PREDICTION OF MACROSCOPIC CROSS-SECTIONS FOR COUPLED NEUTRONICS-T/H ANALYSIS

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Introduction

- **Monte Carlo** (MC) codes are widely used for the accurate modelization of nuclear reactors. However, the efficient inclusion of the thermal-hydraulic (TH) feedback within the MC calculation sequence is still an open problem.

- How can we perform coupled **MC-TH**?
  - Picard Iteration (PI)
  - Quasi-Newton's Method (QNM)
  - Modified PI, based on predictor-corrector (MPI)

- We propose a new prediction block for the MPI:
  - Cross-sections predicted with perturbation theory
  - Power obtained through fast deterministic solver

Picard Iteration

- Relaxation factors based on Robbins-Monro's stochastic approximation [1]:

$$P_1 = \left(1 - \frac{1}{n}\right) P_0 + \frac{1}{n} P_1^*.$$

- Benefits and drawbacks:
  - Easy to implement
  - Slow convergence

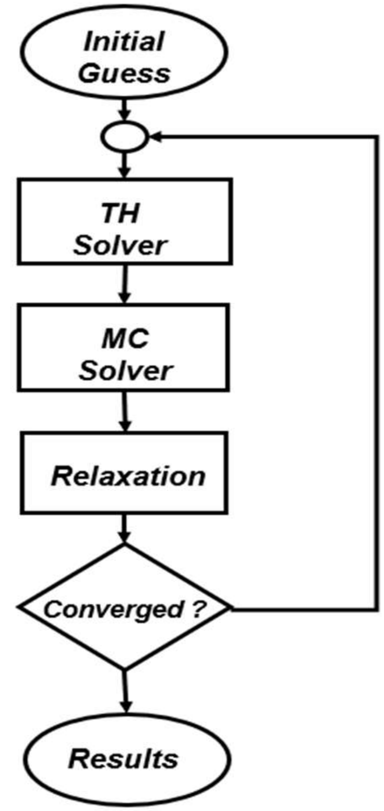

Fig 1. Picard Iteration for MC-TH coupling

Modified Picard Iteration

- A prediction block is added to obtain a better guess of power distribution, therefore enhancing the convergence rate of the whole algorithm. [2]

- The same logics can be applied with a batch-by-batch logics.

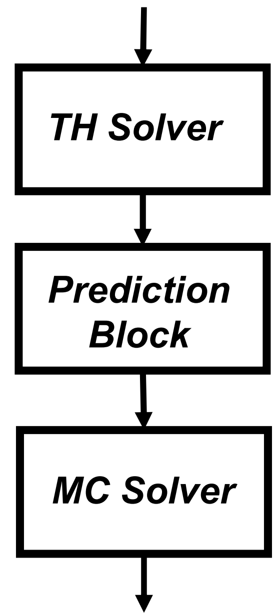

Fig 2. Modified Picard Iteration for MC-TH coupling

Prediction Block

- Prediction block composed by three repeated stages:
  - Cross-Sections Predictor
  - Nodal Power Solver
  - TH calculation

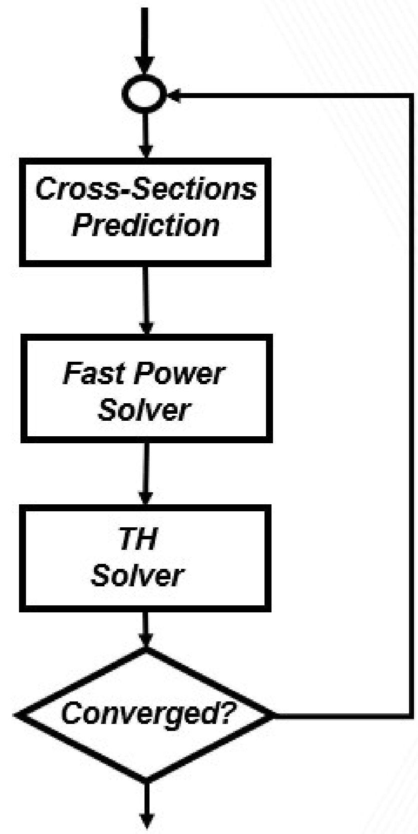

Fig 3. Prediction Block.

