# Multi-Physics simulations for Nuclear Reactor Analysis

**Christian CASTAGNA** on behalf of the collaboration between
the **Nuclear Reactors Group, Politecnico di Milano**
and the **INFN Milano-Bicocca Group**

POLITECNICO MILANO 1863

UNIVERSITA' DEGLI STUDI DI MILANO BICOCCA

INFN Istituto Nazionale di Fisica Nucleare

# Outline

1. Introduction
2. Multi-Physics Modelling
3. Test case
4. Time evolution of neutron fluxes and fissions
5. Burnup analysis
6. Conclusions

# Introduction

- Accurate determination of **reactor antineutrino spectrum** is mandatory for **single-detector** medium-baseline oscillation experiments, like JUNO.
- In the absence of a near detector, the antineutrino flux must be evaluated using **simulations** of nuclear reactors.
- Nuclear reactors are very **complex systems** evolving in time and the emitted antineutrino flux depends on reactor neutronics, thermal-hydraulics and burnup that are involved in a single environment.
- We are investigating the **uncertainties** related to reactor simulations.

# Introduction



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**OPEN ISSUE**

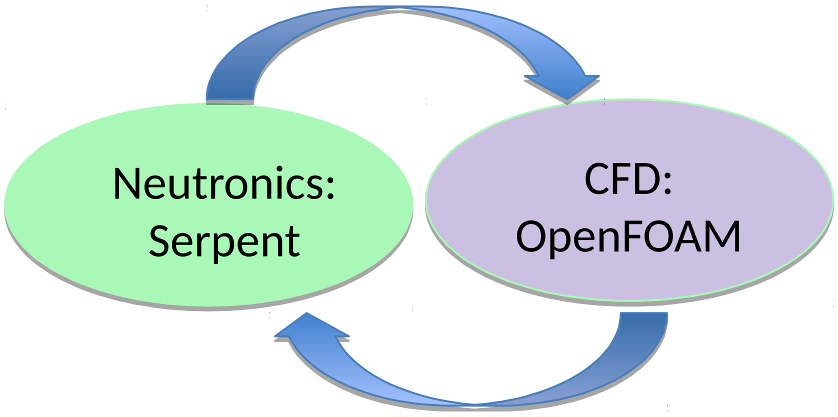
How much detail is needed in reactor simulations to achieve enough accuracy in the evaluation of **fluxes distribution** and **fission fractions** as function of time/burnup?

# Multi-Physics Modelling

- Traditionally, **temperature** and **density** fields are approximate with **uniform** distributions for burnup calculations.
- Depending on the type of reactor, the **thermal-hydraulics can have significant** effects **on neutronics/fuel burnup.**
- In burnup analysis, **Multi-Physics (MP) modelling** of neutronics and thermal-hydraulics are fundamental to achieve a suitable global description of nuclear systems.
- Applying the MP modelling for burnup calculations is a **challenging task** **(lack of systematic studies)**.

# Coupling Code Technique (CCT)

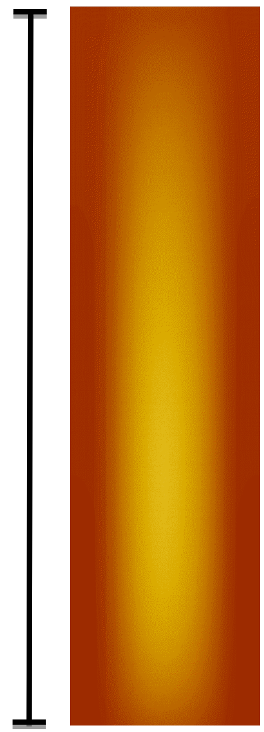
- We developed a MP approach, based on a Coupling Code Techniques (CCT), in which **Serpent Monte Carlo code (neutronics)** and the **OpenFOAM toolkit (T-H)** are run separately. The process of data and variables are passed between them until the **convergence of the power**
- **Serpent implements an interface** to include temperature and densities from external solvers.



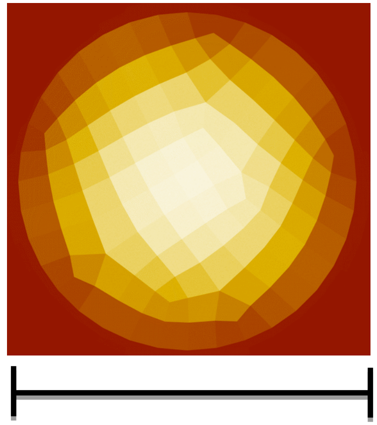
# STUDY OF A SIMPLE TEST CASE

We **preliminary tested** the MP coupling on a **simple geometry**: an infinite lattice of fuel pins with typical parameters of a PWR reactor with high burnup.

- $UO_2$ pin surrounded by water
- Diameter: 8.19 mm
- Active height: 3.66 m
- Pitch (center-to-center): 1.6 cm
- Thermal power: 94.14 kW
- Density: 10.45 g/cm$^3$
- Enrichment: 3.2% $^{235}$U
- 100 cm of water reflector at top/bottom of fuel pin




*Vertical and horizontal sections of fuel pin, taken* by the mesh-plot of temperature distribution during the neutron transport in Serpent.



# BURNUP ANALYSIS

We compare the results of burnup simulations in which neutronics and thermal-hydraulics are coupled (*coupled* case) with the ones from a non-coupled simulation (*uniform* case).

