Advanced Multi-Physics simulations for Burnup Analysis

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collaboration between
the **Nuclear Reactors Group, Politecnico di Milano**
and the **INFN Milano-Bicocca Group**

Outline

1. Introduction
2. Multi-Physics Modelling
3. Reduce Order Methods for Burnup Analysis
4. Conclusions

Introduction

- Determination of **reactor antineutrino spectrum** is mandatory for detector oscillation experiments, like JUNO.
  The **computational modelling of nuclear reactors** is an useful tool to simulate nuclear systems and predict antineutrino flux from fission fractions.

- Because the antineutrino spectrum changes over the time, **fuel burnup analysis** is needed in reactor simulations.

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 for Fuel Burnup

To **reach a high level of accuracy** in the modelling, it is important to **simulate the different "physics"** of a nuclear reactor, i.e. **neutronics** and **Thermal-Hydraulics (T-H)**, taking into account the **mutual feedback** between them.

Multi-Physics (MP) approach

Applying the **MP modelling for burnup calculations** is a **challenging task:**

- **high computational cost**
- **numerical instabilities**
- **lack of systematic studies.**

MP-Burnup Activities

Our activities…

1. Investigation of local and global effect of MP in fuel burnup, for a PWR fuel pin (**update from JUNO-Italia meeting 2018**)

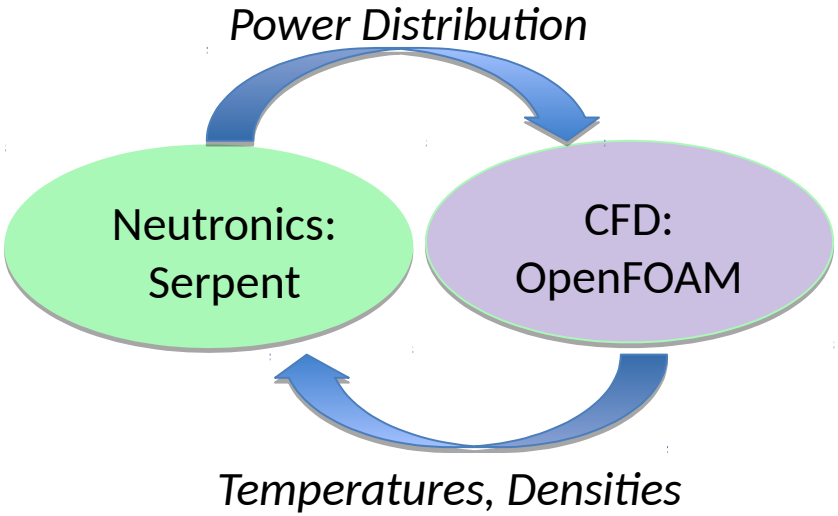
2. Development of numerical methods, **Reduce Order Methods (ROM), to decrease the computational cost** of burnup simulations in PWR.

Coupling Neutronics/T-H

- We developed a MP approach, based on the coupling between **Serpent Monte Carlo code (neutronics)** and the **OpenFOAM toolkit (T-H)**

- Serpent and OpenFOAM **run separately**, the process of data and variables are passed between them until the **convergence of the power**

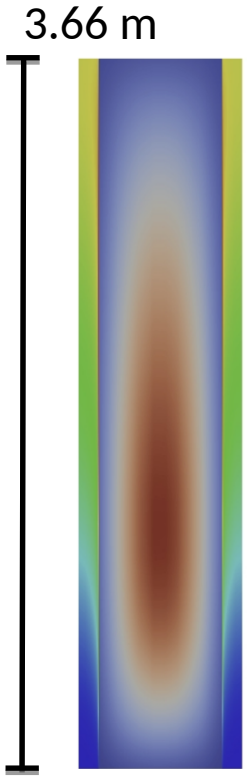
- **Serpent implements an interface** to include temperature and densities from OpenFOAM.