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Prediction of Cross-sections

- Nodal MG macroscopic cross-sections are generated for many points in the operational space, *i.e.*, **branching calculations**.
- Interpolation is used to reconstruct the cross-sections from known points.
- **Issues** with branching**:**
  - Pre-generation phase
  - Usually 2D generation

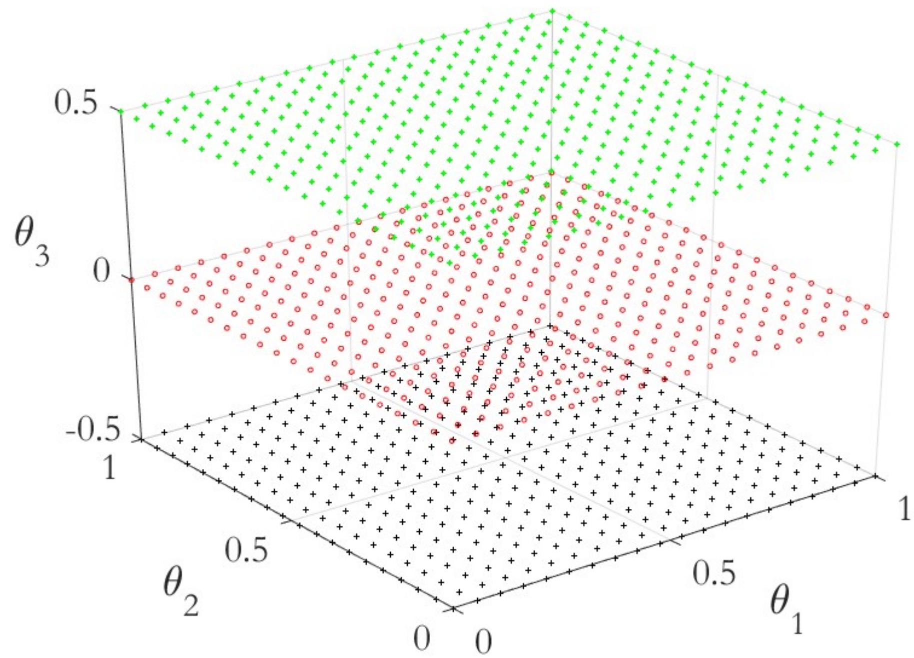

Fig. 4. Rectilinear Grid for Normalized Variables $\theta_1, \theta_2, \theta_3$

Expansion of T/H fields

- **New method:**
  - No pre-generation phase
  - It accounts for 3D effects

- Based on calculation of **generalized transfer functions (GTF)** to map variation in TH spatial distributions on cross-sections fields

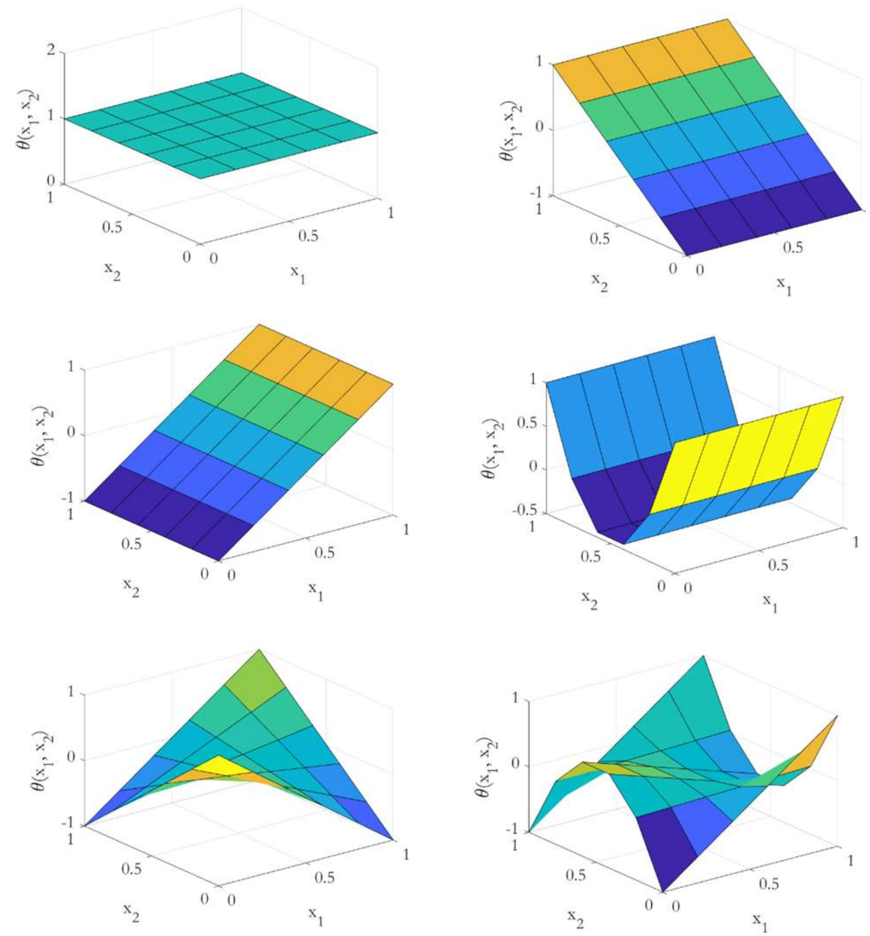

Fig. 5. Example of spatial basis functions for $\theta_i(x_1, x_2)$

Generalized Transfer Function (GTF)

$$\boldsymbol{\rho}(\boldsymbol{x}) \Longrightarrow \boxed{\boldsymbol{H}} \Longrightarrow \boldsymbol{\Sigma}(\boldsymbol{x})$$