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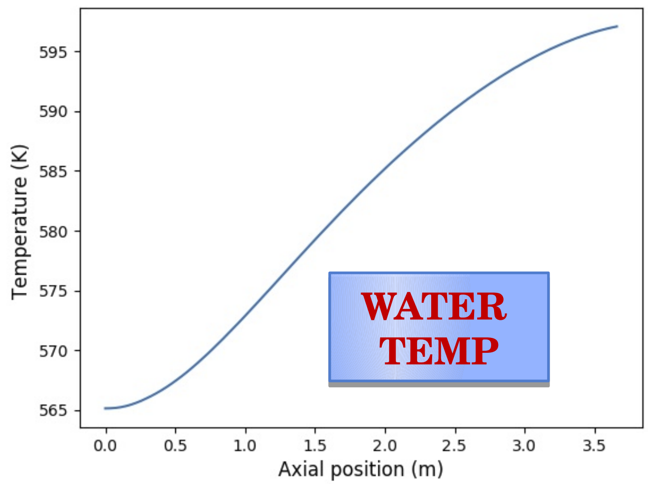
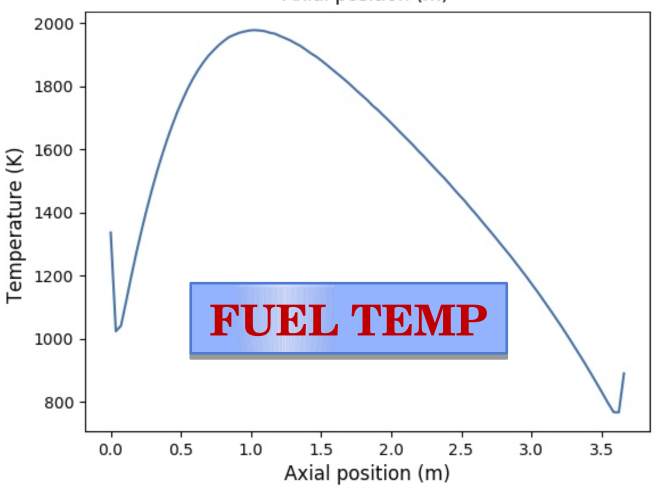
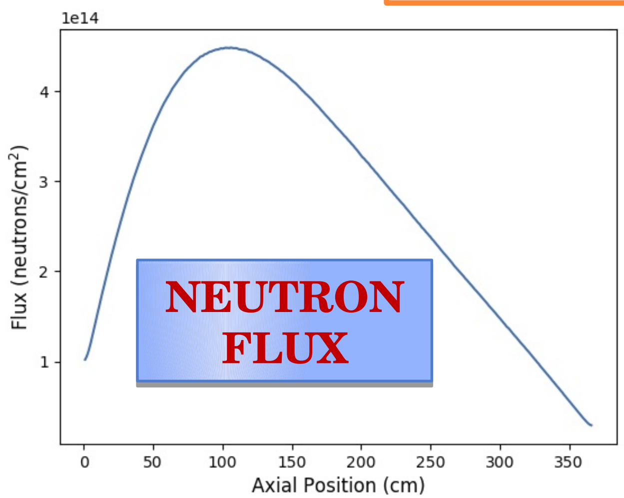
- We carry out the **burnup analysis** with the following time steps (in days): 1, 2, 7, 15, 30, 60, 90, 120, 150, 180, 240, 300, 365, 420, 480, 600, 730, 910, 1095, 1460
- The fuel pin is subdivided in 50 depletion zones (5 radial × 10 axial)
- In the *coupled* case, **temperature and density** distributions are calculated at **fresh fuel** and *updated* at **1, 2, 3 and 4 years**.
- In the *uniform* case, $T_{WATER}$ = 587 K, $T_{FUEL}$=1082 K , $\rho_{WATER}$ = 703 kg/m
- In the transport calculations, we simulate $2*10^8$ neutron histories
- In order to evaluate the statistical uncertainties of nuclide concentrations, we run 8 burnup independent simulations for each case

# SIMULATION OF FRESH FUEL

**After the convergence of the MP coupling** at fresh fuel, we obtain the distribution of **temperatures and neutron flux** in the **axial direction**.



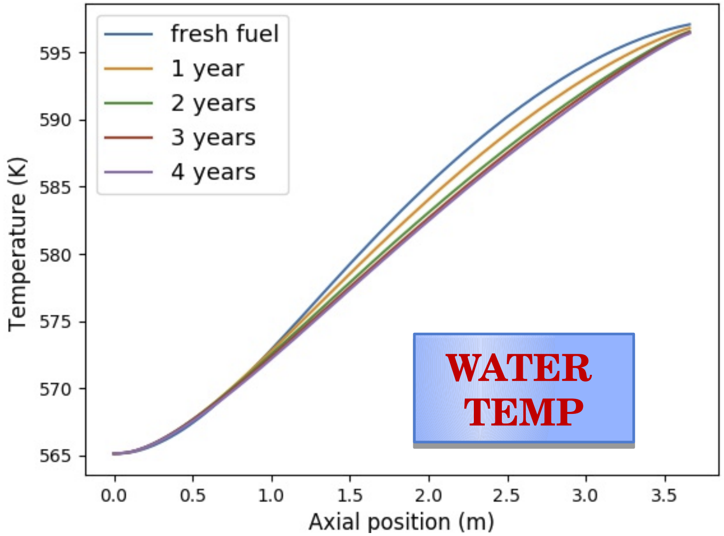




Water is injected from below and heats up as it flows through the active zone.

In the lower part of the pin, higher water density results in more moderation of the neutrons that increase the number of fissions.

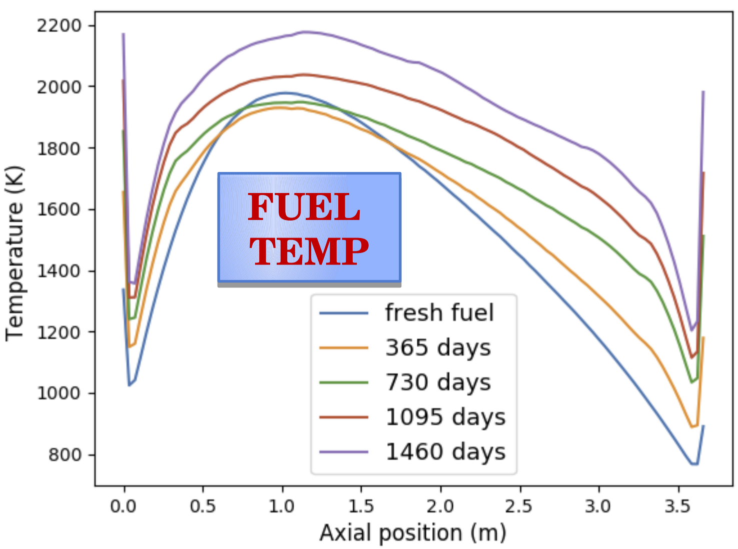
Asymmetric profile of fuel temperature and neutron flux.

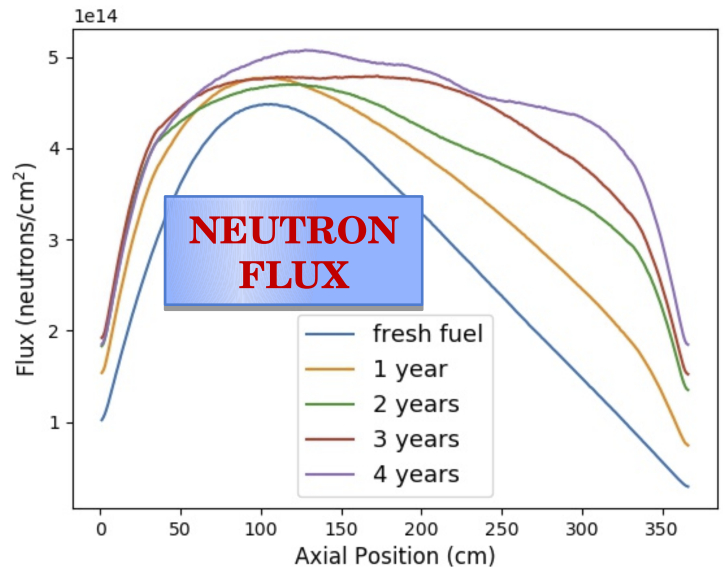
# T-H FEEDBACK AT DIFFERENT TIME STEPS




During the burnup, the <u>MP coupling is updated</u>. The profile of the fuel temperature and neutron flux flattens out.

