of instrumentation guide tubes	1
Total active core flow (kg/sec)	15849.4
Active fuel length (cm)	365.76
Assembly pitch (cm)	21.42
Pin pitch (cm)	1.26
Baffle thickness (cm)	2.52
Design radial pin-peaking (F _H)	1.528
Design point-wise peaking (F _O)	2.5
Core loading (tHM)	81.6
Target cycle length (GWd/tHM) (months)	21.564 (18)
Capacity factor (%)	90.0
Target effective full power days	493
Target discharge burnup (GWd/tHM)	40.0-50.0
Maximum pin burnup (GWd/tHM)	62.0
Shutdown margin (SDM) (% Δρ)	1.3

Core design parameters.



1/4 Core configuration.

OECD/NEA AND U.S. NRC PWR MOX/UO2 (Cont'd)

- XS data from Benchmark
- More complex geometry and composition: Good for testing correct implementation of the coupling
- 3D core calculation: 193 Fuel Assemblies with different burn-up, discretized in 20 axial nodes

FA TYPE MAP

		1	2	3	4	5	6	7	8
FA #	Burnup points	1	1	1	2	2	3	2	1
1 U 4.2	0.15	1	1	2	3	1	1	3	2
2 U 4.5	17.5	1	2	1	1	1	4	2	4
3 M 4.0	20	2	3	1	3	1	2	4	2
4 M 4.3	22.5	2	1	1	1	1	2	1	0
	32.5	3	1	4	2	2	4	2	0
	35	2	3	2	4	1	2	0	0
	37.5	1	2	4	2	0	0	0	X
		0	0	0	0	0	X	X	X