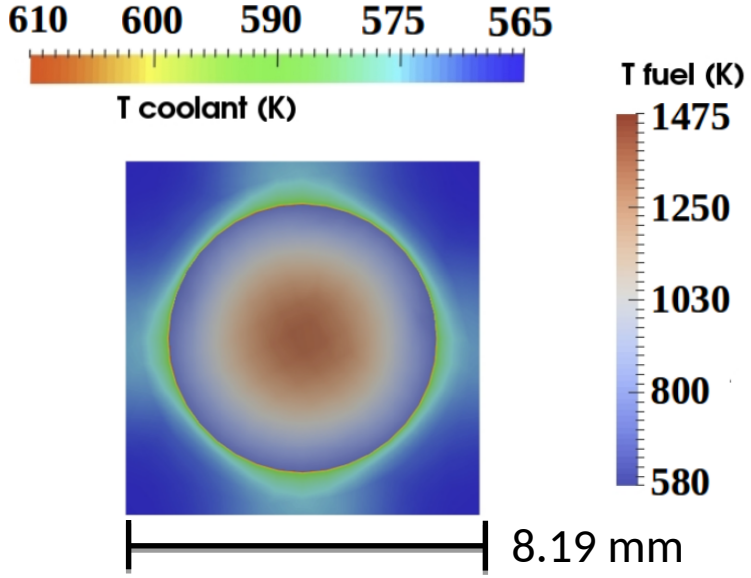
PWR Fuel pin

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: 65 kW
- Density: 10.45 g/cm^3
- Enrichment: 3.2% ^{235}U
- 30 cm of axial reflectors made by **mixture of stainless steel and water (not only water)**



Vertical and horizontal sections of fuel pin, taken by the mesh-plot of temperature distribution in OpenFOAM.



BURNUP ANALYSIS

We compare the results of burnup simulations until 1 year, in which neutronics and thermal-hydraulics are coupled (*coupled* case) with the ones from a non-coupled simulation (*uniform* case).

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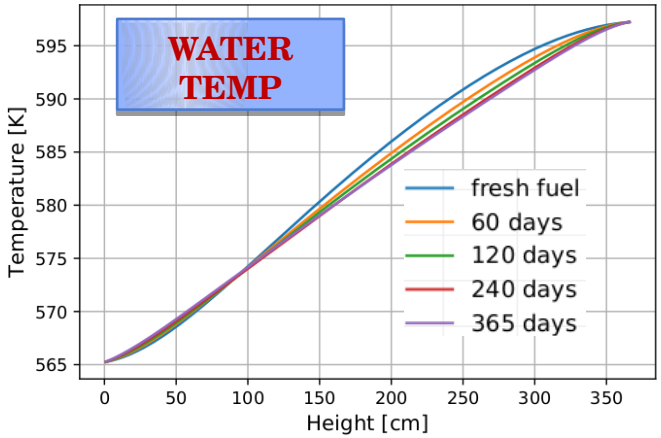
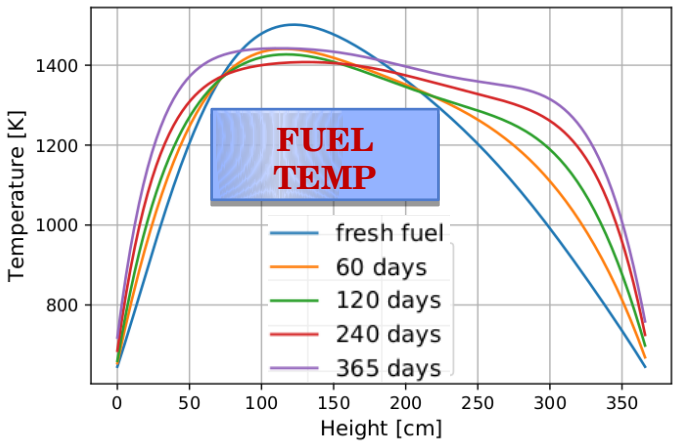
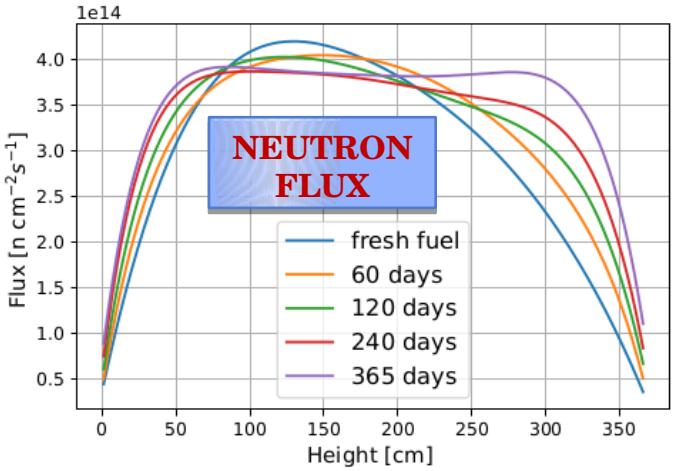
- The fuel pin is subdivided in 90 depletion zones (5 radial × 18 axial)
- In the *coupled* case, **temperature and density** distributions are calculated at **fresh fuel** and *updated* at **60, 120, 240 and 365days**.
- In the *uniform* case, T_{WATER} = 585 K, T_{FUEL}=895 K , ρ_{WATER} = 703 kg/m
- 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

T-H FEEDBACK DURING FUEL BURNUP

After the convergence of the MP coupling at different time steps, we obtain the distribution of **temperatures and neutron flux** along 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.

