KIT Advanced Multiphysics Schemes for LWRs Applications

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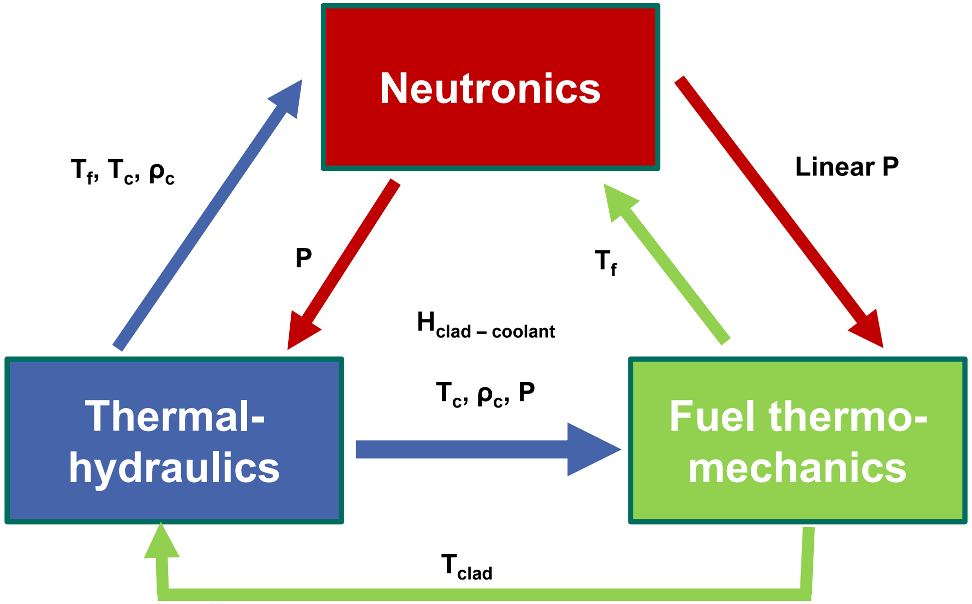
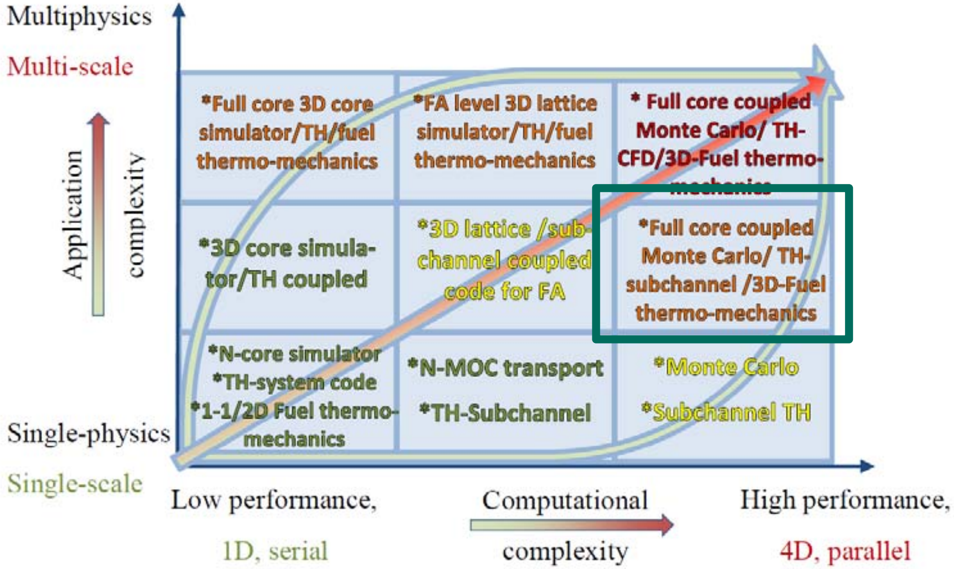
The coupled problem





→ need to simultaneously determine the neutron density field, the flow field and the fuel temperature field

- **Assumption**: the problem can be linearized over some interval and iterations are performed between the different solvers
- **High fidelity solvers**: focused on achieving better predictions by reducing the approximations in the equations and having a better description of the problem domain

KIT approach: High-Fidelity MC-based multi-physics

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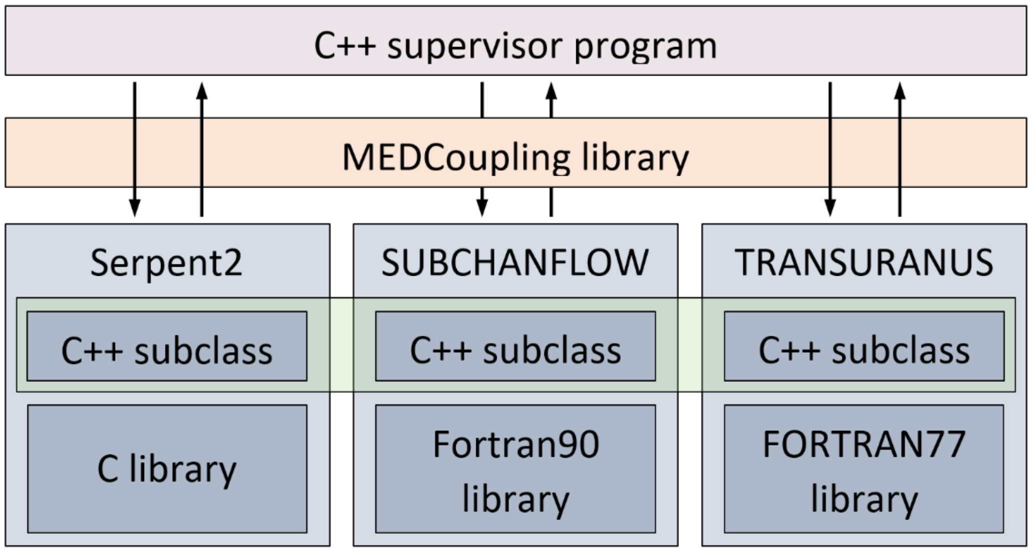
- Objectives:
  - **Avoid approximation** (multi-scale approach) **in neutronics**
  - **Pin-by-pin burnup**
  - **Transient scenarios** (REA-type)
  - **Calculate local safety parameters** directly
  - Provide **reference solutions** for low order methods
- Neutronics (**Serpent 2**)
  - Continuous-energy Monte Carlo neutron transport
  - Pin-by-pin power tallying and burnup calculation
- Thermal-hydraulics (**SUBCHANFLOW**)
  - Pin-level subchannel TH
  - Coolant and fuel safety parameters
- Fuel performances (**TRANSURANUS**)
  - Pin-level thermo-mechanic analysis
  - Fuel safety parameters

Software design for multi-physics analysis

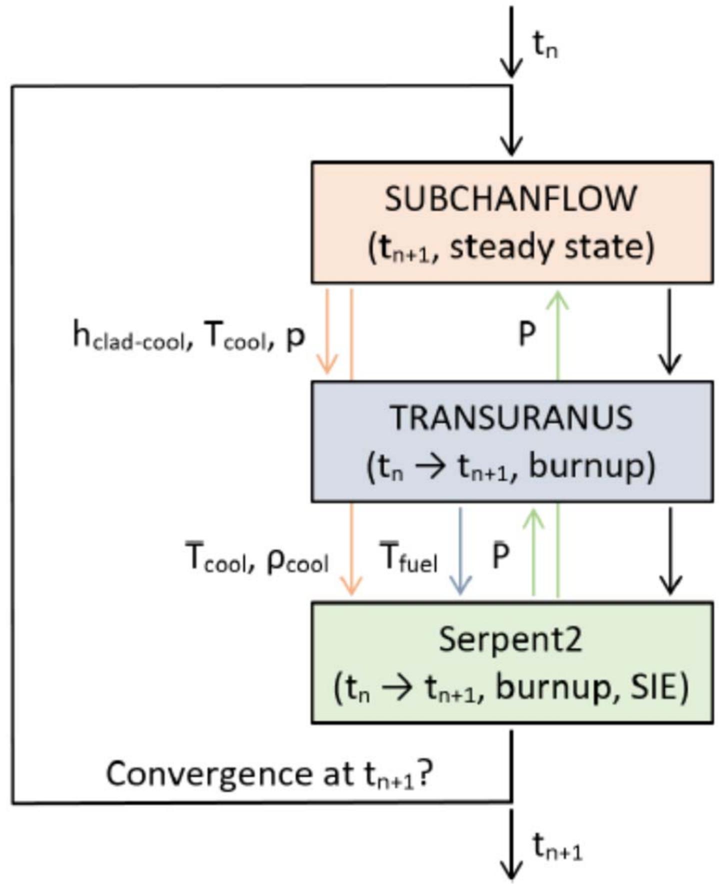
- **Master-slave internal coupling:**
  - **SCF and TU (slaves) modularized and embedded in Serpent2 (master)**
  - **Traditional approach, reference for performance**
- **Object-oriented coupling:**
  - **Serpent2, SCF and TU modularized and coupling scheme implemented in a separate supervisor program**
  - More innovative approach, potential benefits from the object-oriented design
  - Main features:
    - Inheritance-based APIs
    - Object-oriented supervisor
    - Mesh-based feedback



- **Numerical methods:**
  - Operator splitting
  - Picard iterations
  - Pin-by-pin feedback

The Serpent2/SCF/TU depletion coupling scheme

- **SCF simplified fuel model replaced by the more sophisticated one of TU**
- **Semi-implicit iterative scheme** (code to code feedback is done using the **fields at EOS and convergence at EOS achieved iterating each burnup steps**)
    1. **SCF steady state to get cooling conditions for the Serpent power distribution at EOS**
    2. **TU solves a burnup step using SCF solution as BC and Serpent power as heat source**
    3. **Serpent burnup with TH condition at EOS**
- **Pin-level feedback**
- Burnup in Serpent (full set of Bateman equations) and TU (simplified model suitable for fuel performance analysis)
- Traditional N-TH scheme can also be used w/o TU

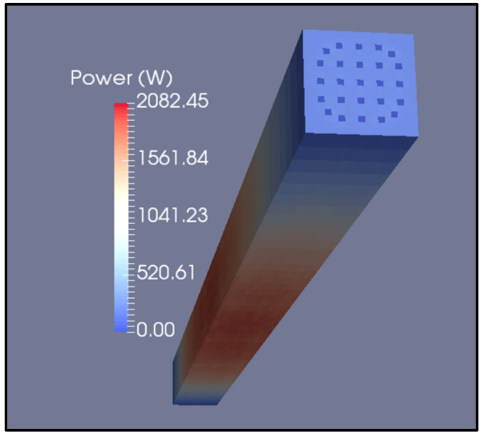


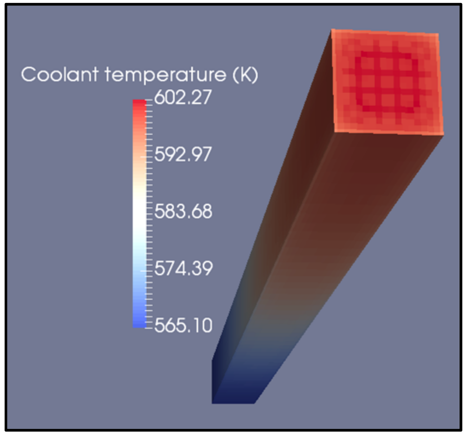
Fully coupled depletion scheme

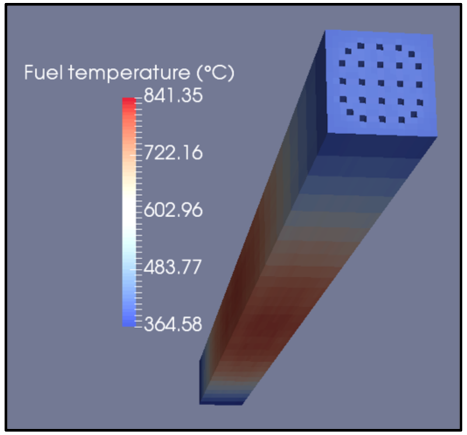
M. Garcia et al.; "A Serpent2-SUBCHANFLOW-TRANSURANUS coupling for pin-by-pin depletion calculations in Light Water Reactors", ANE **139** (2020)