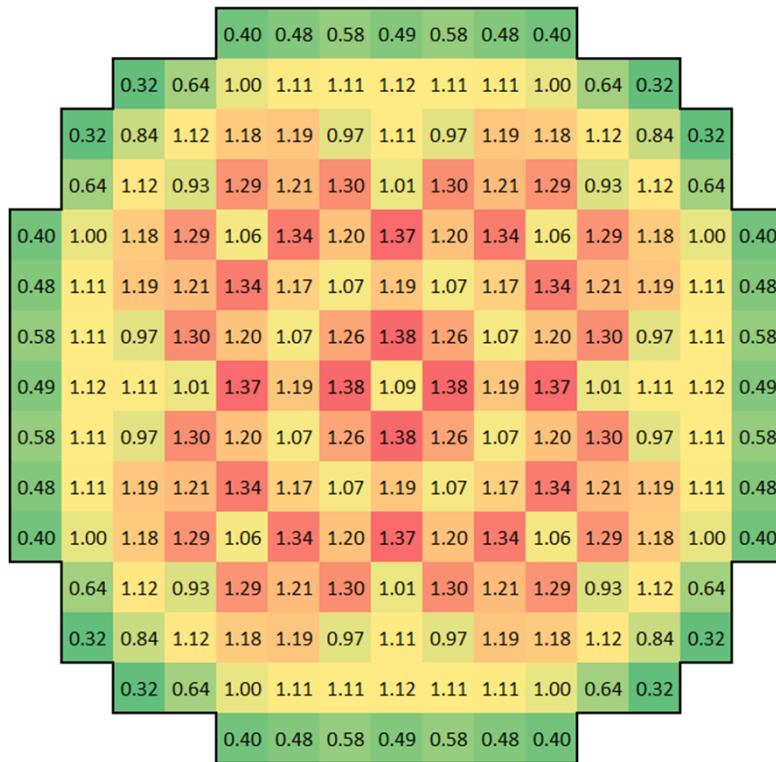
PWR Core: FA radial map

BURNUP MAP

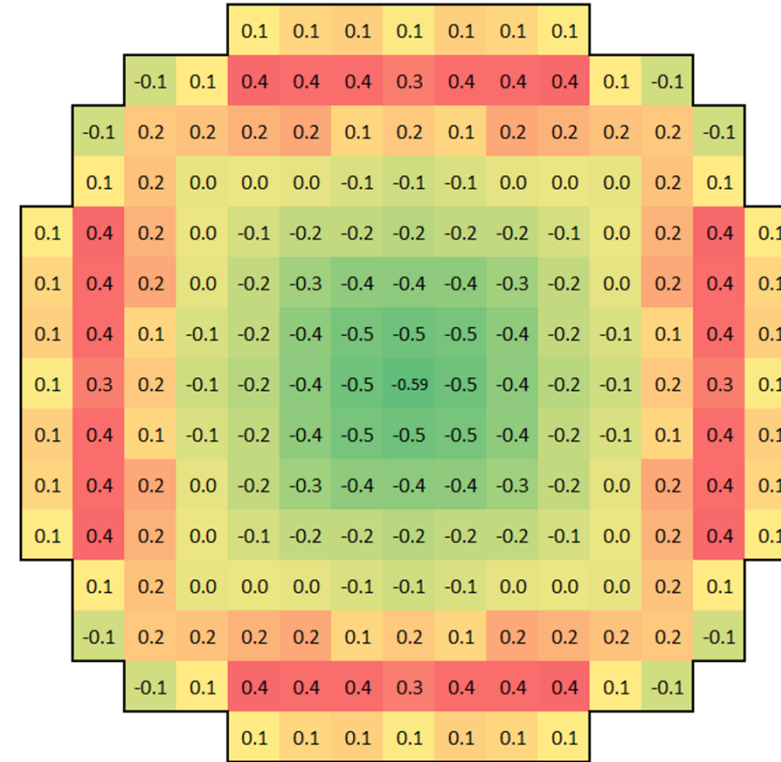
		1	2	3	4	5	6	7	8
a		35	0.15	22.5	0.15	37.5	17.5	0.15	32.5
b		0.15	17.5	32.5	22.5	0.15	32.5	0.15	17.5
c		22.5	32.5	22.5	0.15	22.5	17.5	0.15	35
d		0.15	22.5	0.15	37.5	0.15	20	0.15	20
e		37.5	0.15	22.5	0.15	37.5	0.15	17.5	
f		17.5	32.5	17.5	20	0.15	0.15	32.5	
g		0.15	0.15	0.15	0.15	17.5	32.5		
h		32.5	17.5	35	20				

PWR Core: Burn-up radial map

Results: PARCS w/ internal TH vs PARCS/SCF Assembly-wise Power distribution comparison



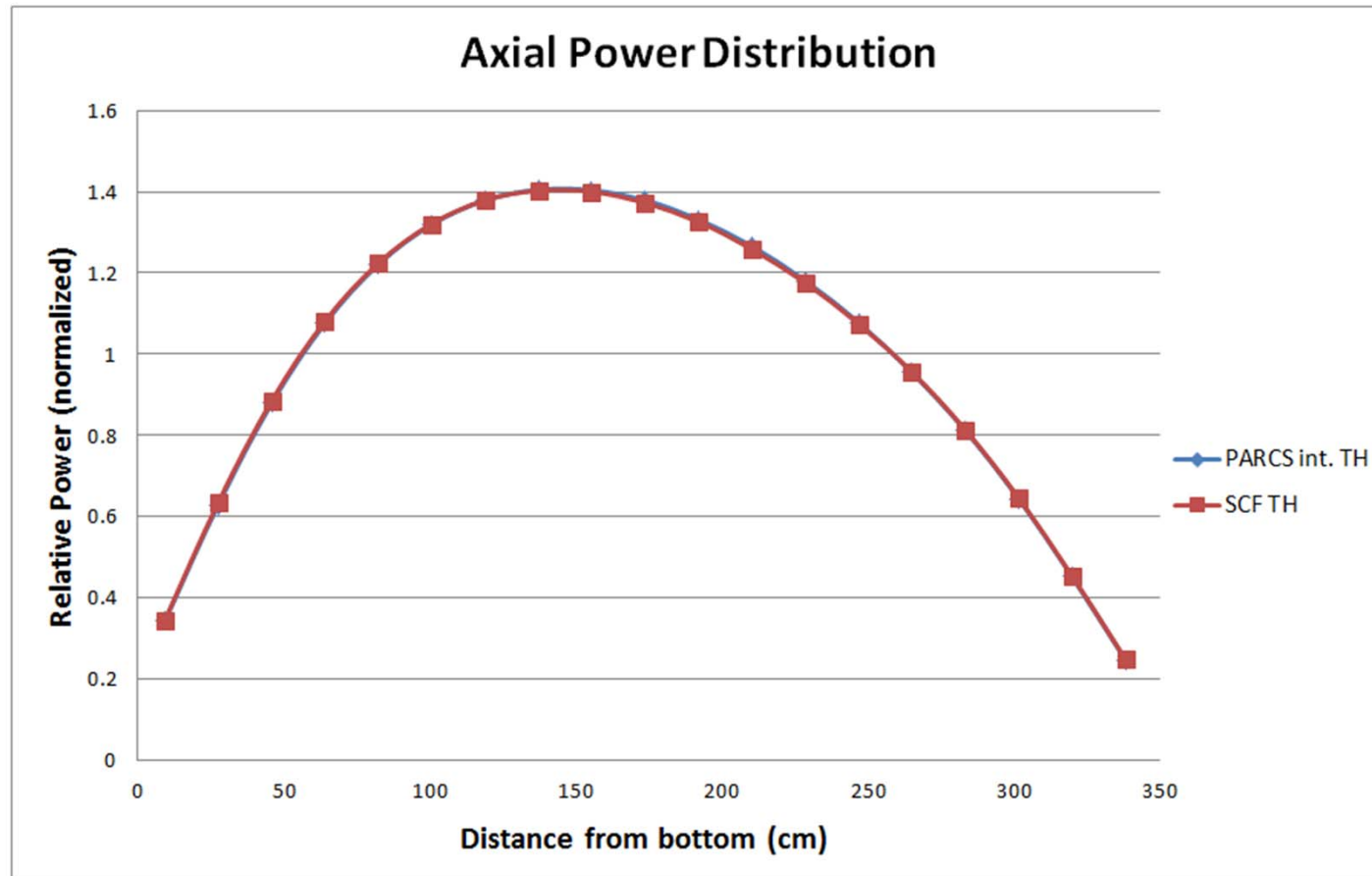
PARCS+Internal TH: axially integrated
Power Distribution (AU)