This is due to the change of the composition of fuel material at different axial zones.



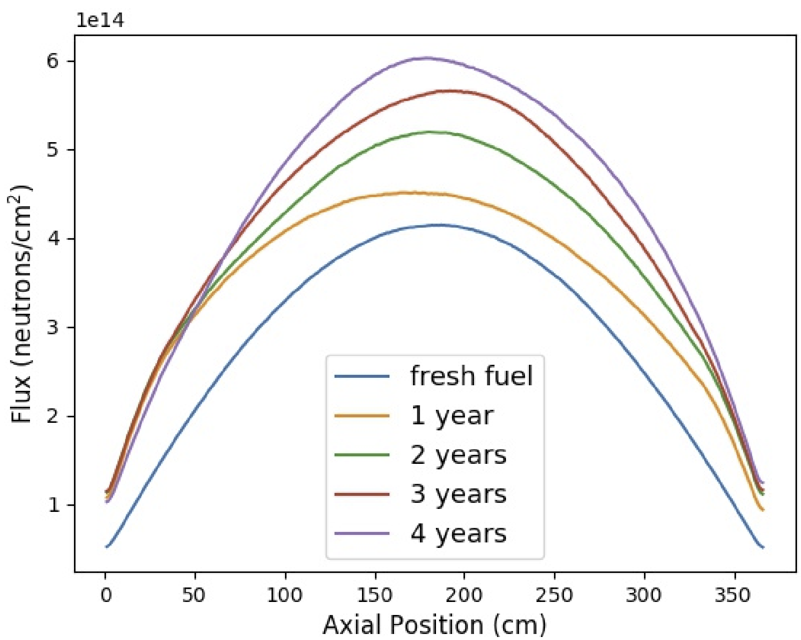



# TIME EVOLUTION OF NEUTRON FLUX

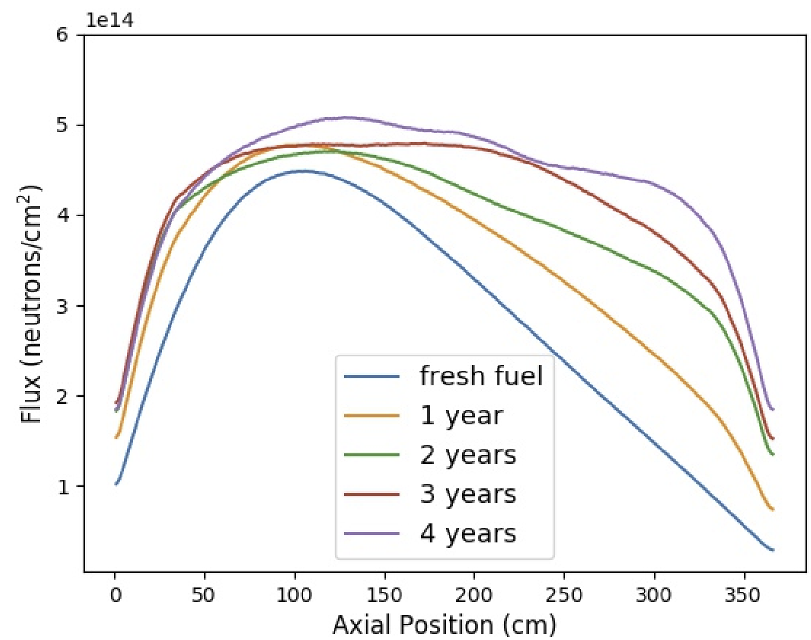
At each time step, the axial profile of the neutron flux is symmetric for the *uniform* case, asymmetric for the *coupled* case.

This difference is due to the change of fission rate density along the axial direction.

**UNIFORM**




**COUPLED**

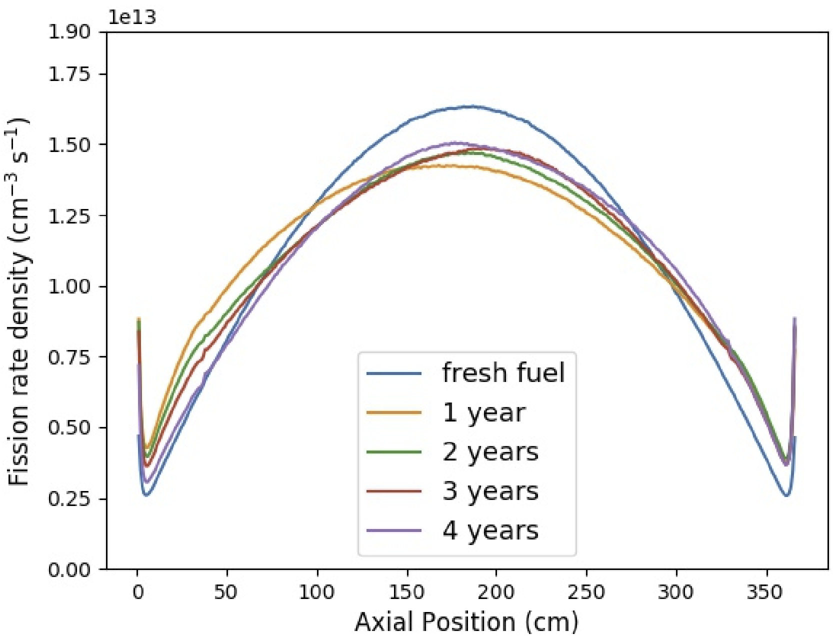


# TIME EVOLUTION OF FISSION RATE

At each time step, the fission rate density is symmetric for the *uniform* case, asymmetric for the *coupled* case.

Fission rate density profile influences the local fuel consumption.

