

# NON-IDEAL CONVERGENCE OF FISSION MATRIX FUNDAMENTAL EIGEN-PAIR IN MONTE CARLO CALCULATIONS

STEFANO TERLIZZI

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# OUTLINE



## INTRODUCTION

Fission matrix definition and how to obtain it from Serpent 2.1.29.

## CONVERGENCE PROBLEMS

Issues with the convergence of fission matrix fundamental eigen-pairs as a function of the mesh size (*e.g.* Does it exist an optimum value of the mesh-size such that the relative error on both the eigenmode and eigenvalue is minimized?)

## NUMERICAL RESULTS

The convergence of the eigen-pair is investigated.

## CONCLUSIONS AND FUTURE WORK

Answers to questions raised in the convergence problems sections.

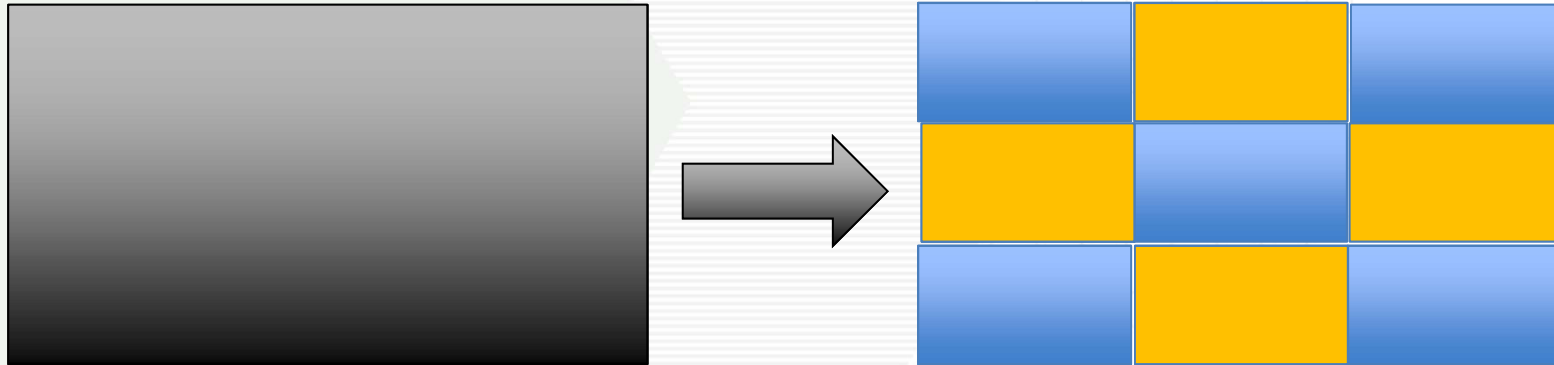


# INTRODUCTION

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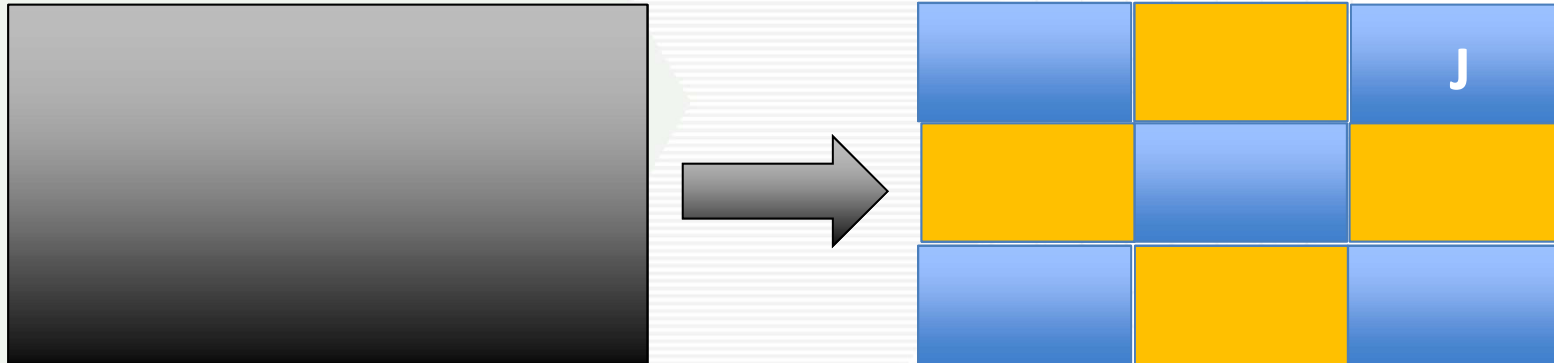
# FISSION MATRIX THEORY FOR CRITICALITY CALCULATIONS

- Domain discretization in non-overlapping cells.
- Every cell must contain fissile/fissionable material.



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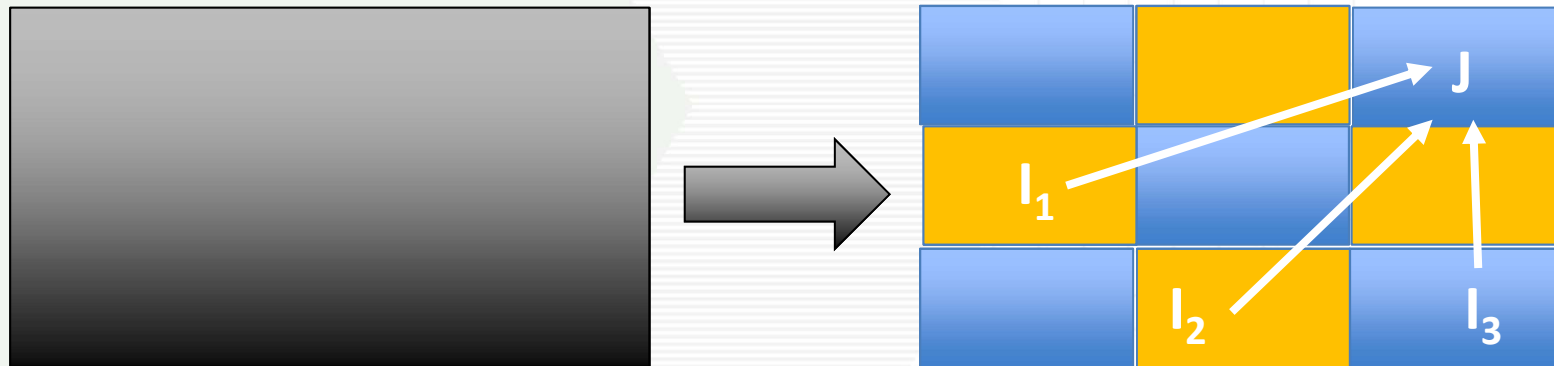
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# FISSION MATRIX THEORY FOR CRITICALITY CALCULATIONS

- Domain discretization in non-overlapping cells.
- Every cell must contain fissile/fissionable material.



(1) 
$$S_j^{(n)} = \frac{1}{k^{(n)}} \sum_{ij} F_{ij}^{(n-1)} S_i^{(n-1)}$$

# FISSION MATRIX THEORY FOR CRITICALITY CALCULATIONS



- The fission matrix element at the  $n^{\text{th}}$  cycle and the corresponding fission source are [1]:

$$(2) \quad \mathbf{F}_{i,j}^{(n)} = \frac{\int_J dr' \int_I dr \hat{\mathbf{F}}(r \rightarrow r') \mathbf{S}^{(n)}(r)}{\int_I \mathbf{S}^{(n)}(r) dr}$$

$$(3) \quad \mathbf{S}_i^{(n)}(r) = \int_I dr \int dE' \nu(r, E') \Sigma_f(r, E') \phi^{(n)}(r, E')$$

# HOW TO GENERATE THE FISSION MATRIX IN SERPENT 2.1.29?



- Fission Matrix (FM) generation is an undocumented feature in Serpent 2.1.29. The Discussion Forum is the only source of information [2].



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IN PRACTICE ...

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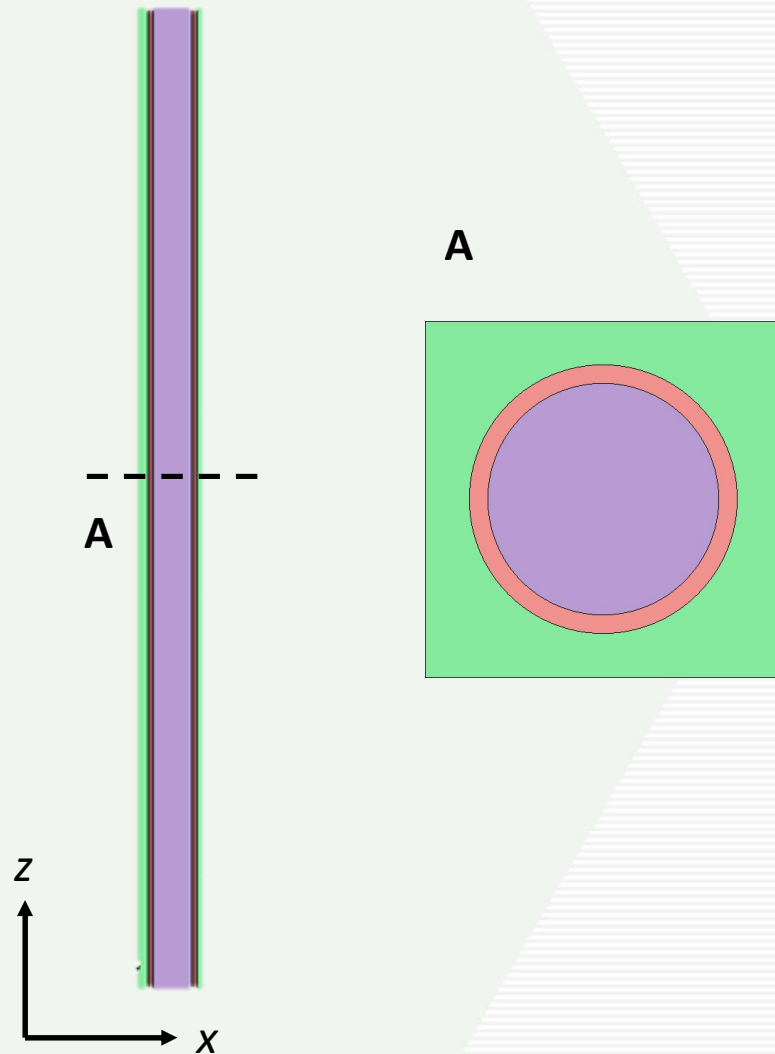
## IN PRACTICE

- The following line must be added to the input file to generate the FM:

```
set fmtx <type> <keyword1> <keyword2> ...
```

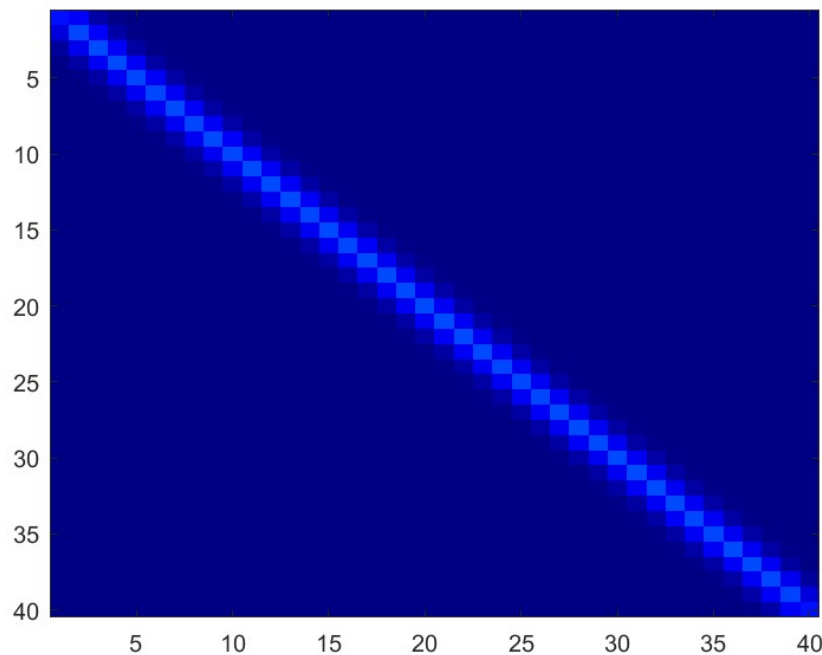
- `<type>` can assume 4 different values, *e.g.* `<type>=4` for Cartesian mesh
- `<input>fmtx<bu>.m` is the output