Relative error (%) $100 \cdot \frac{P_{intern.TH} - P_{SCF}}{P_{inter.TH}}$

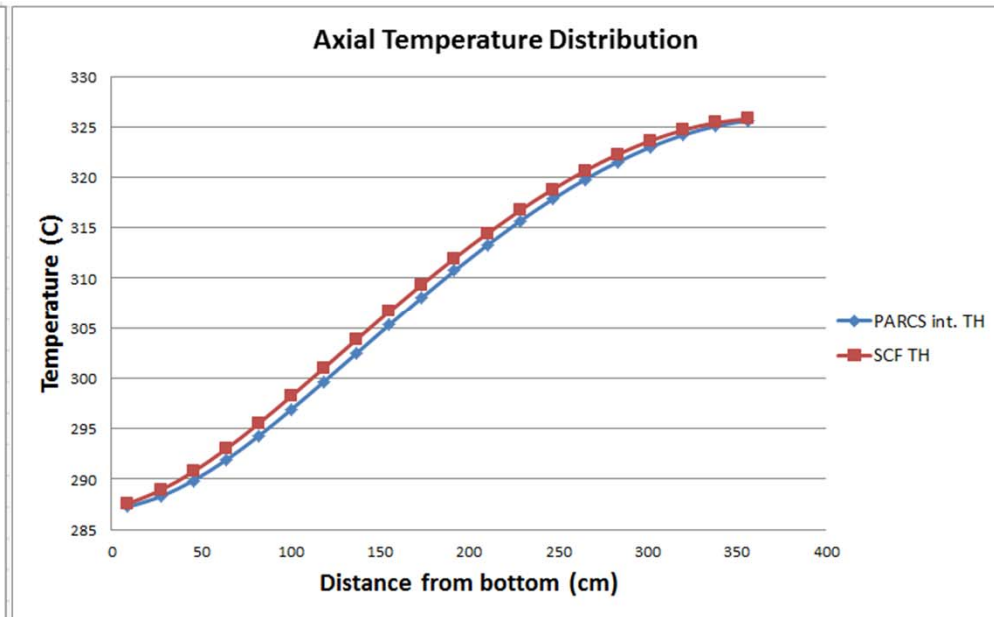
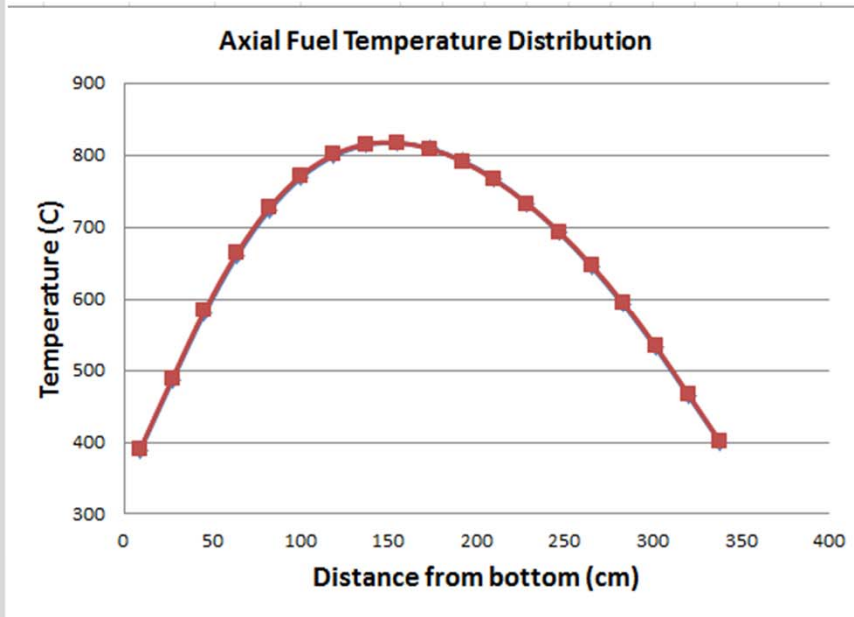
Relative Error < **0.6%**