Pin-by-pin Serpent2/SCF/TU coupling verification

PWR: VERA Benchmark Problem 6



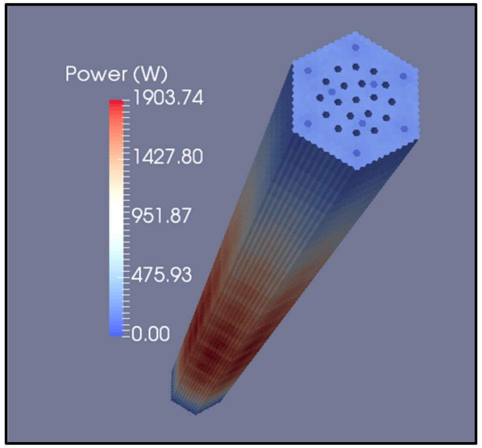


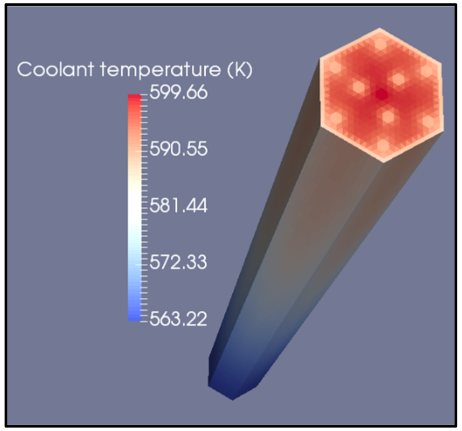


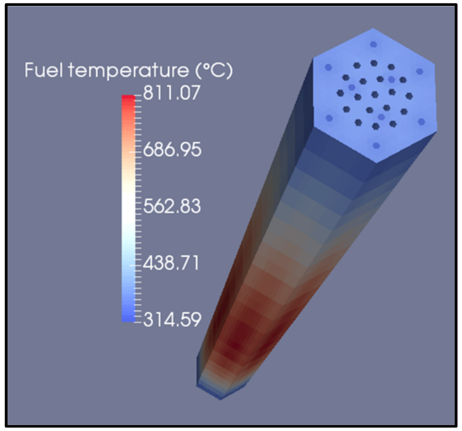
Serpent + SCF / Reported VERA-CS / Difference [%] (color scale 0.935 – 1.055)

	1.0347 1.0355 -0.07	1.0355 1.0357 -0.02		1.0328 1.0342 -0.13	1.0313 1.0311 0.02		1.0103 1.0114 -0.11	0.9798 0.9764 0.34
1.0335 1.0355 -0.20	1.0082 1.0096 -0.14	1.0094 1.01 -0.06	1.0358 1.0359 -0.01	1.0085 1.0088 -0.03	1.0036 1.0057 -0.21	1.0240 1.0252 -0.11	0.9889 0.989 -0.01	0.9734 0.973 0.04
1.0339 1.0355 -0.15	1.0091 1.01 -0.09	1.0094 1.0102 -0.08	1.0367 1.0371 -0.03	1.0091 1.011 -0.19	1.0080 1.009 -0.10	1.0269 1.0265 0.04	0.9880 0.989 -0.10	0.9731 0.9724 0.07
	1.0342 1.0359 -0.16	1.0359 1.0371 -0.12		1.0426 1.0436 -0.10	1.0427 1.0436 -0.09		1.0110 1.0115 -0.05	0.9754 0.974 0.14
1.0339 1.0342 -0.03	1.0072 1.0088 -0.16	1.0108 1.011 -0.02	1.0430 1.0436 -0.06	1.0311 1.0328 -0.16	1.0480 1.0509 -0.28	1.0340 1.0363 -0.22	0.9832 0.9842 -0.10	0.9680 0.9654 0.27
1.0295 1.0311 -0.16	1.0040 1.0057 -0.17	1.0080 1.009 -0.10	1.0433 1.0436 -0.03	1.0484 1.0509 -0.24		1.0161 1.0169 -0.08	0.9659 0.9649 0.11	0.9585 0.956 0.26
	1.0252 1.0252 0.00	1.0256 1.0265 -0.08		1.0348 1.0363 -0.15	1.0156 1.0169 -0.13	0.9743 0.9743 0.00	0.9505 0.9488 0.18	0.9496 0.9473 0.24
1.0116 1.0114 0.02	0.9890 0.989 0.00	0.9880 0.989 -0.10	1.0120 1.0115 0.05	0.9843 0.9842 0.01	0.9655 0.9649 0.07	0.9487 0.9488 -0.01	0.9411 0.9403 0.09	0.9449 0.9434 0.15
0.9783 0.9764 0.19	0.9725 0.973 -0.05	0.9733 0.9724 0.09	0.9755 0.974 0.15	0.9669 0.9654 0.15	0.9568 0.956 0.08	0.9488 0.9473 0.16	0.9461 0.9434 0.28	0.9517 0.9493 0.25

VVER: 30AV5 VVER-1000 FA type (Lötsch benchmark)



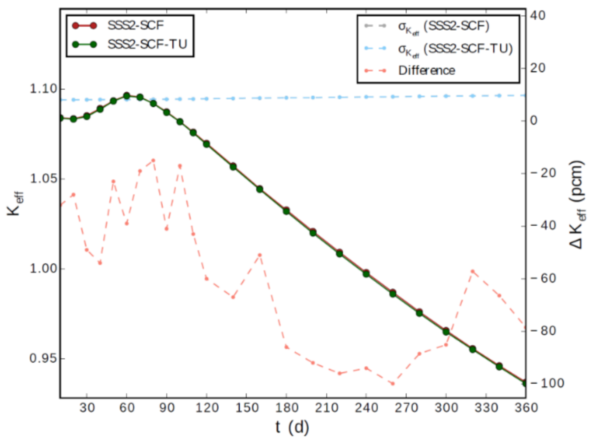


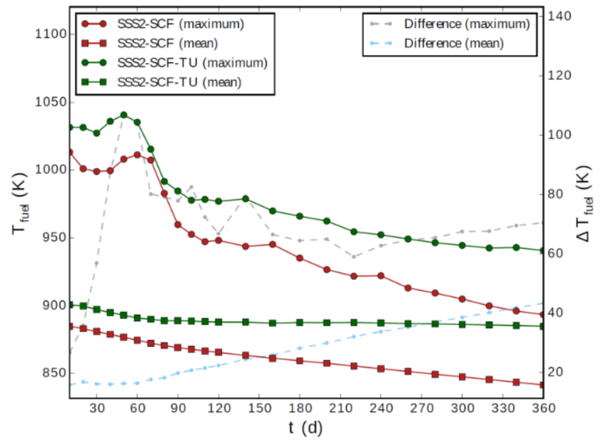


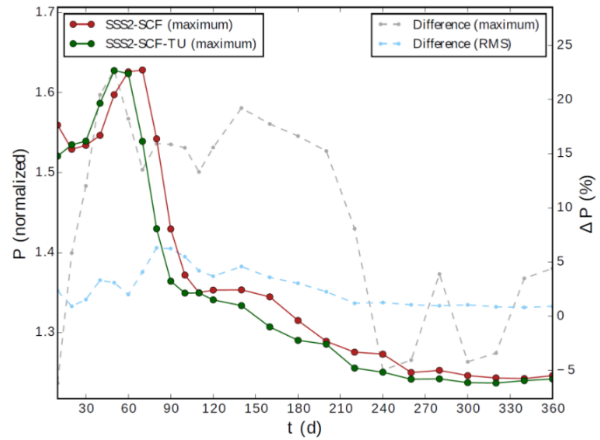
Serpent + SCF / Reported VERA-CS / Difference [°C] (color scale 320°C – 330°C; ○ GT or IT)

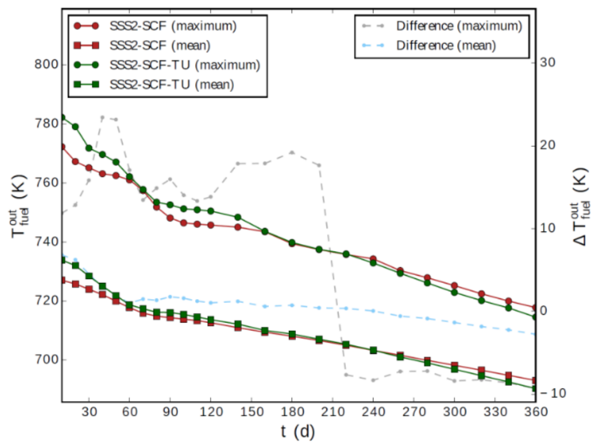
328.5 327.2 1.3	329.1 328.2 0.9	328.4 327.2 1.2	328.3 327.2 1.1	329.0 328.1 0.9	328.1 326.9 1.2	327.4 326.5 0.9	327.0 326.8 0.2	324.6 325.0 -0.4
329.1 328.2 0.9	329.1 328.5 0.6	329.1 328.2 0.9	329.1 328.2 0.9	329.1 328.4 0.7	328.8 328.0 0.8	328.2 327.6 0.6	327.0 326.9 0.1	324.5 325.0 -0.5
328.4 327.2 1.2	329.1 328.2 0.9	328.4 327.2 1.2	328.5 327.3 1.2	329.2 328.3 0.9	328.3 327.1 1.2	327.5 326.5 0.9	326.9 326.7 0.2	324.5 325.0 -0.5
328.3 327.2 1.1	329.1 328.2 0.9	328.5 327.3 1.2	328.8 327.4 1.4	329.5 328.3 1.2	328.5 327.0 1.5	327.4 326.4 1.0	326.8 326.6 0.2	324.4 324.8 -0.4
329.0 328.1 0.9	329.1 328.4 0.7	329.2 328.3 0.9	329.5 328.3 1.2	328.8 327.4 1.4	328.1 326.7 1.4	327.9 327.2 0.7	326.5 326.5 0.0	324.1 324.6 -0.5
328.1 326.9 1.2	328.8 328.0 0.8	328.3 327.1 1.2	328.5 327.0 1.5	328.2 326.7 1.4	327.4 326.4 1.0	327.4 327.0 0.4	326.1 326.2 -0.1	323.7 324.3 -0.6
327.4 326.5 0.9	328.2 327.5 0.7	327.5 326.5 0.9	327.4 326.4 1.0	328.0 327.2 0.8	327.4 327.0 0.4	326.7 326.6 0.1	325.6 325.8 -0.3	323.3 324.0 -0.7
327.0 326.8 0.2	327.0 326.9 0.1	326.9 326.7 0.2	326.8 326.6 0.2	326.5 326.5 0.0	326.1 326.2 -0.1	325.6 325.8 -0.3	324.7 325.1 -0.4	322.6 323.4 -0.8
324.6 325.0 -0.4	324.5 325.0 -0.5	324.5 325.0 -0.5	324.4 324.8 -0.4	324.1 324.6 -0.5	323.7 324.3 -0.6	323.3 324.0 -0.7	322.6 323.4 -0.8	320.9 321.9 -1.0

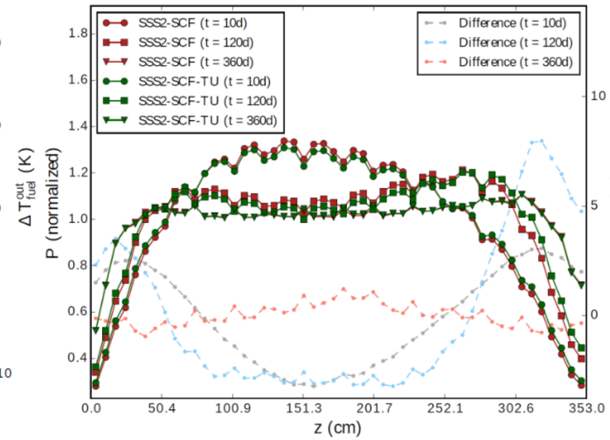
Pin-by-pin Serpent2/SCF/TU coupling verification (VVER-1000 FA)









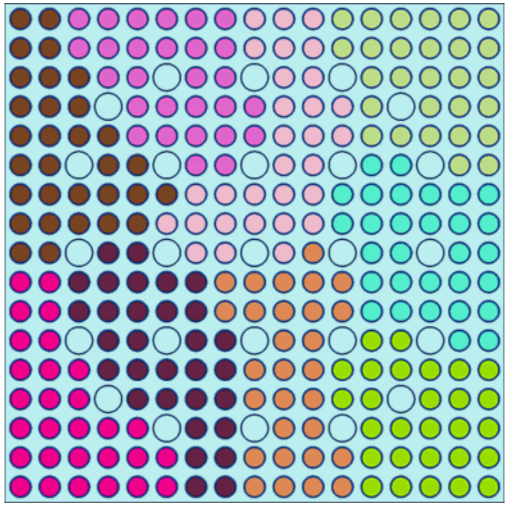


- Negligible impact on neutronics (~100 pcm), peaking factor and outer fuel temperature (~20K)
- Significant differences for fuel-cladding gap and centerline fuel temperature (investigation at higher BU is required)