## TEST PROBLEM: FUEL ROD



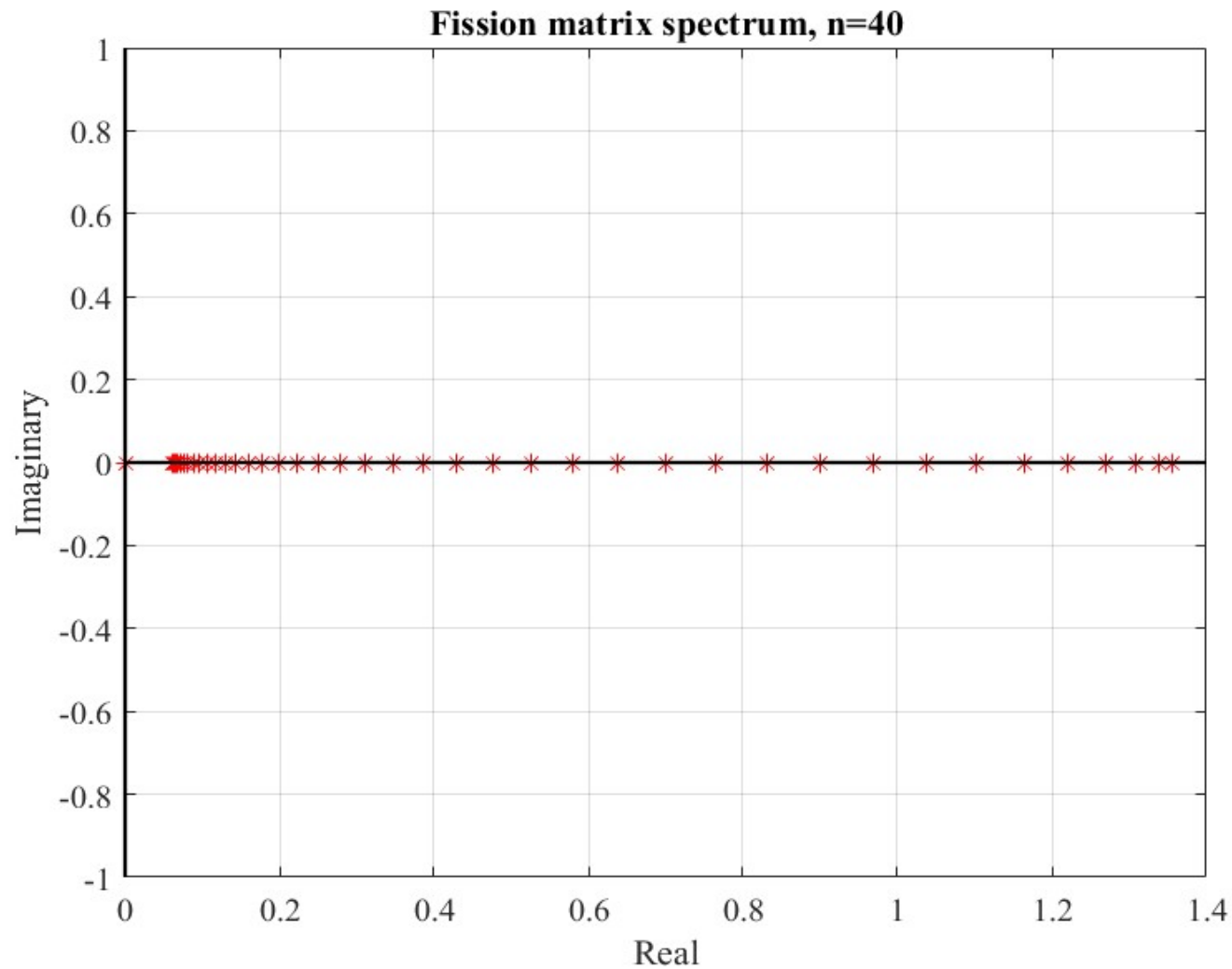
Parameter	Value
Height (cm)	366
Pellet diameter (cm)	0.819
Cladding diameter (cm)	0.950
Pitch (cm)	1.26
H <sub>2</sub> O density (gr/cm <sup>3</sup> )	0.7
Zr Cladding density (gr/cm <sup>3</sup> )	6.55
UO <sub>2</sub> density (gr/cm <sup>3</sup> )	10.4
Enrichment	4.5 wt%

# FISSION MATRIX STRUCTURE



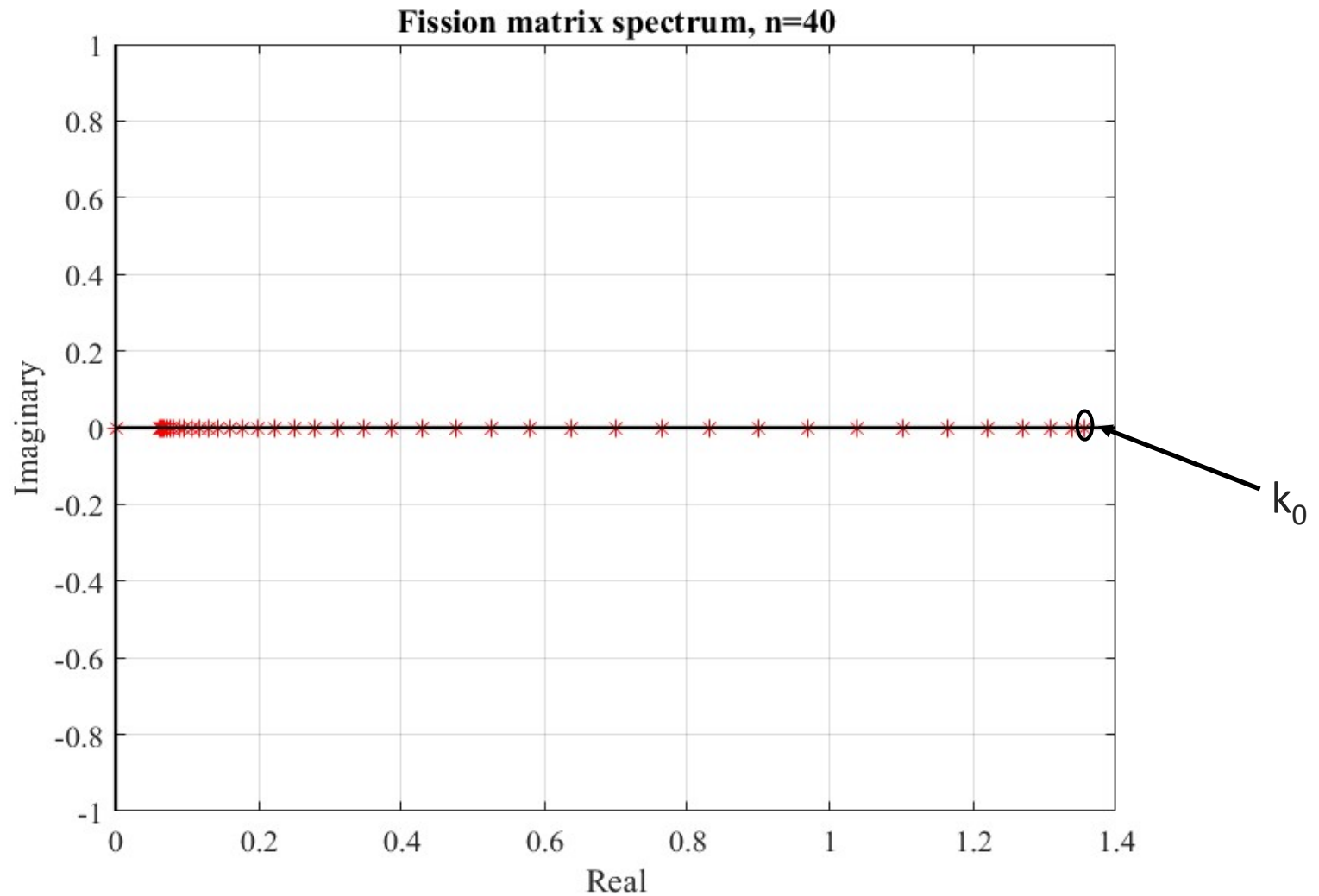
- The fuel rod is discretized with a homogeneous axial Cartesian mesh
- 40 mesh used
- Notice: the fission matrix has a band structure ( keep it in mind ...)

# SPECTRUM OF THE FISSION MATRIX



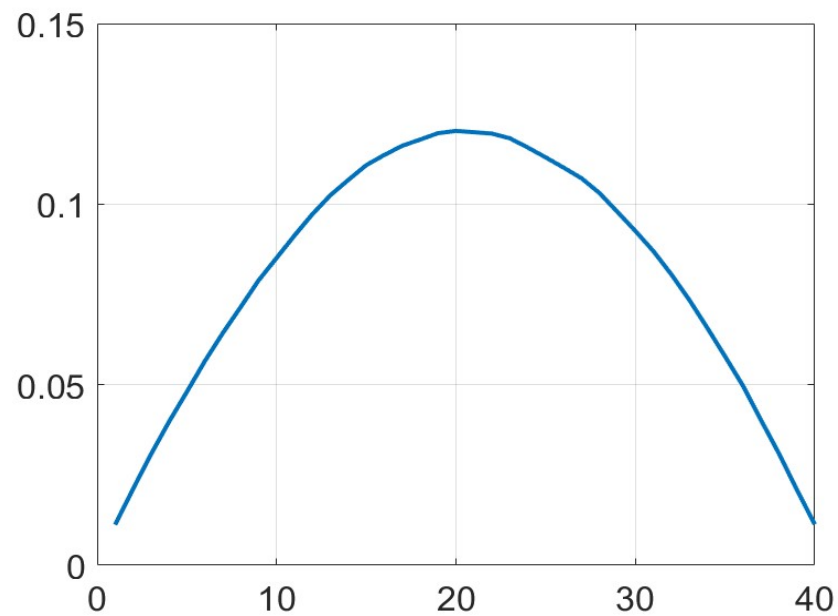


# SPECTRUM OF THE FISSION MATRIX

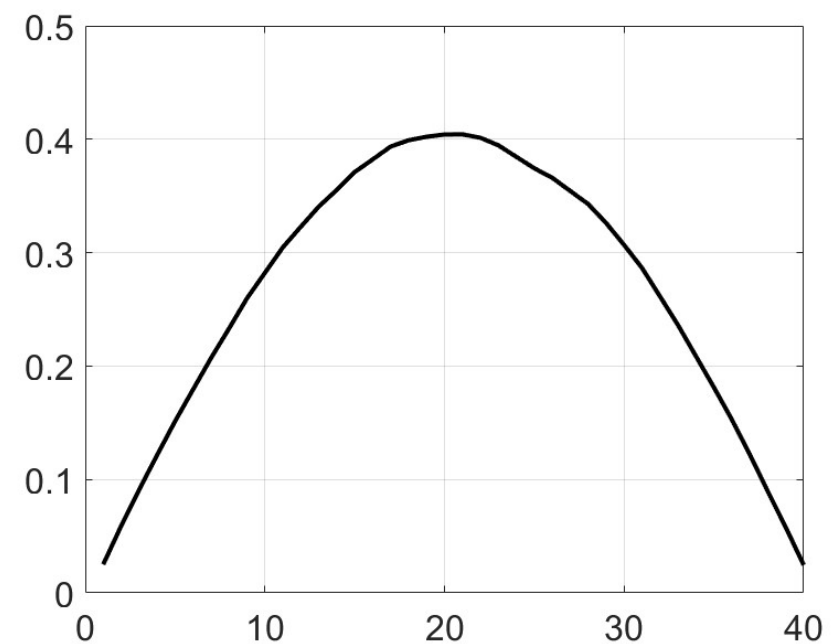


$N = 1$

Forward Eigenmode (Fission  
source distribution)