Axial Power Distribution comparison



Comparison of relative axial Power

Axial Coolant and Fuel Temperature Distribution comparison



Comparison of Fuel temperature

Comparison of Coolant temperature

■ Remarks:

- Good agreement for Power Distribution and Fuel temperature.
- Small differences in coolant temperature distribution encountered. This can be caused by different models in TH calculation e.g. different Look up tables, heat transfer correlation, constitutive equation.

Agenda

- Motivation
- Subchanflow (SCF)
 - Short introduction
 - Previous work done at KIT
- PARCS v3.2 /Subchanflow v2.6 Internal Coupling
 - Coupling Steps
 - Coupling Description:
 - Programming approach
 - Flowchart
 - Convergence criteria
 - Mapping
 - Current Status
- Testing and Results
 - 3x3 minicore
 - OECD PWR MOX UO₂ benchmark (Part II)
- Summary and Outlook

Summary

- Steady state nodal level SCF internal coupling implemented.
- Good agreement with internal solver, some differences product of different correlations and look up tables.
- Special attention is given to the implementation of a good programming.
- The intention is to implement an easy to use new solver that requires not much extra effort from the user.

Outlook

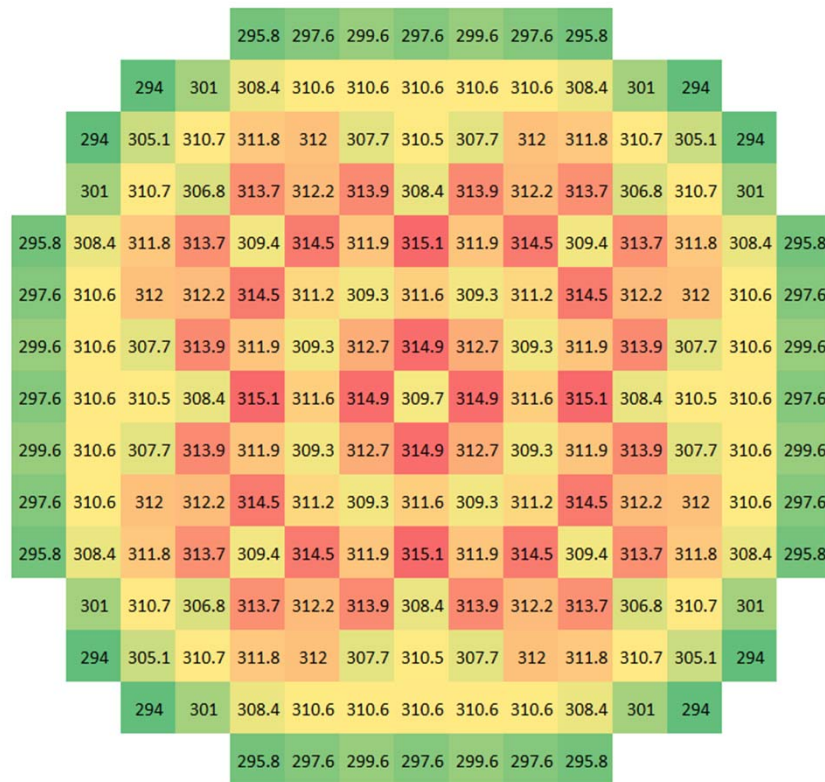
- Implement flexible mapping (axial, radial)
- Implementation of the transient coupling of PARCS and SCF
- Implement the coupling at pin-level (based on KIT experience with DYNSUB)
- Implementation of preprocessor for SCF in case of pin-level coupling.
- Verification and validation against DYNSUB and MC/SCF coupling

