The development of the 3D fuel behavior code OFFBEAT

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PSI 07/11/2019

Motivations for a novel fuel performance code

- ***O***pen***F***OAM ***F***uel ***BE***havior ***A***nalysis ***T***ool (OFFBEAT):
  - developed since 2 years at the LRS-EPFL and at the PSI.
  - main focus are local **multi-physics** and **multi-dimensional** aspects of fuel behavior.

- Recent fuel failure (Swiss NPP) and followup analysis at PSI.
  - need for higher-fidelity tools.

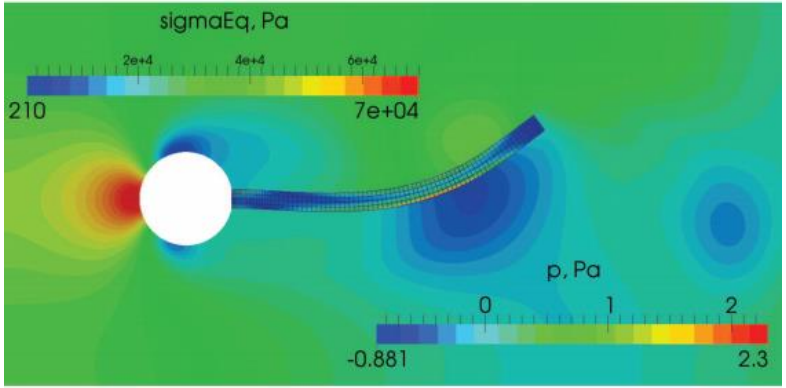
- Existing 2D/3D codes (BISON, ALCYONE, DIONISIO etc.) not easily accessible.

- Lab expertise with OpenFOAM® C++ library

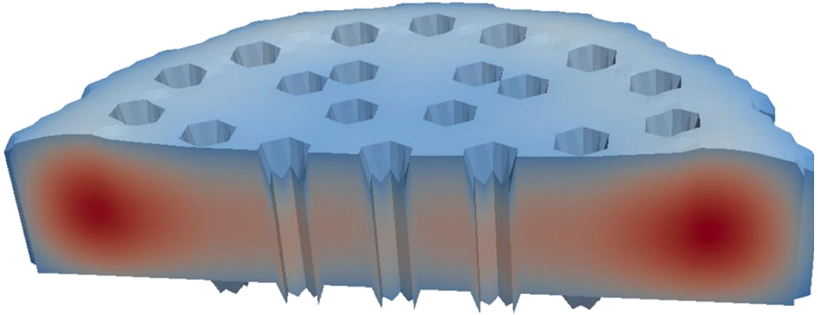
OpenFOAM as a toolbox for engineering applications

- Not “just" CFD! OpenFOAM is a toolbox for PDEs solution and multi-physics problems.

- Many applications outside of CFD, e.g.:
  - Chemistry and combustion or fluid-structure Interaction.
  - Nuclear Reactor Analysis (GeN-Foam at EPFL-PSI).



Z. Tukovic et al. “OpenFOAM Finite Volume Solver for Fluid-Structure Interaction”, 2018



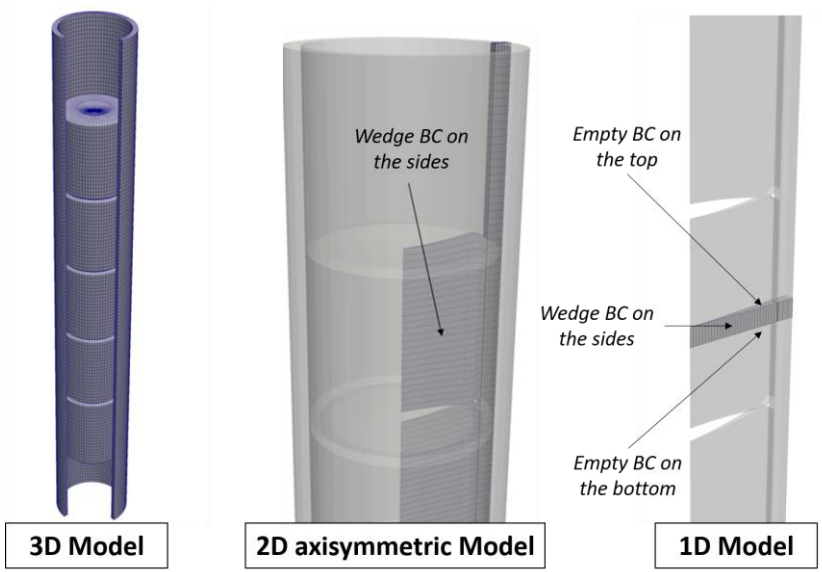
C. Fiorina et al. “GeN-Foam: a novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors”, 2015

OpenFOAM as a toolbox for engineering applications

- OpenFOAM comes with useful features:
  - **inherently 3D library**, but 2D and 1D is also possible;
  - unstructured meshes and arbitrary geometry;
  - data pre- and post-processing;
  - equation discretization, meshing and **parallel solution**.

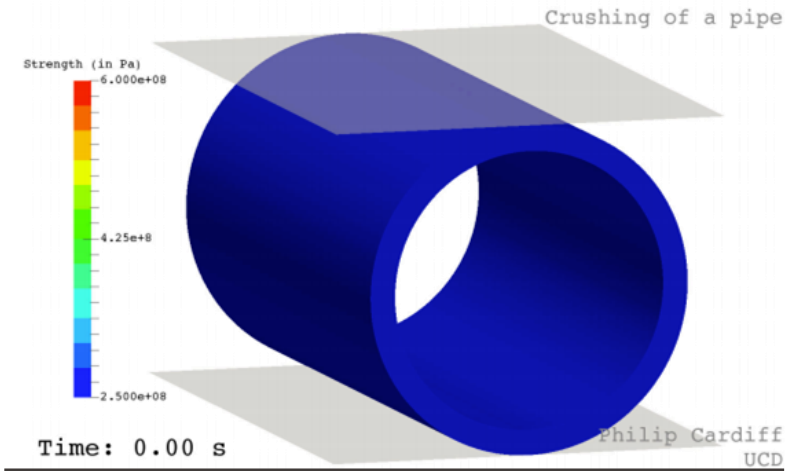
- **<u>No need to modify underlying numerics</u>**!

- Open-source code
  - EPFL now collaborating center on a new IAEA project.



Finite Volume Method and segregated approach

- OpenFOAM based on the **FVM**:
  - simple problem definition and implementation.
  - strongly conservative.
- FVM and FEM share a number of features[1].
- FVM is gaining momentum for solid mechanics applications[2].



P. Cardif et al. "A Lagrangian cell-centred finite volume method for metal forming simulation", 2016

- **Segregated** approach: each physics or component solved separately.
- Iterations take care of explicit terms: **solution is still implicit!**

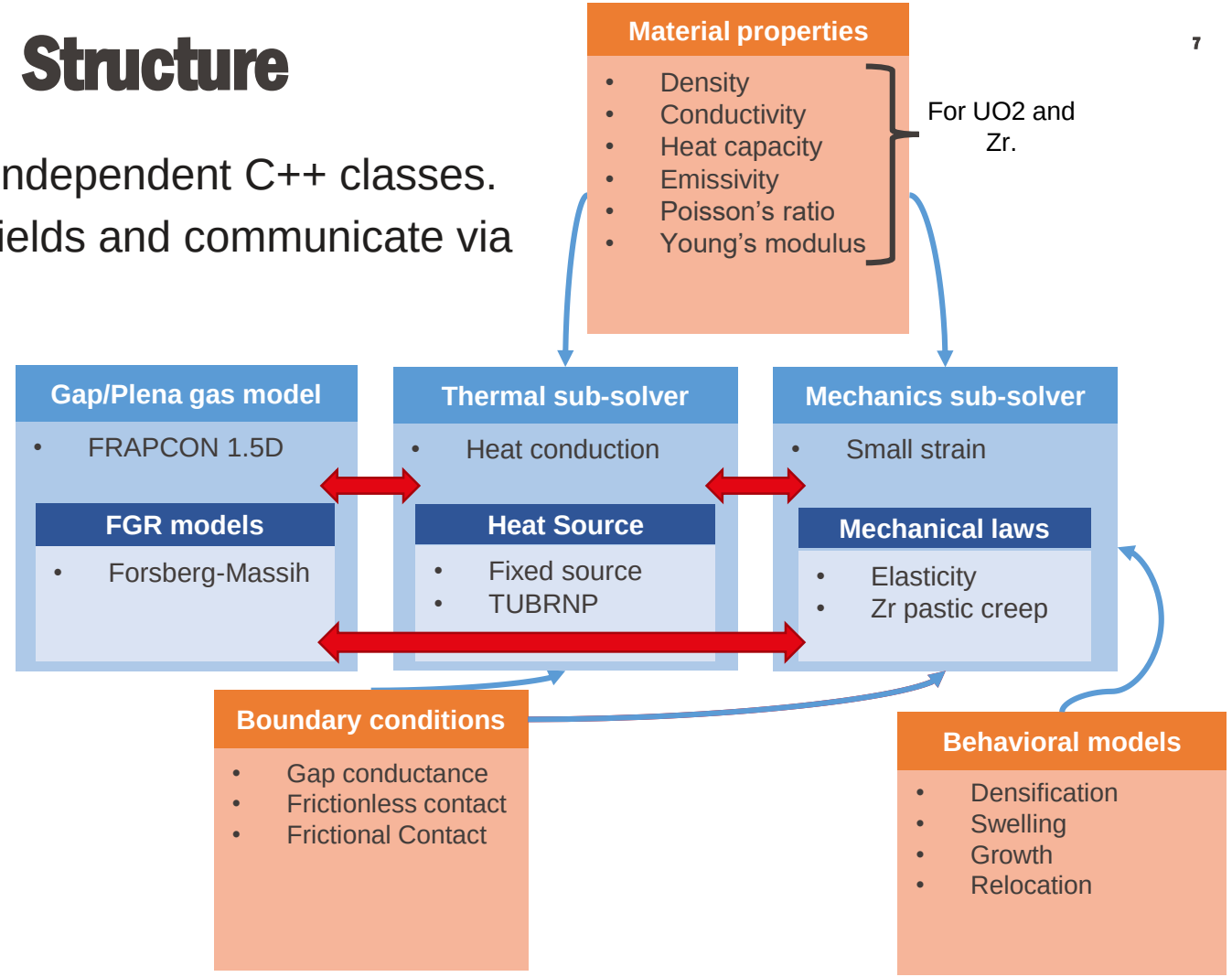
[1] Idelsohn, Onate, ***Finite volumes and finite elements: Two 'good friends'***, 1994
[2] P. Cardif, ***Thirty years of the finite volume method for solid mechanics***, 2018

Outline

- Motivations and main features
- OFFBEAT structure
- OFFBEAT development summary
- Coupling and interaction possibilities
- Conclusions