**UNIFORM**

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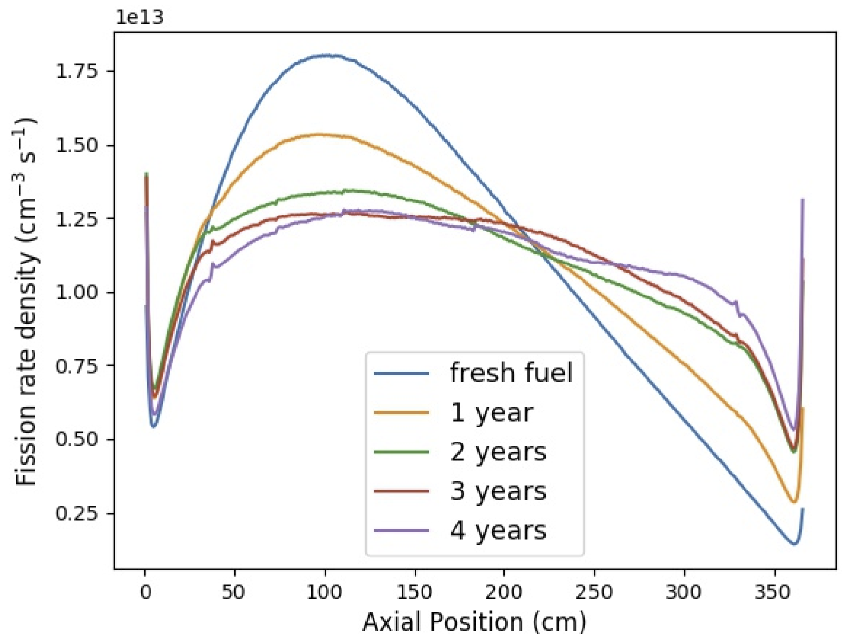
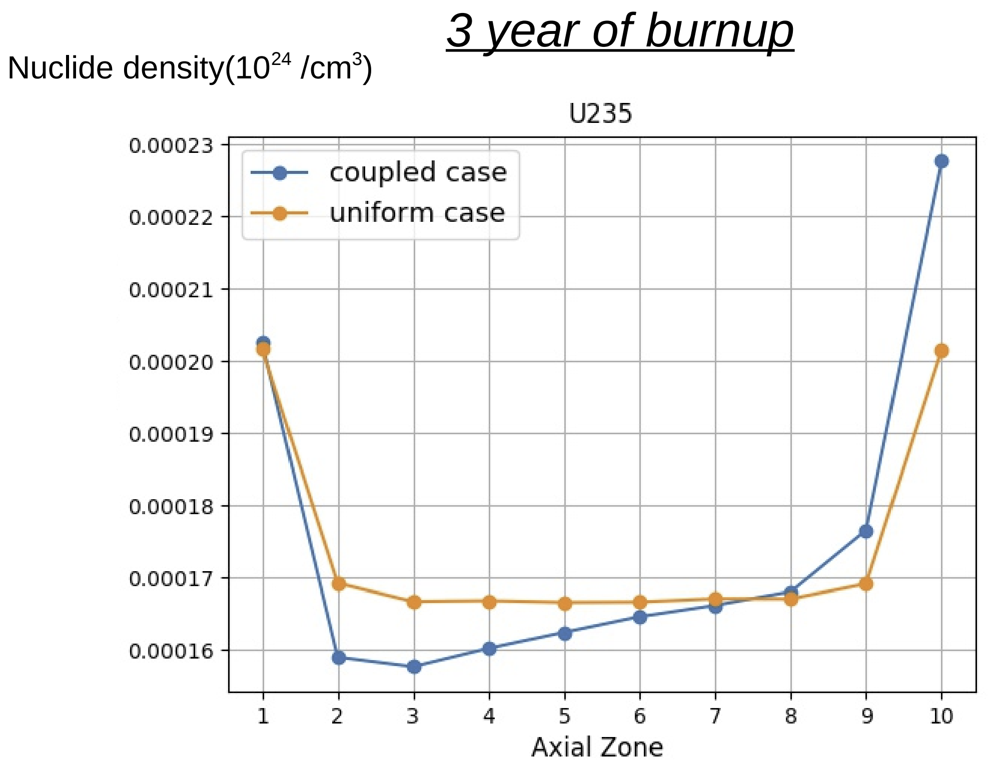


# AXIAL DISTRIBUTION OF THE NUCLIDES

In the axial direction, for the coupled case, the consumption of $^{235}U$ is higher in the lower half, where the fission rate density is higher .
For the uniform case, the consumption is symmetric.

The % variations of the local densities are >5%.