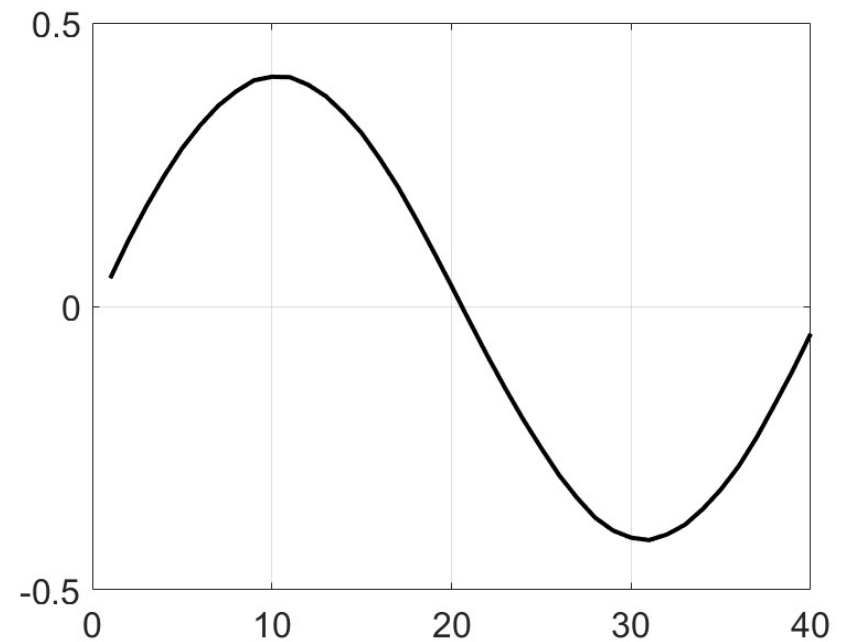
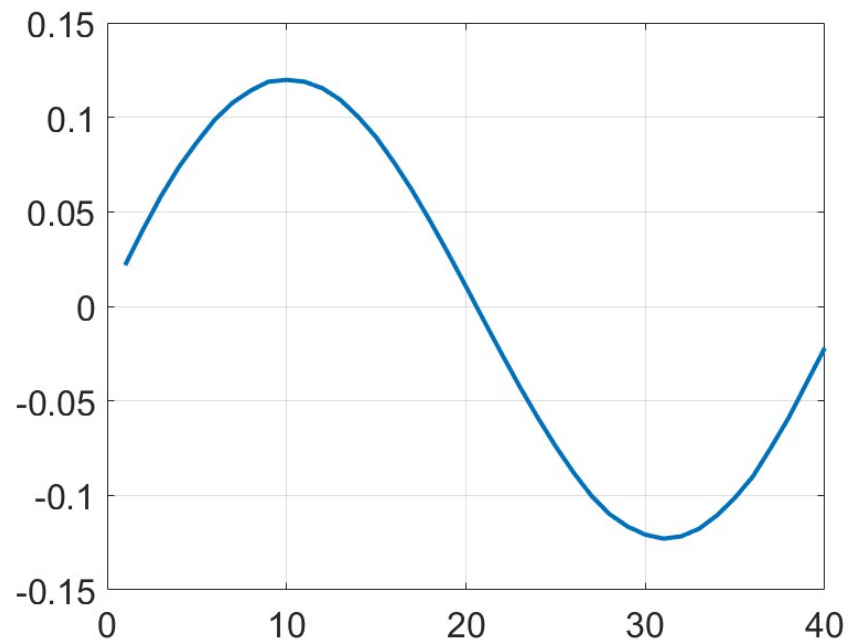
Adjoint Eigenmode  
(Importance distribution)



$N = 2$

Forward Eigenmode

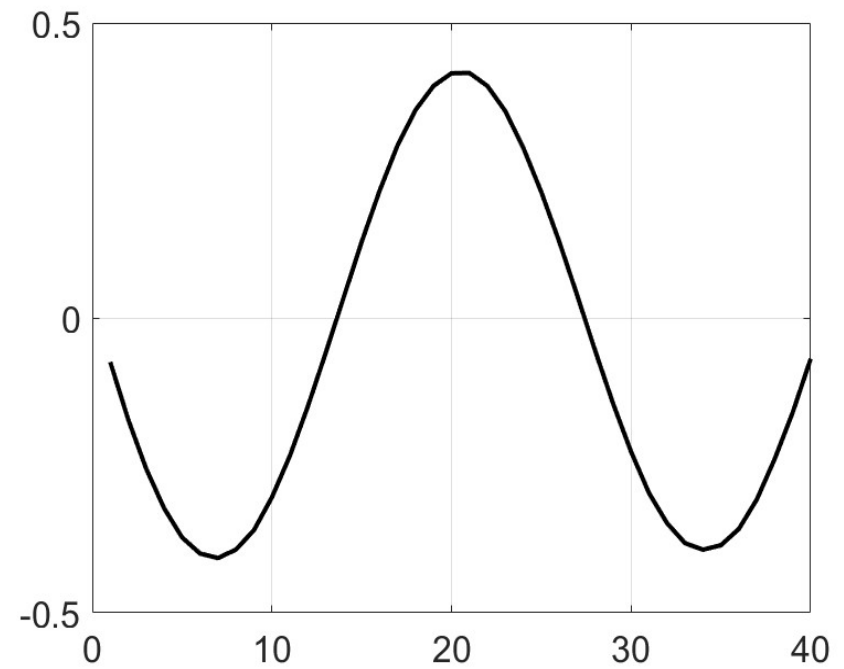
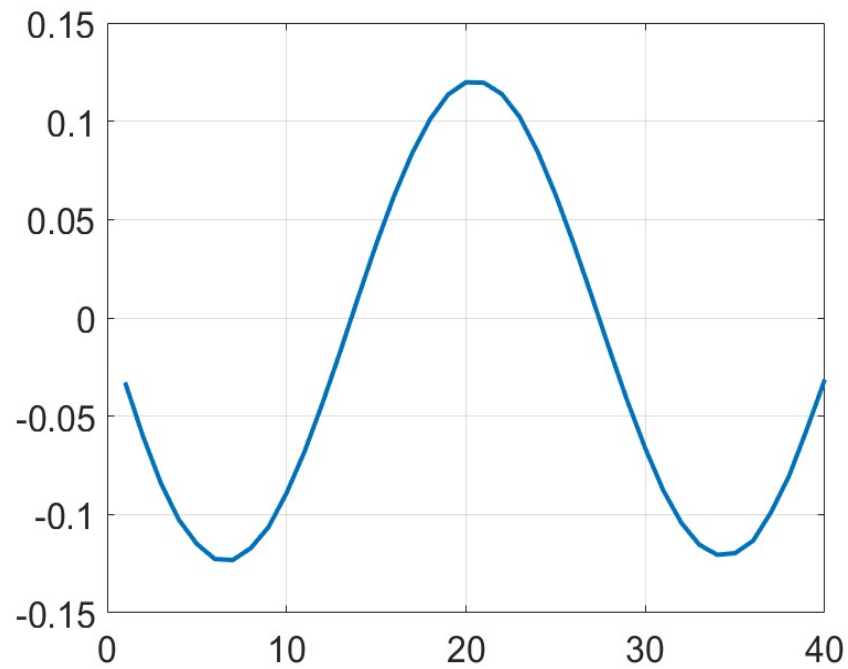
Adjoint Eigenmode



$N = 3$

Forward Eigenmode

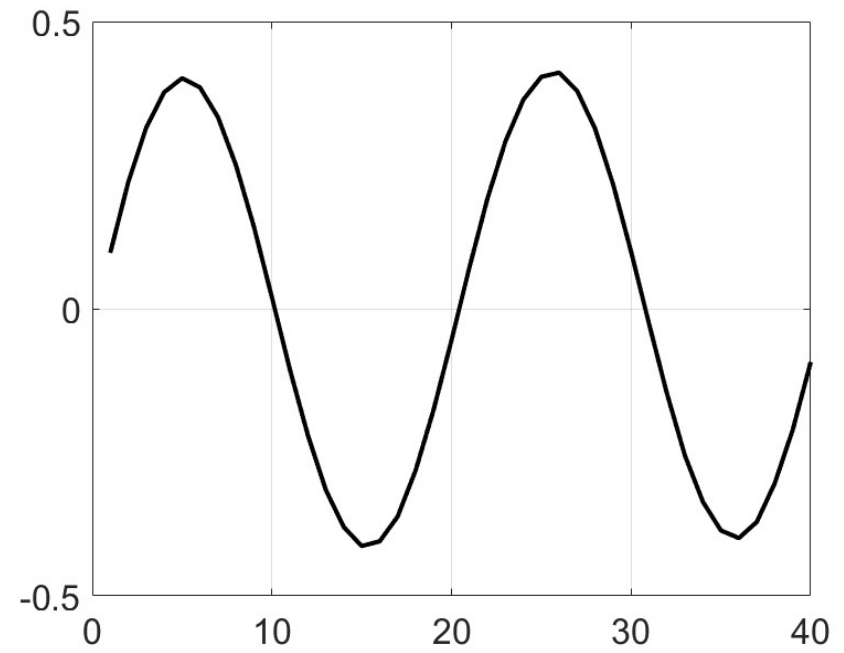
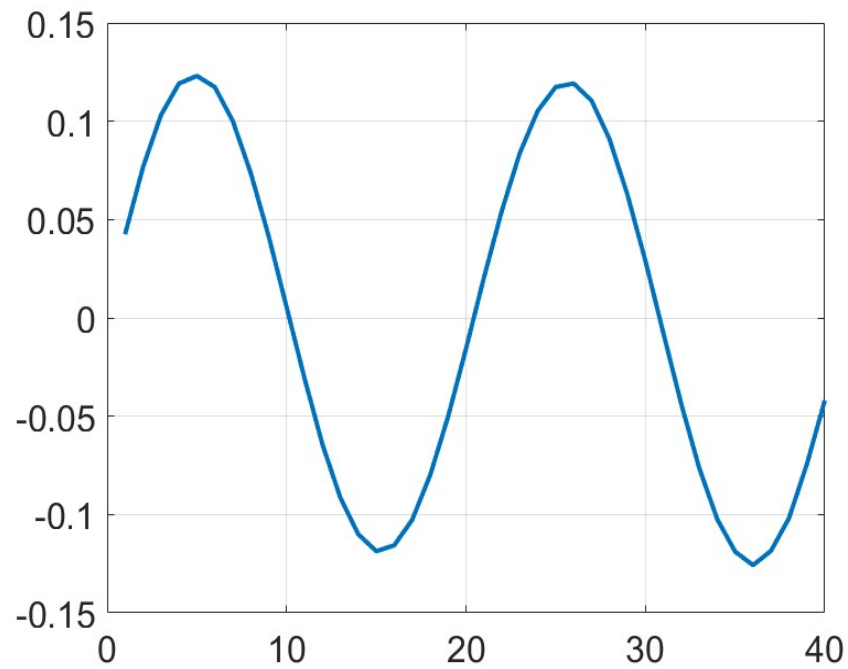
Adjoint Eigenmode