OFFBEAT – Structure

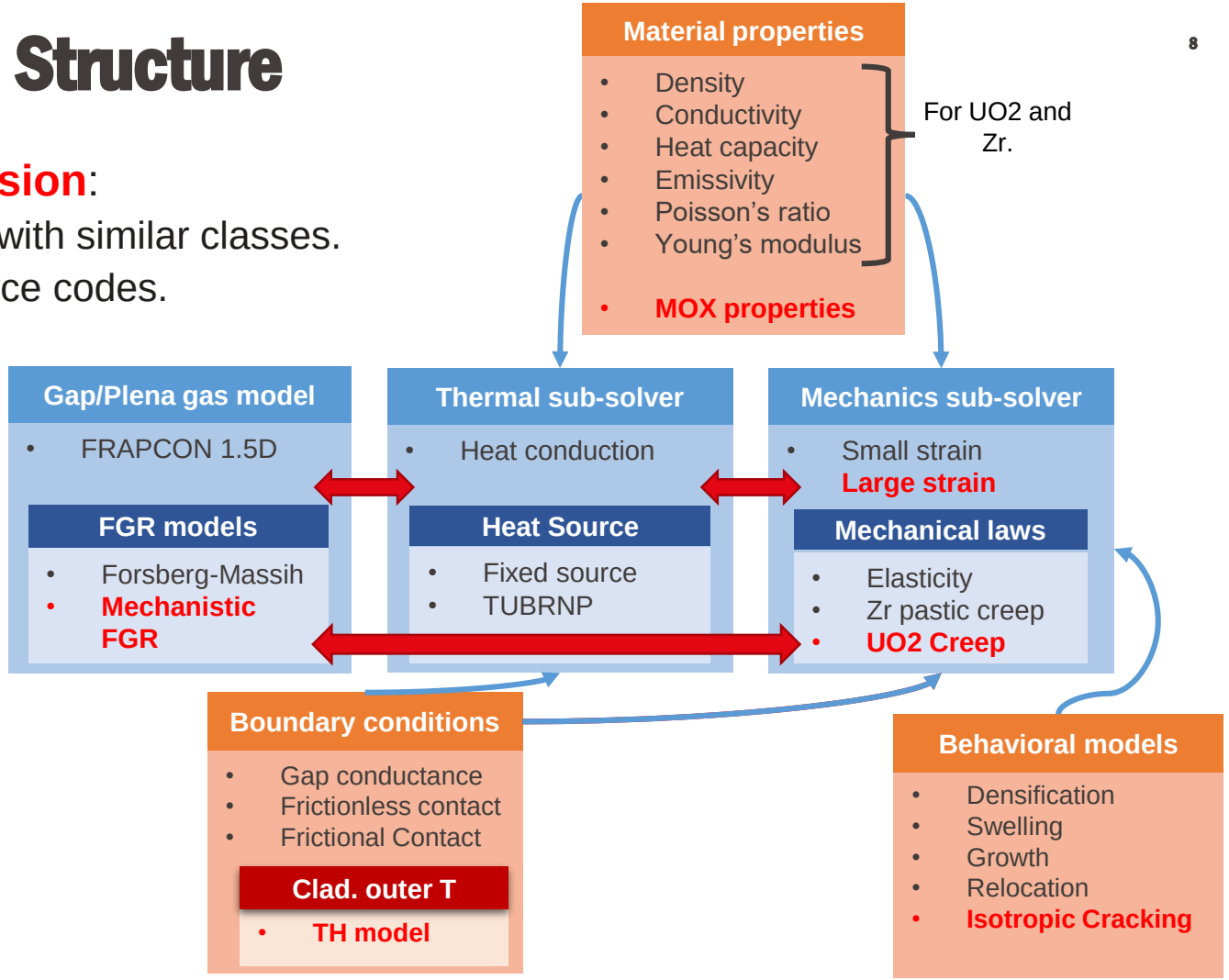
- Modular approach: independent C++ classes.
- Classes exchange fields and communicate via functions.



OFFBEAT – Structure

Straightforward **extension**:

- Swapping existing with similar classes.
- Reusing open-source codes.



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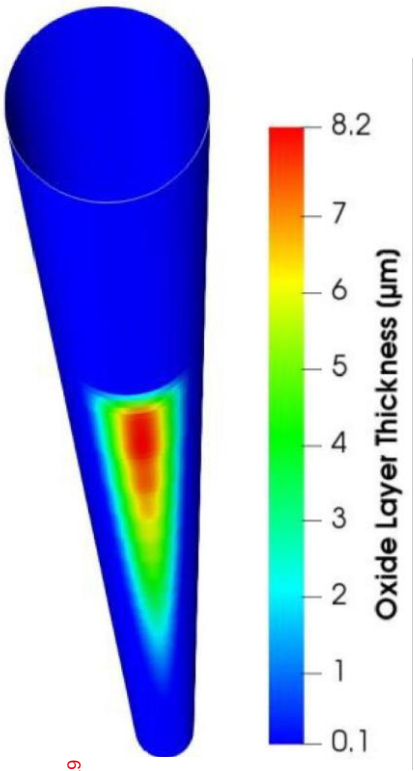
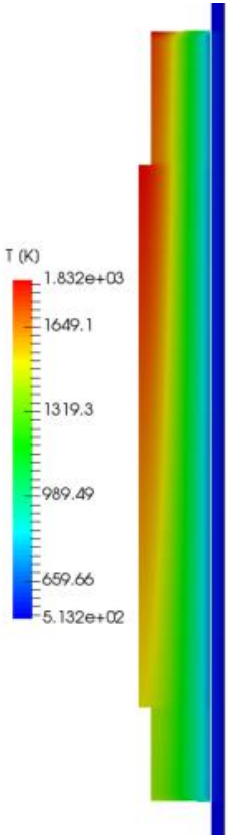
Previous works under linear-elastic framework



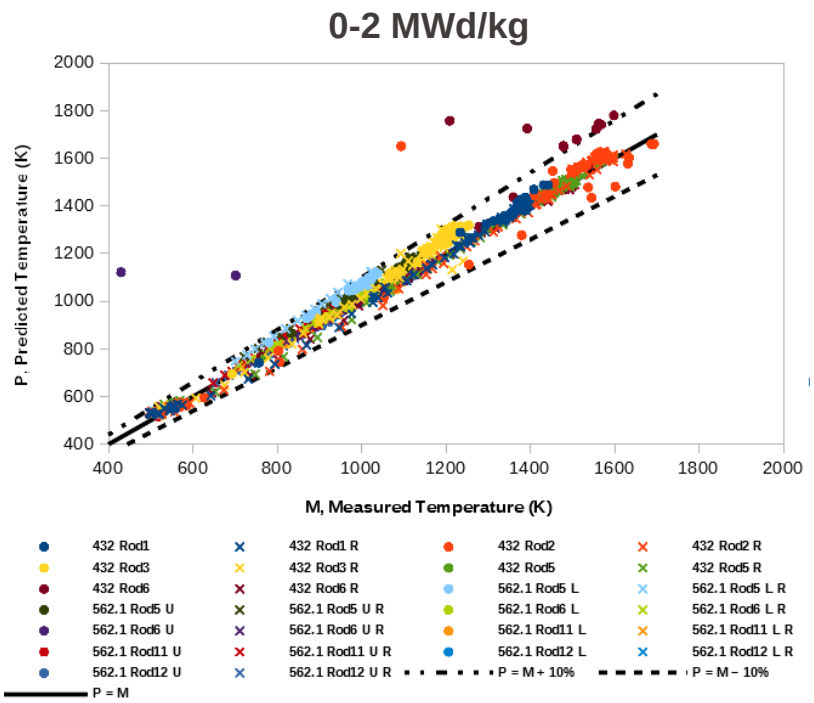
- Asymmetric heat exchange under dryout conditions [1].

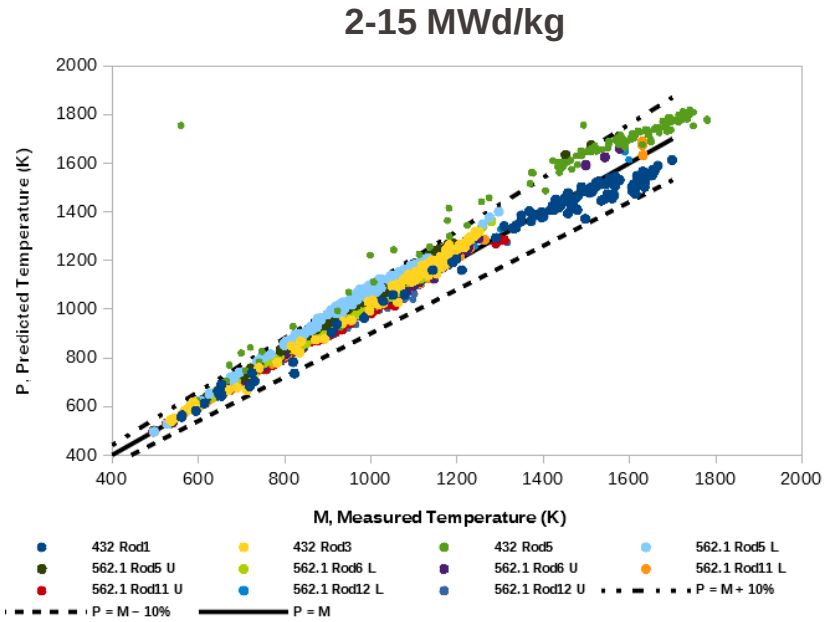
- Preliminary validation of fuel centerline for 8 rods low burnup rods of the IFPE database[2].
- Fuel modeled as linear-elastic axisymmetric fuel rods



[1] I.Clifford et al.,***Studies on the effects of local power peaking on heat transfer under dryout conditions in BWRs***, 2019
[2] A.Scolaro et al., ***The OFFBEAT multi-dimensional fuel behavior solver***, (soon available on NED)

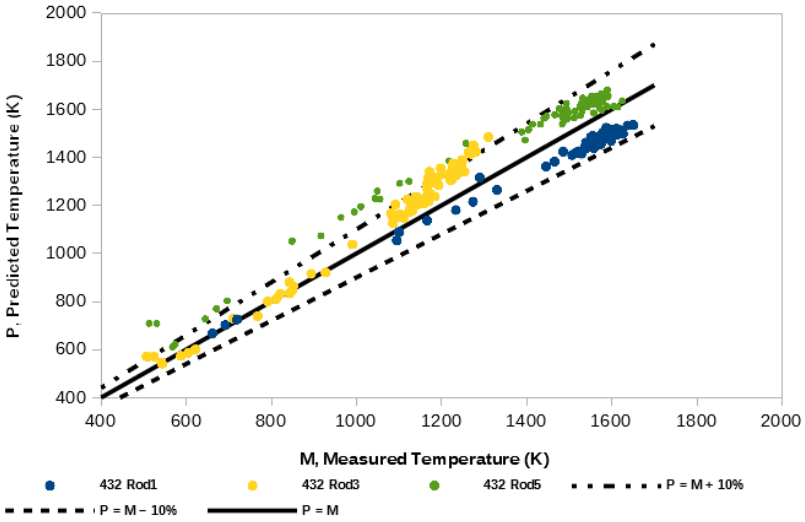
Preliminary FCT Validation – Results (1)



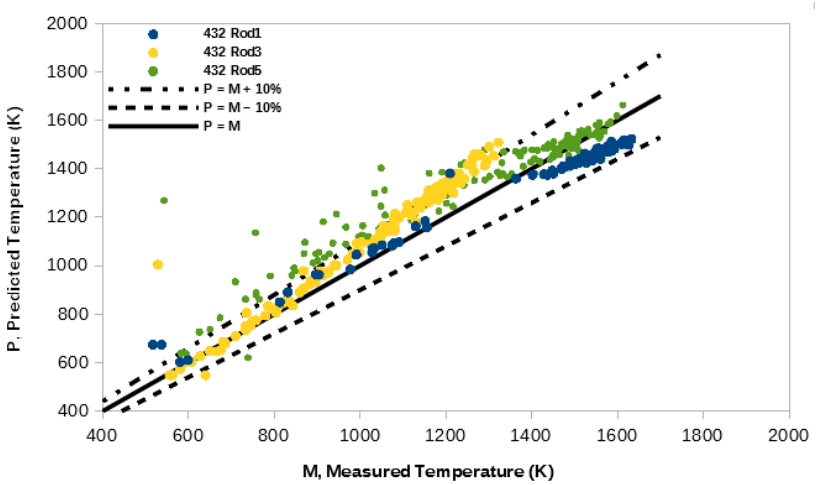


Preliminary FCT Validation – Results (2)

15-25 MWd/kg



25-40 MWd/kg



Current Main Focus – Analysis of PCMI/PCI Scenarios

- Renovated industrial and research interest.
- Optimal **testing ground** for many important features.

- Necessary ingredients for PCMI scenario analysis:
  - Pellet-Cladding contact model
  - Zircaloy rate-independent plasticity model;
  - Zircaloy thermal and irradiation creep;
  - Fuel isotropic cracking and creep.
  - Frictional contact force

Starting Nov 2019

Contact Model

- Penalty method contact model with **conservative surface mapping (AMI)**:

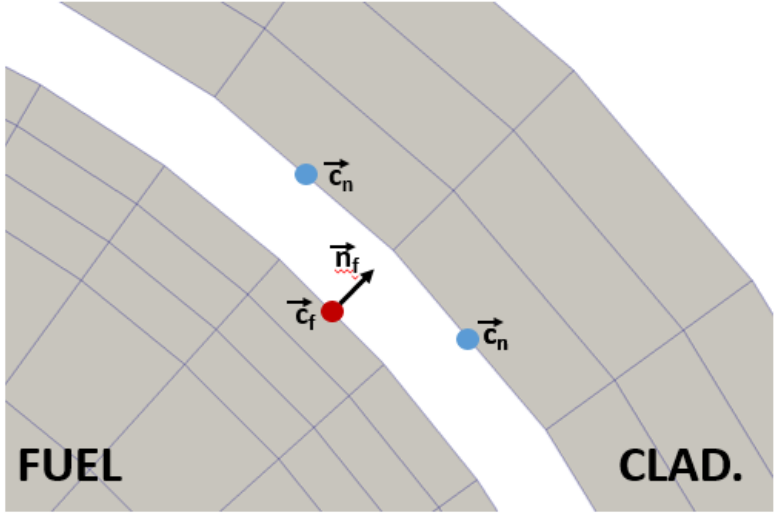
$$p = \alpha * g * E$$

α = penalty factor, g = penetration, E = stiffness

- Low penalty factor: helps convergence but might change the physics.