- The input density is projected on a suitable basis set, based on TH-computed profiles.

$$\rho(x) = \sum_n \rho^{(n)} \psi_n(x)$$

$$\widetilde{H}(\nu, \rho) = \frac{\sum_n [\rho^{(n)} \tilde{\Sigma}_n(\nu)]}{\tilde{\rho}(\nu)}$$

FFT-based Approximation

$$\boldsymbol{\rho}(\boldsymbol{x}) \Rightarrow \boxed{\boldsymbol{H}} \Rightarrow \boldsymbol{\Sigma}(\boldsymbol{x})$$

- If the change is limited, ψ_n are close enough and the transfer function can be approximated by the following relation:

$$\widetilde{H} \approx \frac{\tilde{\Sigma}_0}{\tilde{\rho}_0}$$

Prediction of Power

- The power is predicted using perturbation theory:

$$\delta\psi_0 = \sum_{m=1}^{N} a_m \psi_m.$$

$$a_m = \frac{\left\langle \psi_m^\dagger, \delta\mathcal{L}\psi_0 - \lambda\delta\mathcal{M}\psi_0 \right\rangle - \delta\lambda \left\langle \psi_m^\dagger, \mathcal{M}\psi_0 \right\rangle}{\left\langle (\lambda - \lambda_m)\psi_m^\dagger, \mathcal{M}\psi_0 \right\rangle}.$$

- In this work, the flux modes are assumed to coincide with the modes of the fission matrix produced by Serpent. In addition, the simplification $M = \nu\Sigma_f$ and $\mathrm{L} = \Sigma_a$ are introduced [3].

Test Problem

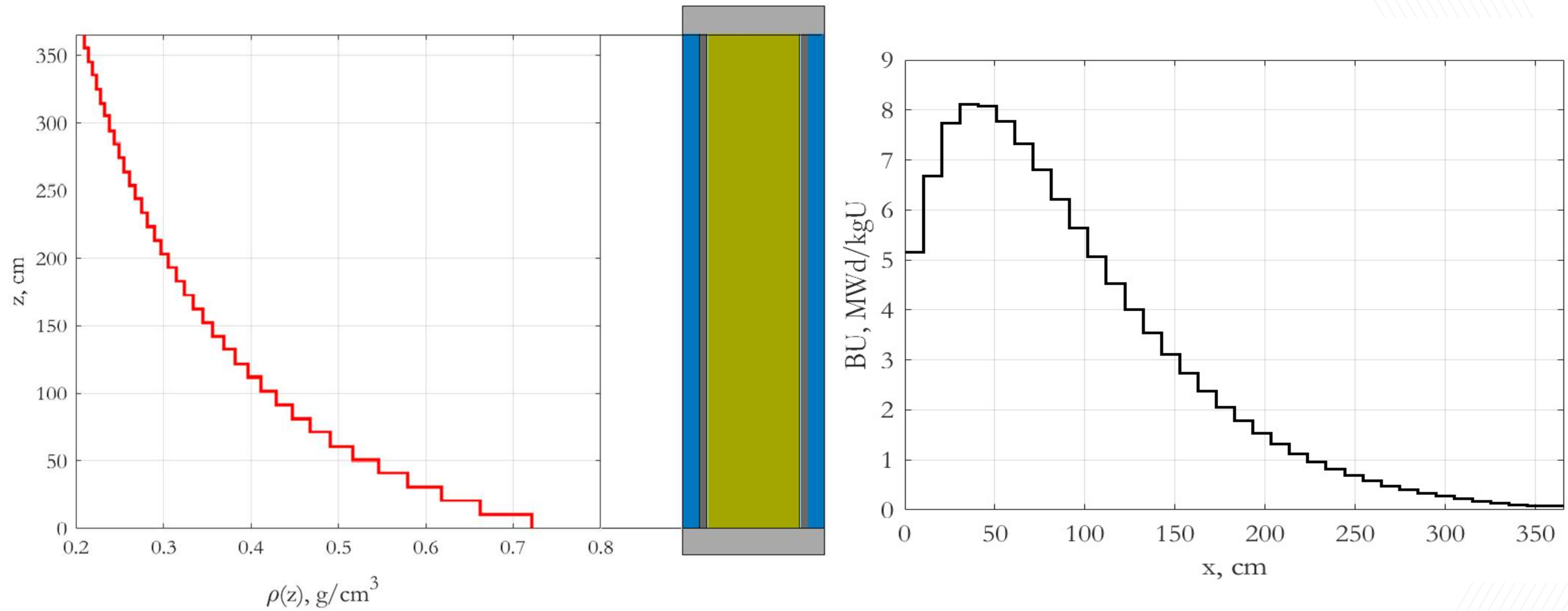

Fig 6. BWR 3D unit cell with realistic density profile and axial reflectors. The same unit-cell is depleted for 3.0 MWd/kgHM.