$N = 4$

Forward Eigenmode

Adjoint Eigenmode

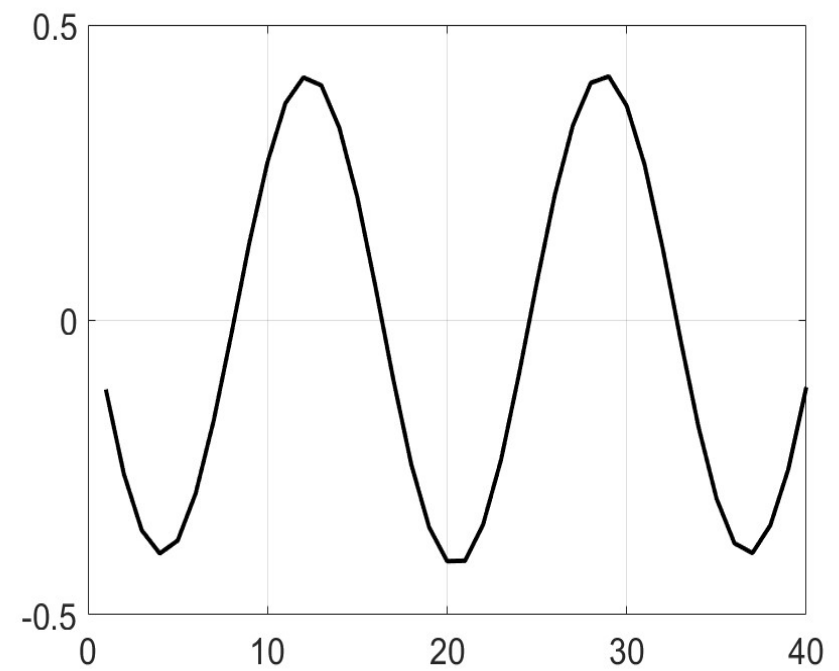
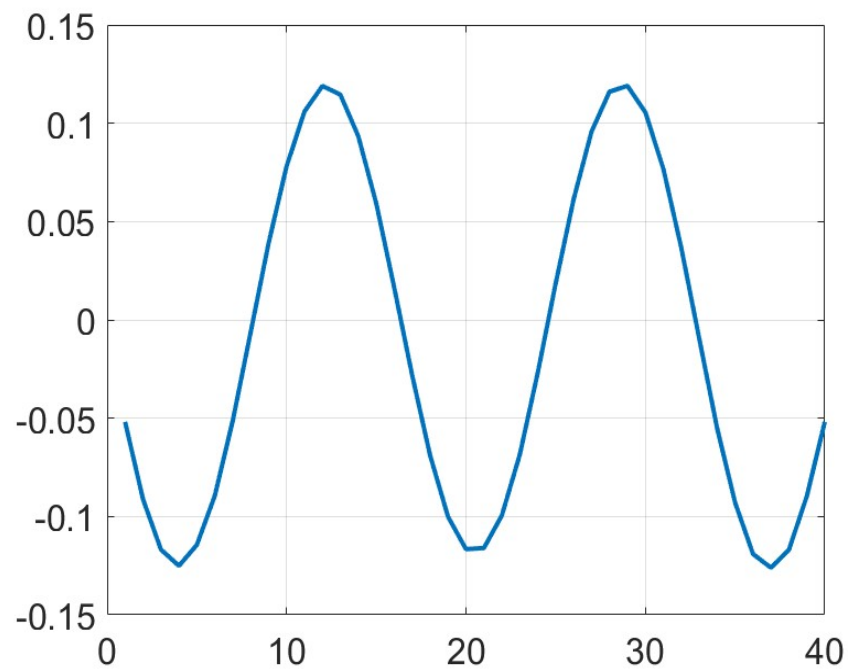




$N = 5$

Forward Eigenmode

Adjoint Eigenmode



## APPLICATIONS OF FISSION MATRIX



The fission matrix can be used for several purposes. For example:

- Acceleration of the source iteration scheme
- Calculation of the higher eigenmodes for sensitivity analysis
- Extraction of the fundamental eigen-pair directly from fission matrix

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*This presentation discusses the convergence of the fission matrix eigen-pair as a function of the mesh size.*

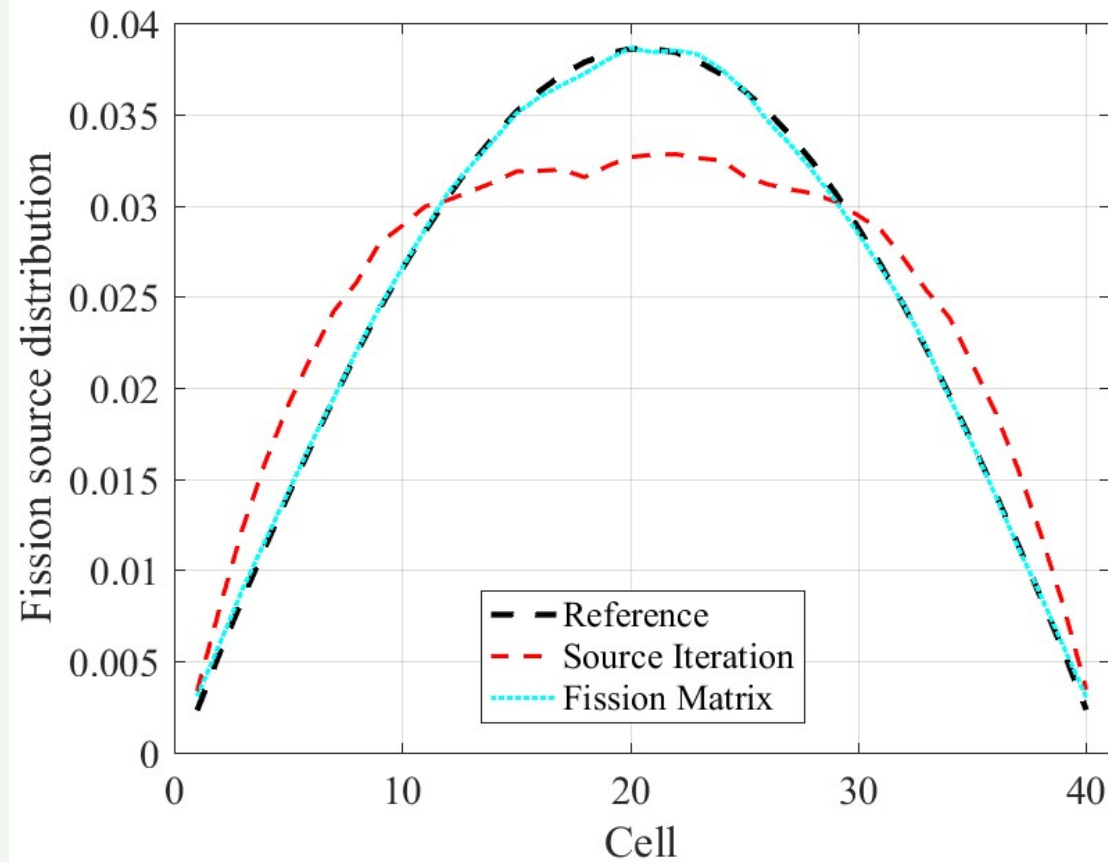
## REFERENCE SOLUTION VS. FISSION MATRIX SOLUTION OF THE FUEL ROD PROBLEM



- Serpent 2.1.29 was used to generate the reference solution.
- The fission matrix and the corresponding eigen-pair are computed using 30 cycles (10 skipped) with 100,000 particles.
- To generate the FM, **1/1000<sup>th</sup>** of the reference histories are run.

Parameter	Value
Total number of neutron histories	3,3x10 <sup>9</sup>
Number of independent simulations	20
Number of particles/simulation/cycle	150,000
Cycles/simulation	1100
Active cycles	700
$\sigma(k\text{-eff})$	0.2 pcm
$\sigma(S)$	<0.1%

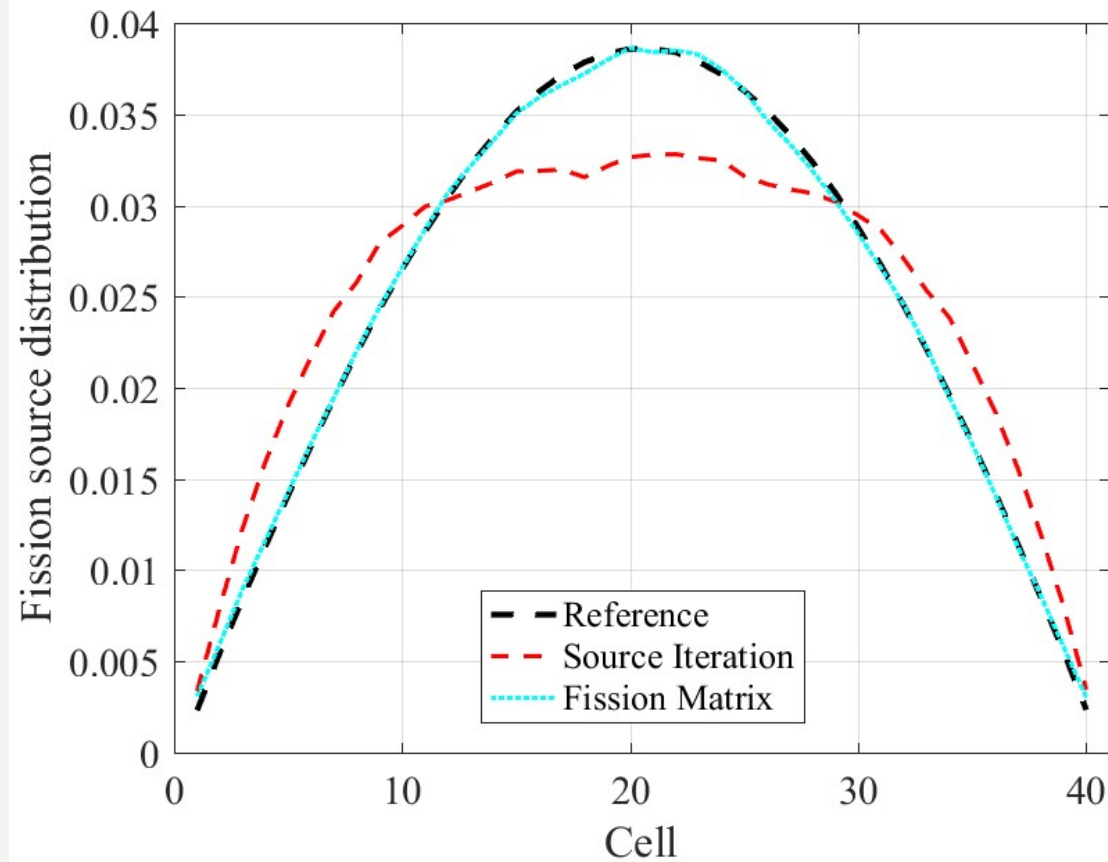
# FUEL ROD SOLUTION



We hit the reference solution with only 30 cycles!!