M. Garcia et al.; “A Serpent2-SUBCHANFLOW-TRANSURANUS coupling for pin-by-pin depletion calculations in Light Water Reactors”, ANE **139** (2020)

Collision based domain decomposition

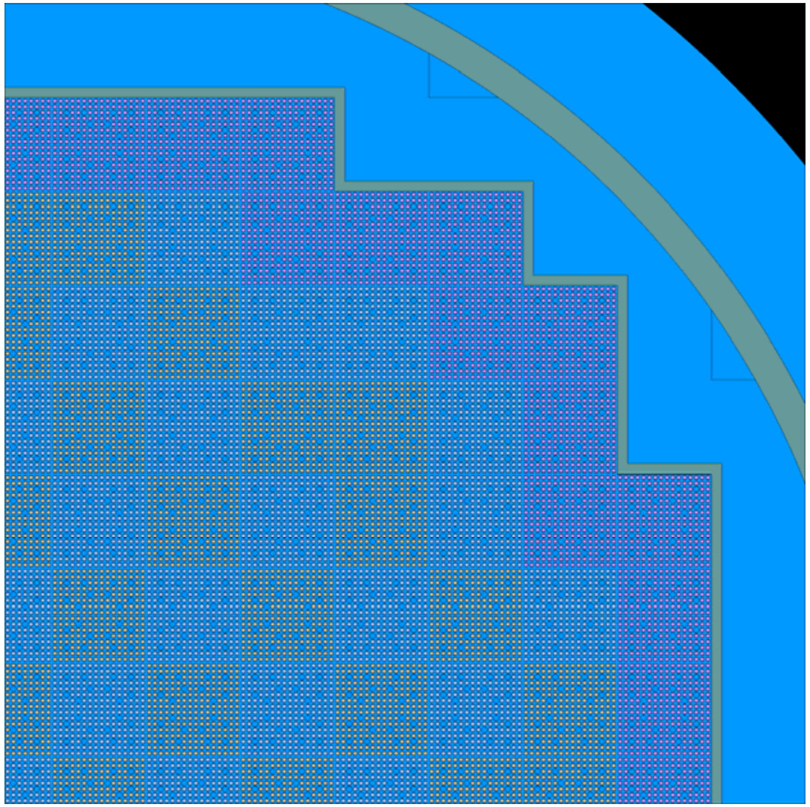
- **Full-core pin-by-pin burnup:**
  - **Hugh calculation times (~10^9 neutron histories per transport cycle)**
  - **Massive memory demand (~TB, larger than the in-node memory in HPC)**
- **Collision-based Domain Decomposition (CDD):**
  - **Memory scalability in burnup calculations:**
    - **Burnup materials decomposed in domains (MPI tasks)**
    - **All other data replicated across domains**
  - Tracking scheme:
    - Particle transfers across domains
    - Asynchronous MPI communications
    - Optimized tracking termination control
    - No physical or numerical approximations

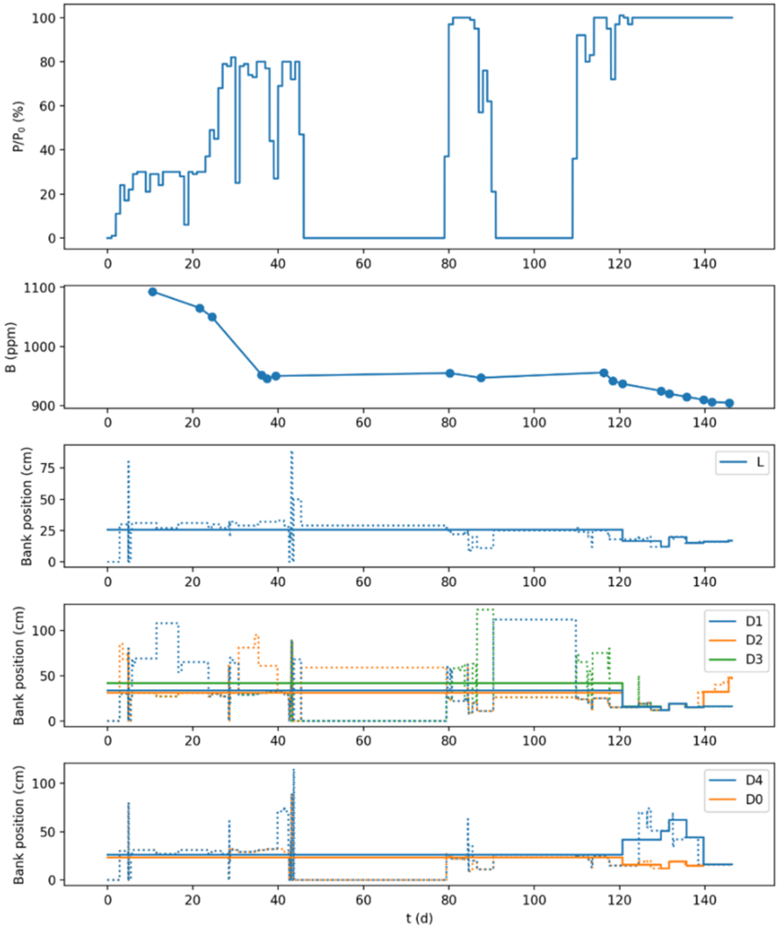


M. Garcia et al.; "A Collision-based Domain Decomposition scheme for large-scale depletion with the Serpent 2 Monte Carlo code", ANE, 152 (2021)

PWR – Validation (1)

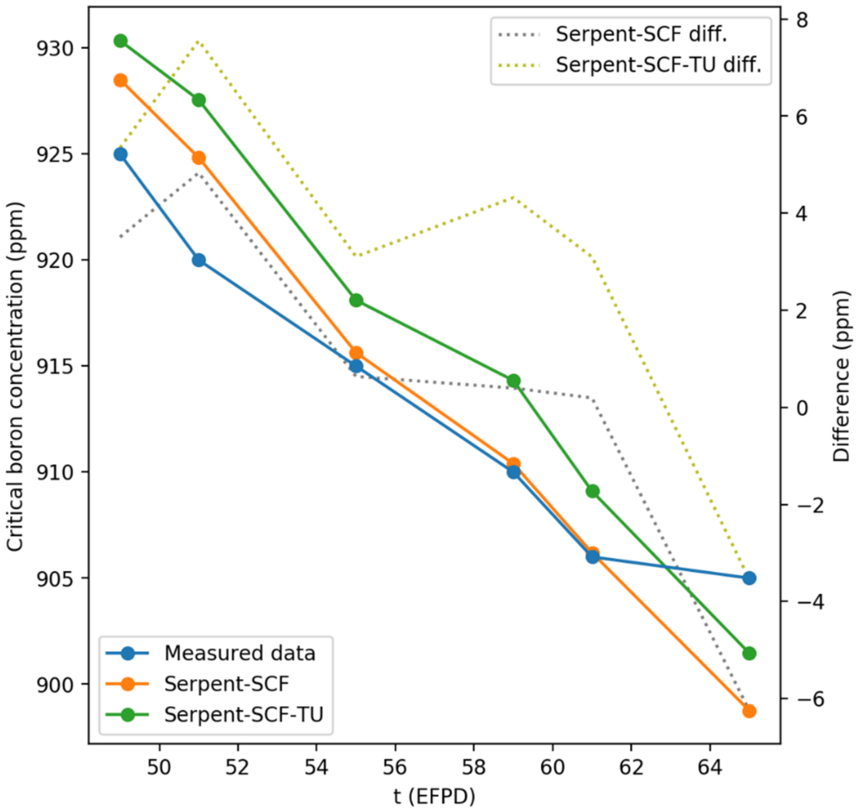
- Full-core pin-by-pin depletion
- Operating history up to 65 EFPD
- Critical boron and flux data

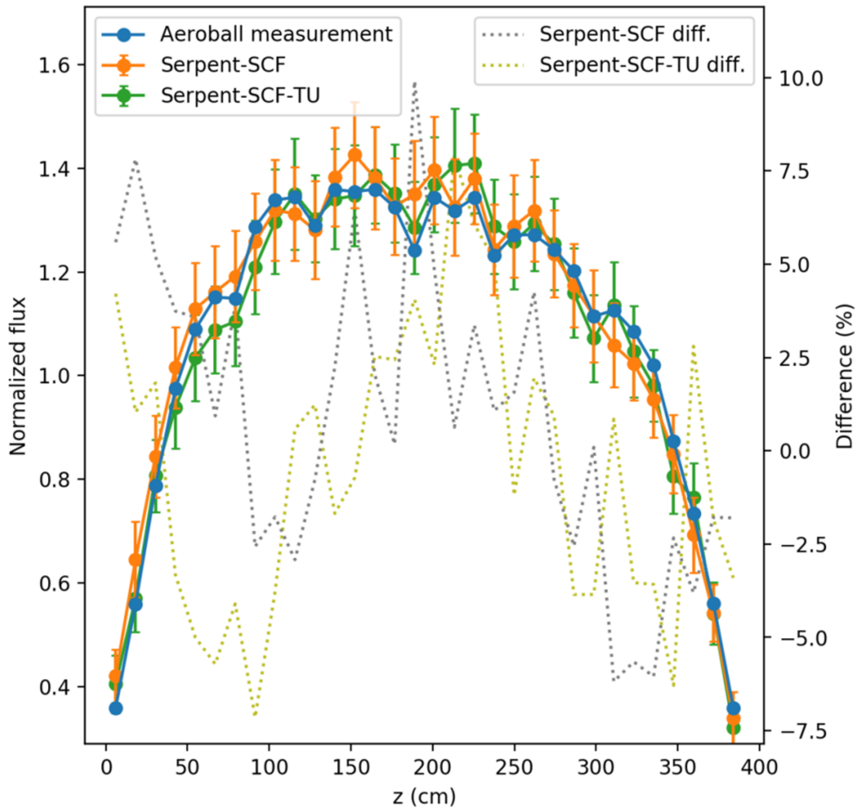




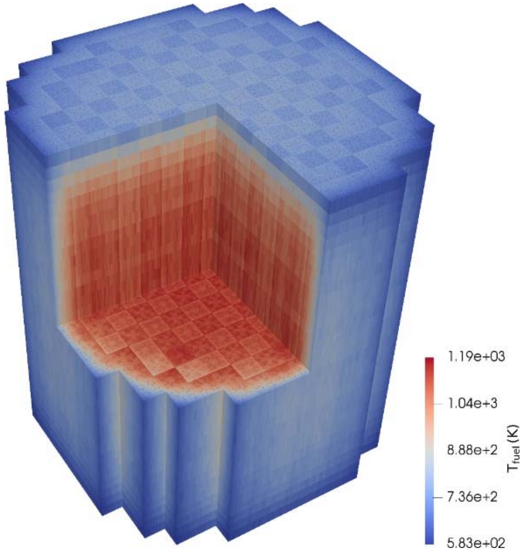
PWR – Validation (2)

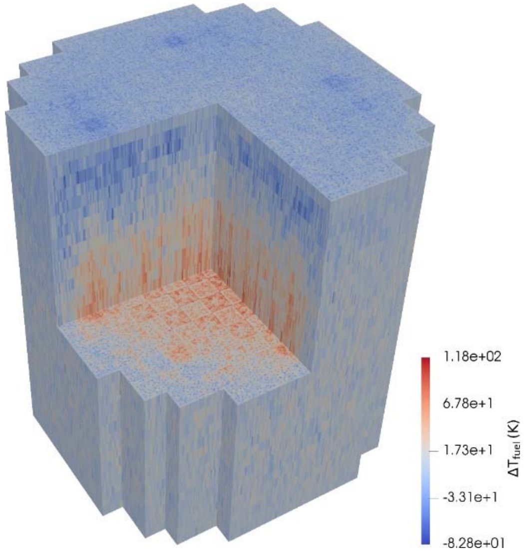
- Good agreement between results and experimental measurements.
  - Differences in critical boron concentration within a few ppm
  - Aeroball neutron flux profiles within the statistical range of the results