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Test Problem

- Simplifications:
  - Only the density feedback is considered
  - Uncertainty is not propagated through the calculations

- Computational Environment:
  - Serpent 2.1.30 is used for MC calculations
  - THERMO for TH calculations
  - MATLAB for linkage code
  - MC calculations carried out on a Linux cluster using twenty-eight Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40GHz node,

Reference Solution

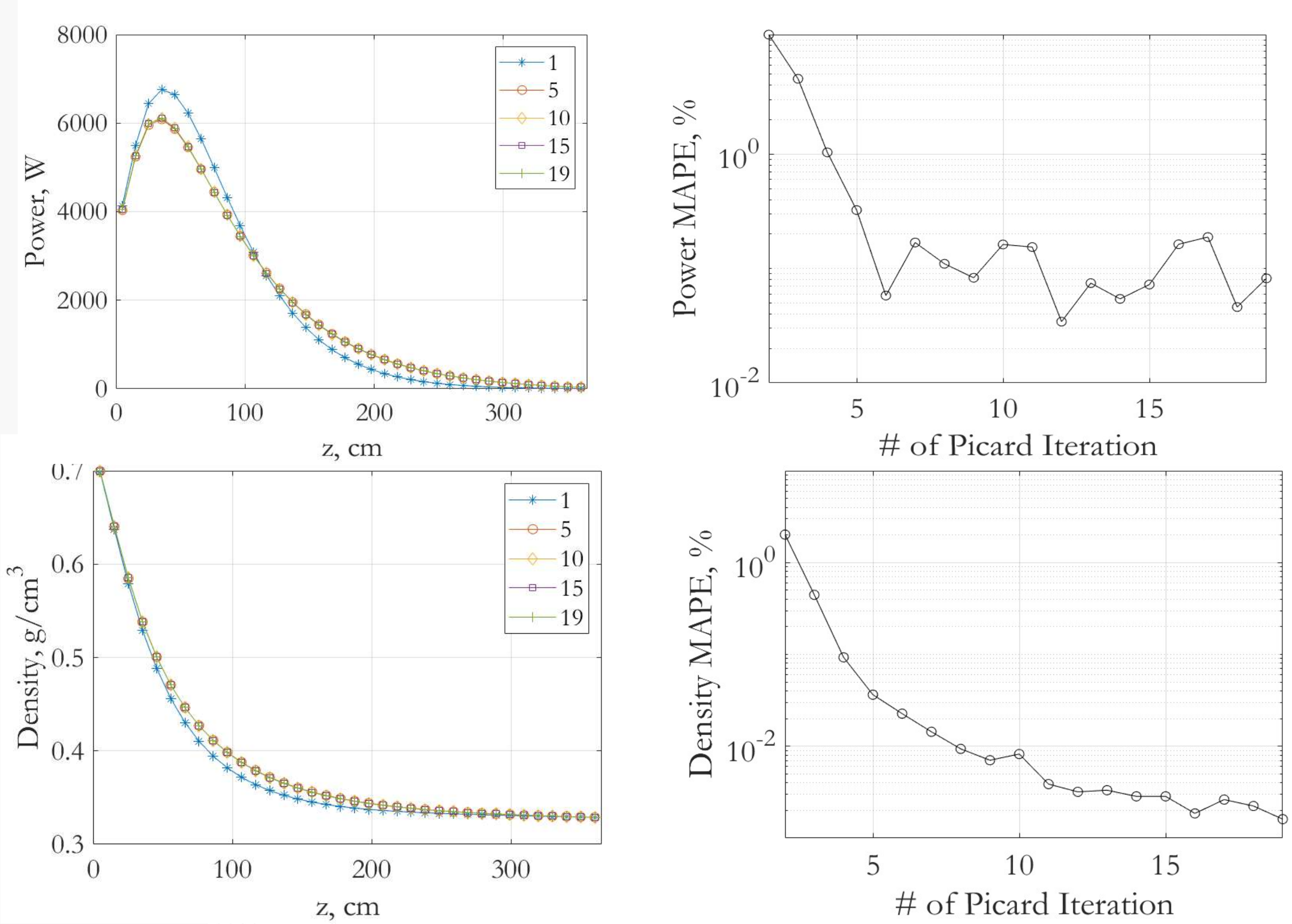

Fig 7. Convergence of power and density as a function of the number of iterations.