Over the time, fuel temperature and neutron flux flatten out, because of the fuel consumption.

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JUNO-Italia, INFN Ferrara,
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Nuclear Reactors Group

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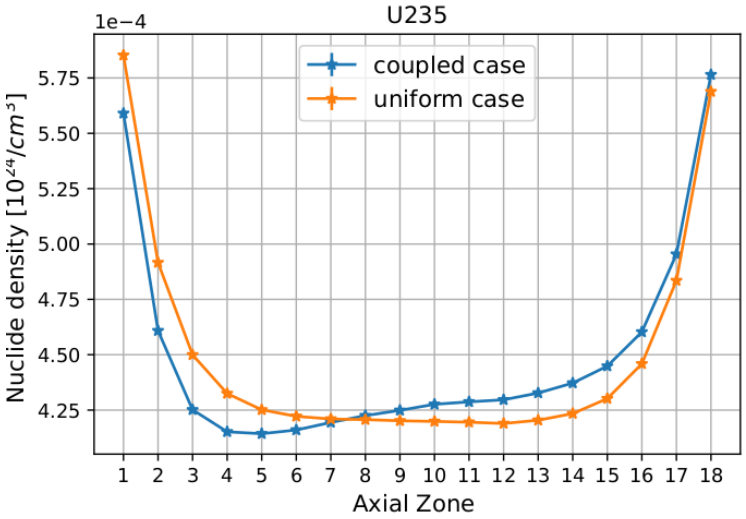
RESULTS: LOCAL EFFECTS

By the comparison with uniform temperature approach:

- **Local differences** of fissile nuclide densities until **> 5 %**, after 1 year of burnup



NEXT STEP: EXTENSION TO FA AND FULL CORE

CRITICAL POINTS OF BURNUP SIMULATIONS

The most critical aspect is the **high computational** cost of burnup simulations:

- **Burnup itself: Monte Carlo** calculations (neutronics), estimation of nuclide density from solution of **Bateman equation** (memory req.)
- **MP Coupling**: calculation of **cross sections at different temperatures** (neutronics), **CFD** simulation (thermal-hydraulics)

The issue gets **worse for assembly and full core** calculations.

PROPOSED SOLUTION

- Development of **Reduce Order Modelling (ROM)** to reduce computation of burnup (new for burnup, **presented here**)
- Adoption of **porous media approach for TH**, instead of CFD (literature, **under development** at PoliMi)

REDUCE ORDER METHODS (ROM)

- The goal of a **ROM method** is to **capture the essential features** of the behaviour of a system in a reliable way by **improving computational performance**

- The assumption is that the **behaviour of a system** can be well described **by a small number of dominant modes**. Historically, the earliest attempt of a reduction strategy is the truncated Fourier series (1806).

- These methods are **applied successfully in several fields**, from aerospace and mechanical engineering, to life science

REDUCE ORDER METHODS FOR FUEL BURNUP

- **Let consider burnup calculation for a single region**, we solve the **Bateman equation**:

$$\boldsymbol{n}' = \boldsymbol{A}\boldsymbol{n} \quad , \quad \boldsymbol{n}(0) = \boldsymbol{n}_0$$

$\boldsymbol{n}(t) \in \mathbb{R}^n$ = nuclide concentration vector

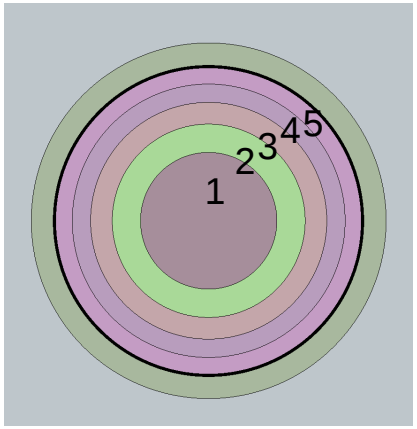
$\boldsymbol{A} \in \mathbb{R}^{n \times n}$ = burnup matrix containing the decay and transmutation coefficients of the nuclides under consideration.