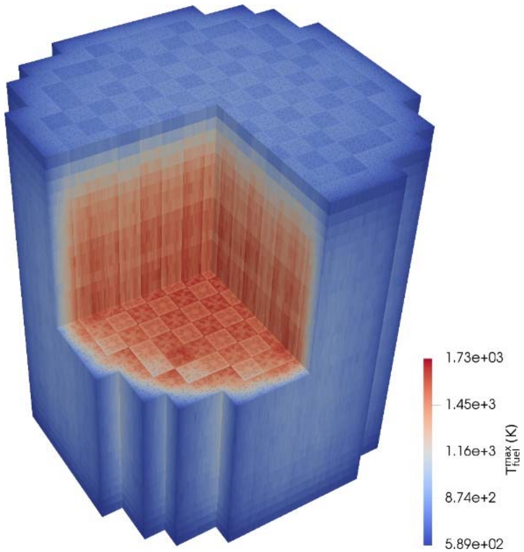


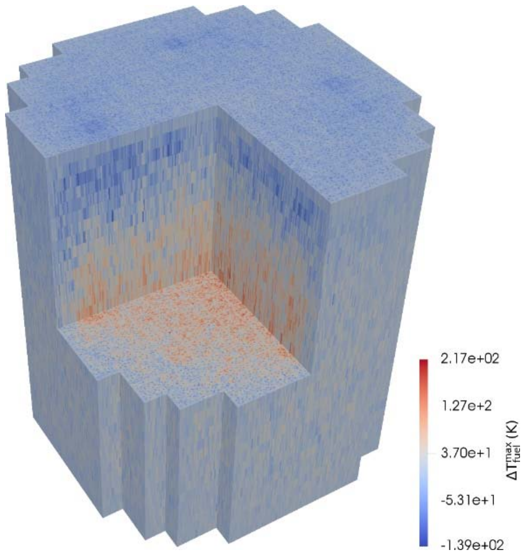
PWR – Validation (3)





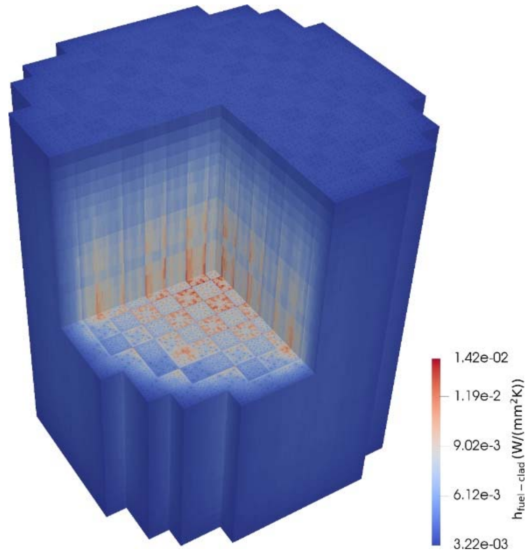
Fuel T
BU=2.35 MWd/kgU

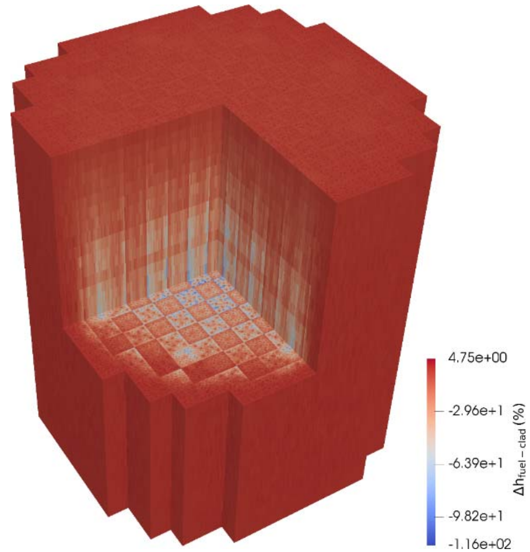




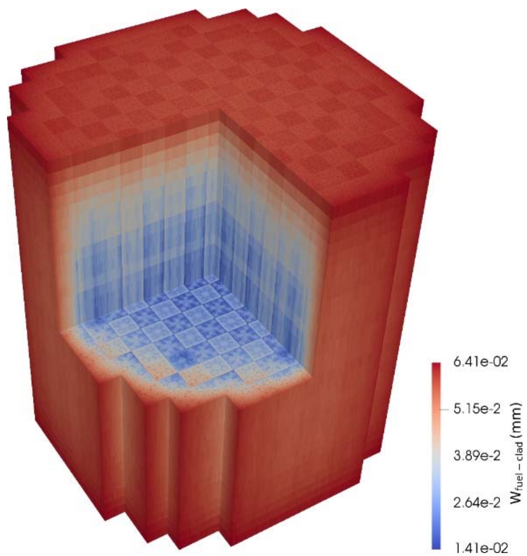
Fuel centerline T
BU=2.35 MWd/kgU

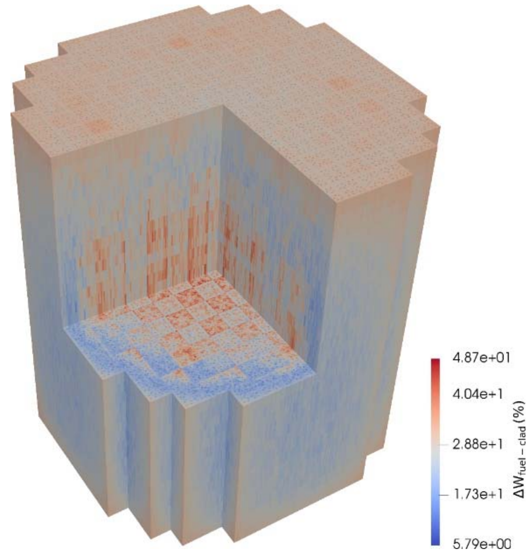
PWR – Validation (4)





Fuel-clad gap heat transfer coefficient BU=2.35 MWd/kgU

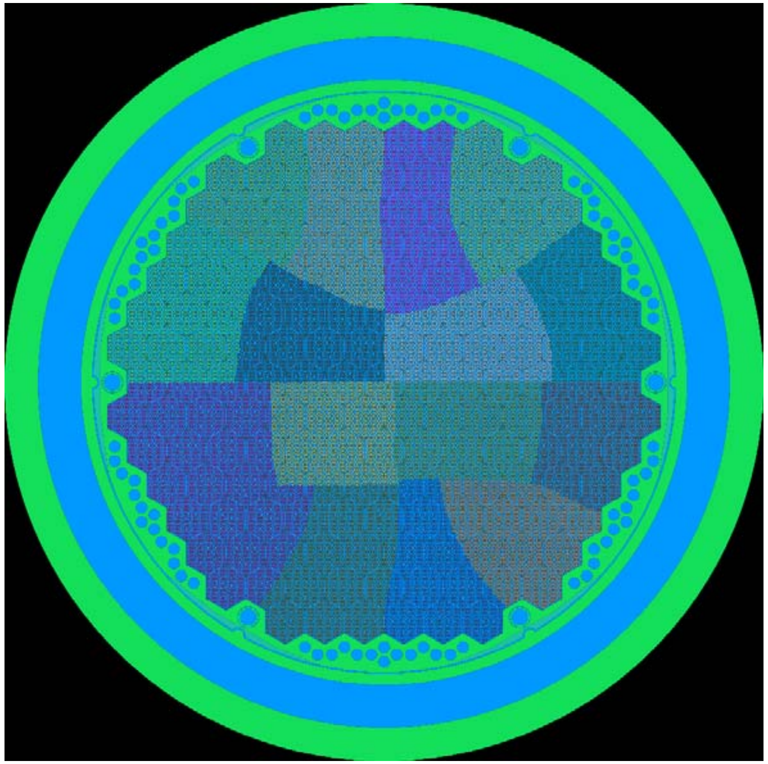


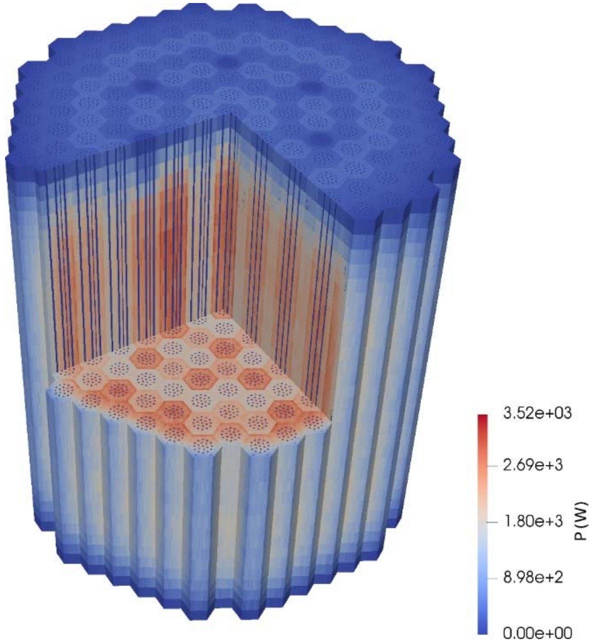


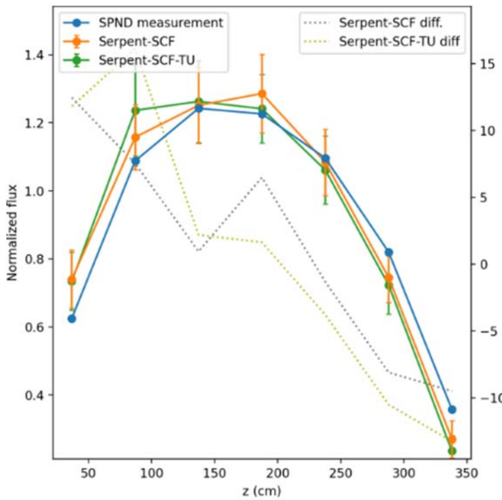
Fuel-clad gap width BU=2.35 MWd/kgU

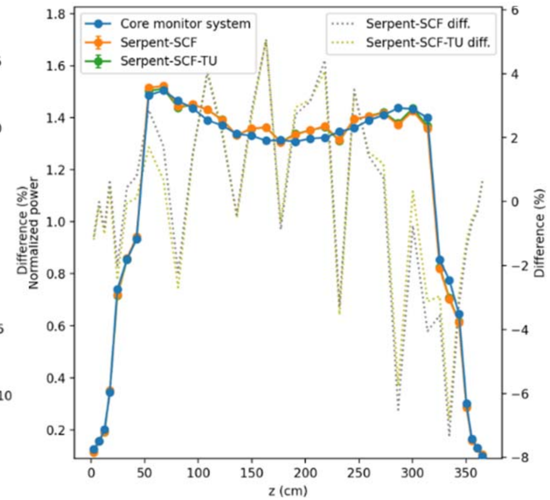
VVER – Validation

- Full-core pin-by-pin depletion
- Operating history up to 280 EFPD
- Critical boron and flux data
- Runtime: 7 days (1280 CPUs, 64 nodes)









The Serpent2/SCF internal coupling

- Based on a “new philosophy” → **maintainability** + user friendly
- **SCF and TU (slaves) modularized and embedded in Serpent2 (master)**
- **Open doors functions in Serpent2**
- **SCF used as shared library**
- All mapping with ad-hoc files
- Traditional approach, reference for performance

Serpent code official distribution
(Several c routines such as Main.c ... +)
initinternal.c()
internalcouplingsaysstop.c()
iterateinternal.c()
terminateinternal.c()
ifcgetroutines.c
Makefile

Ad- Hoc Coupling C routines
Several C routines to initialization, convergence, etc.
Modified by the coupling (filled)
Accessed by the coupling (as for external supervisor coupling)

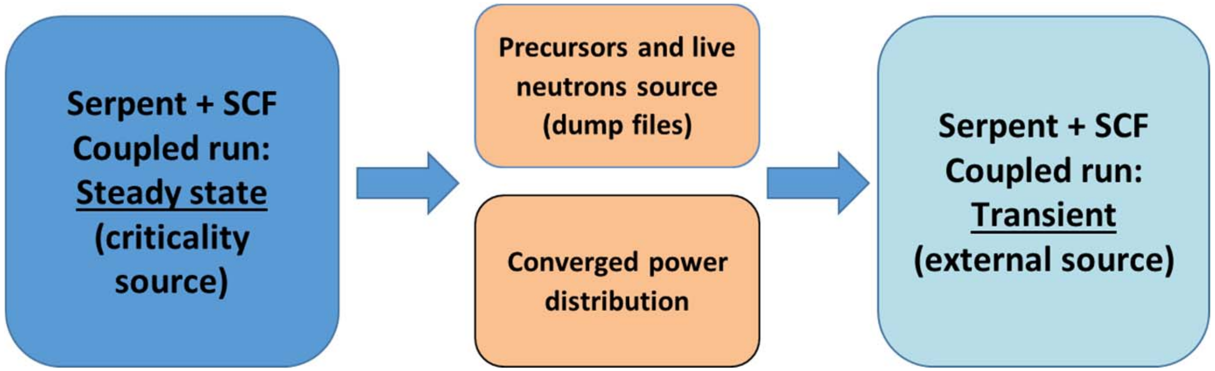
SCF compiled as library (libsubchanflow.so)
Top level functions available in subchannflow.h
*void scf_set_data_file_*
*void scf_set_mpi_rank_*
*void scf_initialize_*
*void scf_get_dimensions_*
*void scf_terminate_*
*void scf_solve_steady_state_*
*void scf_get_present_time_*
*void scf_compute_time_step_*
*void scf_init_time_step_*
*void scf_iterate_time_step_*
*void scf_solve_time_step_*
void scf_terminate_time_step_();
*void scf_is_stationary_*
*void scf_set_field_*
*void scf_get_field_*