Thank you for your attention.

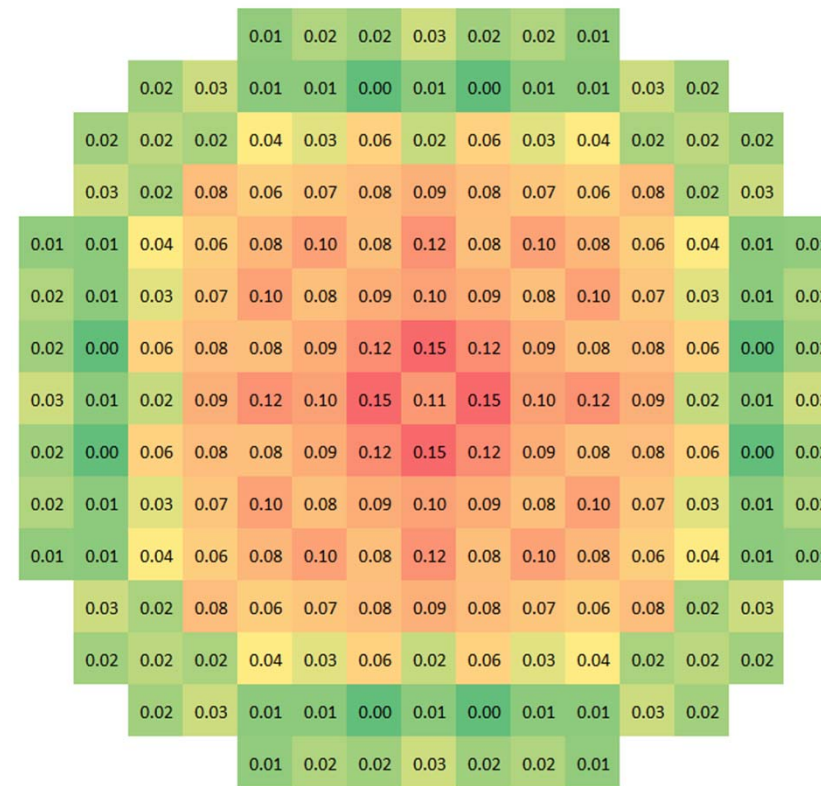
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Outlet moderator temperature