Comparison Metrics

- Percentage Absolute Difference:

(1) $$PAD_i^X = \frac{|X_i - \hat{X}_i|}{\hat{X}_i} \times 100.$$

- Mean Average Percentage Error of QoI X:

(2) $$MAPE_X = \frac{1}{N}\sum_{i=0}^{N} PAD_i^X \times 100.$$

Figure of Merit:

(3) $$FOM_X = \frac{MAPE_X}{MAPE_{X_0}}.$$

Power and Density Distribution

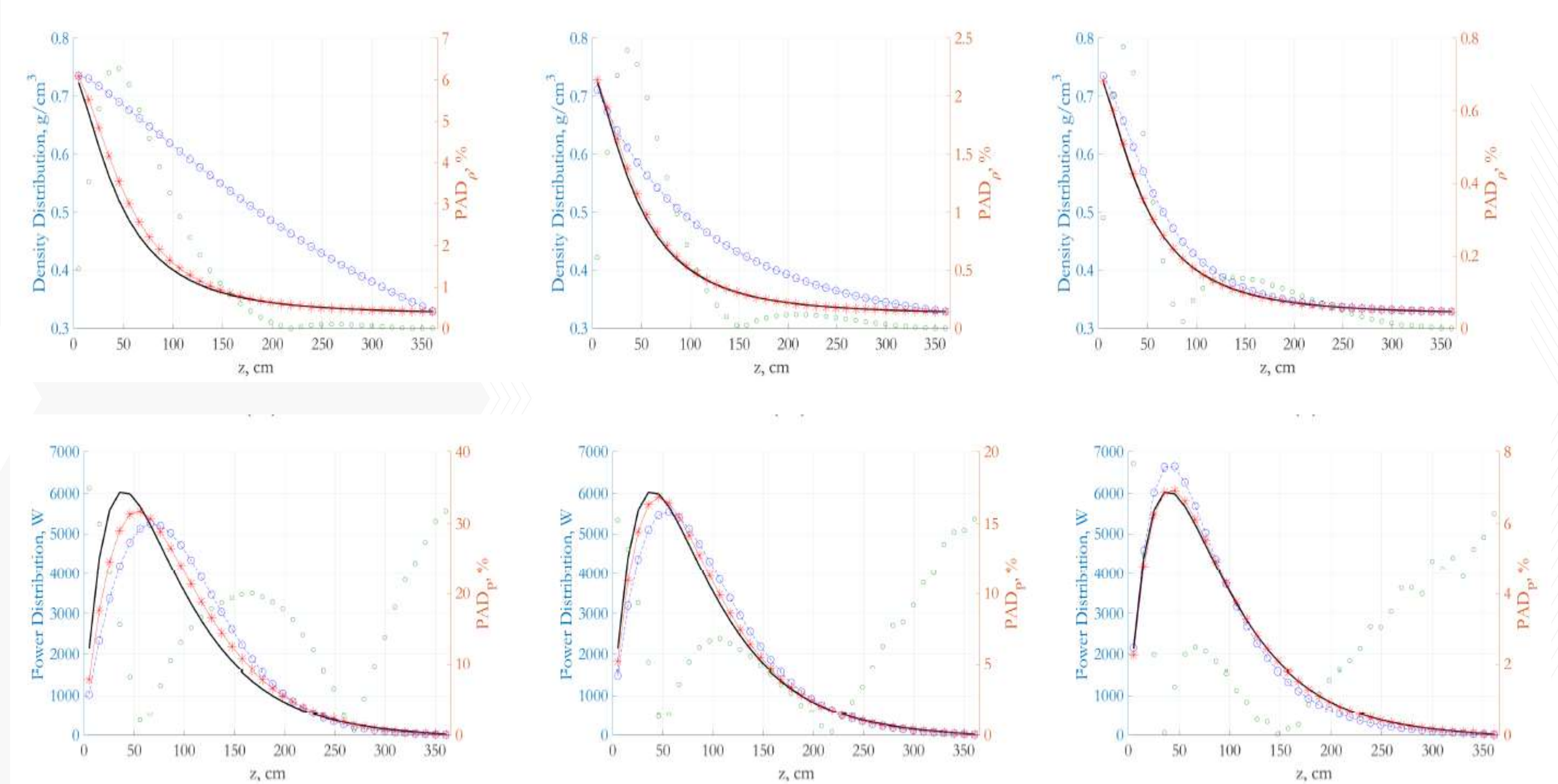

Fig 8. Predicted density and power for different initial density profiles' guess.