- ❖ Codes are kept well separated. Ad-hoc coupled routines
- ❖ Use top level routines in Serpent and SCF (as library)
- ❖ Combined in a single executable

D. Ferraro et al.; “*Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for a PWR minicore*”, ANE 137 (2020)

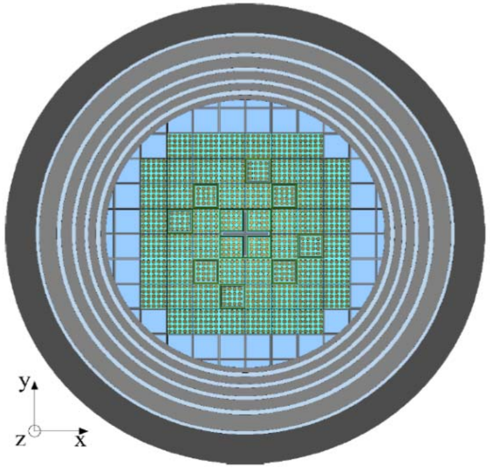
The Serpent2/SCF time-dependent coupling

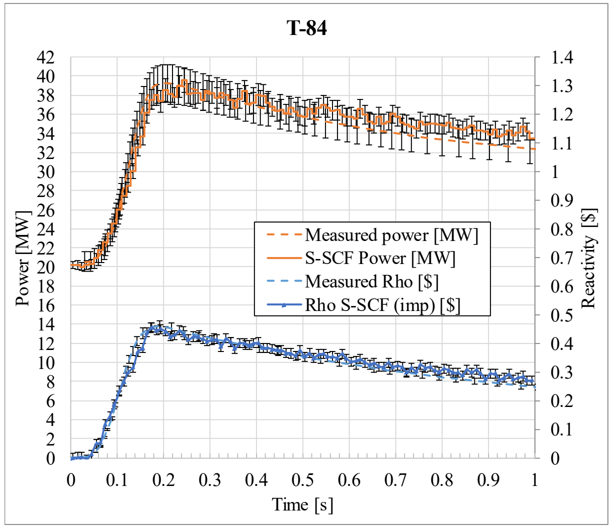
- MC time-dependent simulations:
  - For a given interaction history the distance and energy of the particles is known
  - Traditionally done as external source
- **Different time-scales** of prompt and delayed neutron precursors (~10^{-4} for PWRs)
- Tracking the precursors population that produces the delayed neutrons
- **Two external source simultaneously considered for "*live*" neutrons and for the precursor populations generating the delayed neutrons**
- **Feedback after each time step (fission power + TH fields)**
- **A prior criticality calculation need to be performed**

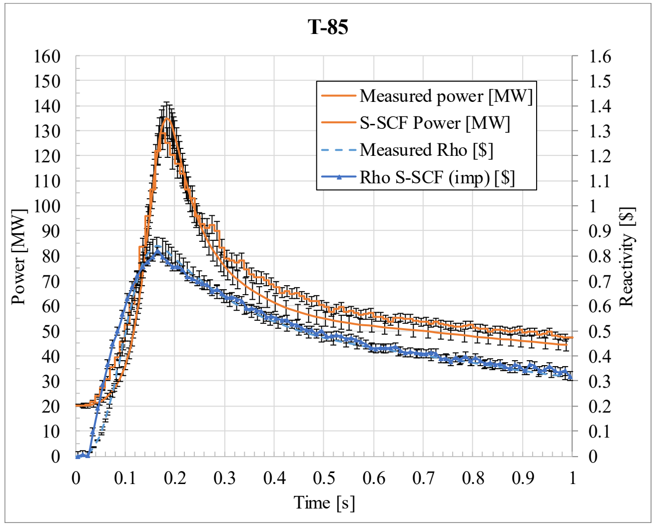


Validation of the Serpent2/SCF internal coupling (1)

- SPERT (PWR-type, RIA-kind scenarios with insertion of 0.5$ - 1.5 $)
- Pin-by-pin models developed and validated for cold and HFP states
- Steady-state and transient calculations for two scenarios (0.46$ and 0.87$)
- 100 steps for a 1 sec scope







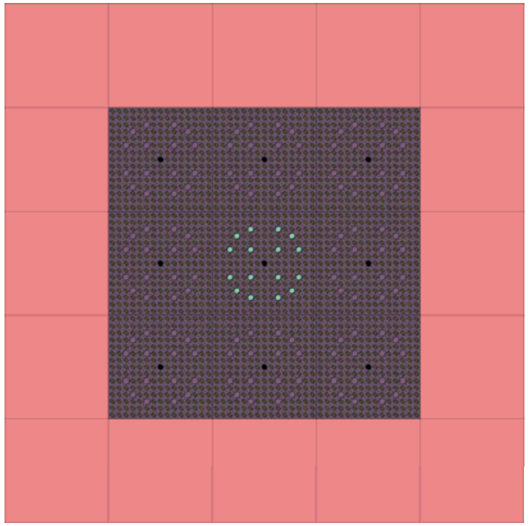
Coefficient	Value per time step [min.CPU@2.6Ghz]	Total [min. CPU@2.6Ghz]
Serpent run time	~4.8e3	4.8e5
SCF run time	~0.4	20

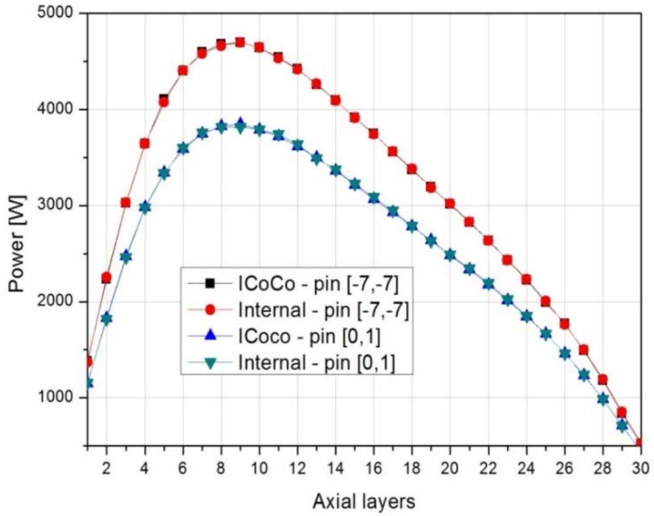
→ 10000h CPU @ 2.6 GHz for each run!

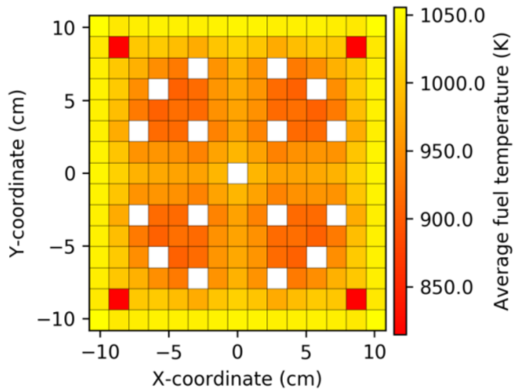
D. Ferraro et al.; „Serpent/SUBCHANFLOW pin-by-pin coupled transient calculationsfor the SPERT-IIIE hot full power tests“, ANE **142** (2020)

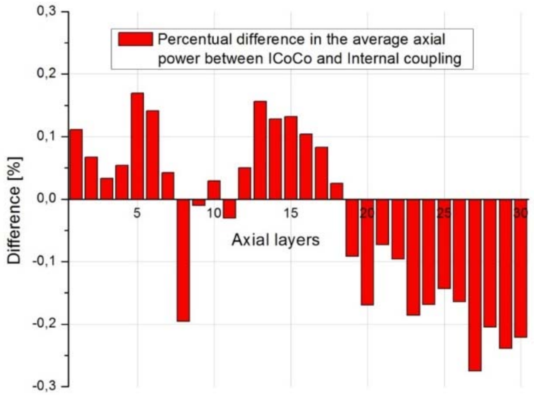
Verification of the two coupling approaches

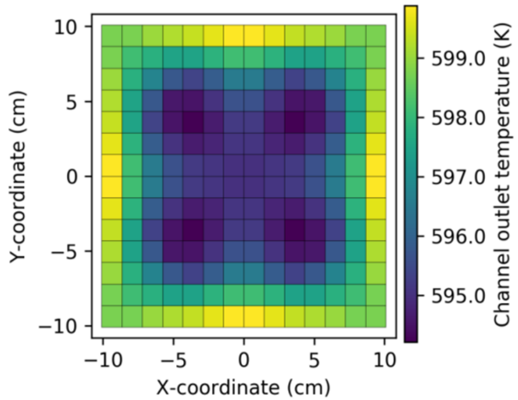
Reflector	Reflector	Reflector	Reflector	Reflector
Reflector	U	U	U	Reflector
Reflector	U	R	U	Reflector
Reflector	U	U	U	Reflector
Reflector	Reflector	Reflector	Reflector	Reflector











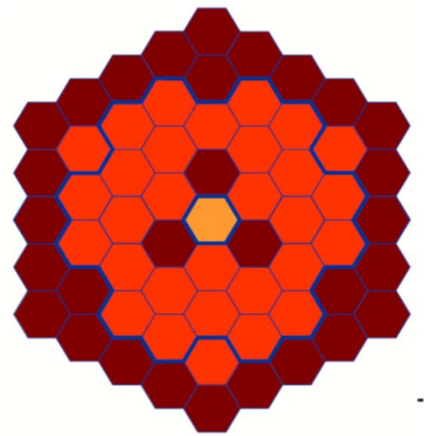
Overall very good consistency between the two approaches

EU Projects

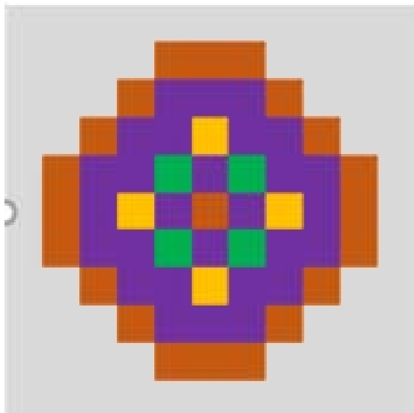
Project	Title	Period
HPMC	High-Performance Monte-Carlo Reactor Core Analysis	2011-2014
McSAFE	High-Performance Monte Carlo Methods for SAFEty Demonstration- From Proof of Concept to realistic Safety Analysis and Industry-like Applications	2017-2020
McSAFER	High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors	2020-2023

The McSAFER Project

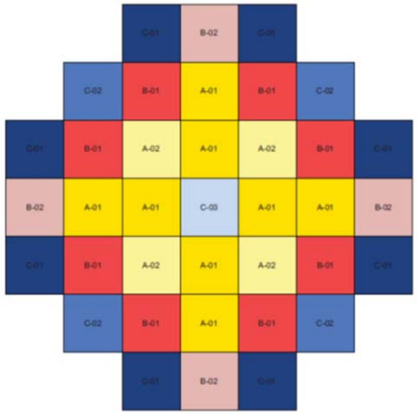
- **Goals:**
  - <u>Advance</u> the safety research for SMR by combining experimental and analytical investigations (numerical simulations)
  - <u>Development, improvement</u> of simulation tools for SMRs (safety evaluations)
  - <u>Validation</u> of simulation tools with experimental data generated within McSAFER (COSMOS-H, MOTEL, HWAT)
  - <u>Application</u> of simulation tools (traditional, advanced low-order and high-fidelity) to four SMR-designs
  - <u>Demonstrate</u> advantages of advanced tools compared to legacy methods



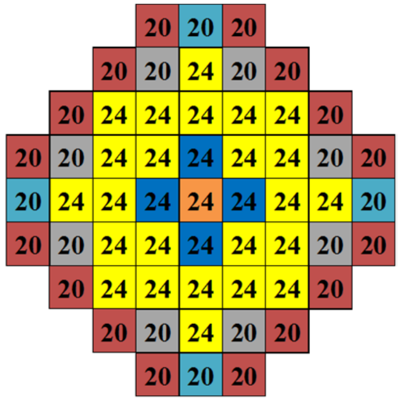
CAREM (Argentine)