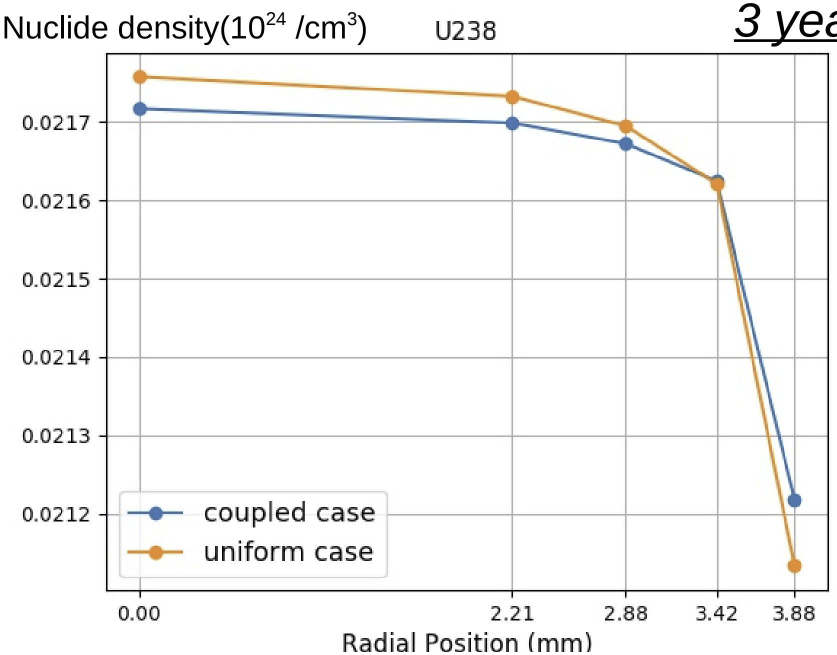

*(*) % variations calculated as (coupled-uniform)/uniform*

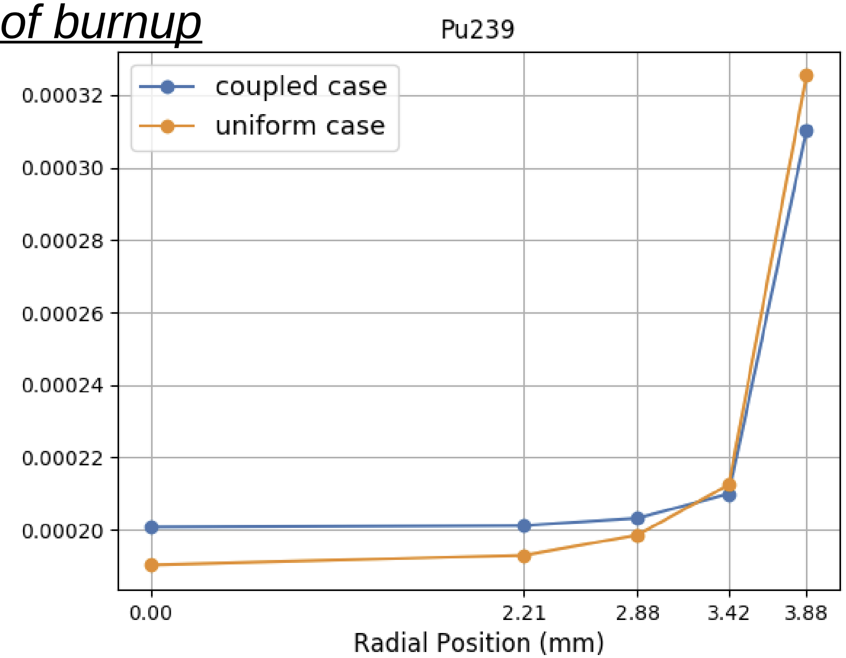
*(**) the relative statistical uncertainties are < 0.01%*

# RADIAL DISTRIBUTION OF THE NUCLIDES

For each case, in the radial direction, the dominant effect on fuel consumption is the self-shelding, i.e. the absorbtion increases for the nuclei near the fuel surface, like $^{238}$U. This directly leads to more production of $^{239}$Pu in the outer region.

*3 year of burnup*

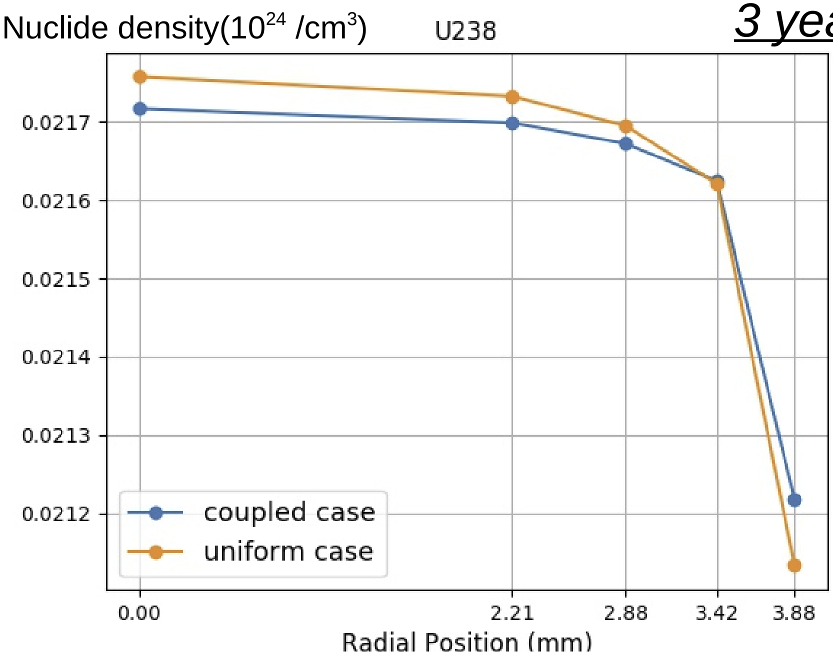


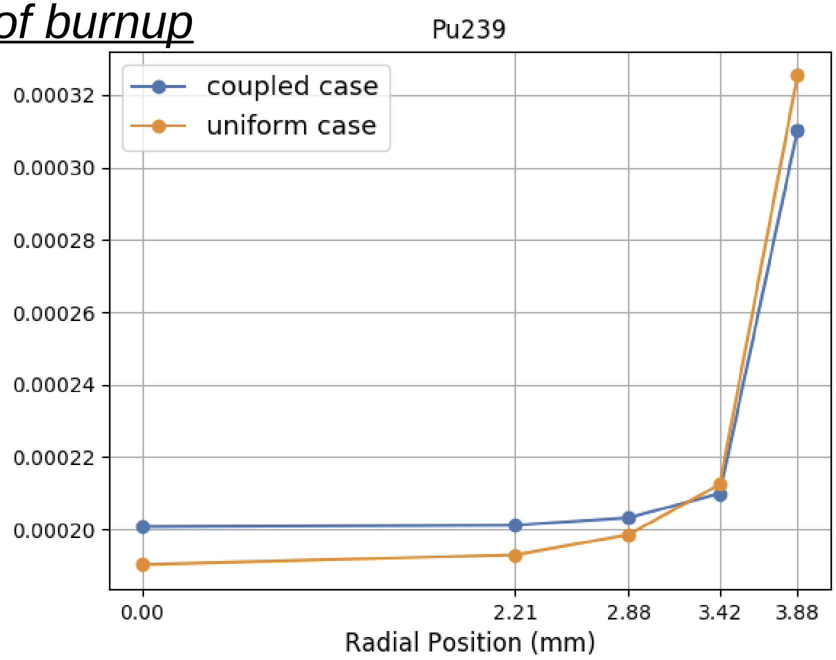



# RADIAL DISTRIBUTION OF THE NUCLIDES

Comparing the 2 cases, in the coupled one, higher fuel temperature in the center of the pin increases the resonance absorption of neutrons by $^{238}U$ (*Doppler effect*), with higher production of $^{239}Pu$(~ 4%) than the uniform one.