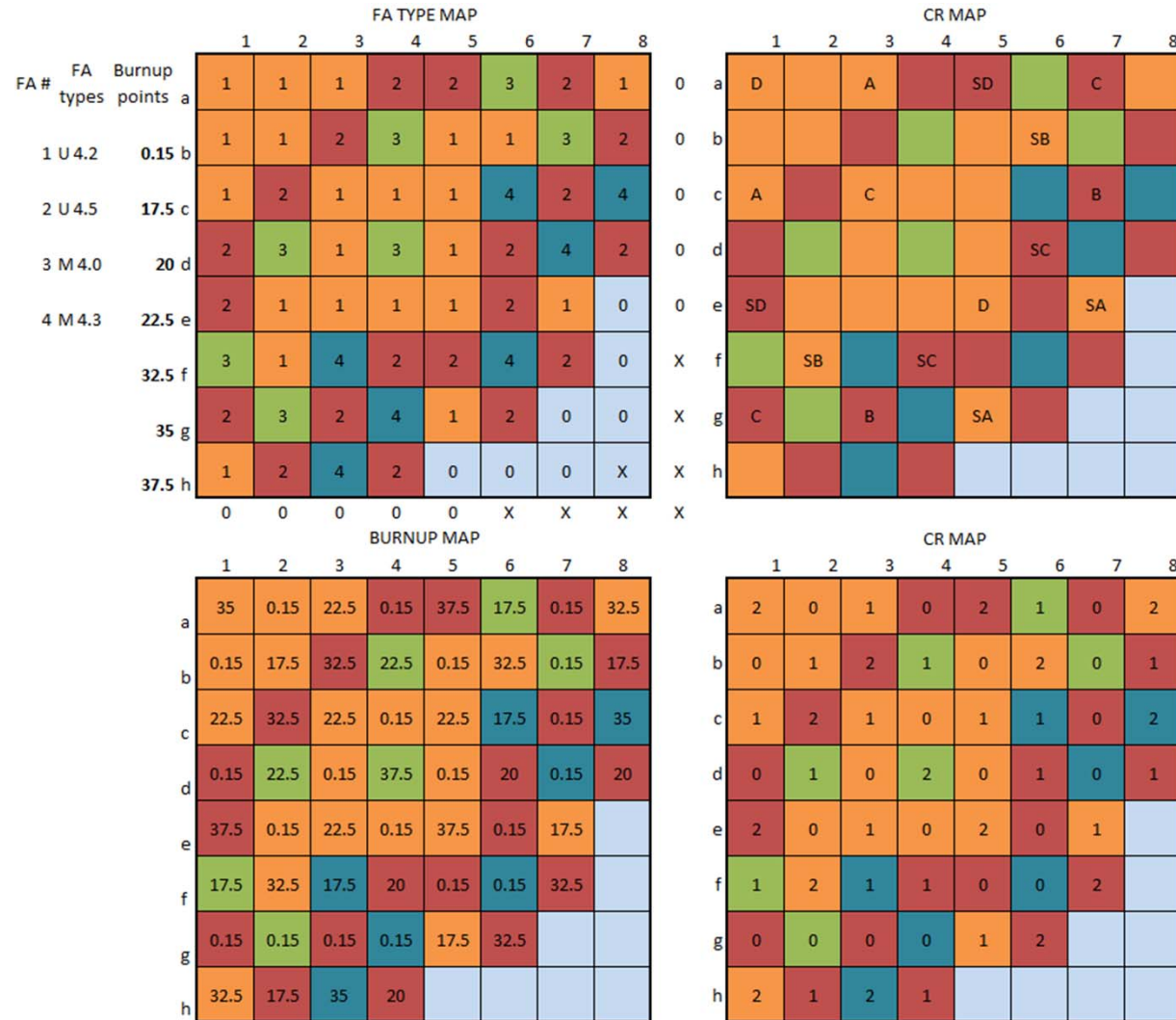


PARCS+Internal TH: outlet moderator temperature



Absolute difference: PARCS/int. TH – PARCS/SCF

Appendix



SCF: Code Features

- Completely programmed in Fortran 95.
- Can be used with WINDOWS or LINUX.
- Dynamic memory management.
- **Modular structure, keyword and table oriented input.**
- Available fluids: water, lead, lead-bismuth sodium, helium, air.
- **Works with SI units.**
- Flexible geometry definition (**square, hexagonal**).
- Sub-channel fuel assembly simulations.
- Fuel assembly or “channel wise” whole core simulations.
- Steady state and transient solution.

Basic Equations and Numerical Solution

- Sub-channel formulation of mass, momentum and enthalpy equation.
- Simplified lateral momentum equation without convection term.
- Forced convection upward flow, no recirculation.
- Two Phase Flow mixture for water and sodium (3 equations with slip).
- Fully implicit solution for pressure, flow, enthalpy.
- Direct pressure matrix inversion for small problems.
- SOR pressure matrix iteration solution for large problems.
- Fully explicit TVD solution for scalar advection (boron).
- Explicit sub-time-step solution of point kinetic equations.
- Iterative procedure to find critical heat flux condition.