Σ_a and $\nu\Sigma_f$

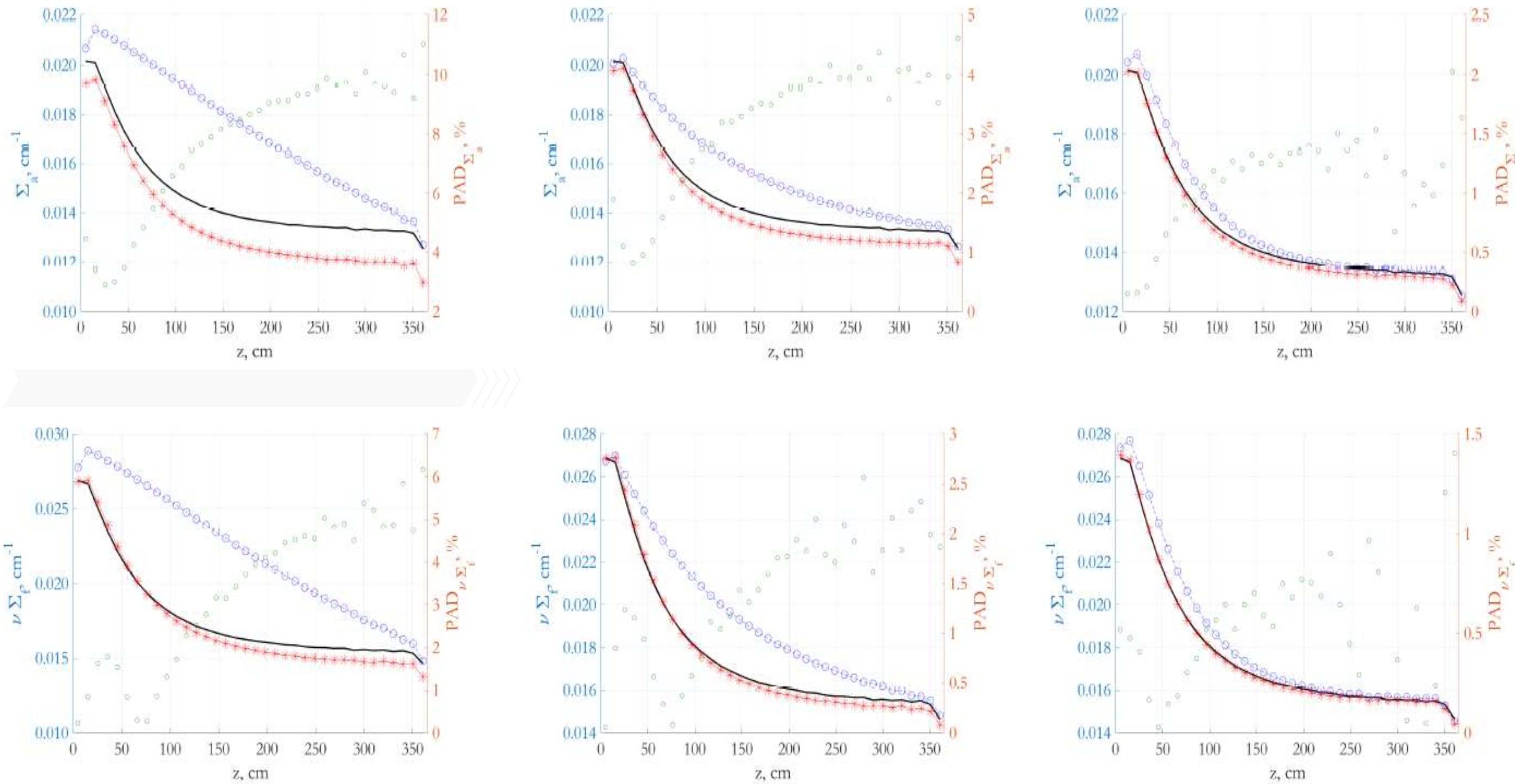

Fig 9. Predicted Σ_a and $\nu\Sigma_f$ for different initial density profiles' guess.