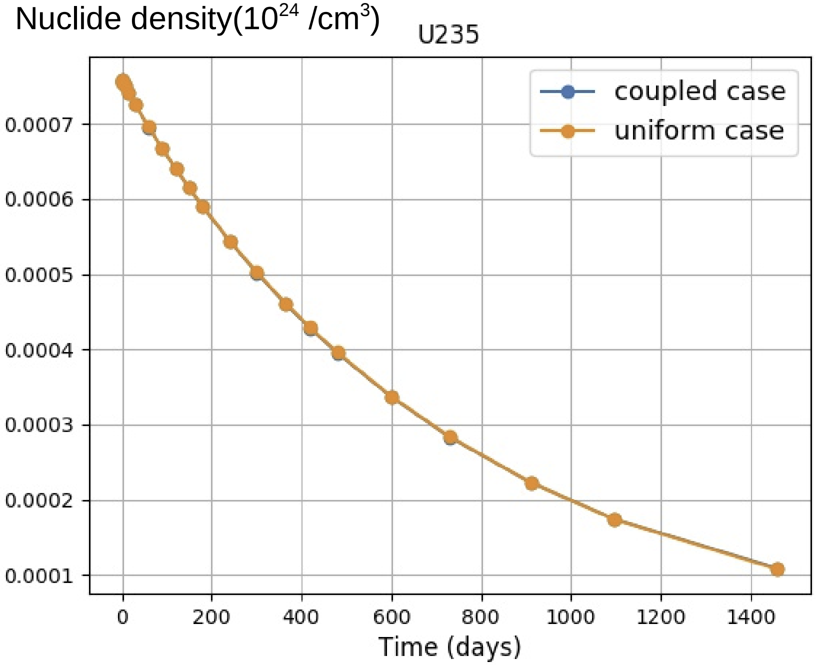
*3 year of burnup*

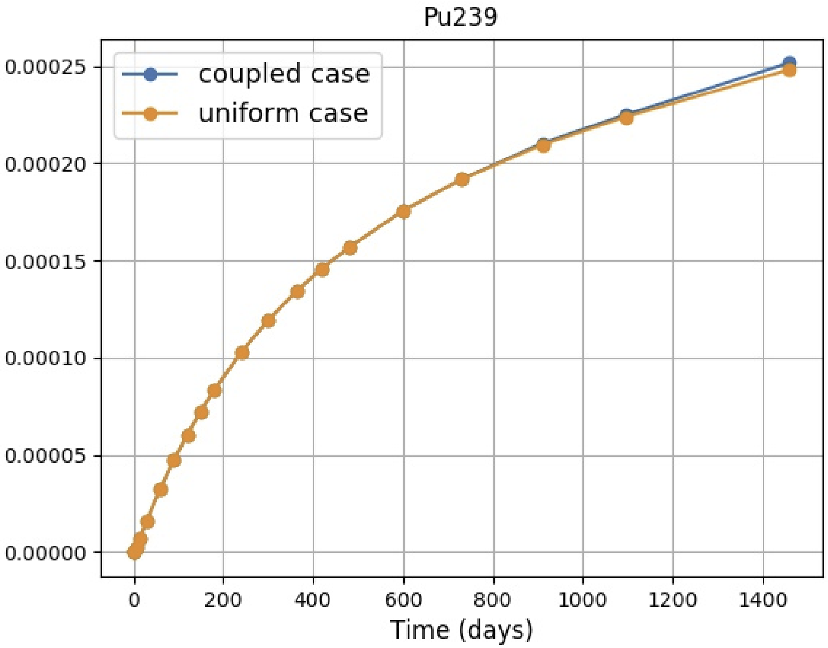


# TIME EVOLUTION OF NUCLIDE DENSITY

Nuclide density($10^{24}$ /cm$^3$)




After 4 years, % variations of global nuclide density* between *coupled* and *uniform* case are 1.0 % for $^{235}U$ and 1.4 % $^{239}Pu$, with relative statistical uncertainties <0.01%

(*) mean over the 50 BU zones

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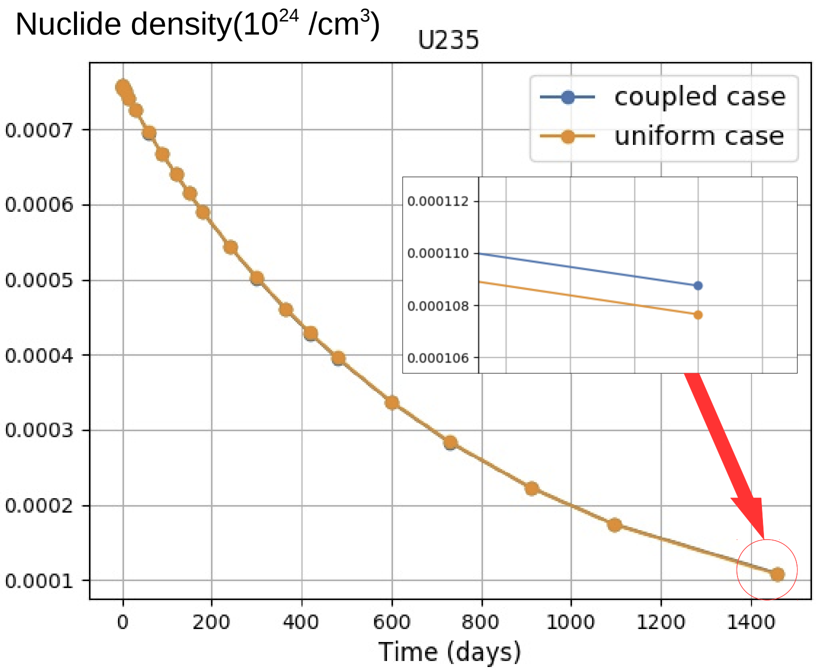


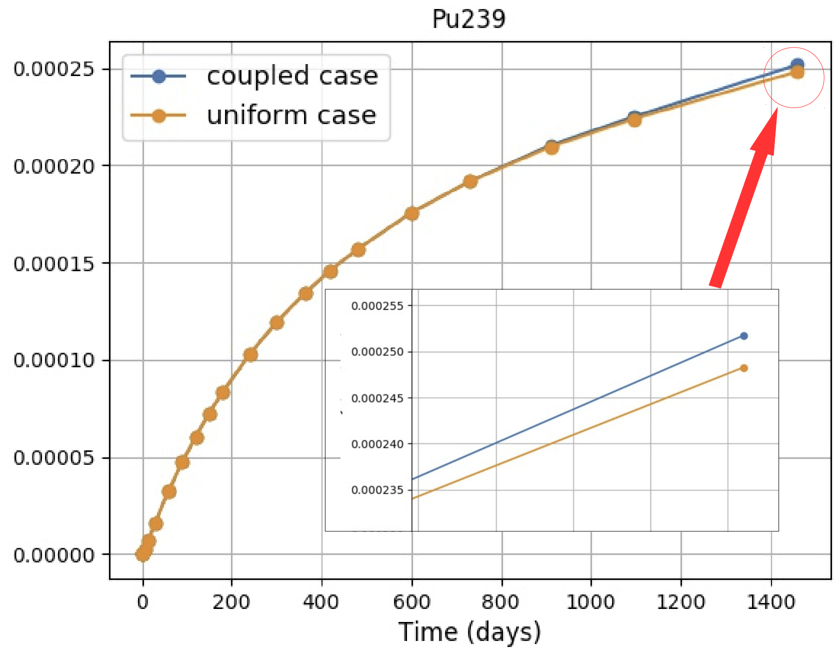


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# CONCLUSIONS

- We developed a multi-physics coupling to obtain accurate simulations for the fuel burnup. Preliminary tested on a fuel pin divided in 50 BU zones