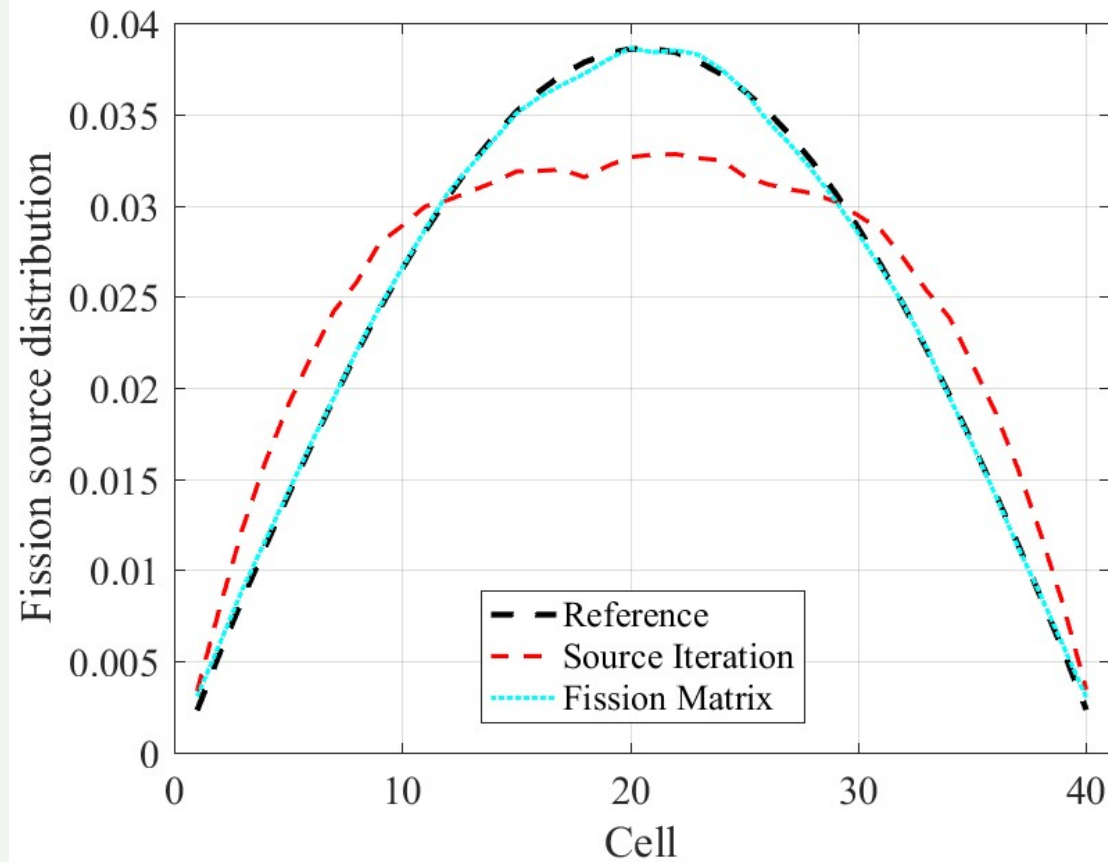


# FUEL ROD SOLUTION



Was it just luck?

# FUEL ROD SOLUTION



Was it just luck? (In brief ... Yes, partially)



# CONVERGENCE PROBLEMS

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## THE ERROR IS DRIVEN BY TWO FACTORS:

- Discretization
- Statistical uncertainty



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Ideally, we should run an **infinite** number of particles and define an infinitely fine mesh to have a perfect solution.



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- Discretization
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Ideally, we should run an infinite number of particles and define an infinitely fine mesh to have a perfect solution.

When the number of particles simulated is **finite** ... non-ideal mesh-wise convergence

## QUESTIONS TO BE ADDRESSED

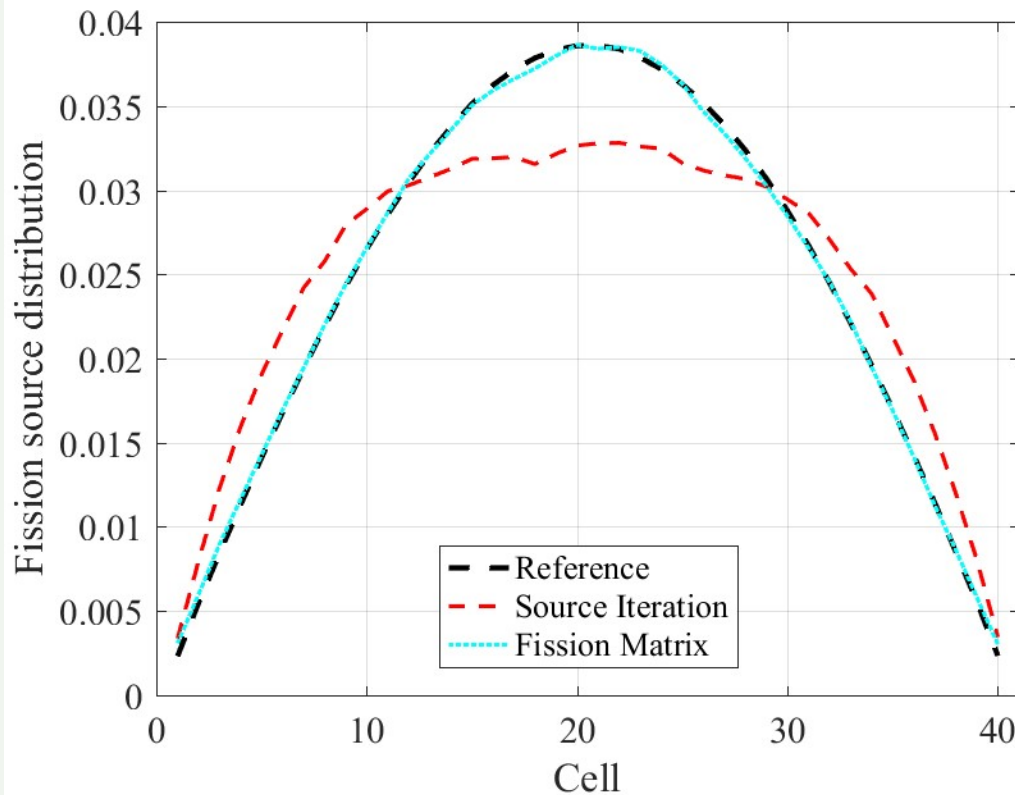


- When the fission matrix eigenvector is cycle-wise converged, does the obtained distribution coincide with the correct solution? Can we have a false convergence?
- Does the trend of the fundamental eigenvalue error coincide with the error trend of the eigenvector as a function of the mesh size?
- Does it exist a value of the mesh such that both the error on the fundamental eigenmode, on the  $k$ -eff and the estimate on the dominance ratio is minimum?

# NUMERICAL RESULTS

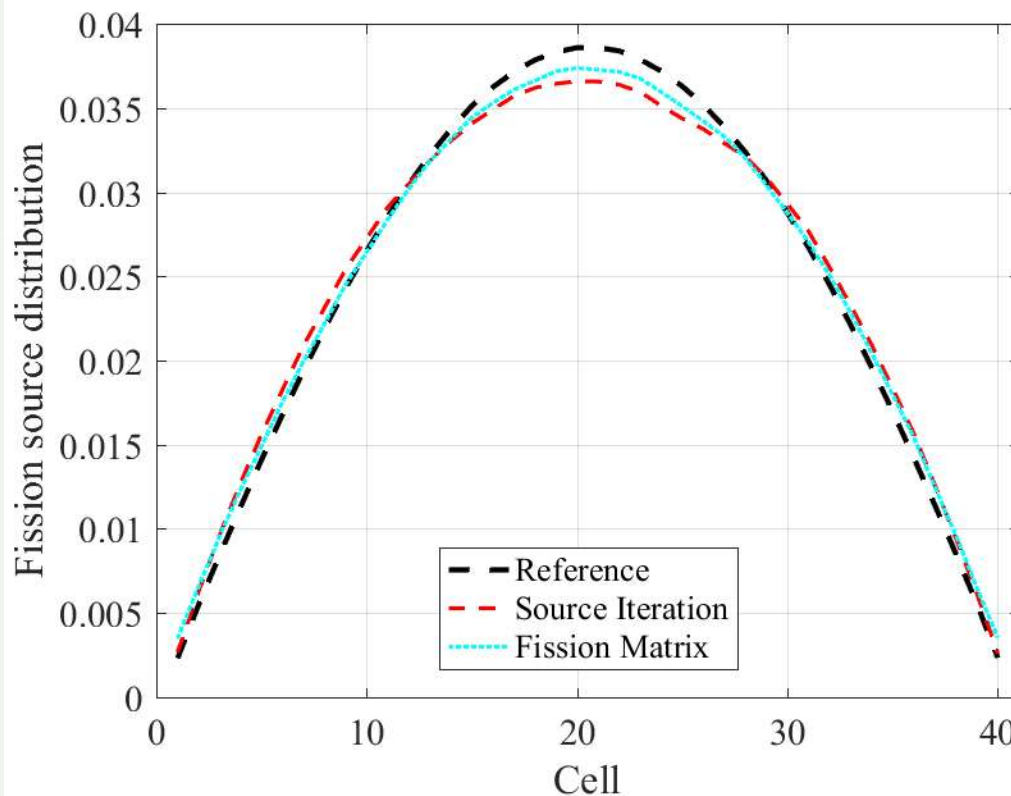
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## CYCLE-WISE DETERIORATION OF THE SOLUTION



- The fission matrix is extracted at the 30<sup>th</sup> cycle
- The fission distribution hits the correct solution!

# CYCLE-WISE DETERIORATION OF THE SOLUTION

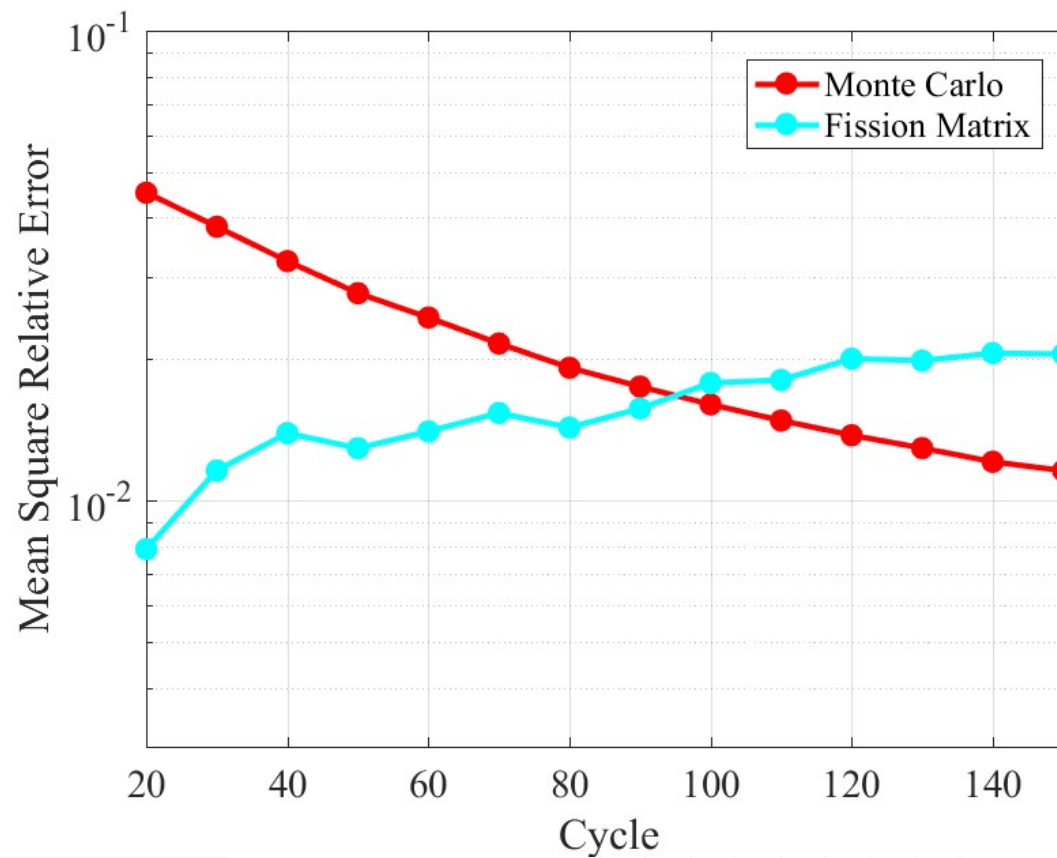


$n = 150$

- The fission matrix is extracted at the 150<sup>th</sup> cycle
- The fission distribution converges to a different distribution!