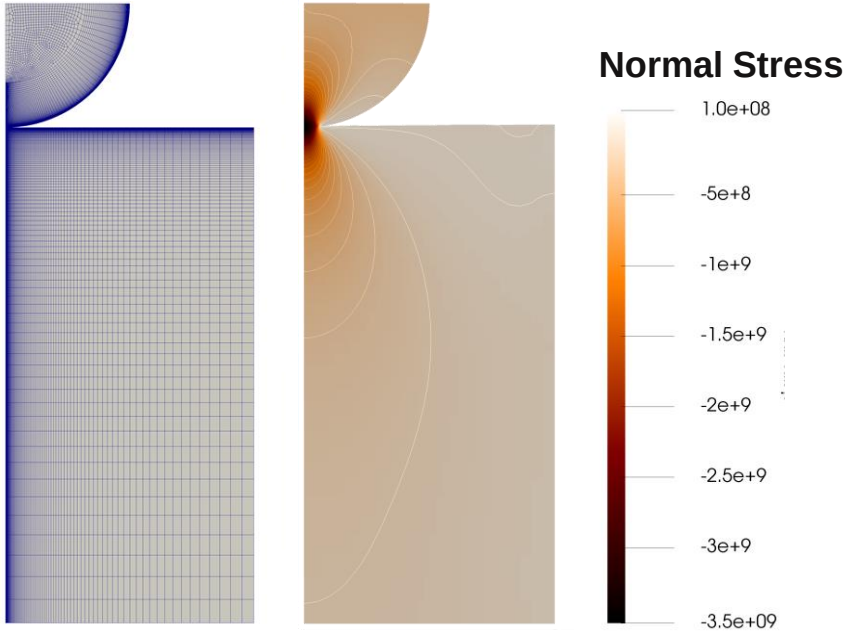
- High penalty factor: more accurate but needs stronger under-relaxation.

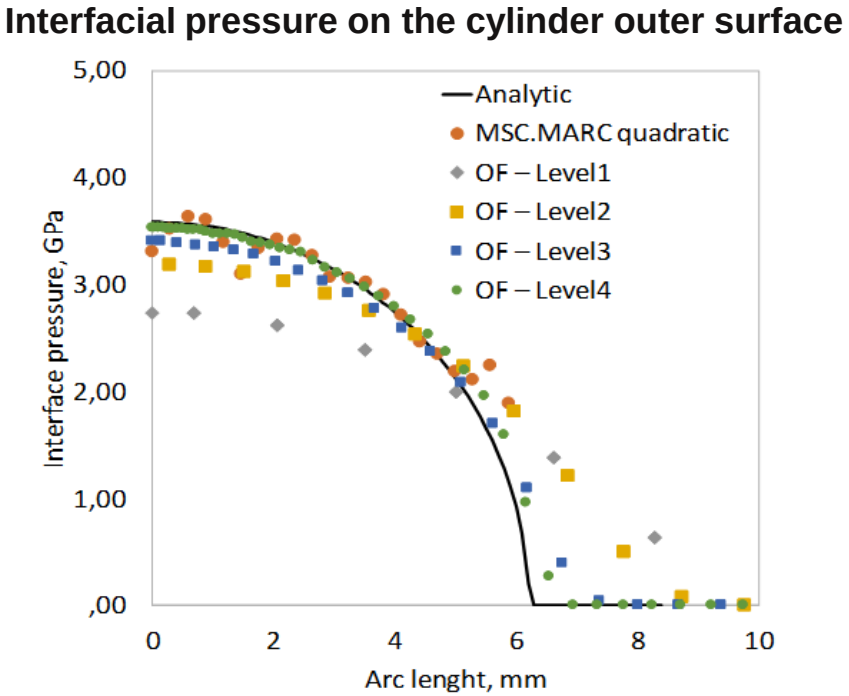
- **Alternative approaches?**



Contact Model Benchmark

- Punch test from the NAFEMS. Hard problem (almost point contact)!



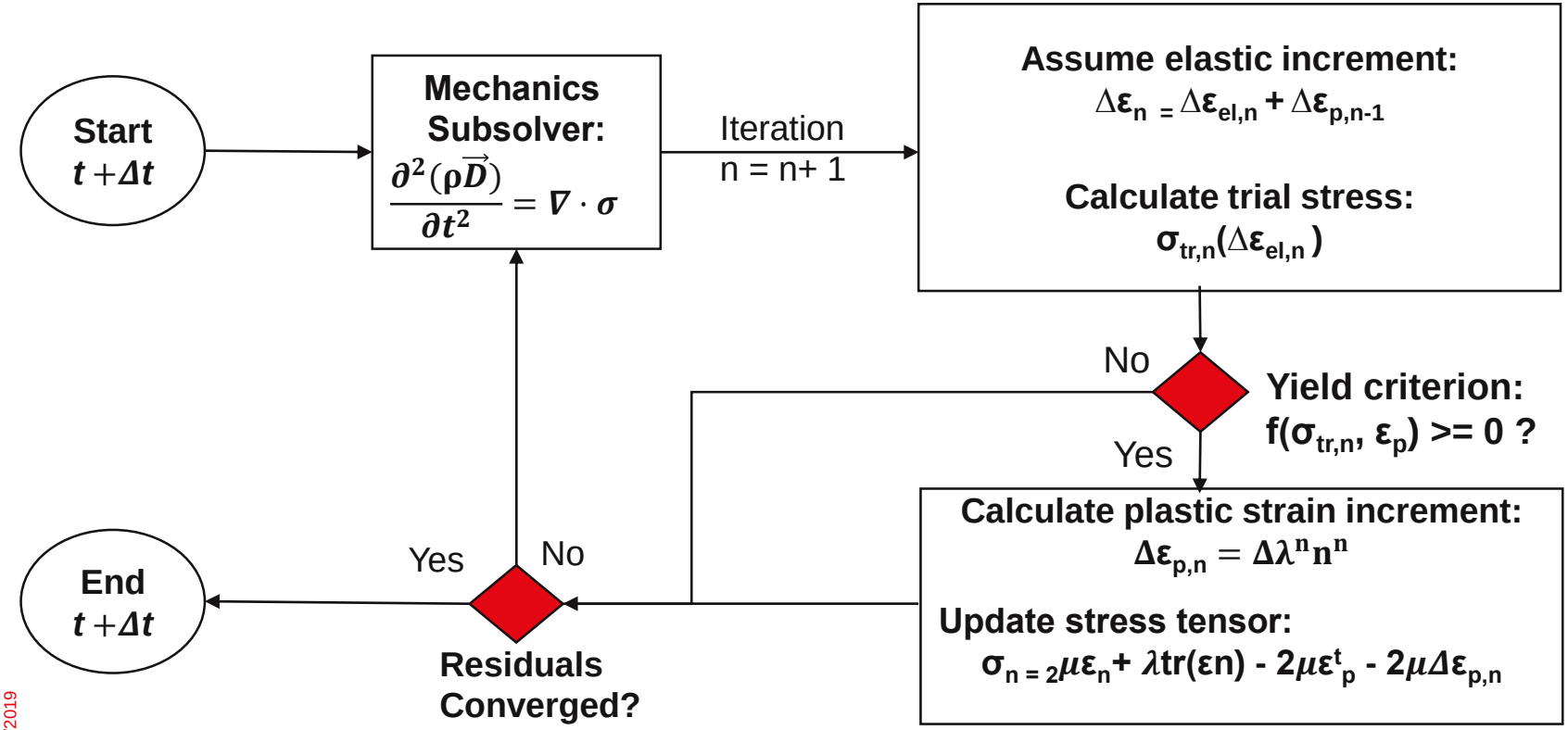


Zircaloy Plasticity and Creep Models

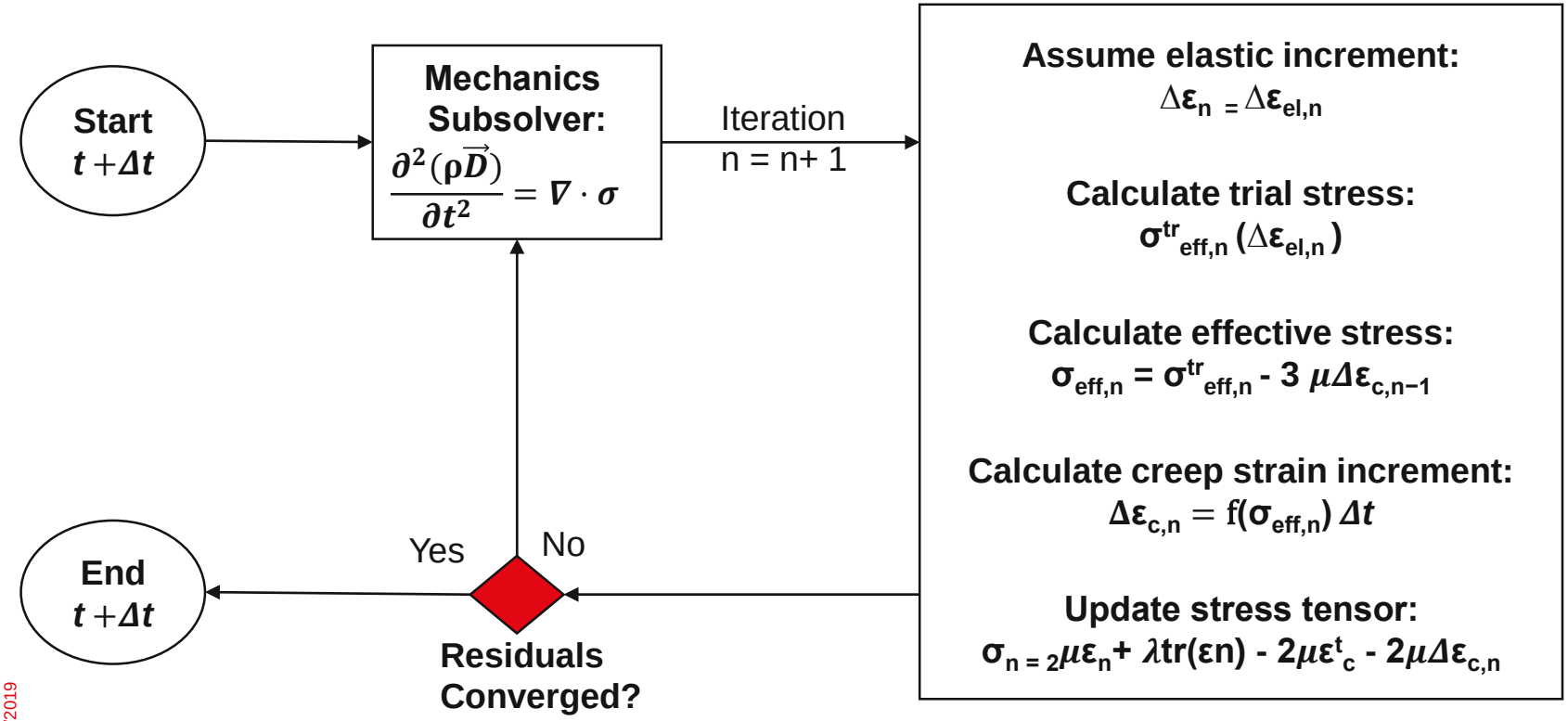
- Rate independent von Mises **plasticity** model with linear strain hardening[1].
- Limbäck-Anderson **creep** model based on implementation in Peregrine [2].
- Prandtl-Reuss flow-rule for multi-axial stress states $\Delta\boldsymbol{\varepsilon}_{c,i} = \frac{3\boldsymbol{\sigma}_{dev}}{2\sigma_{eff}}\Delta\varepsilon_{c,eff}$
- $\boldsymbol{\Delta\varepsilon_c = f(\sigma)}$ … but $\boldsymbol{\sigma = 2\mu\varepsilon + \lambda tr(\varepsilon) - 2\mu\varepsilon^t_c - 2\mu\Delta\varepsilon_c}$

[1] Simo, J.C. and Hughes, T.J.R., **Computational Inelasticity**, 1998
[2] W. Liu et al. ***Numerical method of modeling creep of zirconium-alloy cladding in a multi-physics fuel performance code***, 2013

Plasticity Model Implementation



Creep Model Implementation

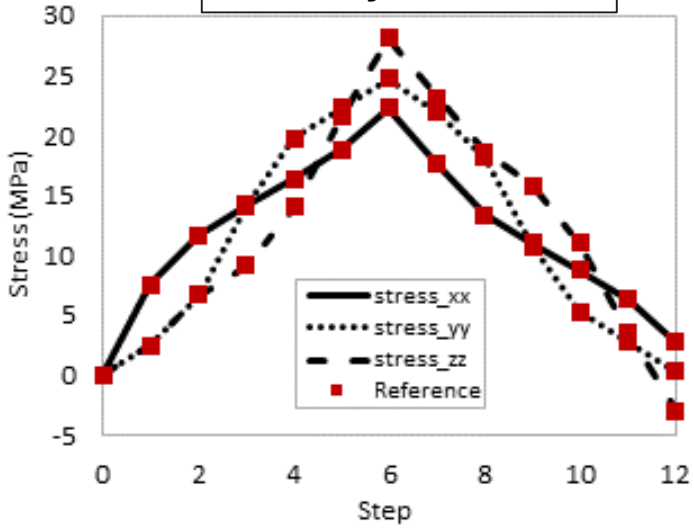


Plasticity and Creep Models Benchmarks

- Plasticity → 3D NAFEMS benchmark
- Creep → benchmark from Liu et al.