- Temperature and density profile of the fuel and the coolant influence the axial profile of the neutron flux and fission rate distribution at different time steps

**COUPLED VS UNIFORM (CLASSICAL) SIMULATIONS**

- Along the axial direction, variation >5 % for $^{235}U$ density with asymmetric consumption (coupled case).
- Along the radial direction, variation ~ 4% for $^{239}Pu$ density, due to the increase of the resonance absorption by $^{238}U$ at the center of the fuel pin (coupled case)
- Global effect on fuel consumption of the order ~ 1 % for $^{235}U$ and $^{239}Pu$

**IN FUTURE WORKS:**

- Extension of the multi-physics modelling to a fuel assembly geometry
- Benchmark analysis with experimental data

# THANKS FOR YOUR ATTENTION!

# BACKUP SLIDES

# Fission fraction and neutrino flux

The fission fraction uncertainty is an indispensable part of the prediction of antineutrino flux of reactor neutrino experiments, especially absolute measurement experiments that use a single detector.

$$S(E_\nu) = \frac{W_{\mathrm{th}}}{\sum_i f_i E_i} \sum_i f_i S_i(E_\nu)$$

$W_{th}$ is the thermal power of the reactor, $E_i$ is the energy released per fission per isotope *i*, f*i* is the fission fraction of the isotope, S*i*(E) is the antineutrino energy spectrum of isotope *i*, which is normalized to one fission.

$^{235}\mathrm{U}$

$^{239}\mathrm{Pu}$

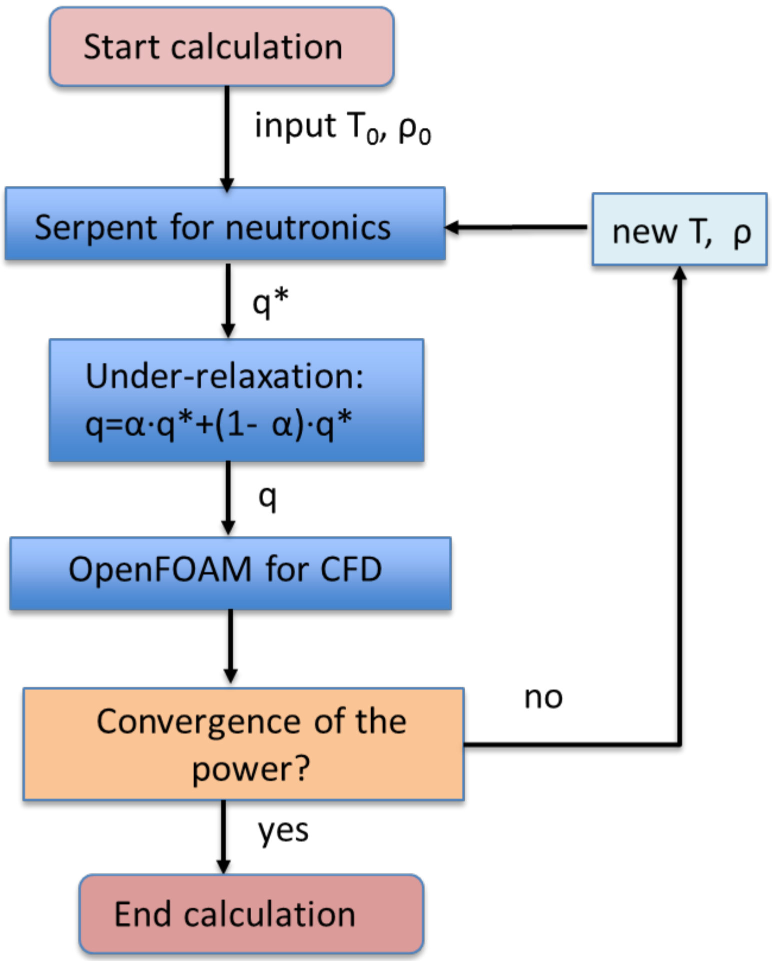
$^{241}\mathrm{Pu}$

# Coupling Code Technique (CCT)

- **Serpent implements a Multi-Physics Interface** to include temperature and densities from OpenFOAM. This could be done because Serpent calculates **cross sections at different temperatures** from the interpolation of the cross section loaded
- **External coupling** by a wrapper script that launches Serpent and OF
- The convergence of the power is stabilized by an under-relaxation step:

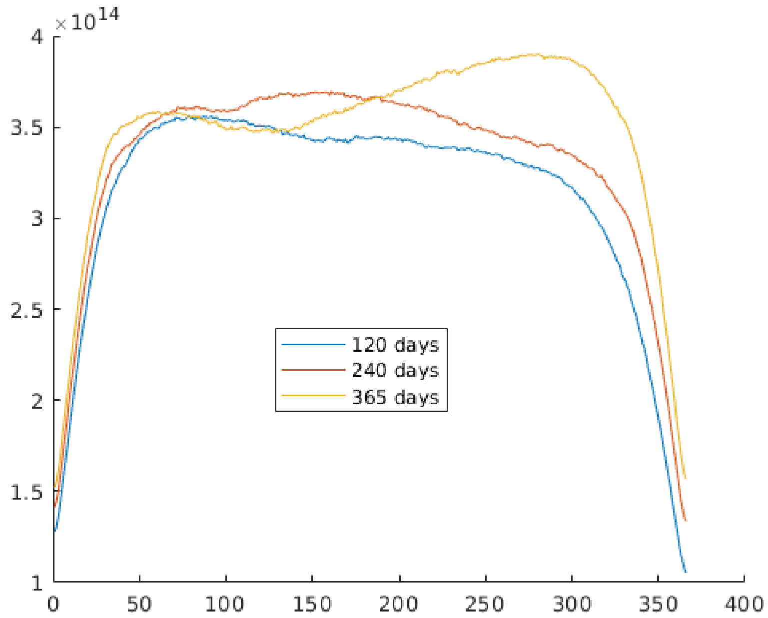
$$q=\alpha\cdot q^{*}+(1-\alpha)\cdot q^{*} \qquad 0<\alpha<1$$