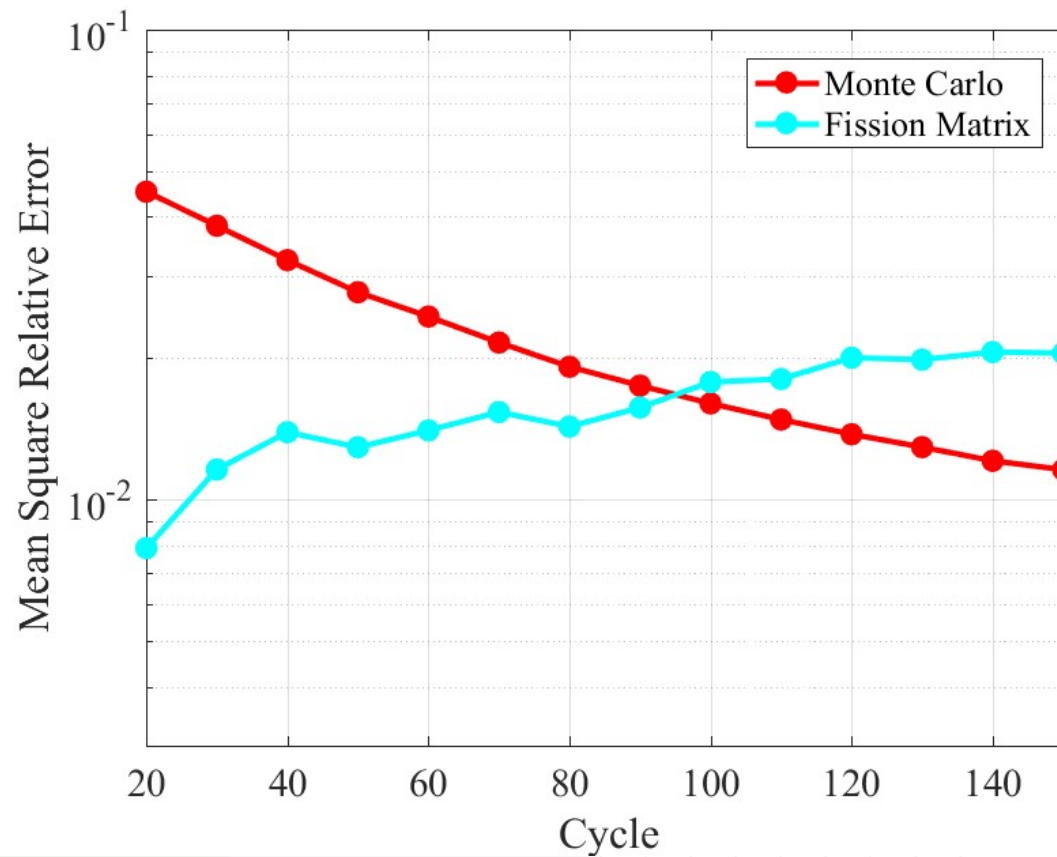
# CYCLE-WISE FUNDAMENTAL EIGENMODE MSRE FROM REFERENCE SOLUTION



The error increases cycle-wise!

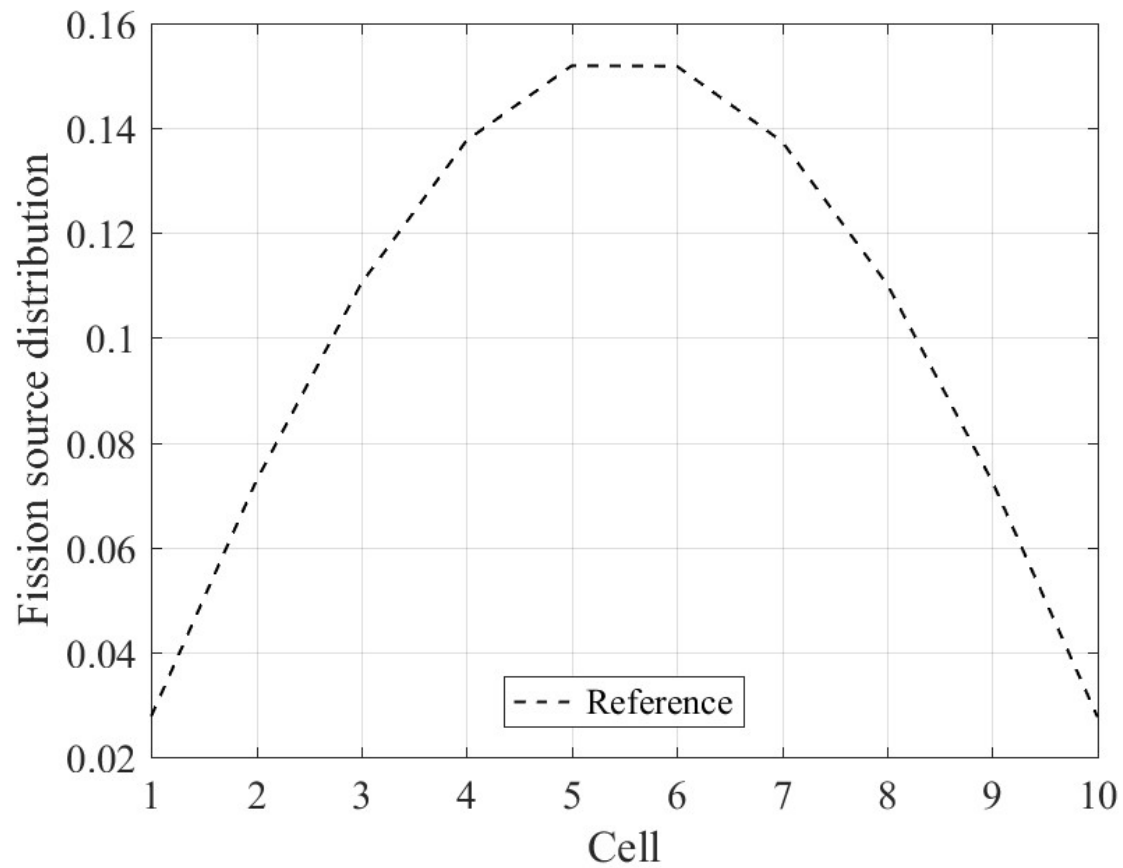


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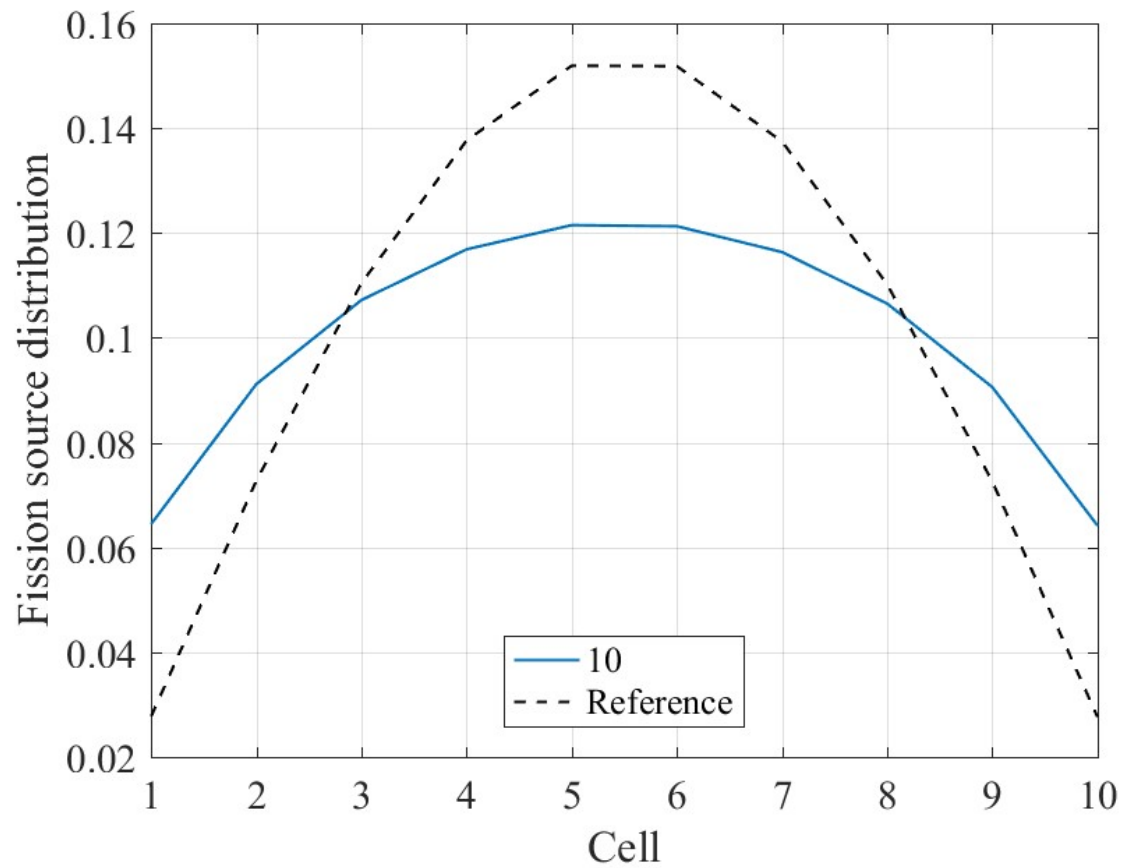