- **Code predictions match analytical results.**

Plasticity benchmark

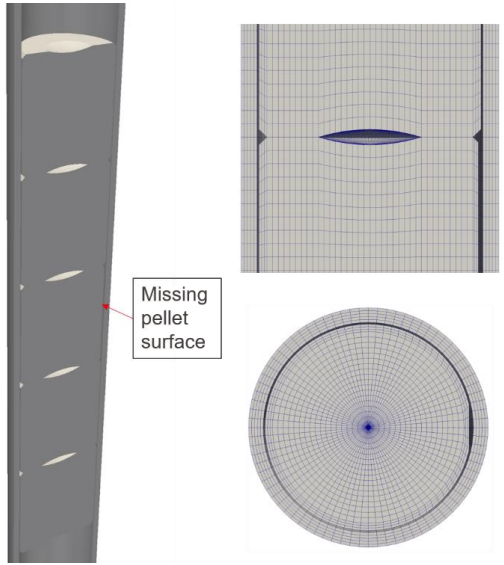


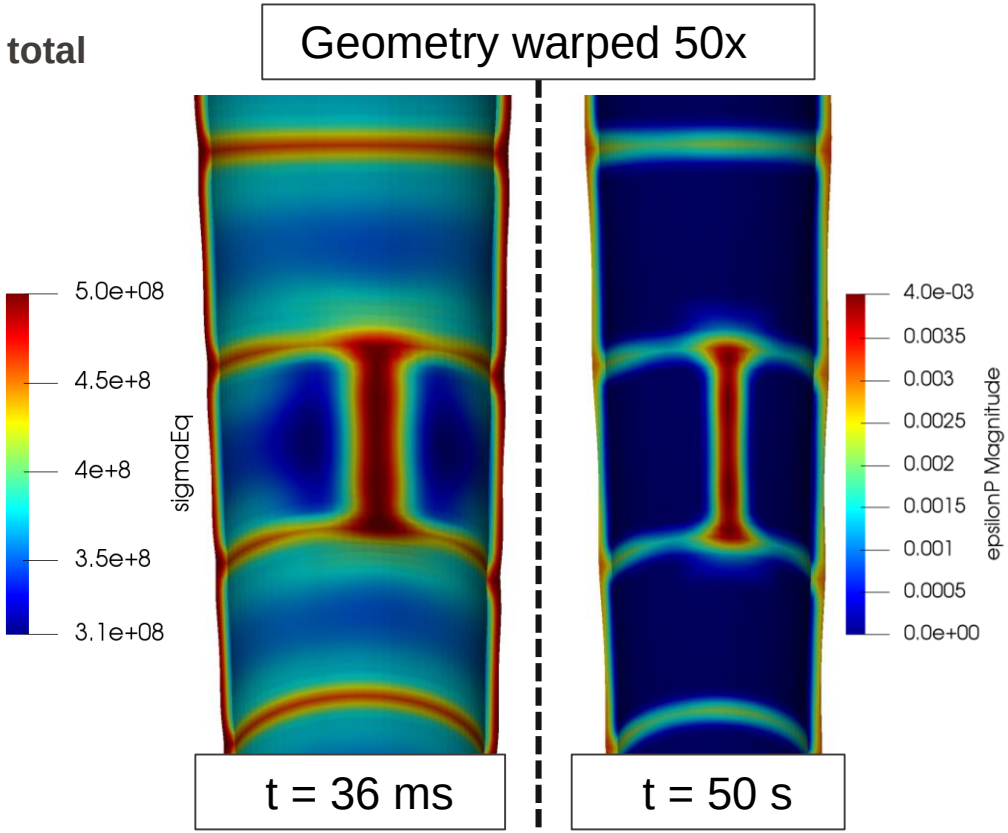
Creep benchmark

Parameter	Analytical Solution	OFFBEAT
$\dot{\varepsilon}_i$ [s^{-1}]	3.08 E-10	3.08 E-10
$\dot{\varepsilon}_{th}$ [s^{-1}]	77.82 E-10	77.86 E-10
ε_p	3.527 E-3	3.529 E-3
$\varepsilon_{c,eff}$	4.336 E-3	4.339 E-3
$\varepsilon_{c,radial}$	1.987 E-3	1.990 E-3
$\varepsilon_{c,azimuth}$	4.331 E-3	4.334 E-3
$\varepsilon_{c,axial}$	2.344 E-3	2.344 E-3

Plasticity Model – Test Case

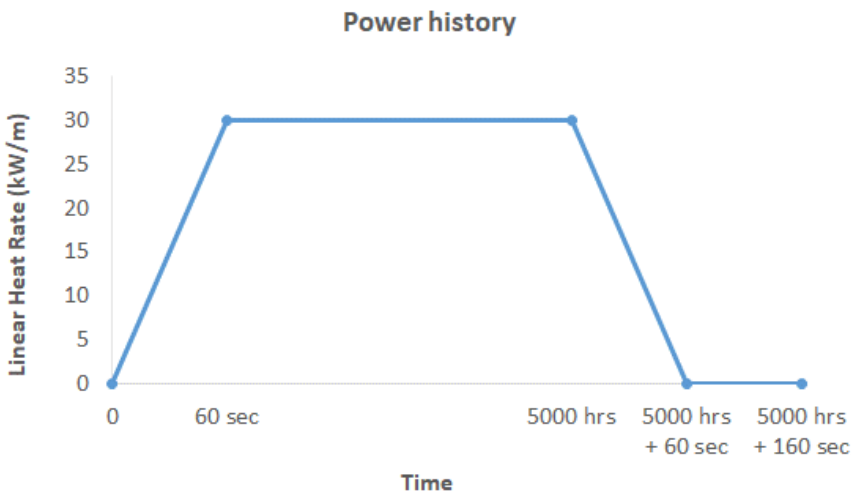
- 6 pellets, MPS in the middle.
- RIA-like scenario: **500 kJ/kg pulse of 40ms, total transient time of 50s.**
- Perfectly plastic cladding.
- Stress concentration in front of defect.

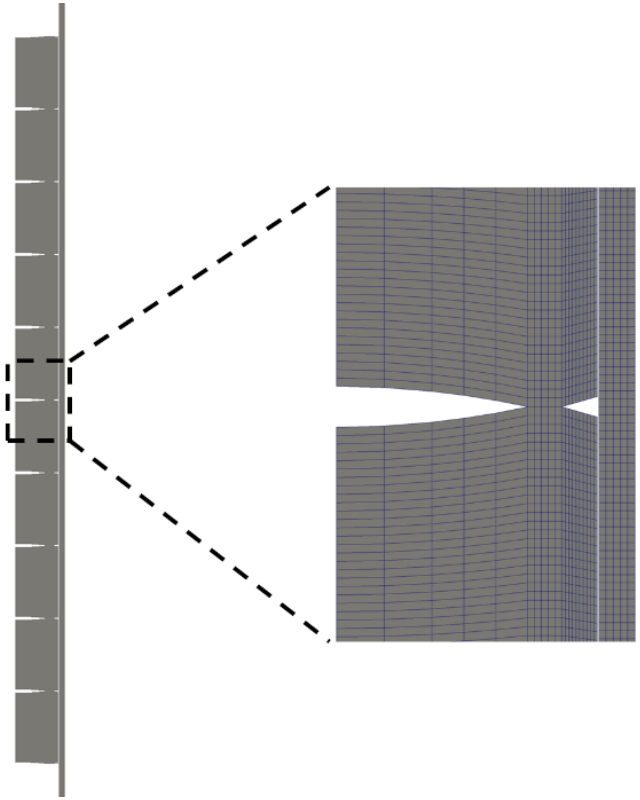




Creep Model – Test Case

- Axi-symmetric model with 10 pellets.
- Dish and chamfers included.
- Pellets attached through land.

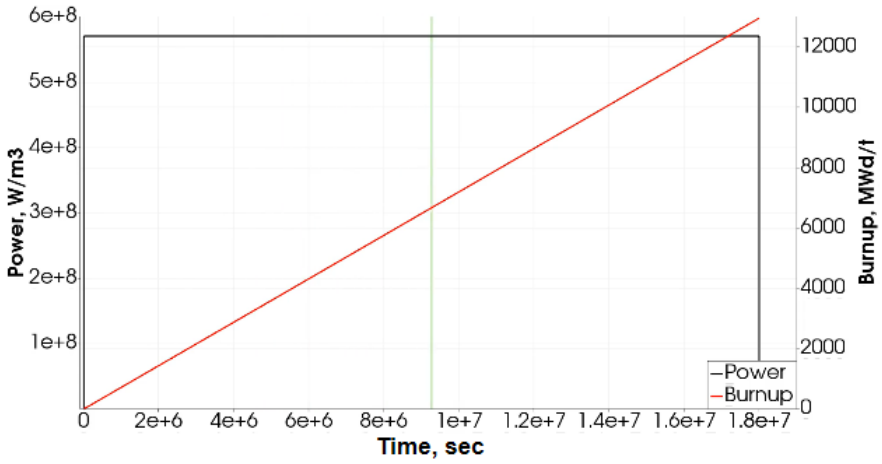


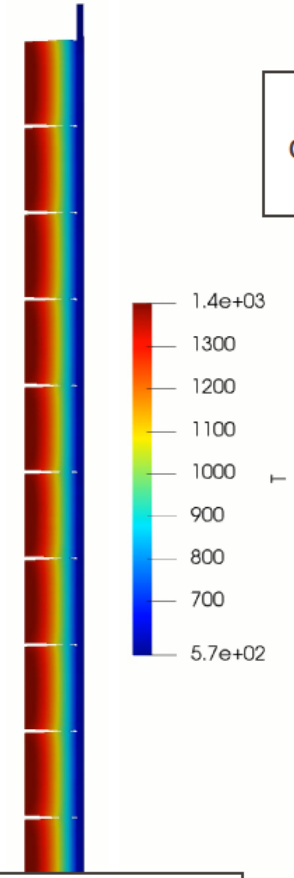


Creep Model – Test Case

- Two simulations: elastic and creep/plastic cladding.
- Penalty factor = 1
- Mesh: 26000 cells.
- 5 hours on one core (Intel® Xeon® CPU E5-1660 v4 with 8 3.2 GHz cores)