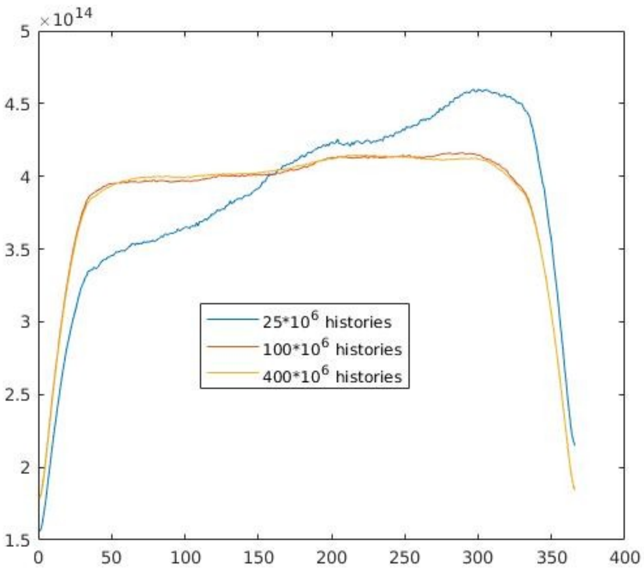
T=temperature, ρ=density, q=local power



# TRANSPORT CALCULATION

-Run with Serpent *restart file* because SIE **do not** generate results from transport calculation
-The instability persists and the calculation needs the increase of neutron histories → increase the number of histories until 200 *$10^8$ of histories



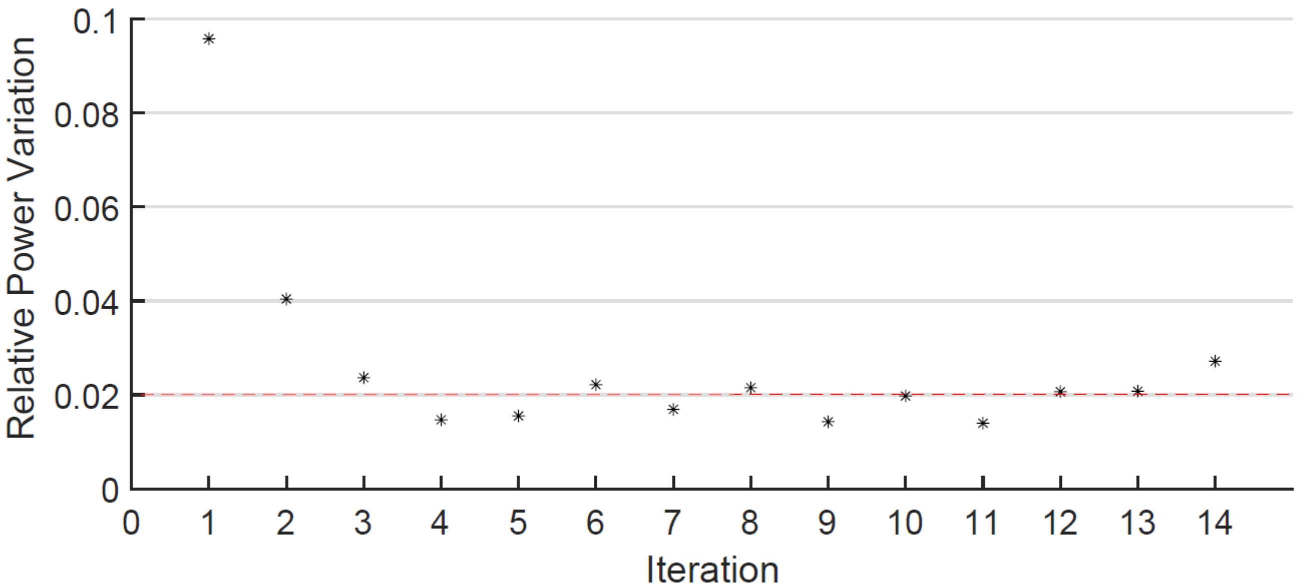



# Test Case: Convergence

In the test case, after 3 iterations, the relative power variation **oscillates around a percentage value of ~2%.** It does not decrease because of the statistical fluctuation of the Monte Carlo method.

To obtain further decrease $C_{\%}$ → Increase number particle histories

For the purpose of this work, the **convergence is reached**.



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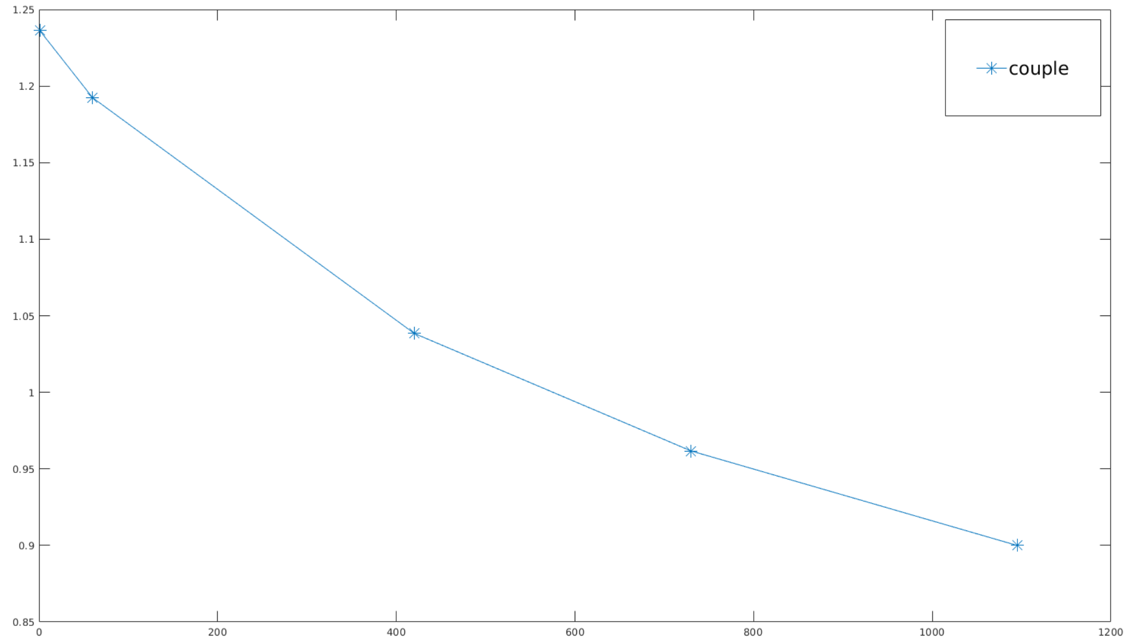
$$^{235}\mathrm{U}$$
$$^{239}\mathrm{Pu}$$
$$^{241}\mathrm{Pu}$$

# KEFF VARIATION

$k_{eff}$=1.24573±0.00025 for fresh fuel



# Density of the water

$$\rho = c_0 + c_1 T$$

$$\rho\left[\mathrm{kg\,m^{-3}}\right] = 2119.3844 - 2.42865 \times T[K]$$

Data from IAPWS: International Association for the Properties of the Water an Steam