- In a **full core calculation, burnup of 10^4-10^6 regions requests hundreds of GB for RAM**: memory problem

- The idea for **ROM is the restriction of the calculation to 10-10^2 virtual regions**, which represent the **basis vectors** to reconstruct the compositions of all 10^4-10^6 *real regions*

APPLICATION OF ROM METHOD TO FUEL BURNUP

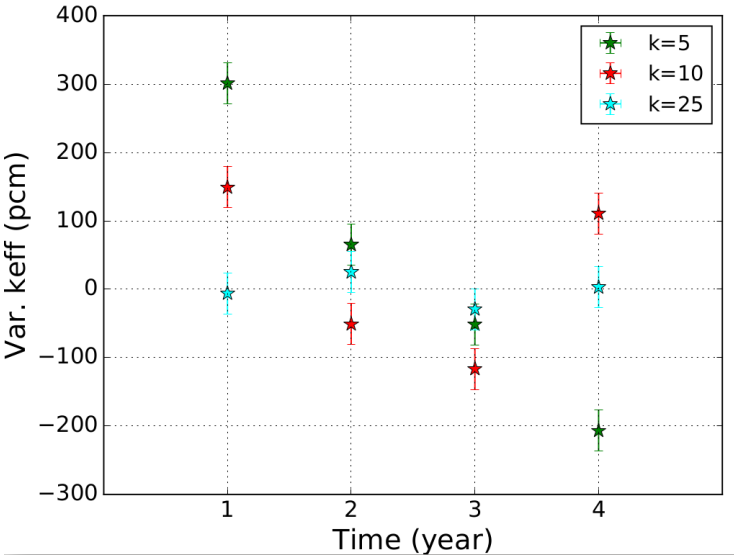
- We are testing the ROM for fuel burnup. At the beginning, we start with **standard** calculation to the case of TMI-1 PWR unit cell
- 2D simulations of 5 burnup regions for 5 power level→ **total 25 BU regions**
- 4 years of burnup with time steps of 30 days→ **Full Order (FO)** model



Radial section of TMI-1 PWR unit cell, with 5 BU regions, taken by geometrical plot of Serpent

RECONSTRUCTION OF NUCLIDE CONCENTRATION FROM BASIS VECTOR (NO BURNUP)

- **From ROM***, we get **5, 10 and 25 basis (virtual materials)**
- **Verification**: we **run criticality (NO BURNUP) calculations with real materials reconstruced** from linear combination of **5, 10 and 25 basis** at different time steps
- **Verification**: accuracy of **keff increases with the level of approximation**. Variation **10-10^2 pcm, respect to keff not approximated** ($2\sigma \approx 30$pcm)



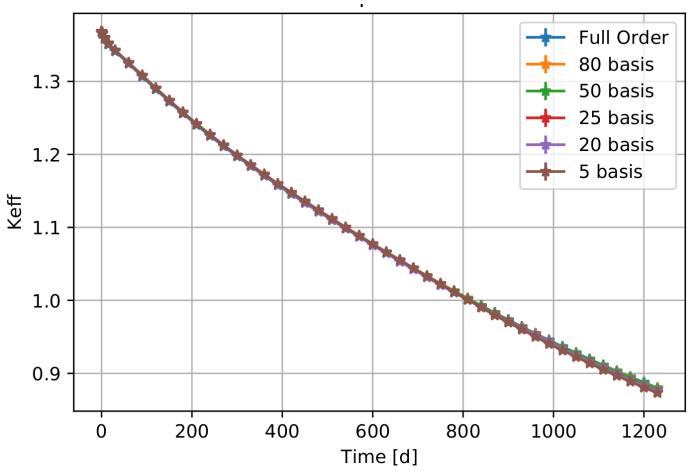
$\Delta k_{eff} = [Keff - Keff_{approx}]_{pcm}$

Difference (pcm) of the multiplication factor between full order and reduce order simulations (reconstruction with approx)

*adoption Singular Value Decomposition (SVD)

PRELIMINARY RESULTS: REDUCE ORDER MODELLING FOR BURNUP

- **Run *reduce order burnup* calculations with the first 80, 50, 25, 10 and 5 basis vectors for burnup matrixes**
- **Decrease of criticality** over time is correctly reproduced by ROM. **Differences** with full order keff (not approx.) of the order of **10-10^2 pcm** ($2\sigma \approx 30$pcm)



- Relative variation of **<1 % for U-238 and few % for U-235,** in case with 5, 20, 25, 50 and 80 basis

Preliminary verification of the methodological approach

CONCLUSION

- Developed MP coupling Serpent/OpenFOAM for 3D burnup calculations with multi regions, able to described local and global effects
- The improvement of the accuracy of burnup simulations (MP, multi-regions) increases the computational cost→ issue for full core calculations
- Ongoing activity: implementation of Reduce Order Methods for burnup analysis.
- The philosophy is to burn few virtual materials to reconstruct the inventory for many real materials.
    - Verification for criticality calculations
    - Preliminary verification for burnup calculations