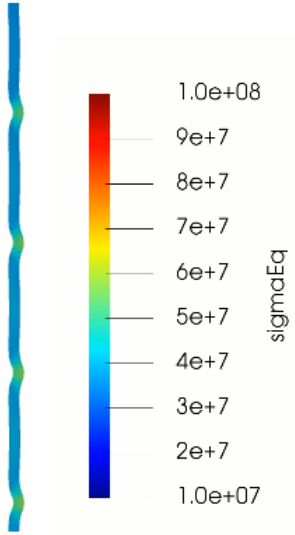
Creep Model – Results





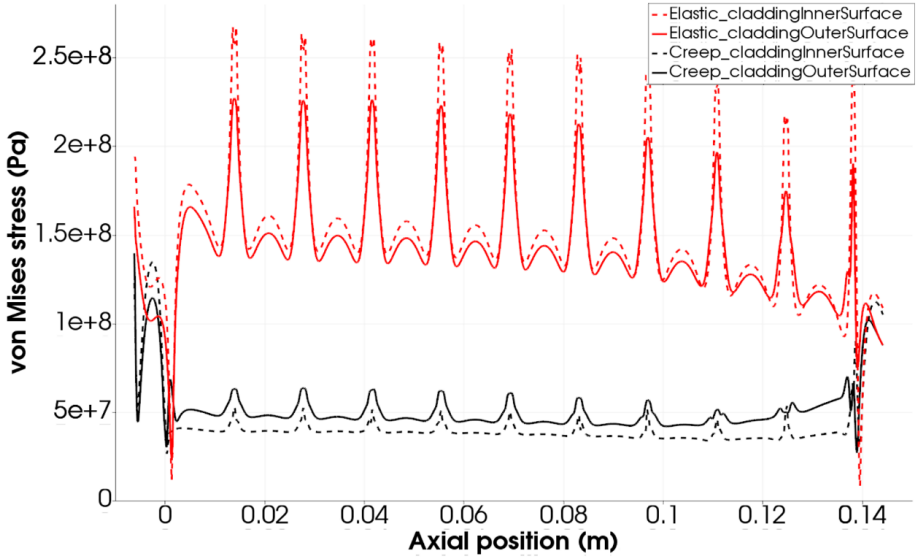
Model Scaled 2x in radial direction

Detail for section of the cladding. Geometry warped with displacement 50x

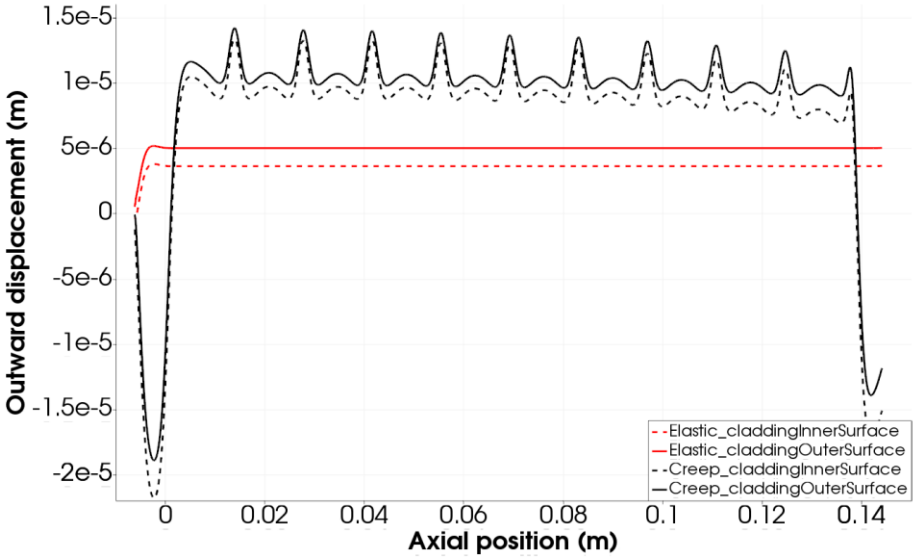


Creep Model – Test Case

End of phase at constant power,
t = 5000 hrs



End of simulation,
t = 5000 hrs + 160 s



Development of OFFBEAT – Near future plans

- Test-cases show feasibility for PCMI scenarios.
  <u>Need for mechanical behavior validation</u>:
  - elongation and cladding deformation.
  - PCMI benchmark from NEA.
  - 3D validation?

- Near future development efforts related to PCMI:
  - Fuel isotropic cracking and creep model.
  - Frictional contact force.

- PCI scenarios:
  - Coupling with thermochemistry (and CFD?)

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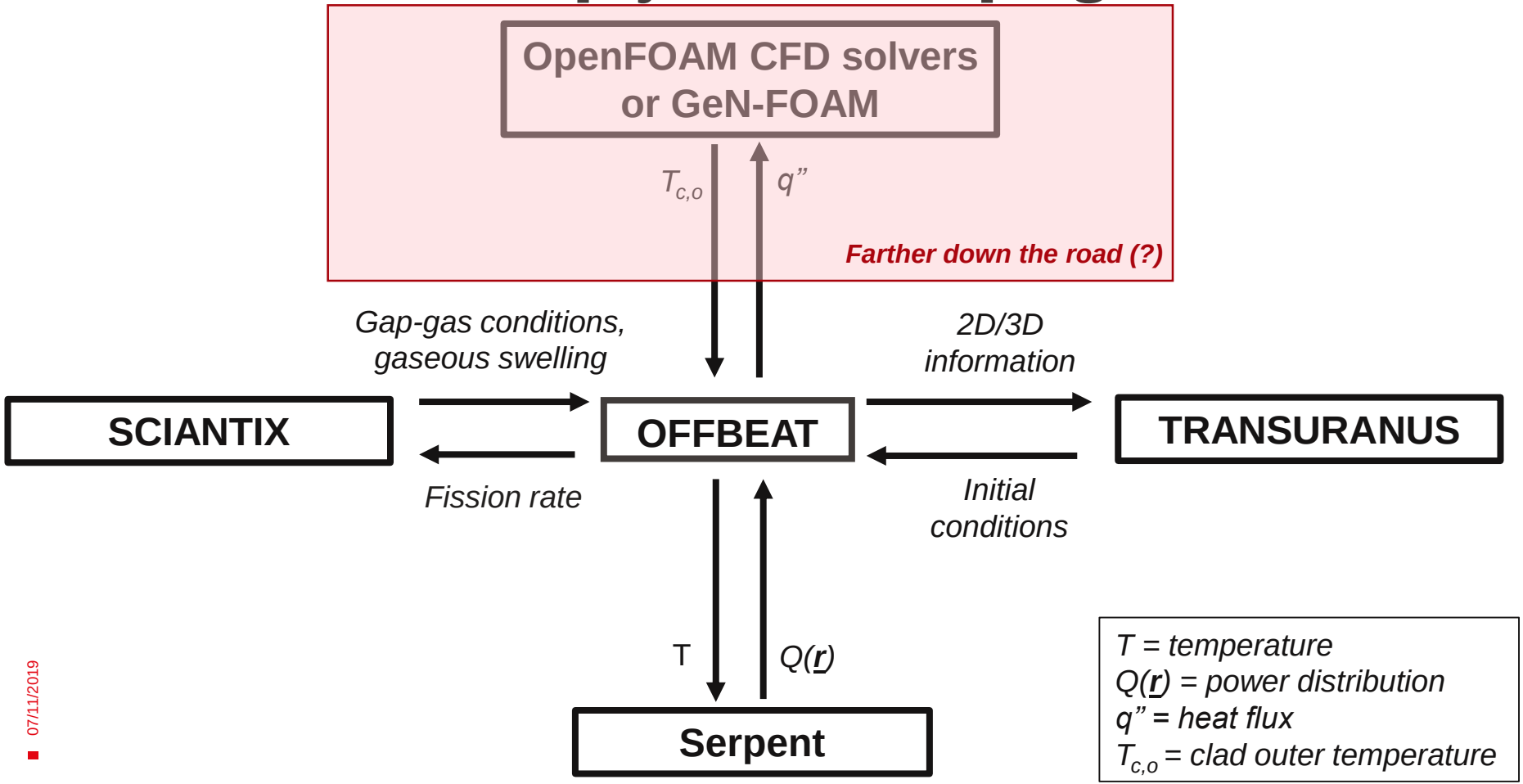
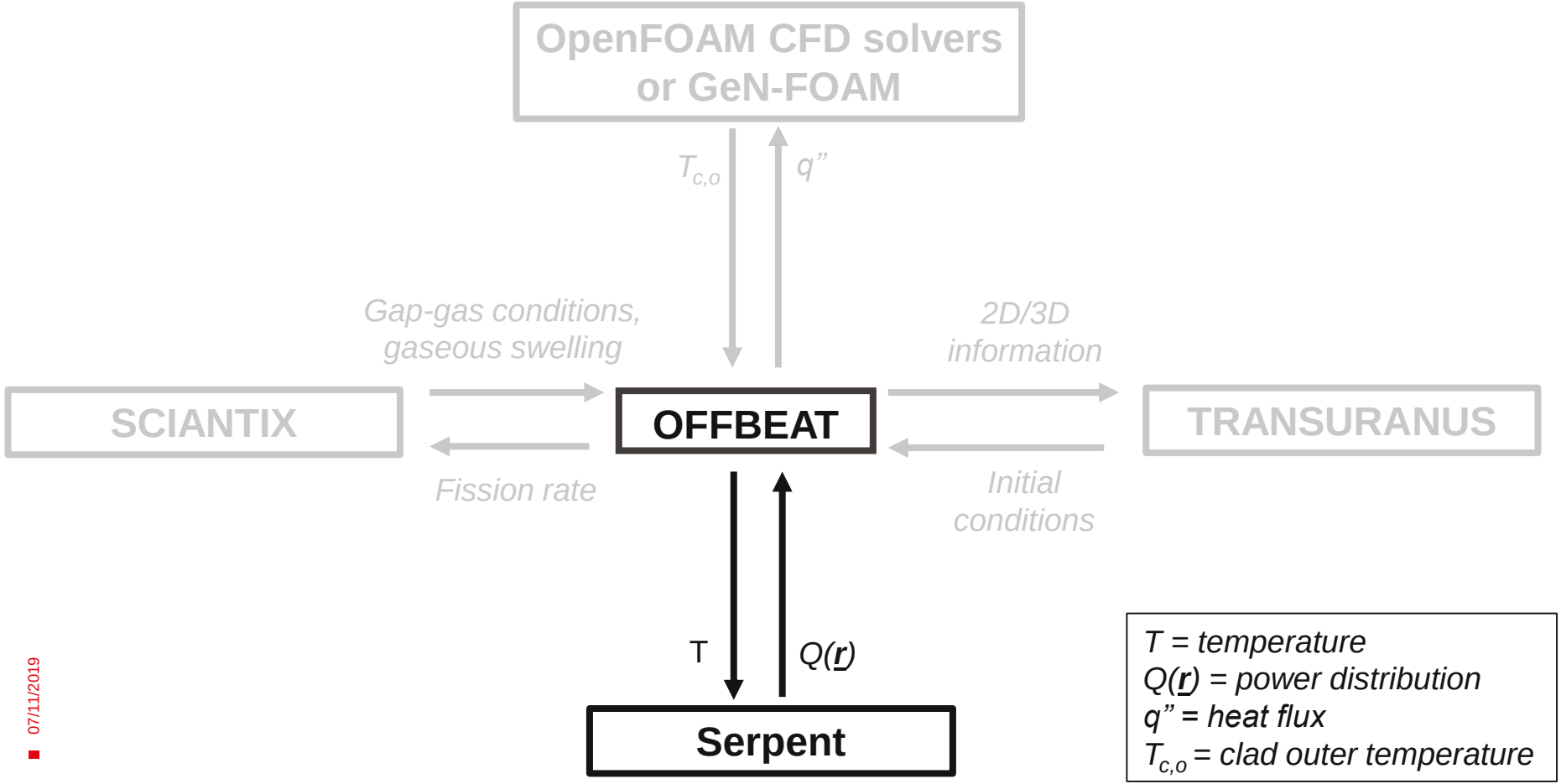
OFFBEAT – Multi-physics and Coupling Possibilities



T = temperature
$Q(\underline{r})$ = power distribution
q'' = heat flux
$T_{c,o}$ = clad outer temperature