Maybe we should refine the mesh

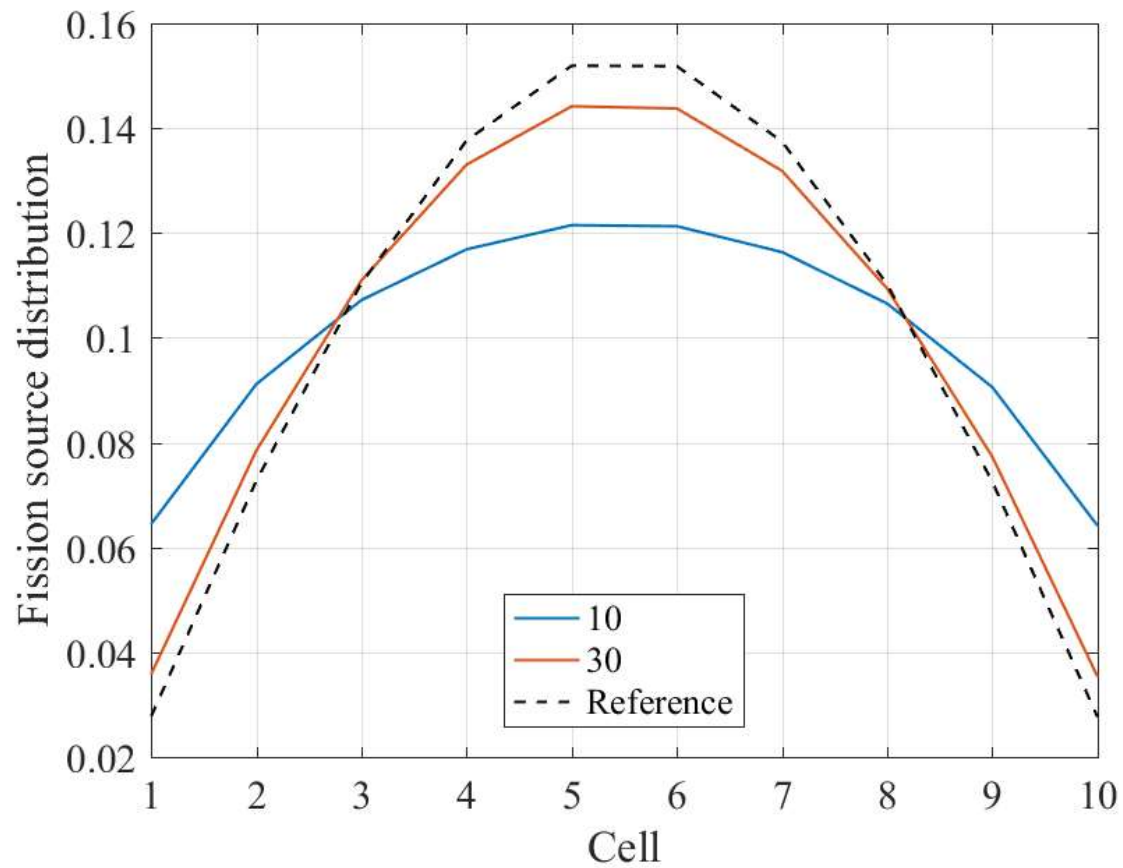
# FUNDAMENTAL EIGENMODE CONVERGENCE



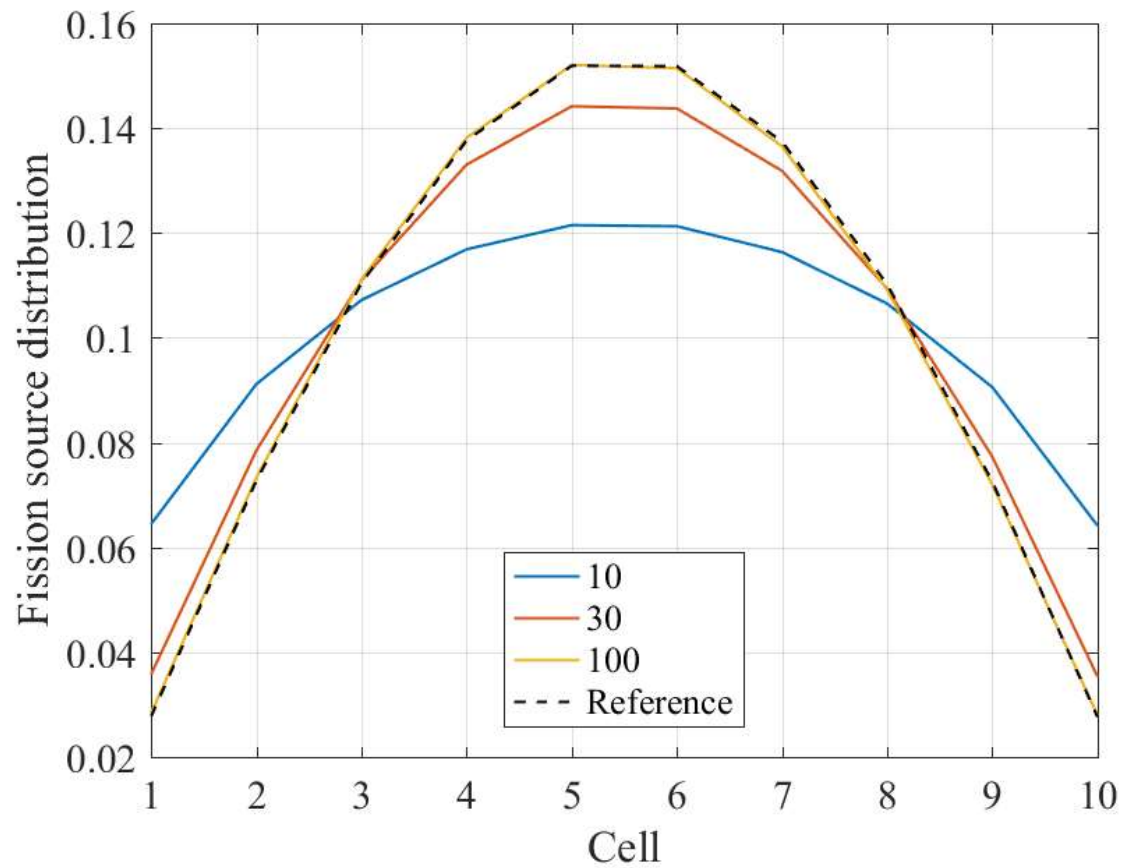
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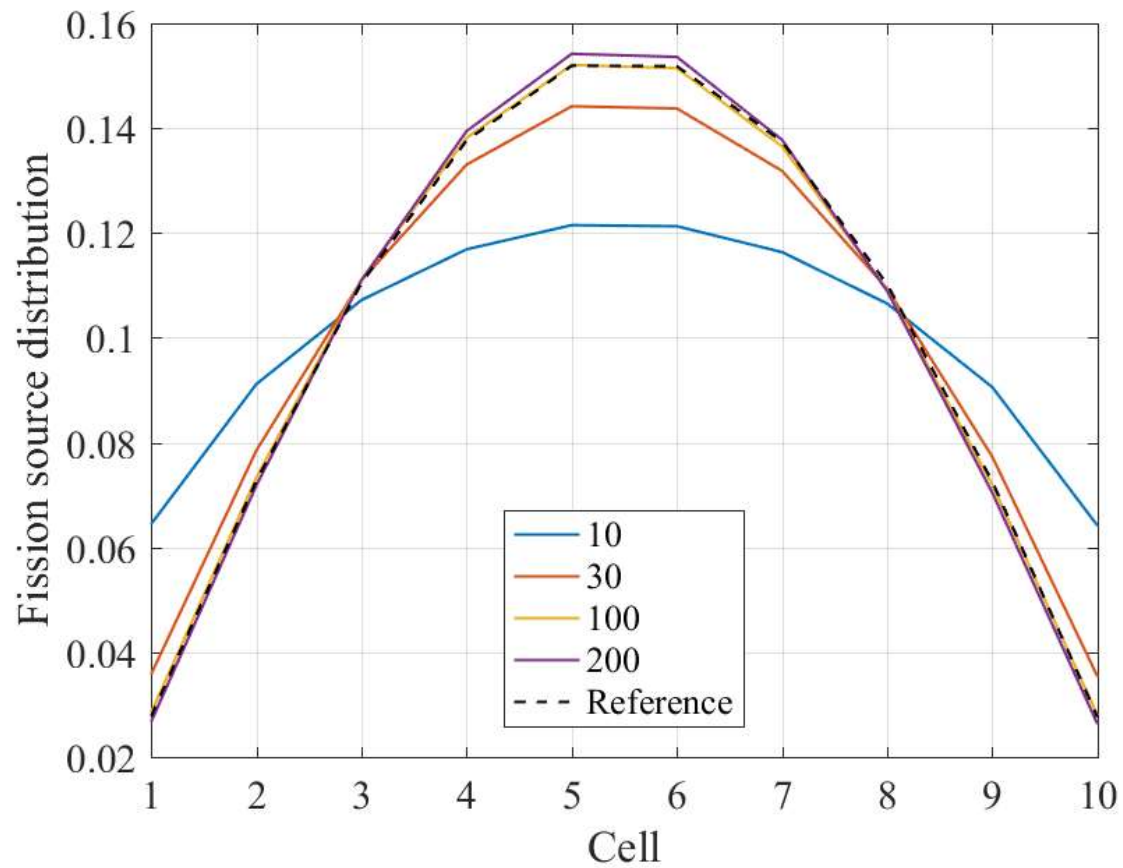
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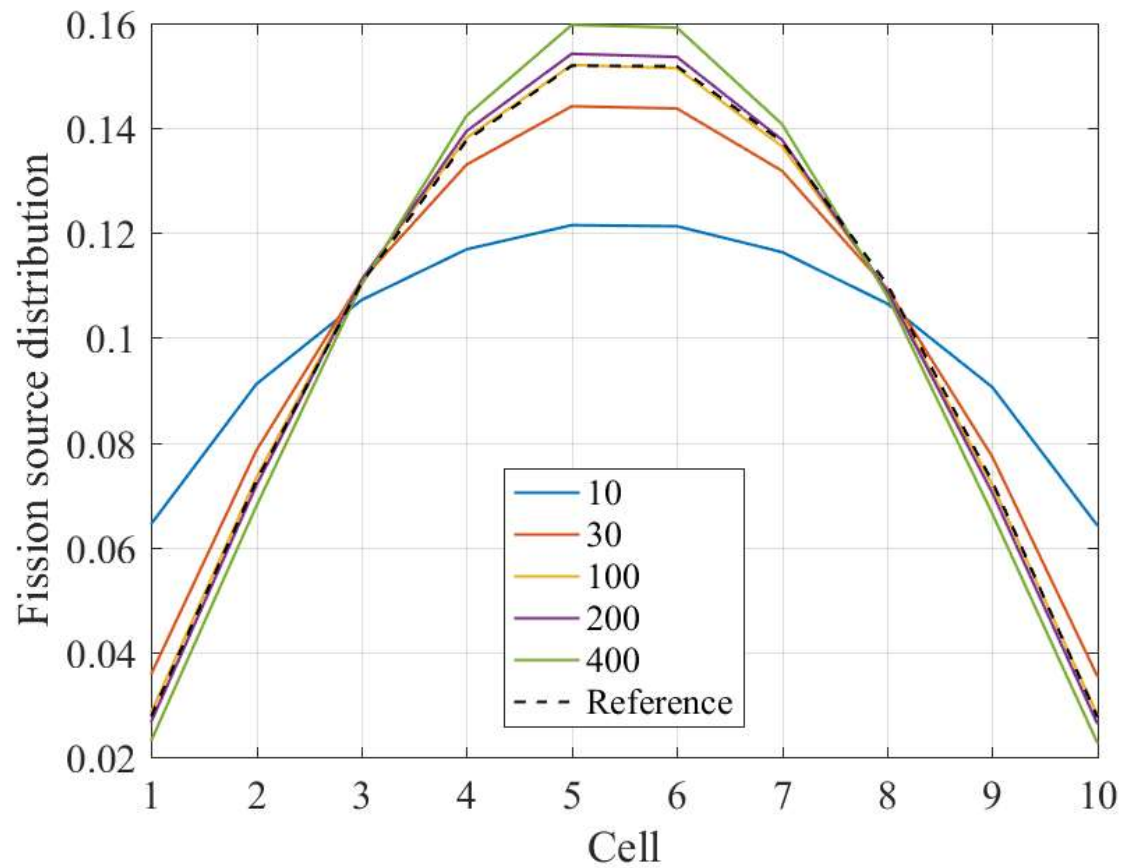


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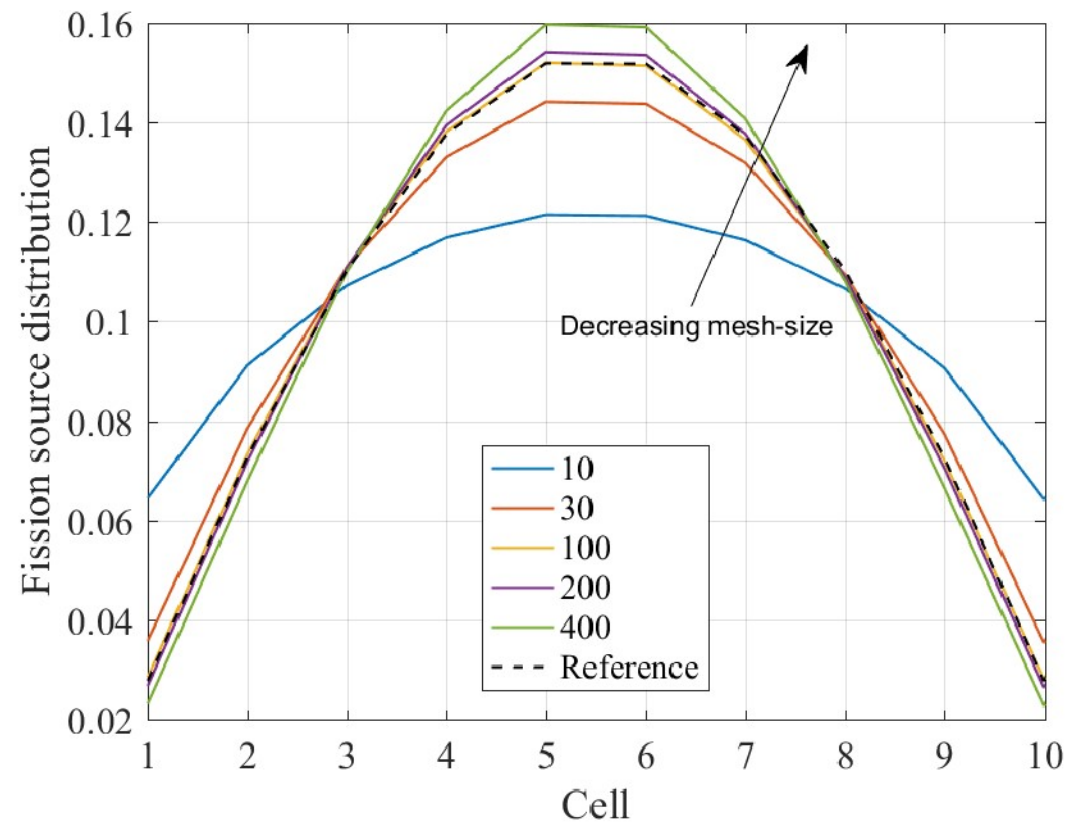