F-SMR (France)



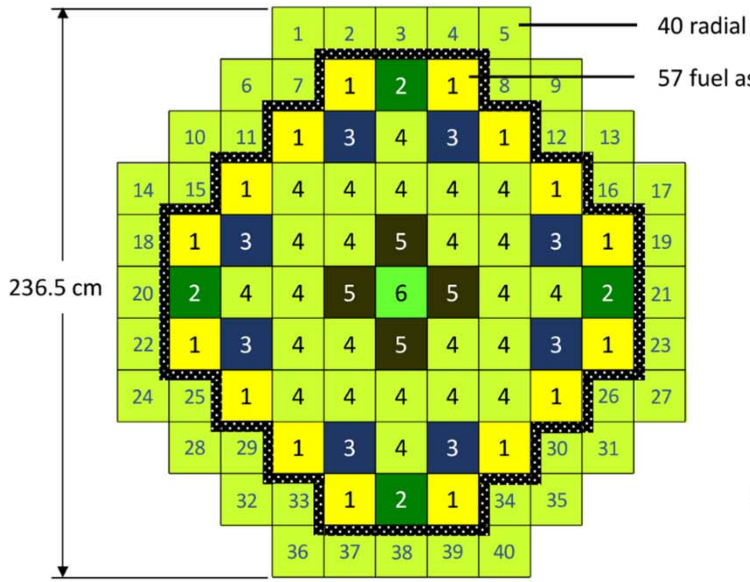
NuScale (USA)



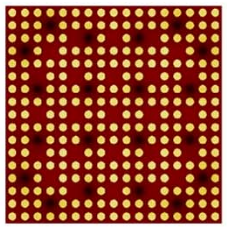
SMART (KSMR, KIT)

The KSMR boron-free core

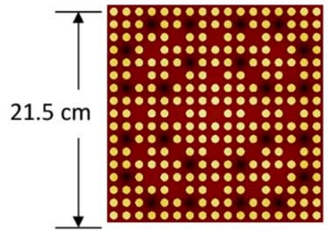
- Based on the SMART concept



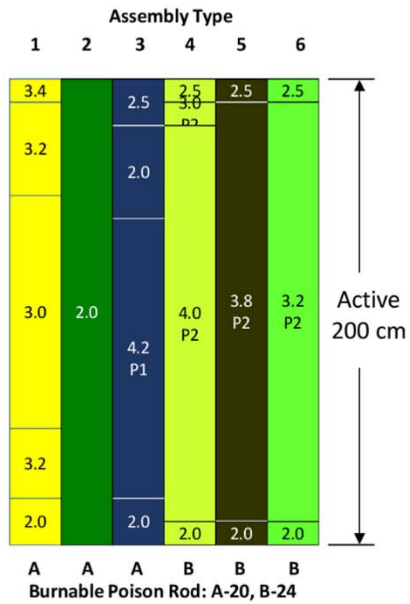
Radial configuration



P1 – Type A 20 poison rods

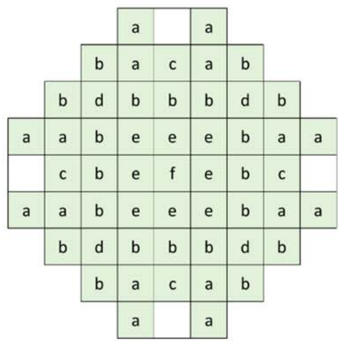


P2 – Type B 24 poison rods

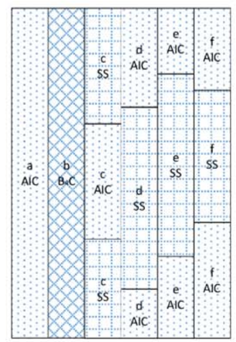


Axial configuration

Y. Alzaben et al.; "Core neutronics and safety characteristics of a boron-free core for Small Modular Reactors," *Annals of Nuclear Energy*, vol. 132, pp. 70–81, Oct. 2019

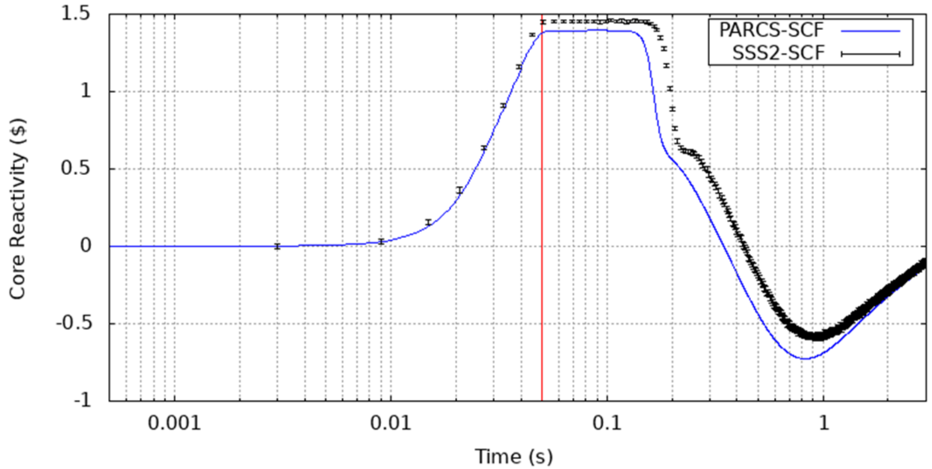


Radial configuration

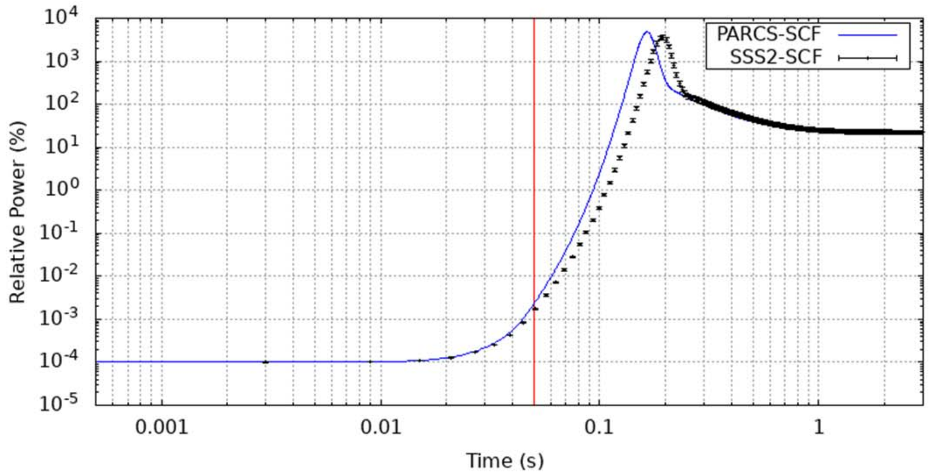


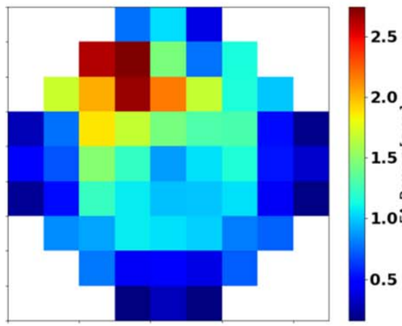
Axial configuration

REA on the KSMR core (1)

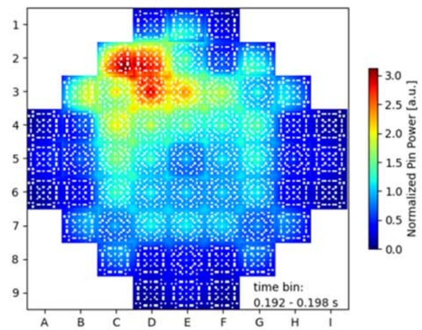


	PARCS-SCF	SSS2/SCF
Peak reactivity	1.395$	1.45$ ± 0.01$
Peak power [ratio to nominal]	48.35	36.2
Time at peak power	0.1645 s	0.192 s – 0.198 s
Final power [ratio to nominal]	0.23	0.22 ± 0.01
ßeff	685 pcm	702 pcm ± 1 pcm
Minimum DNB ratio	1.6154	1.3032
Final minimum DNB ratio	4.5304	3.8892





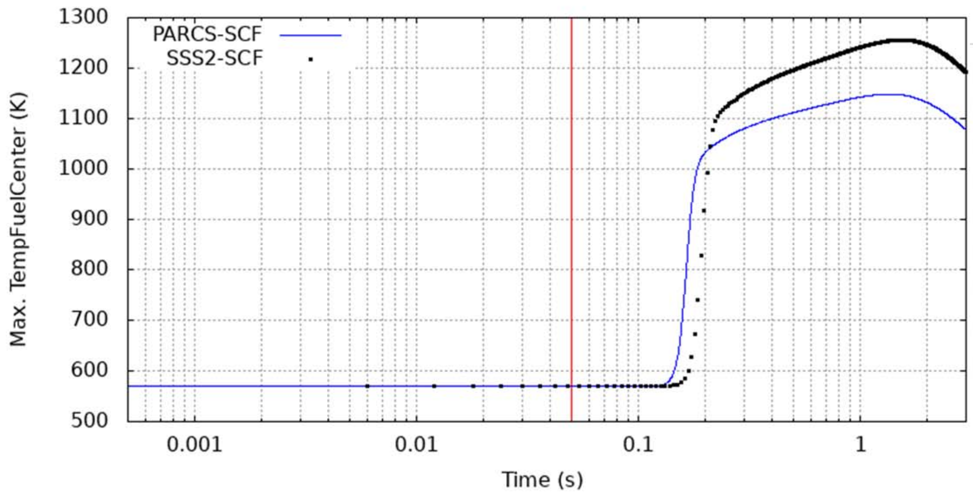
PARCS/SCF

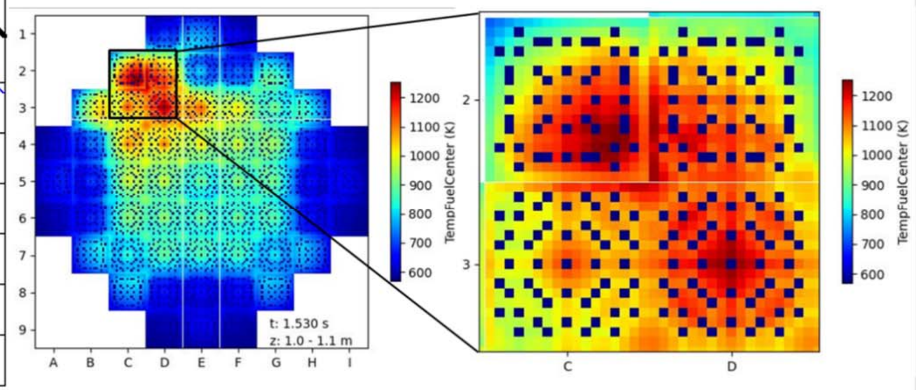


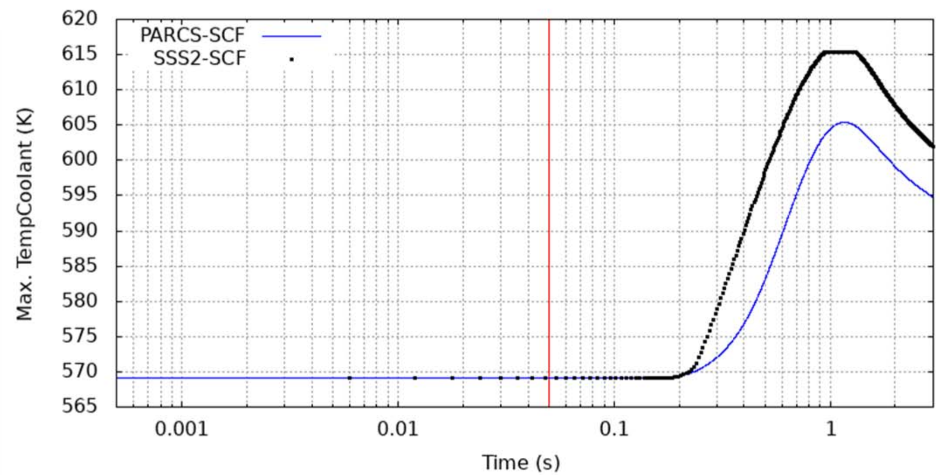
Serpent2/SCF

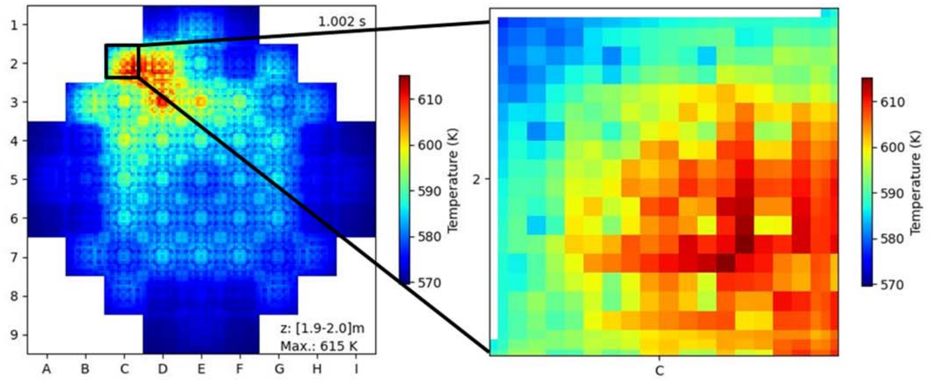
L. Mercatali, G. Huaccho and V.H. Sanchez-Espinoza; “Multiphysics modeling of a reactivity insertion transient at different fidelity levels in support to the safety assessment of a SMART-like Small Modular Reactor”, *Frontiers in Nuclear Energy Research* (Accepted, April 2023)