OFFBEAT – Serpent Coupling



T = temperature
*Q(**r**) = power distribution*
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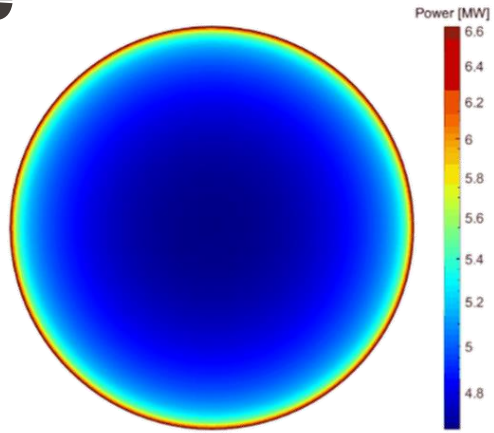
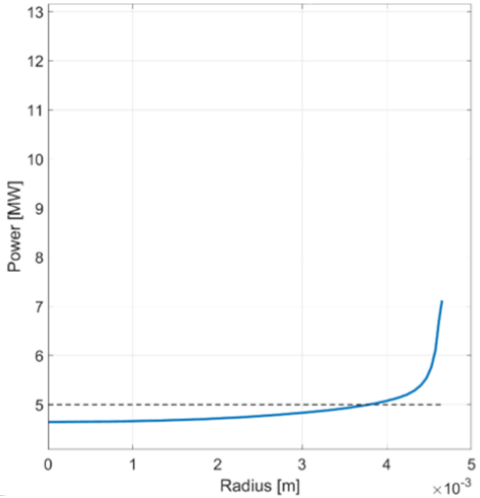
Neutronics effect on fuel performance



- Fuel power profile evolves with burnup!
  - Complicated function of rod (and assembly) design parameters and enrichment.
- Main effect: lower centerline temperature.
- Traditionally in fuel performance codes either:
  - impose radial profile or
  - use simplified neutronics model
    → e.g. **TUBRNP module in TRANSURANUS**

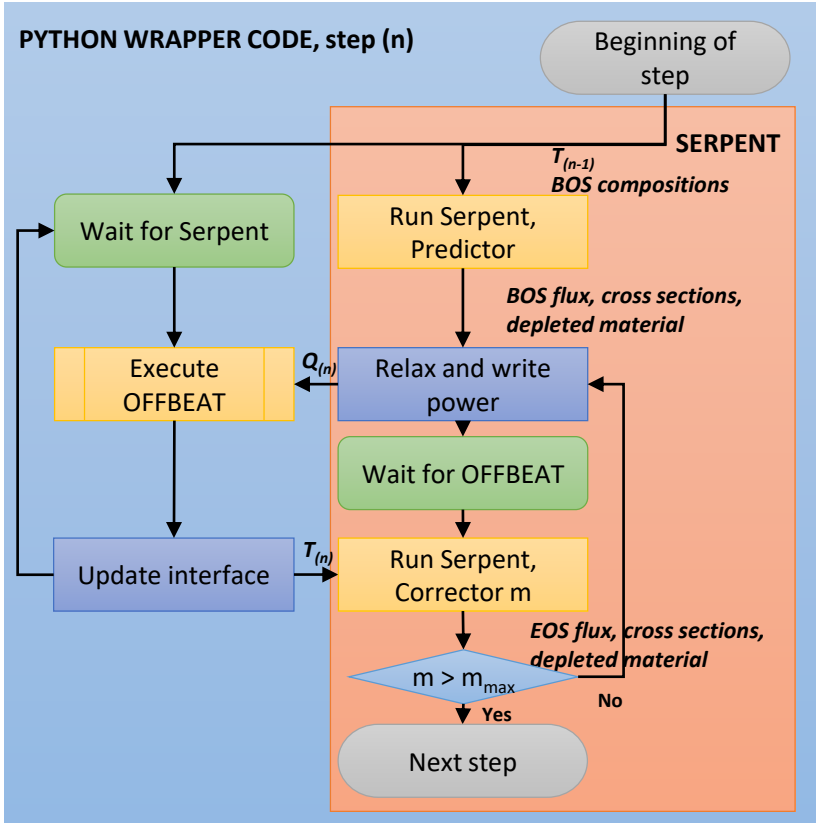


Motivations for OFFBEAT/Serpent Coupling

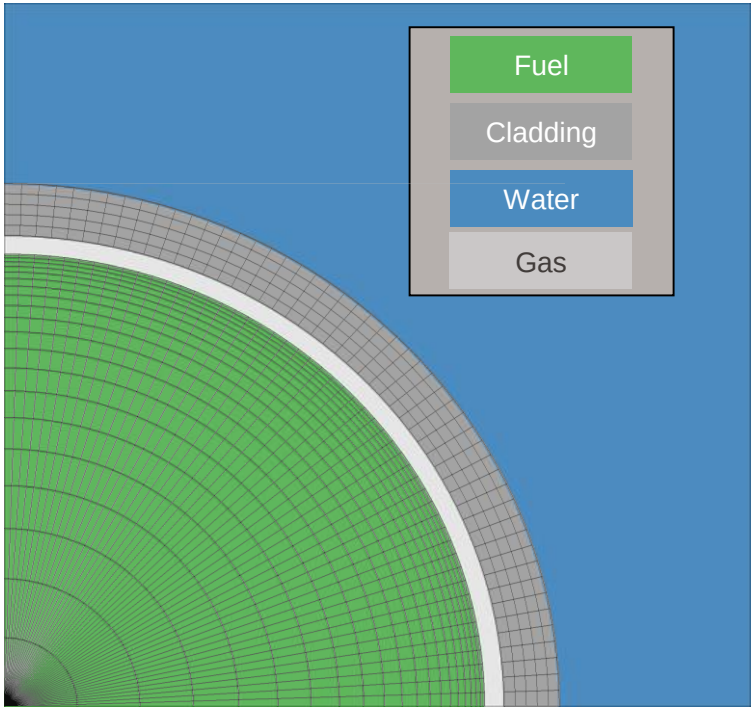
- Traditional approach:
  - + computational cost.
  - + well validated with traditional UO2 fuel in PWRs.
  - - fitting parameters for new fuel.
  - - one-group diffusion with strong absorbers.
  - - asymmetric cases?
- Coupling fuel performance and neutron transport codes:
  - + no need for fitting parameters.
  - + could be used with strong absorbers or in non convential configurations.
  - + could handle asymmetric cases.
  - - computational cost.

OFFBEAT/Serpent Coupling Scheme

- Using the **Serpent Multi-Physics Interface**.
- A Python wrapper code coordinates the two codes
- Temperatures from OpenFOAM to calculate cross sections.
- Power profile from transport calculation.
- Burnup simulation: compositions handled within Serpent.



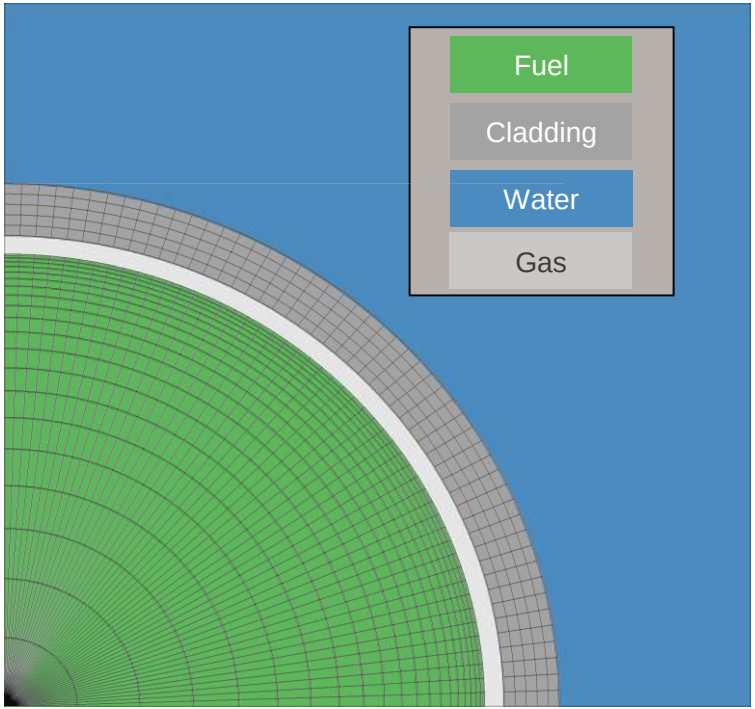
PWR UO2 Rod



Model Details	
Fuel Radius	4.65 mm
Material	UO2 (3.5 wt-% enriched)
Linear power	20 W/mm
Radial mesh	20 burnup zones
Gap width	190 µm
Cladding thickness	0.535 mm
Material	Zircaloy-4
Temperature	600 K
Boron concentration	420 ppm
Pitch	1.496 mm

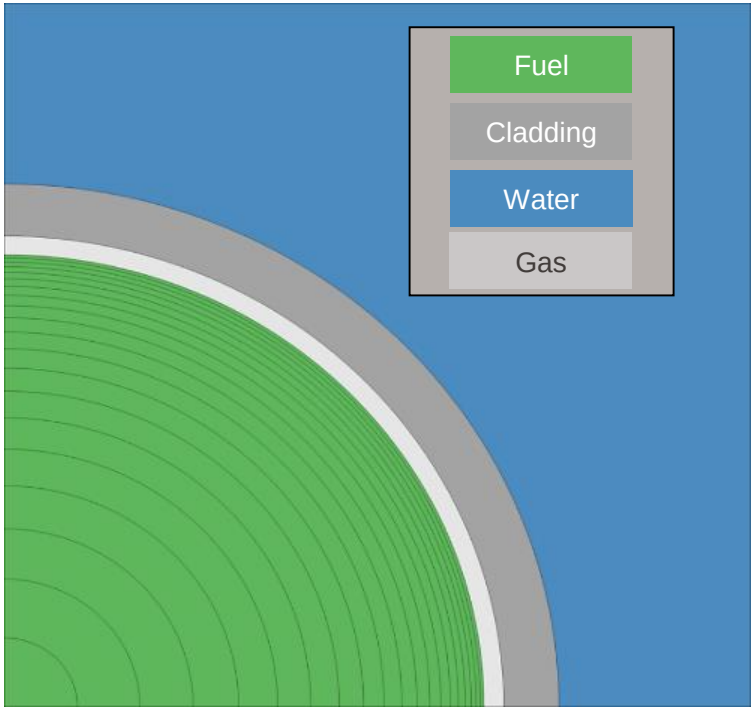
Serpent Parameters	
Neutrons per cycle	50,000
Inactive cycles	50
Active cycles	300
Burnup scheme	CE/LI
Burnup step	2 MWd/kg
Maximum burnup	102 MWd/kg
Substeps	10

PWR UO2 Rod – Adaptive Search Mesh



- Adaptive search mesh algorithm:
  - Check only limited number of OFFBEAT cells for each interaction point.
  - Adaptive algorithm saves memory → gradually refining mesh
- Attention must be paid to statistics of each cells.
- Higher number of cells → more neutrons needed for smooth results.
- Possible problem for asymmetric cases.

PWR UO2 Rod – Adaptive Search Mesh



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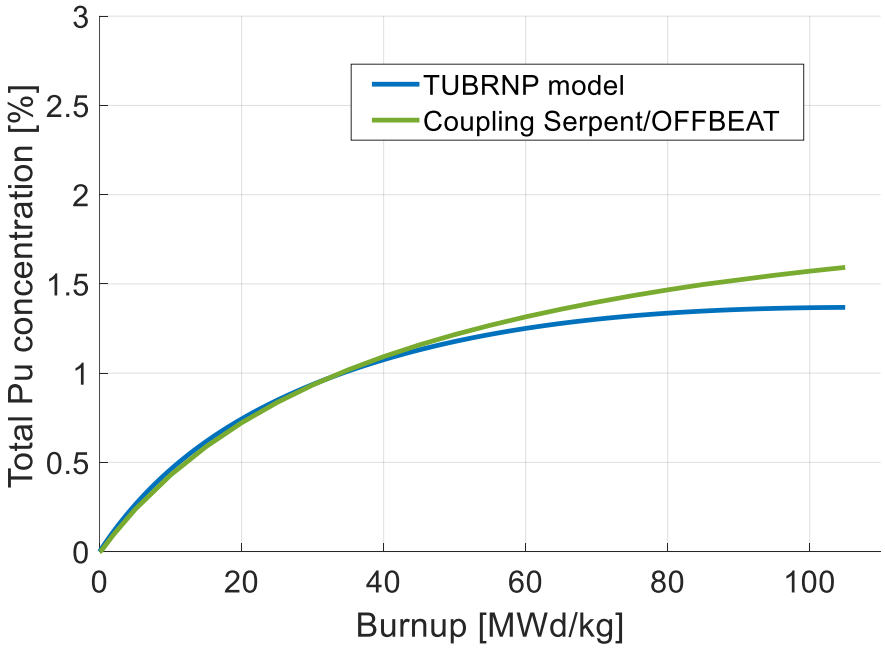
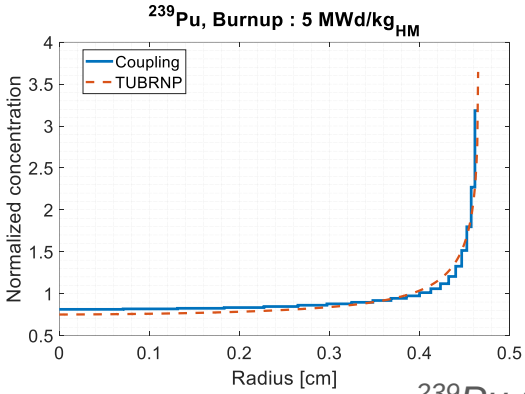
PWR UO2 Rod - Results