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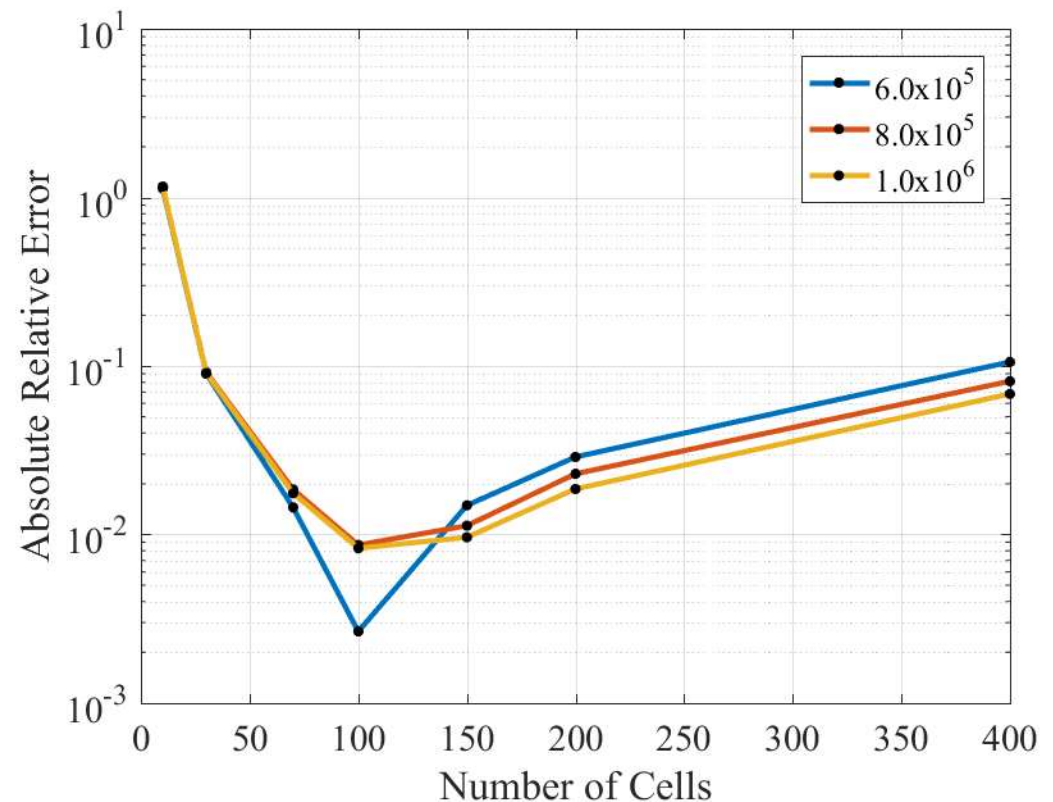
- The distribution does not approach asymptotically the reference solution!
- For finer mesh grids, neutrons are “trapped” in the high importance zone .



# ABSOLUTE RELATIVE ERROR AS A FUNCTION OF MESH FOR DIFFERENT NEUTRON BATCH SIZE



- For a coarse mesh structure, the discretization error dominates over the statistical uncertainty
- For high number of mesh, the opposite holds.
- Slightly different trend for 600,000-particles: probably due to the high statistical noise.



# SEMI-ANALYTICAL MODELIZATION OF THE ERROR



## DISCRETIZATION ERROR

As the volumes of the cells approach zero, the discretization error tends to zero.

$$\epsilon_d(h) = a/N^b$$

- $N$ : number of cells
- $a, b$ : unknown parameters dependent on statistics and system characteristics.

# SEMI-ANALYTICAL MODELIZATION OF THE ERROR



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## STATISTICAL ERROR

It is an aggregate of two terms,

- Transmission term
- Condition-number term.

$$\epsilon_s(h) = cN^2$$

- $c$ : unknown parameters dependent on statistics and system characteristics.

## TRANSMISSION TERM

- The FM generation process is equivalent to solving a set of  $N^2$  fixed source calculations.
- High uncertainty far from diagonal
- Serpent filters out the elements with standard deviation larger than 10%
- The majority of the elements outside the diagonal are set to zero: loss of information

Number of cells	Apparent axial distance (cm)
10	197.6400
30	140.7067
70	119.5804
100	109.5804
150	98.4784
200	90.8137
400	72.7288



## CONDITION-NUMBER TERM

- A consequence of the fission matrix structure
- The condition number increases as the mesh size increases because more elements are set to zero, *i.e.* the FM becomes ill-conditioned
- It can be demonstrated that the condition number bounds the error propagation in matrix-vector multiplication, on which the power method relies.

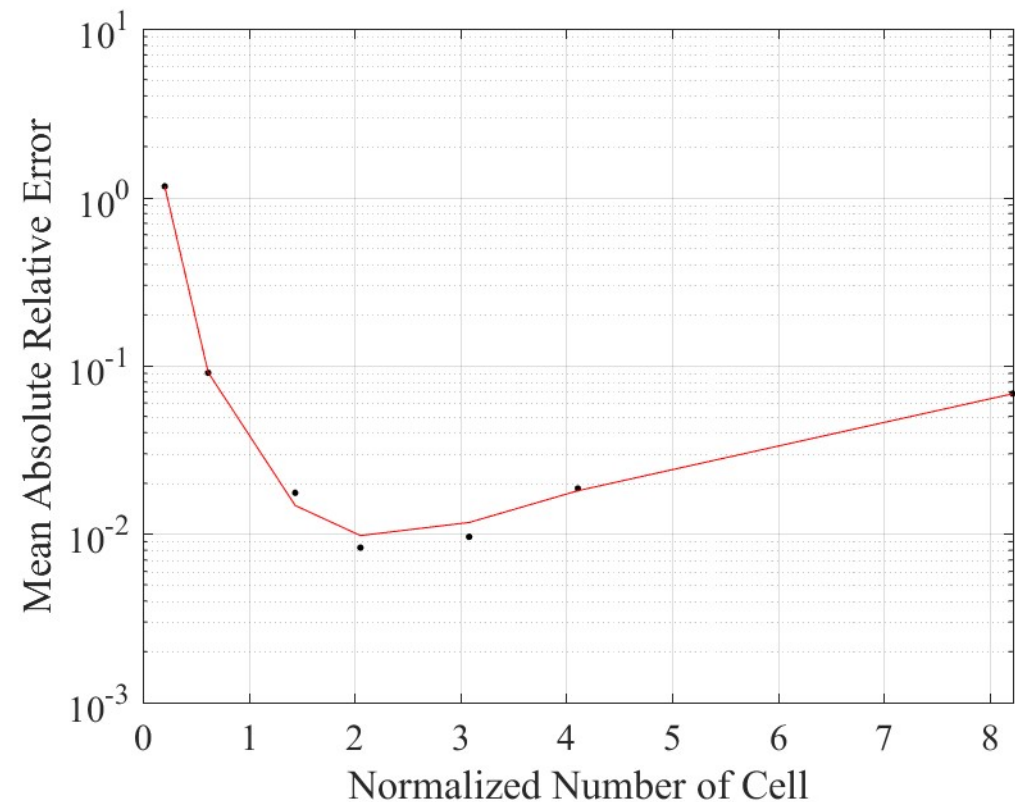
Number of cells	Condition Number
10	1.7559
30	10.0132
70	63.2548
100	91.5687
150	139.3537
200	208.1023
400	798.0571

## MODEL PRELIMINARY EVALUATION

- The error can then be described as :

$$\epsilon(x) = \frac{a}{N^b} + cN^2$$

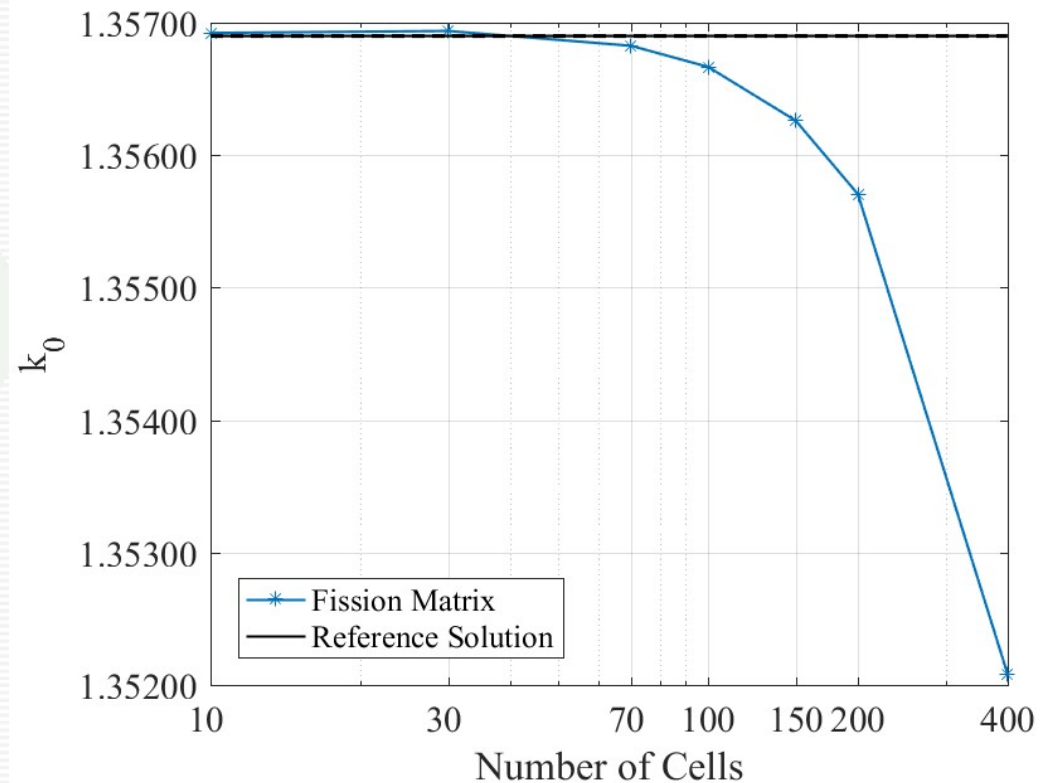
- The 1,000,000-particles curve fit using the Non-Linear Least Square Method ( relative mean square error: 0.0019)



## IS THE POINT OF MINIMUM ERROR COINCIDENT FOR THE EIGEN-PAIR?



- The best estimate is obtained for coarser mesh.
- The fundamental eigenvalue of the fission matrix is only dependent on the statistics, *i.e.* average number of particles per mesh.





## CONCLUSION AND FUTURE WORK

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## CONCLUSIONS



- When the fission matrix eigenvector is cycle-wise converged, does the obtained distribution coincide with the correct solution? Can we have a false convergence?

Yes

- Does the trend of the fundamental eigenvalue error coincide with the error trend of the eigenvector as a function of the mesh size?

No

- Does it exist a value of the mesh such that both the error on the fundamental eigenmode, on the k-eff and the estimate on the dominance ratio is minimum?

No



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## FUTURE WORK



- Error propagation through fission matrix spectral calculations
- Use of fission matrix eigenmode for improved initial guess
- A priori determination of the optimal mesh size/structure
- Can we relate it to the cell-wise diffusion length?

## REFERENCES



[1] Carney, S., Brown, F., Kiedrowski, B., & Martin, W. (2014). Theory and applications of the fission matrix method for continuous-energy Monte Carlo. *Annals of Nuclear Energy*, 73, 423-431. DOI: [10.1016/j.anucene.2014.07.020](https://doi.org/10.1016/j.anucene.2014.07.020)

[2] <https://goo.gl/r3T2Cp>



QUESTIONS?

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