REA on the KSMR core (2)

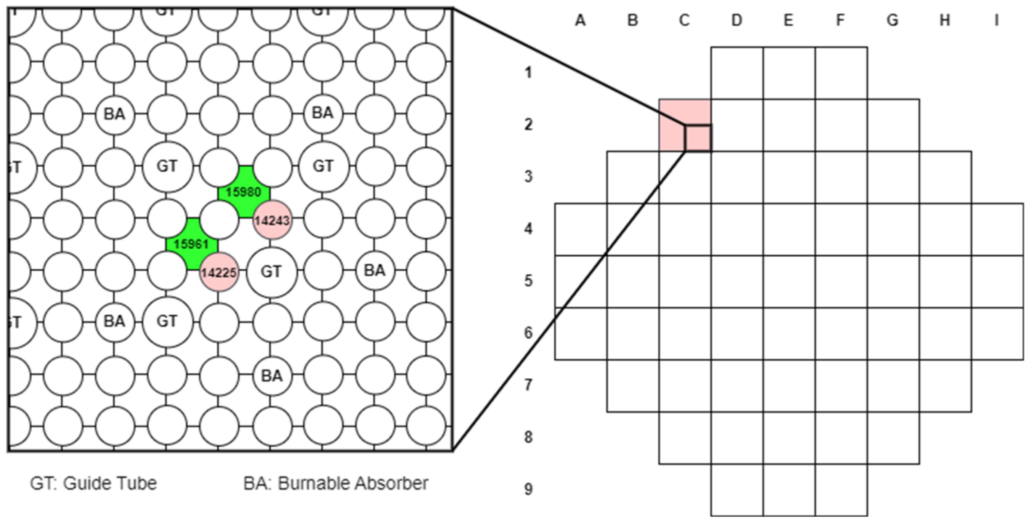




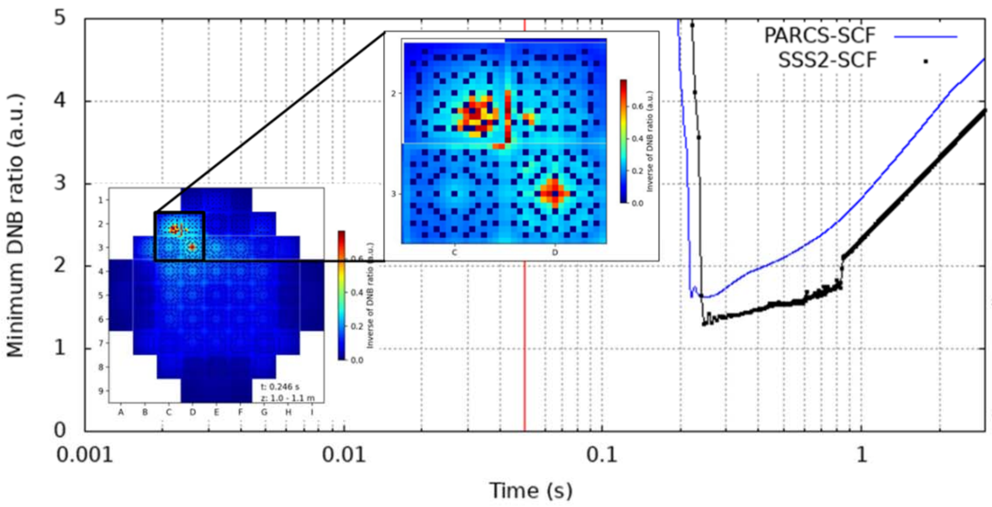


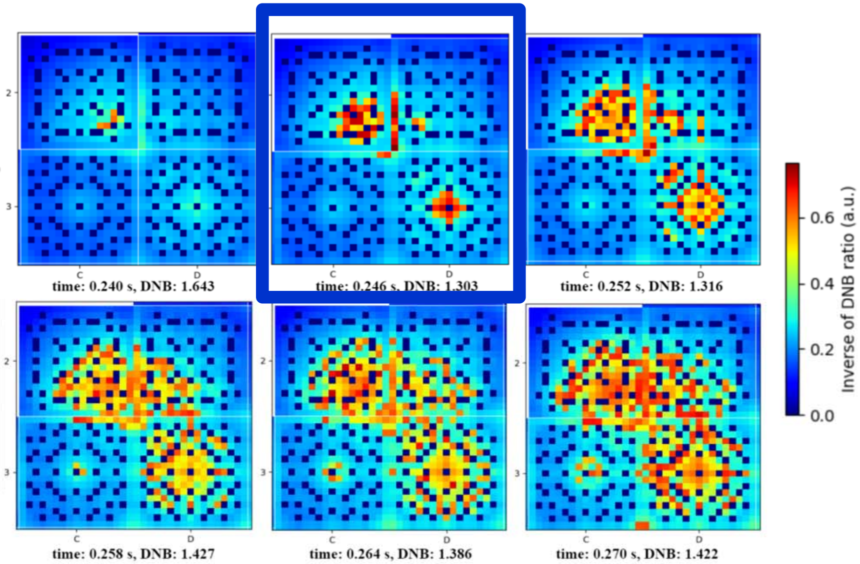


REA on the KSMR core (3)



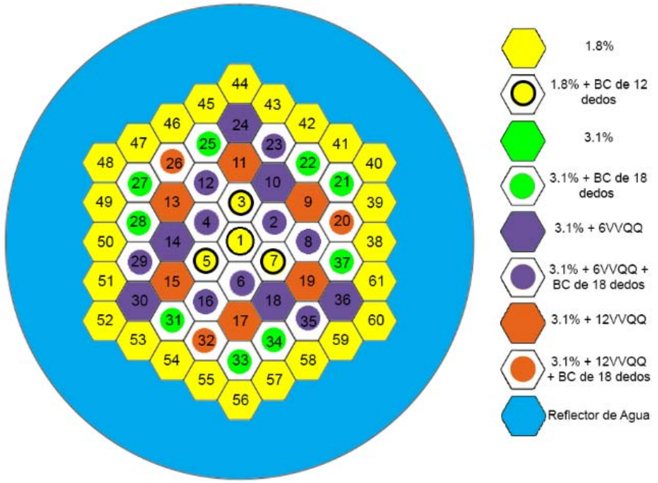
- Nodal solution not conservative (lower local power peak, lower cladding temperature and higher DNBR)
- Fuel rod cladding integrity not challenged during the REA

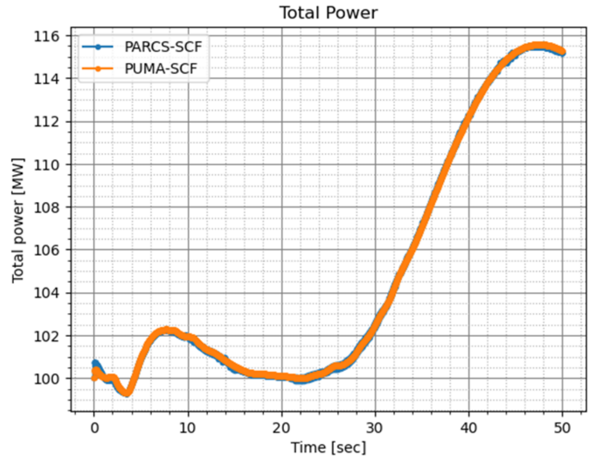


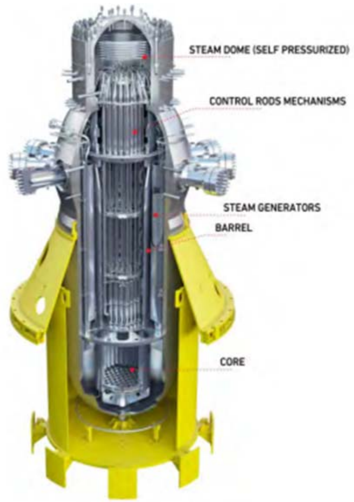


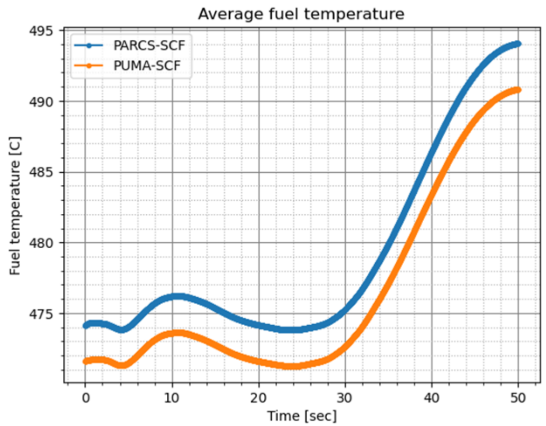
CAREM-like SMR

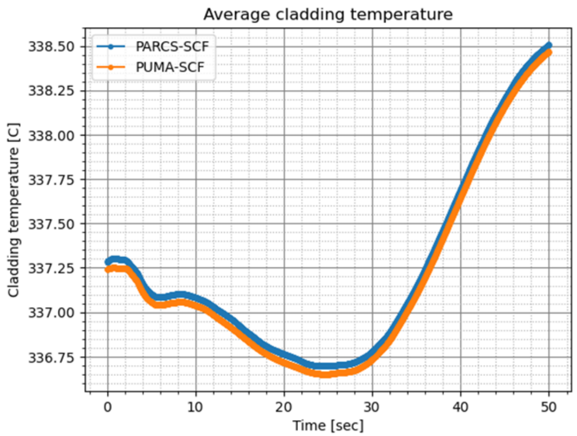
- **Overcooling transient scenario**
- **Solutions: Serpent/SCF (KIT) vs. PARCS/SCF (KIT) vs. PUMA/SCF (CNEA)**