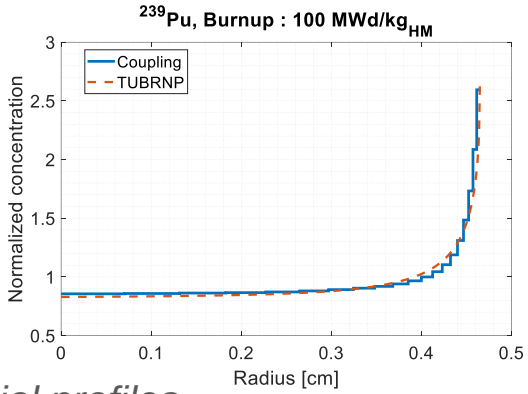


Total Plutonium concentration evolution

- Similar predictions at low/medium burnup.
- Different results at high burnup.
  - Saturation for TUBRNP
  - Buildup for coupling

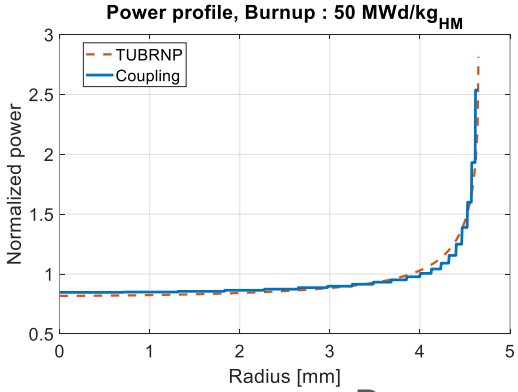
PWR UO2 Rod – Radial Profile

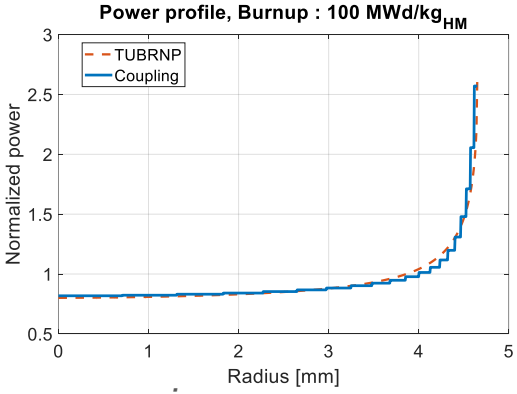




^{239}Pu radial profiles

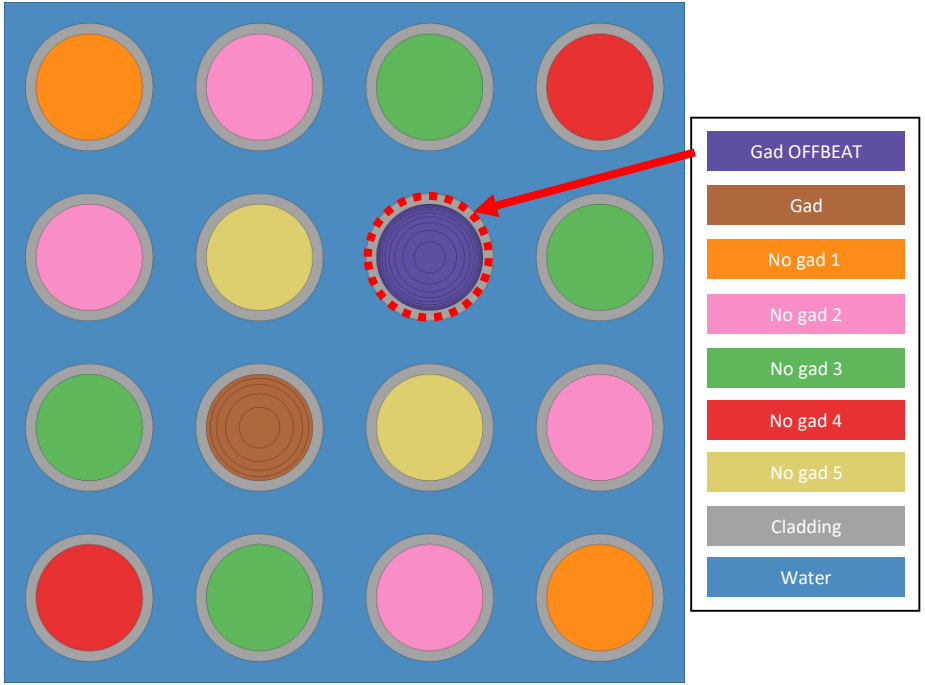
- No significant difference for the radial profiles





Power profiles comparison

BWR UO2 Gd Rod

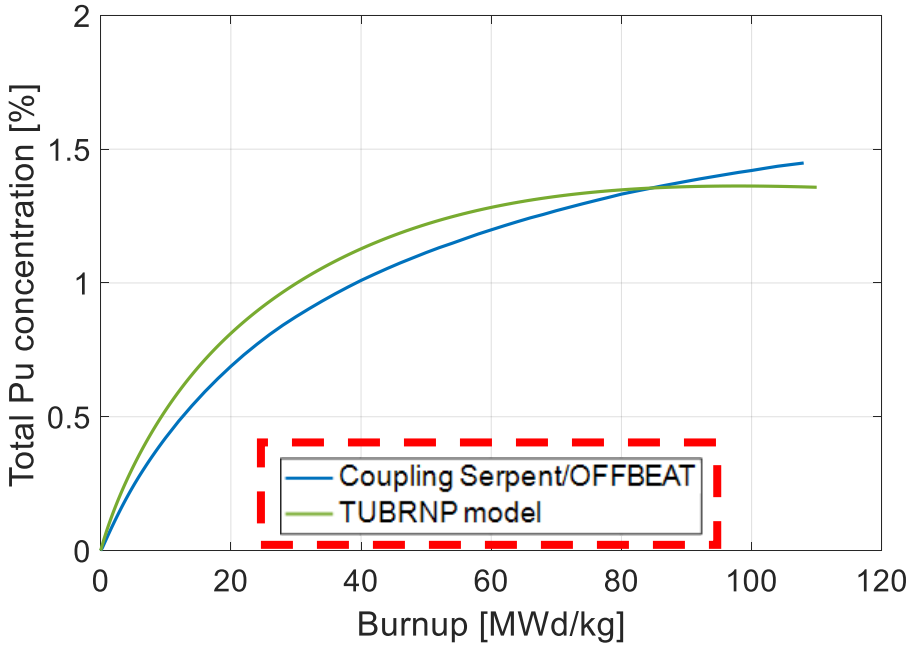


BWR Serpent model

Model Details	
Radius	5 mm
Material	UO2 (3 wt-% enriched)
Power density	20 W/g
Gd-pins content	3 wt-%
Temperature	873.15 K
Radial mesh (coupled)	10 burnup zones
Cladding thickness	0.5 mm
Material	Zircaloy-2
Temperature	573.15 K

Serpent Parameters	
Neutrons per cycle	50,000
Inactive cycles	50
Active cycles	300
Burnup scheme	CE/LI
Burnup step (<10 MWd/kg)	0.25 MWd/kg
Burnup step (>10 MWd/kg)	5 MWd/kg
Maximum burnup	100 MWd/kg
Substeps	10

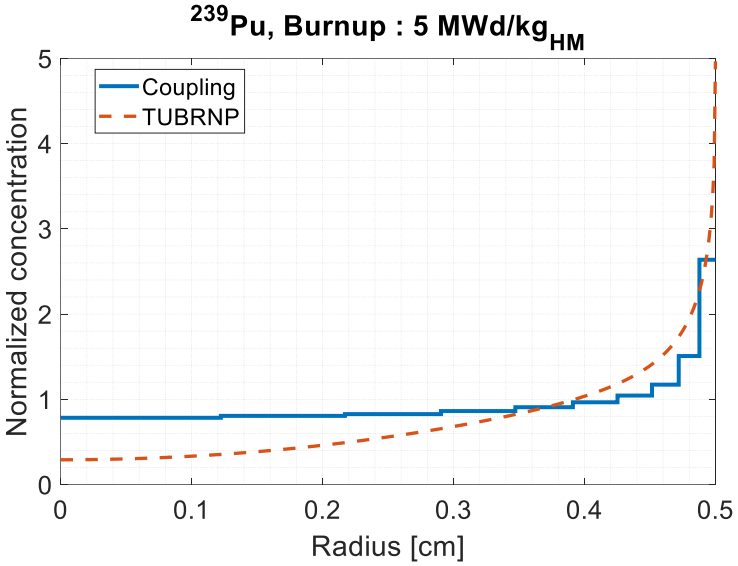
BWR UO2 Gd Rod - Results

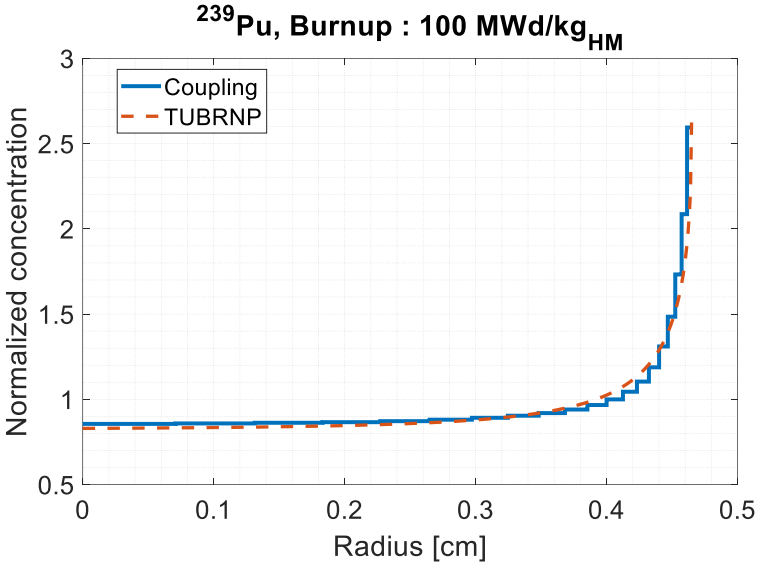


Total Plutonium concentration evolution

- More pronounced differences.
- Differences start at the beginning of the irradiation.