Transfer Functions

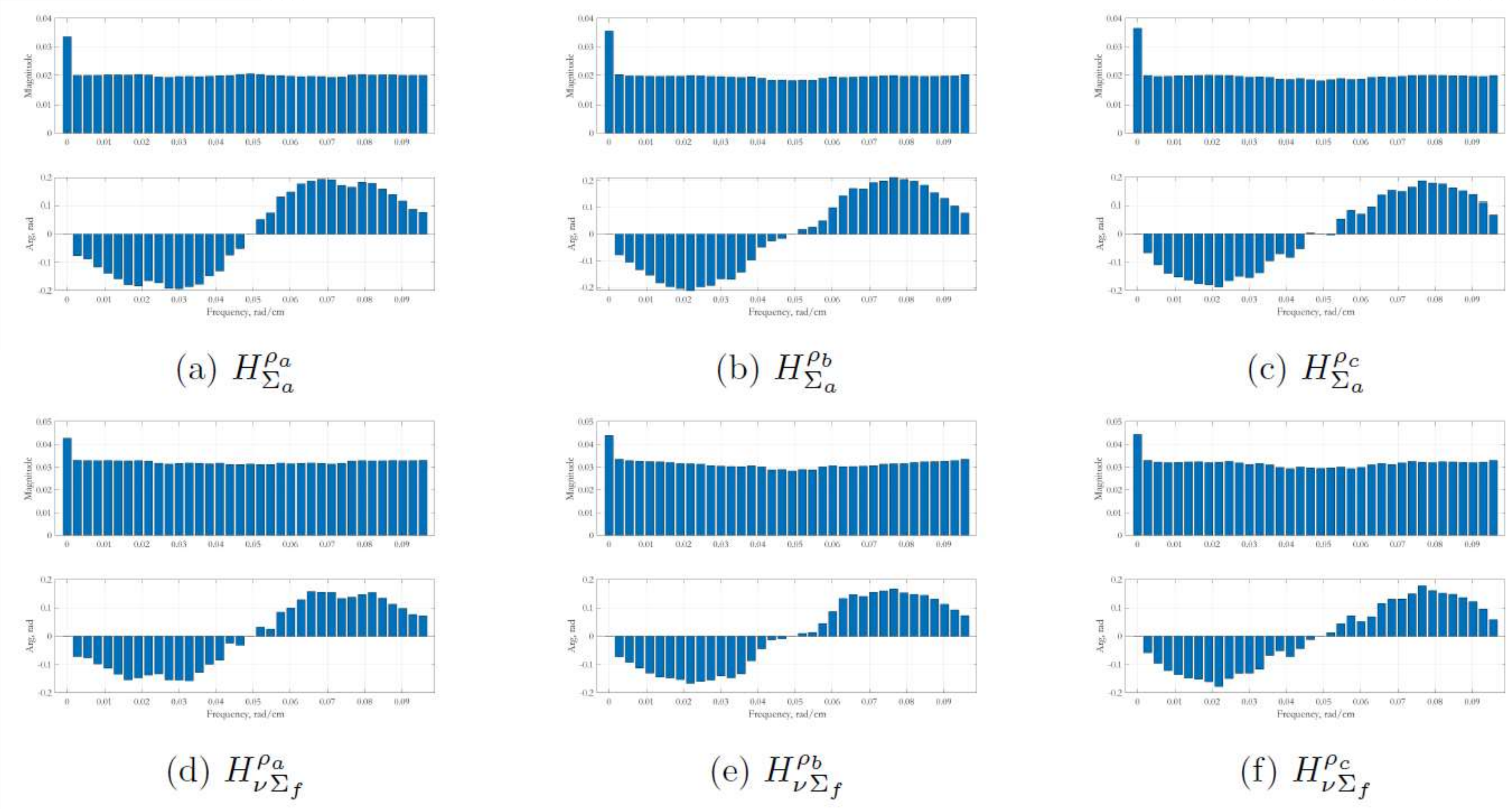

Fig 10. Transfer functions for different initial density profiles' guess.

Power and Density Distribution

Table 1. MAPE for different QoIs for different initial guess.

Parameter/Initial Guess	$H^{\rho_0^{(1)}}$	$H^{\rho_0^{(2)}}$	$H^{\rho_0^{(3)}}$
ρ	1.6076	0.5026	0.1509
Σ_a	7.8030	3.2004	1.1073
$\nu\Sigma_f$	3.3085	1.4260	0.5315
Power	15.9987	6.5554	2.7601

Table 2. FOM for different QoIs for different initial guess.

Parameter/Initial Guess	$H^{\rho_0^{(1)}}$	$H^{\rho_0^{(2)}}$	$H^{\rho_0^{(3)}}$
ρ	5.16e-2	4.50e-2	5.45e-2
Σ_a	4.20e-1	4.66e-1	5.71e-1
$\nu\Sigma_f$	1.32e-1	1.54e-1	2.09e-1
Power	5.12e-1	3.81e-1	1.25e-1