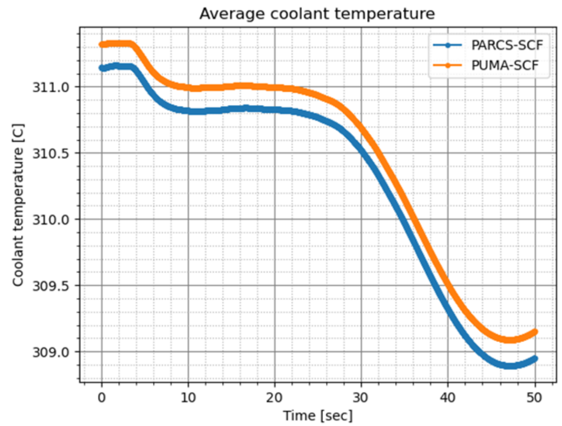










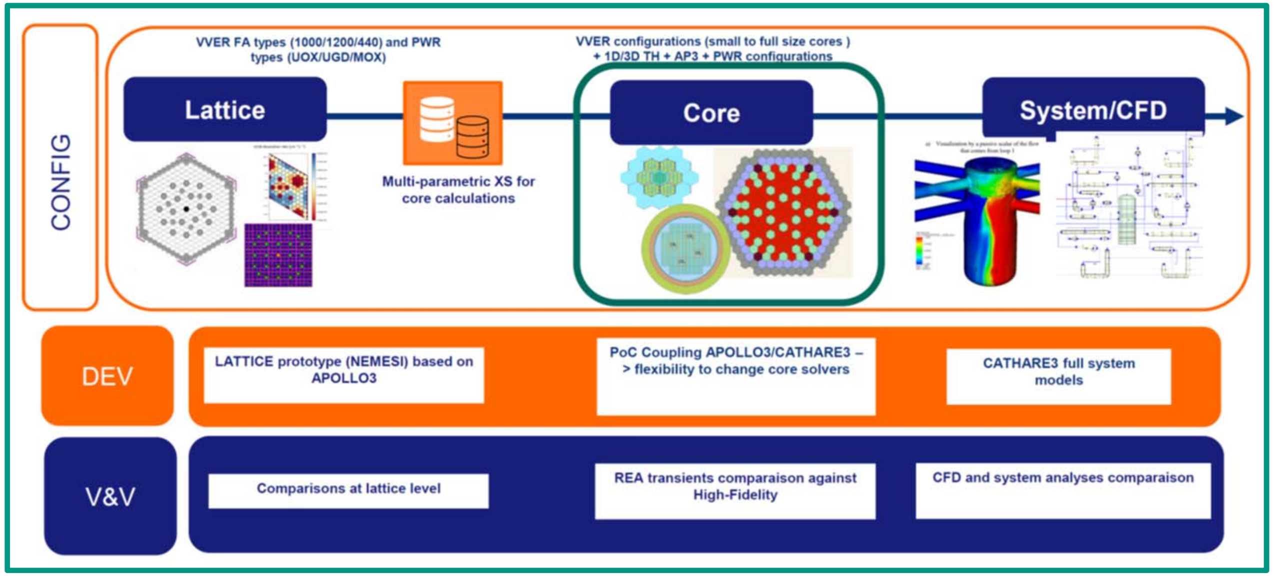


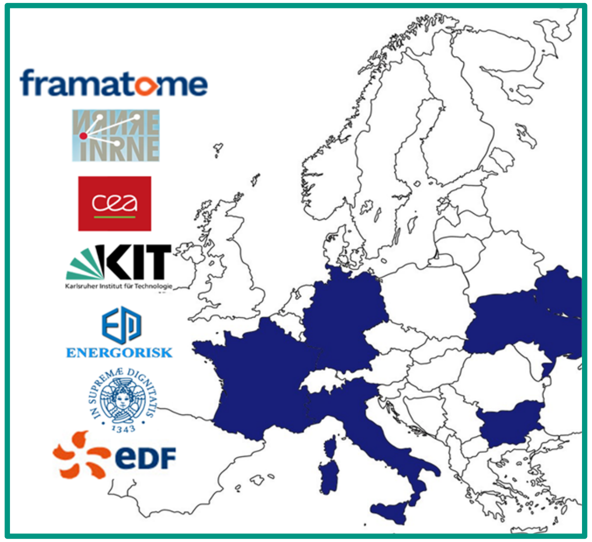
L. Mercatali et al.; “Modeling of an Overcooling Transient Scenario in a CAREM-like Small Modular Reactor”, *NURETH-20 (Washington – USA, 2023)*

The EU *CAMIVVER* Project (1)

Code And Methods Improvements for VVER safety assessment

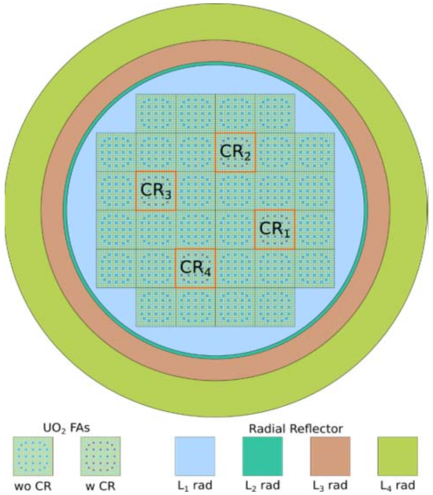
- Safety Authorities requirements are pushing towards Verification and Validation (V&V) activity -> Rare transient data at full scale system push to a more extensive use of benchmarks, statistical libraries, and sensitivity analysis techniques for consolidating the full system response prediction
- European state-of-the-art computer codes became a priority for preserving EU sovereignty and nuclear independence
- VVER type constitutes a dynamic and growing part (stronger issue since February 2022)
- A first step toward the industrialization of new generation codes

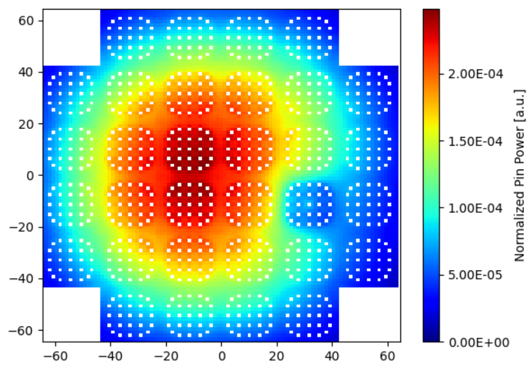


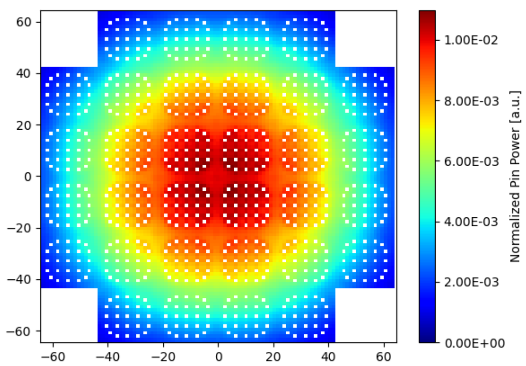


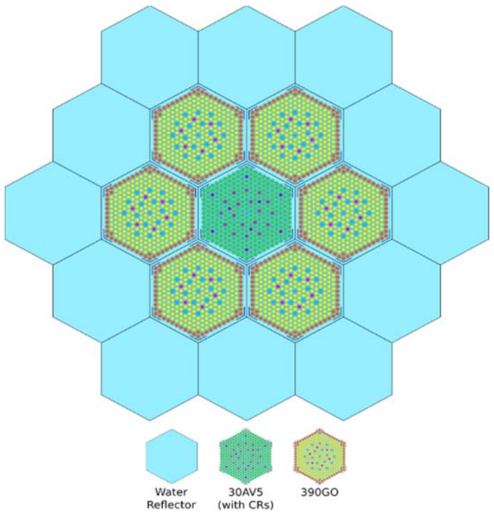
The EU *CAMIVVER* Project (2)

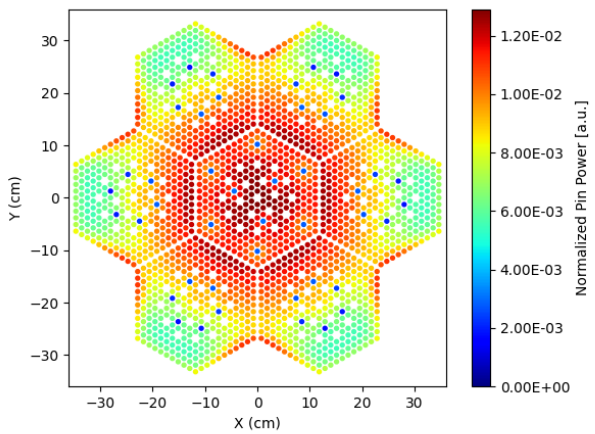
- **REA on two two theoretical minicore cases**

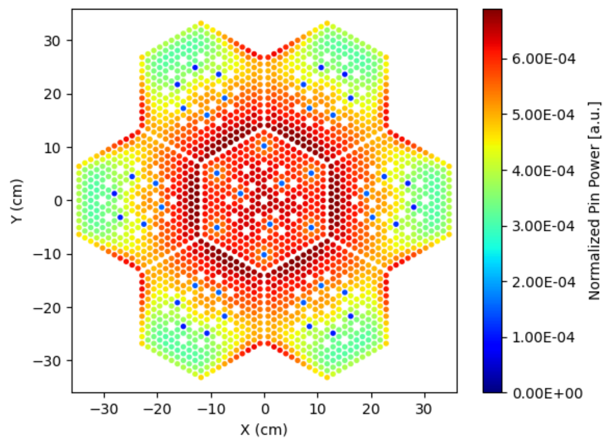






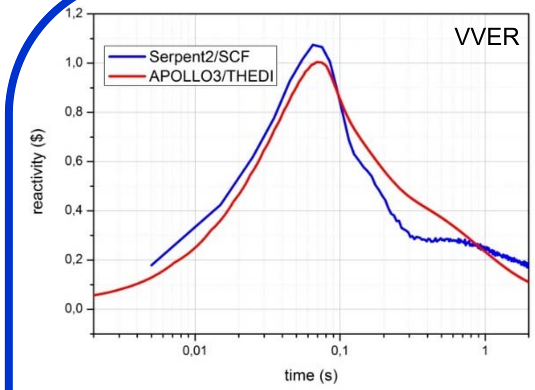


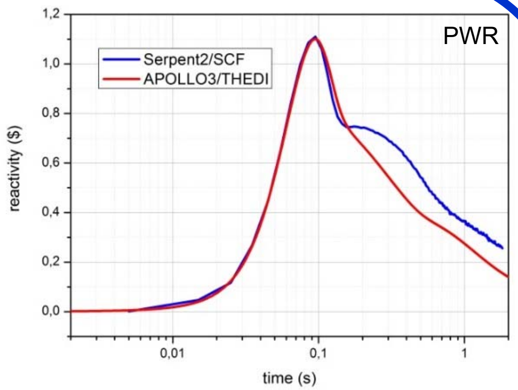


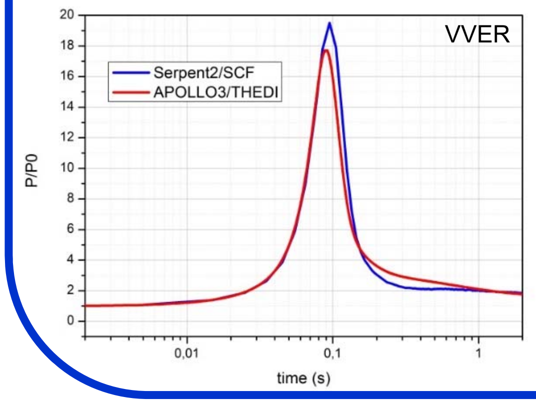


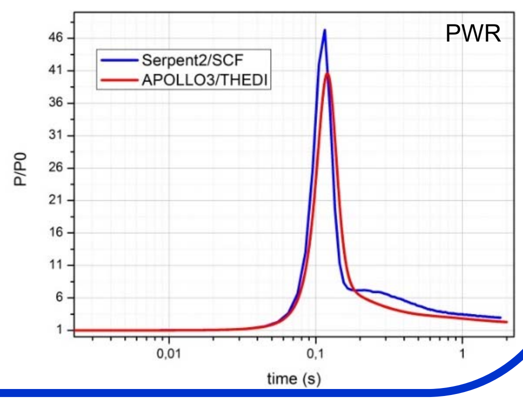
L. Mercatali et al.; "Advanced Multiphysics Modeling for VVER and PWR Applications", ICAPP2023 (April 2023)

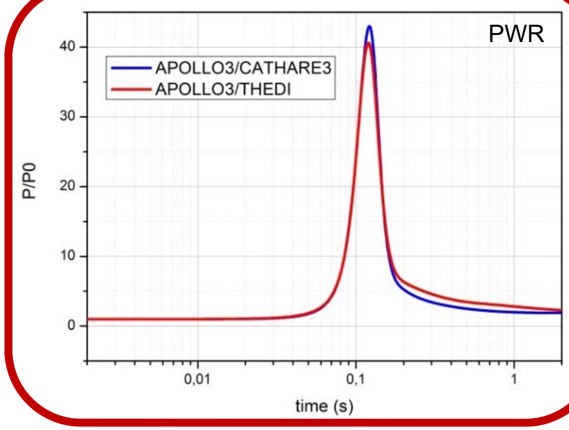
APOLLO3®/THEDI & APOLLO3®/CATHARE3 vs. Sepent2/SCF











	Minicore	Peak factor [P/P0]	Peak time [s]
Serpent2/SCF	PWR	47.27	0.115
	VVER	19.55	0.095
A3/T	PWR	40.60	0.1198
	VVER	17.74	0.0895
A3/C3	PWR	43.00	0.1220

The *CAMIVVER* Project Final Workshop

www.camivver-h2020.eu

Most Project deliverables are public and can be downloaded

On LinkedIn

camivver-h2020-european-project

Karlsruher Institut für Technologie

Thank you!

INR