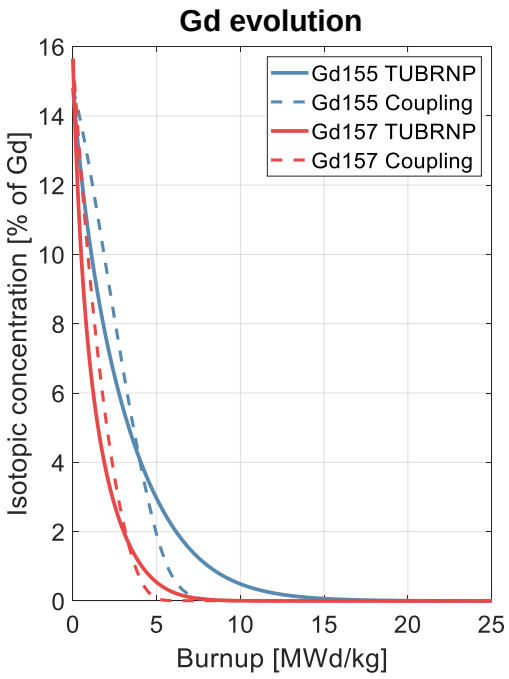
BWR UO2 Gd Rod – Radial Profile



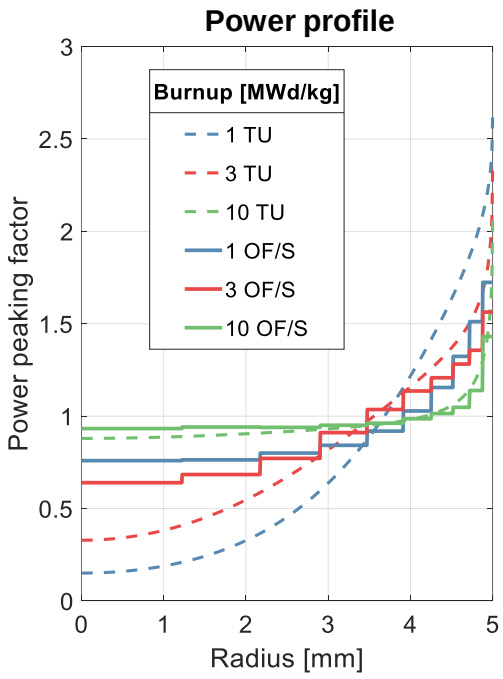


^{239}Pu radial profiles

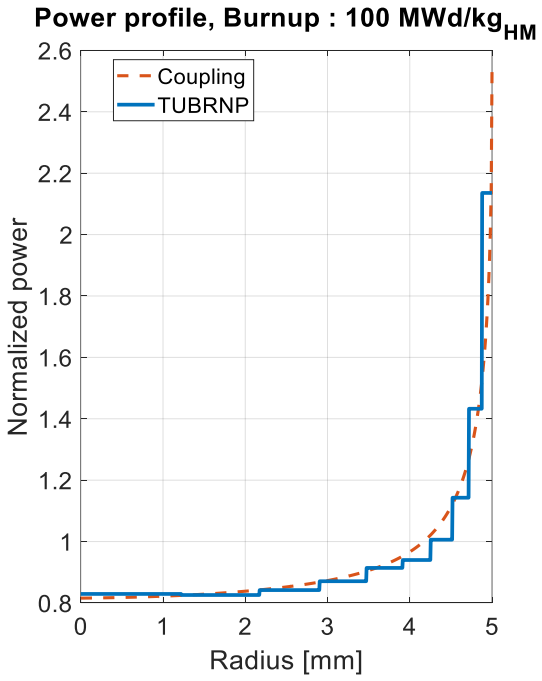
BWR UO2 Gd Rod – Radial Profile



Gd evolution with burnup



Power profiles comparison
Low burnup



Power profiles comparison
High burnup

OFFBEAT/Serpent Coupling – Follow up

- Preliminary tests provide promising (and expected) results.

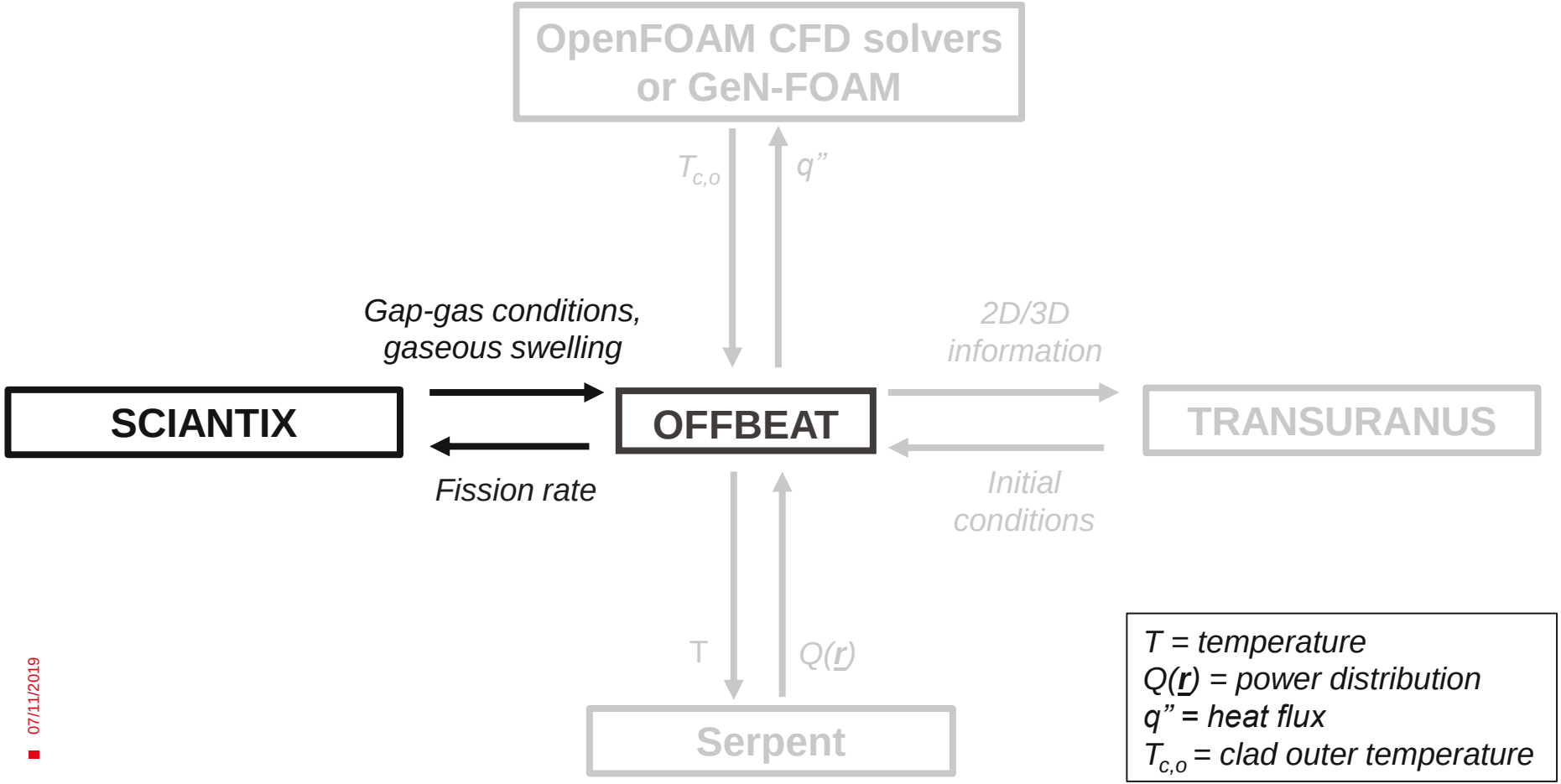
- **Computational cost is high** → no relevant gain for traditional fuel.
- **Interesting solution for:**
  - new fuel types → obtaining fitting parameters?
  - experiments with non-traditional features.
  - asymmetric scenarios.

- Y. Robert (now PhD student at Berkley) will continue to work on the project.

- Aim is to prove feasibility of OFFBEAT/Serpent coupling **for more realistic scenarios.**

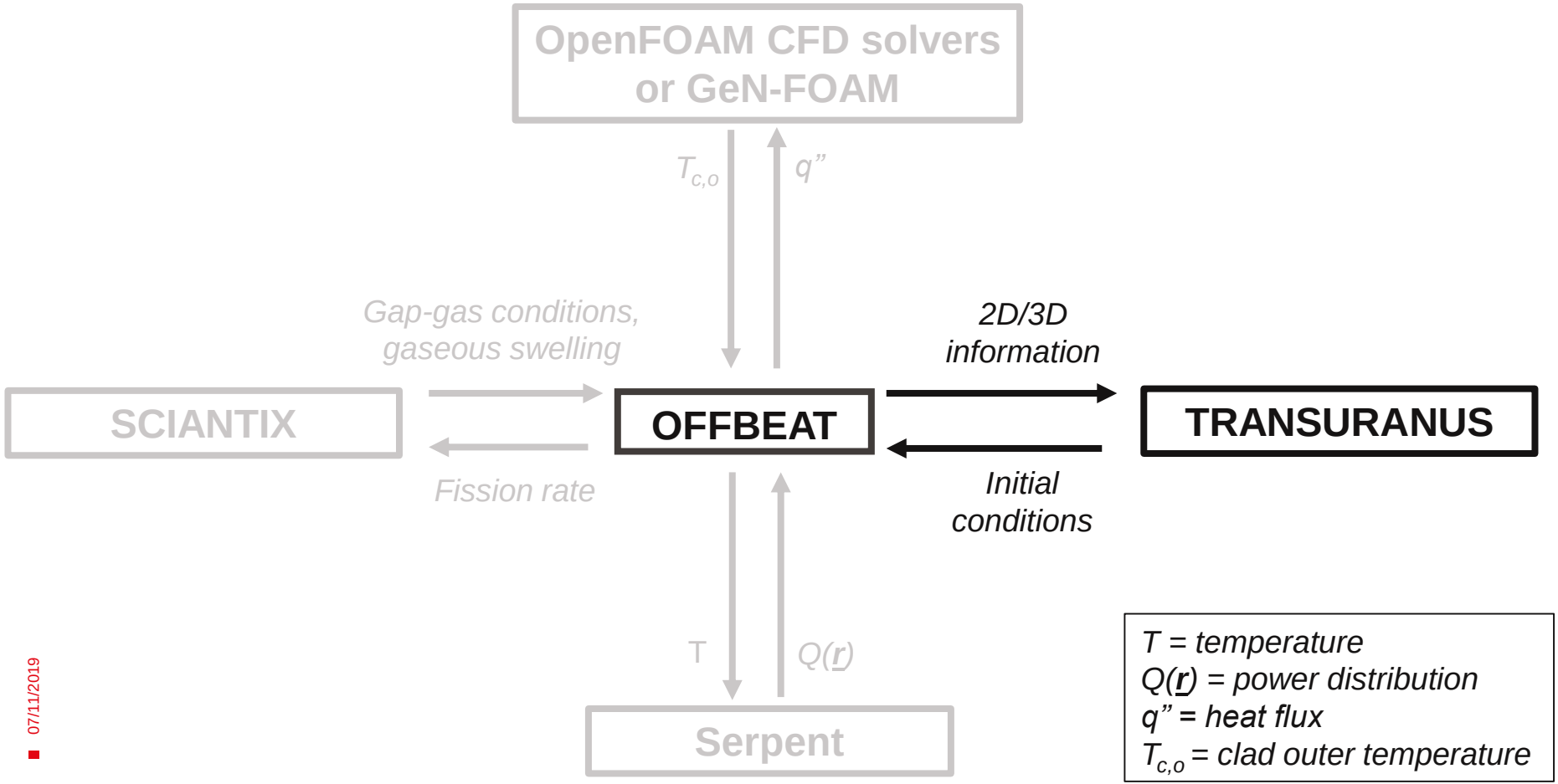
- Examples:
  - 2D assembly with Gd-rods or void channel with angular binning of neutron flux.
  - 3D partial insertion of control rods in PWR.

OFFBEAT – SCIANTIX Coupling



T = temperature
*Q(**r**) = power distribution*
q” = heat flux
$T_{c,o}$ = clad outer temperature

Collaboration with the JRC Karlsruhe



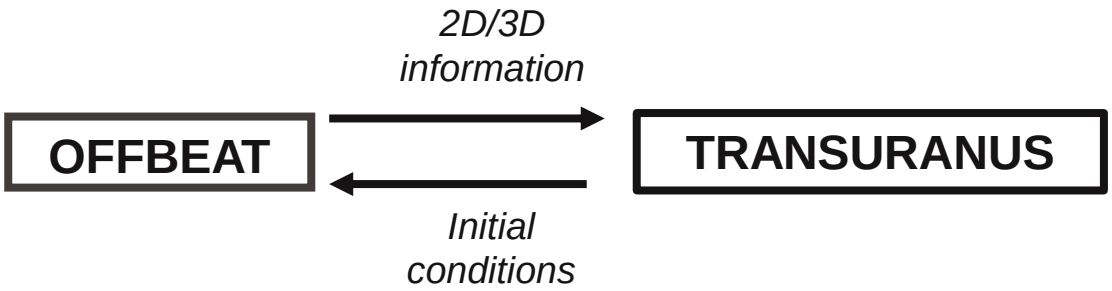
T = temperature
*Q(**r**) = power distribution*
q” = heat flux
$T_{c,o}$ = clad outer temperature

Collaboration with the JRC Karlsruhe

- Visiting stay starting soon (thanks to ENEN+).

- Primary objective: analysis of fuel creep experimental results.
  → **use advanced tools for designing and interpreting non-traditional experiments?**

- Secondary objective: first strategy for OFFBEAT-TRANSURANUS coupling.



Conclusions

- OFFBEAT, a new open-source fuel behavior solver with focus on **multi-dimensional and multi-physics** aspects of fuel behavior.
- Efforts have focused on implementation, mainly for PCMI/PCI capabilities.
- ***Need for more validation and applications!***
- OFFBEAT is open to various coupling possibilities:
  - OpenFOAM CFD (or GeN-Foam)
  - SCIANTIX
  - Serpent

EPFL

Merci