First Results For Heterogeneous Fuel

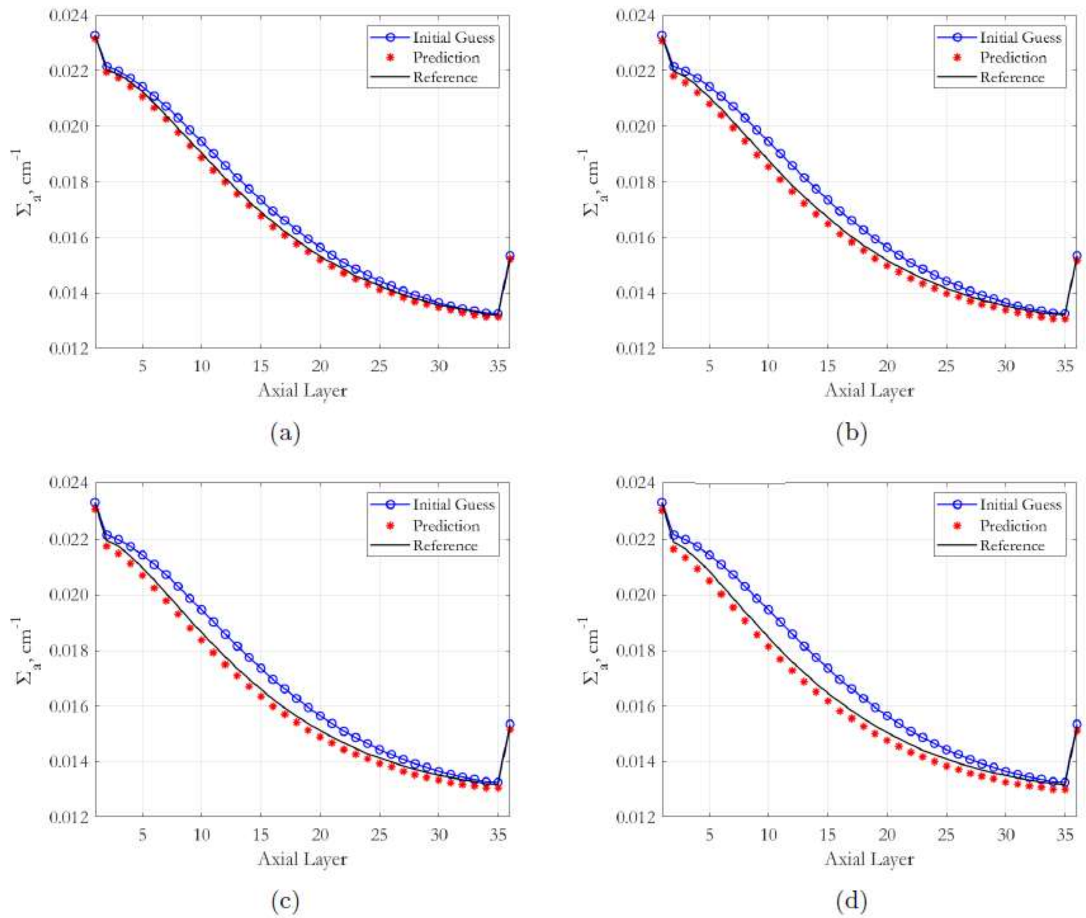

Fig 11. Selected results for depleted BWR unit-cell.

Power and Density Distribution

Table 3. MAPE for different convolution of density profile and transfer functions..

TF/Density	ρ_1	ρ_2	ρ_3	ρ_4	ρ_5
$H_{\rho_1}^{\Sigma_a}$	0.00	0.76	1.18	1.66	1.37
$H_{\rho_2}^{\Sigma_a}$	0.76	0.00	0.43	0.91	0.61
$H_{\rho_3}^{\Sigma_a}$	1.20	0.43	0.00	0.49	0.19
$H_{\rho_4}^{\Sigma_a}$	1.69	0.92	0.49	0.00	0.30
$H_{\rho_5}^{\Sigma_a}$	1.39	0.62	0.19	0.30	0.00

Conclusions

- A new method, called GTF, was introduced for the prediction of the cross-sections variation due to perturbations in the T/H scalar fields.
- A simple FFT-based approximation of the GTF was then obtained and used to formulate a new prediction block to be used in the modified Picard iteration scheme.
- The block was tested against a 3D BWR unit-cell problem showing good agreement with the reference solution.

Ongoing and Future Work

- Considering alternative deterministic power solvers, *e.g.*, diffusion.
- Considering alternatives to FFT, *e.g.*, wavelets.
- Integration into full MC-T/H sequence.

References

[1] Jan Dufek & Waclaw Gudowski (2006) *Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors*, Nuclear Science and Engineering, 152:3, 274-283.

[2] Bryan R. Herman, Benoit Forget, Kord Smith (2015), *Progress toward Monte Carlo–thermal hydraulic coupling using low-order nonlinear diffusion acceleration methods*, Annals of Nuclear Energy, 84, 63-72,

[3] Terlizzi Stefano and Kotlyar Dan (2019), *On-the-fly Prediction of Macroscopic Cross-sections' Spatial Response to TH Perturbations Through Transfer Functions: Theory and First Results,* Nuclear Science and Engineering, DOI: 10.1080/00295639.2019.1698239

QUESTIONS?