Physical models

- Flow regime dependent heat transfer models.
- Slip model for boiling including sub-cooled boiling.
- Several “Critical Heat Flux” correlations.
- Pressure drop models including spacers and wire-wraps.
- Flow regime dependent turbulent cross-flow mixing models.
- (equal mass or equal volume).
- 2D (r-z) fuel pin heat conduction, axially for transients, only.
- **Simplified correlation based fuel pin behaviour.**
- (cracking, swelling, fission gas release).
- Gap conductance model for fuel-cladding gap.
- Water EOS and properties: **IAPWS-97 formulation.**
- Point kinetic model based transient power calculation.

User Friendly

- Compilation with standard Fortran compiler.
- Fast running on Desktop-PC or Notebooks.
- Input based on clear text keywords and tables.
- **Fixed input template, error handling.**
- Reading of external tables prepared by pre-processors.
- Amount of output controlled by simple input keyword.
- **Output for graphical tools (1D, 2D, 3D) in simple table e.g. ParaView.**
- **Online visualization possible with GNUPLOT.**
- **Direct support from U. Imke (uwe.imke@kit.edu).**

Example: COBAYA3/SCF Boron Dilution Problem

- A. Gomez and e. al., "On the Influence of Shape Factors for CHF Predictions with the Sub Channel Code SUBCHANFLOW during a Rod Ejection," in *NUTHOS-9*, Kaohsiung, Taiwan, 2012
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- W. Jaeger, J. P. Manes, U. Imke, J. J. Escalante and V. S. Espinoza, "Validation and comparison of two-phase flow modeling capabilities of CFD, sub channel and system codes by means of post-test calculations of BFBT transient tests," *Nuclear Engineering and Design*, vol. 263, pp. 313-326, 2013

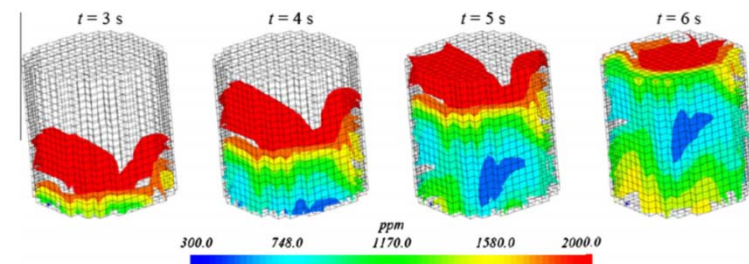
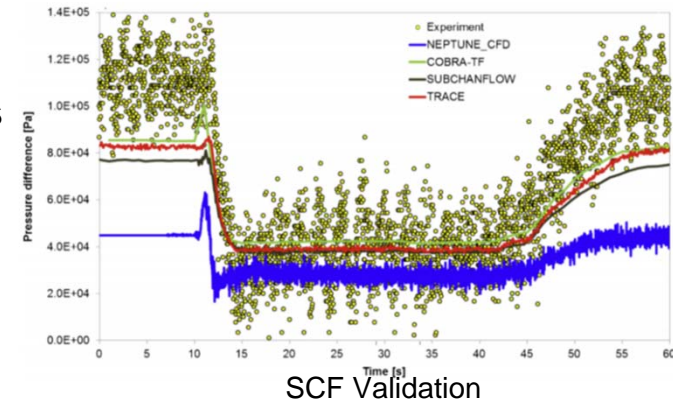


Fig. 13. Evolution of the boron concentration during the transient for the slug size 1 ($t = 3-6$ s).

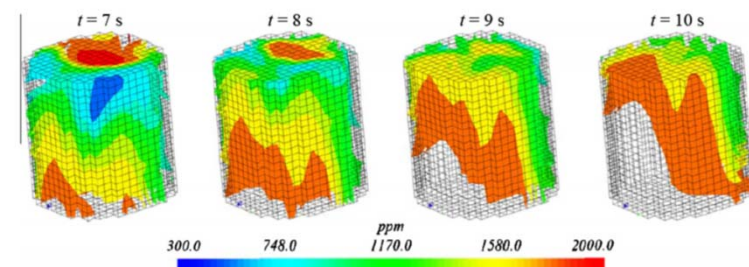


Fig. 14. Evolution of the boron concentration during the transient for slug size 1 ($t = 7-10$ s).