BACKUP SLIDES

RECONSTRUCTION OF NUCLIDE CONCENTRATION FROM BASIS VECTOR (NO BURNUP)

- From Full Order (FO) calculations, we get a **nuclide inventory** represented by a matrix **M of 1555 (nuclides)* 1325 (5 regions*5 power level*53 time steps)**

$$M=\sum_{i=1}^{1325} \sigma_i v_i^t u_i$$

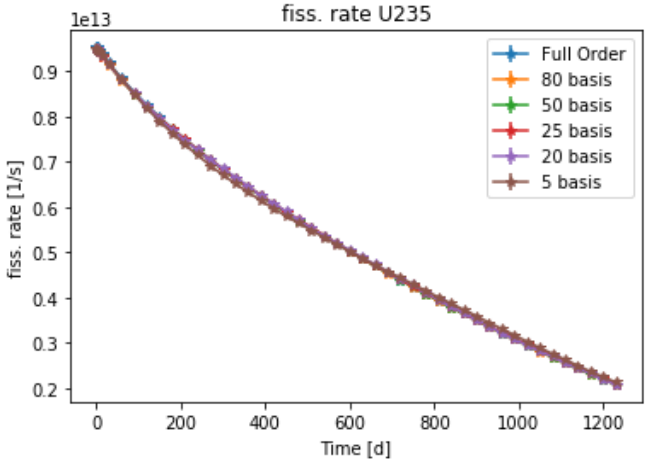
- M is decomposed* in a finite sum of 1325 vector basis **material (virtual)**.
  The **k-th truncation is the level of approximation adopted (k=25, k=10, k=5)** to reconstruct the compositions of **real materials**:

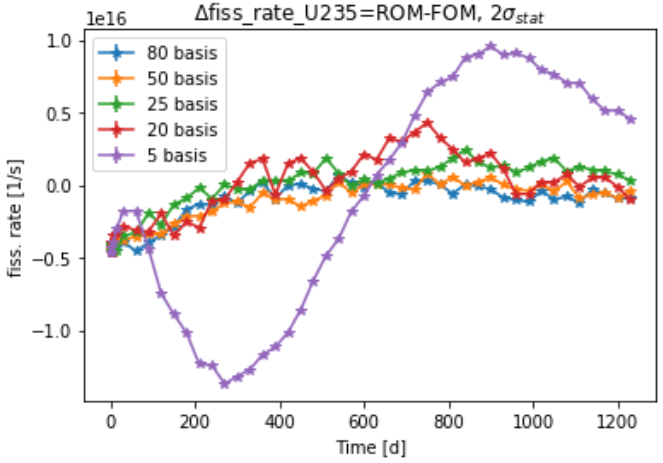
$$M_k=\sum_{i=1}^{k} \sigma_i v_i^t u_i \quad \textbf{[k=25, k=10, k=5]}$$

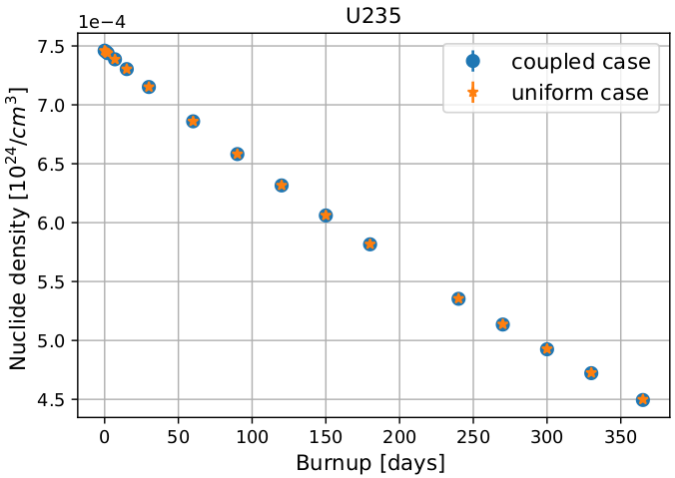
*SVD decomposition of linear algebra

Simulation	Time
Burnup Uniform Case Serpent	30 min.
Burnup Coupled Case Serpent	60 min.
Coupling iteration Serpent (criticality)	25 min.
Coupling iteration OpenFOAM	15 min.

FISS. RATE U-235






U235
1e−4
coupled case
uniform case
Nuclide density [$10^{24}/cm^3$]
Burnup [days]
7.5
7.0
6.5
6.0
5.5
5.0
4.5
0
50
100
150
200
250
300
350