Incomplete Parabolic Short Characteristics in IDT

Mathématiques pour la neutronique
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Outline

- Introduction;
- Incomplete Parabolic Short Characteristics;
- Numerical results;
- Reduction of the memory imprint by Von Neumann series expansion;
- Numerical results;
- Conclusion and future developments.

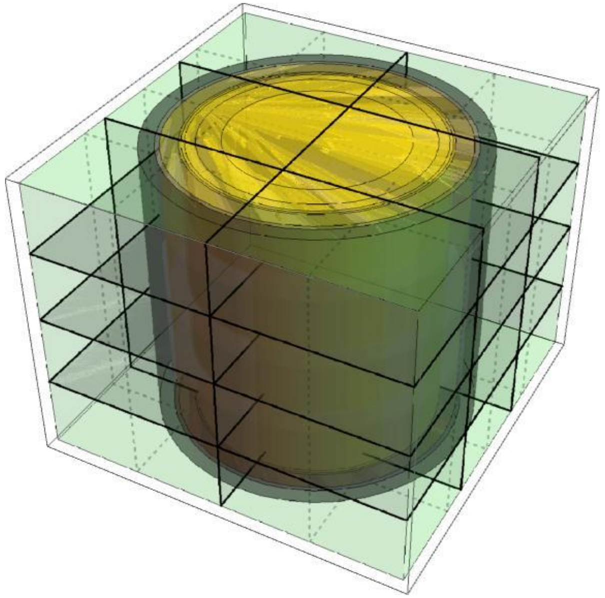
Generalities on the IDT solver

- Discrete-ordinate solver for the Multigroup Boltzmann Equation;

- Spatial solution by Constant, Linear or Incomplete Parabolic Short Characteristics;

- The spatial domain is discretized by a Cartesian grid, hosting Heterogeneous Cartesian Cells (HCCs);

- Each HCC is equipped with an inner mesh (cylinders + X/Y/Z-mesh) and its surfaces discretized by a Cartesian grid.



Method of Short Characteristics (MOSC)

One-group integral transport equation along direction *d*,

$$\varphi_d(\boldsymbol{r}_t^- + x\boldsymbol{\Omega}_d) = \varphi_d(\boldsymbol{r}_t^-)e^{-\tau_t(x,0)} + \int_0^x q_d\left(\boldsymbol{r}_t^- + y\boldsymbol{\Omega}_d\right) e^{-\tau_t(x,y)} dy$$

Polynomial expansion of the source and the surface angular flux,

$$q_{d,\alpha}(\boldsymbol{r}) = \sum_c P_{\alpha,c}(\boldsymbol{r})\, q_{d,\alpha,c} = \boldsymbol{P}_\alpha(\boldsymbol{r}) \cdot \boldsymbol{q}_{d,\alpha}$$

$$\varphi_{d,s}(\boldsymbol{r}_t^\pm) = \sum_b P_{s,b}(\boldsymbol{r}_t^\pm)\, \varphi_{d,s,b}^\pm = \boldsymbol{P}_s(\boldsymbol{r}_t^\pm) \cdot \boldsymbol{\varphi}_{d,s}^\pm$$

Method of Short Characteristics

The solution of MOSC reads as

$$\boldsymbol{\varphi}_{d,\alpha}(\boldsymbol{r}) = \sum_{s'(\alpha)} \boldsymbol{I}_{\alpha,s'}(\boldsymbol{\Omega})\, \boldsymbol{\varphi}^{\pm}_{d,s'} + \sum_{\beta(\alpha)} \boldsymbol{C}_{\alpha,\beta}(\boldsymbol{\Omega})\, \boldsymbol{q}_{d,\beta}$$

$$\boldsymbol{\varphi}^{+}_{d,s}(\boldsymbol{r}) = \sum_{s'(s)} \boldsymbol{T}_{s,s'}(\boldsymbol{\Omega})\, \boldsymbol{\varphi}^{\pm}_{d,s'} + \sum_{\beta(s)} \boldsymbol{E}_{s,\beta}(\boldsymbol{\Omega})\, \boldsymbol{q}_{d,\beta}$$

MOSC suffers from large memory occupation due to the angular probability matrices,

$$Collision \propto N_d \cdot N_g \cdot N_{cells} \cdot N^2_{r/cell} \cdot N^2_c$$

Reduction of the memory imprint

In the Integro-Differential Transport code IDT,

- Reduction of the number of stored directions by symmetry and reciprocity relations;
- Reduction of the number of cells by Von Neumann expansion;
- Reduction of the number of regions per cell by Incomplete Parabolic Short Characteristics.

Incomplete Parabolic Short Characteristics

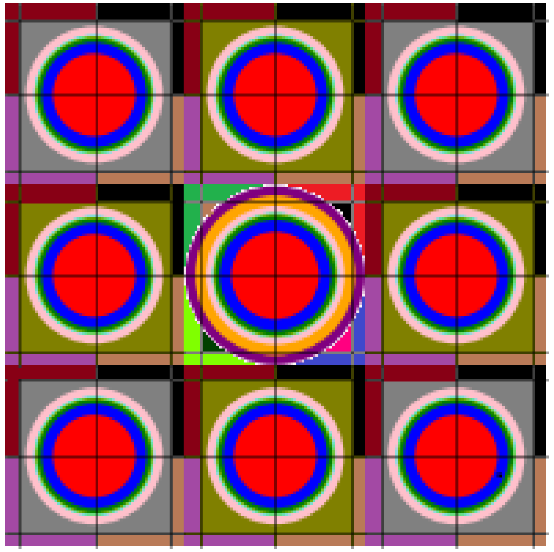
- The polynomial expansion has been extended up to parabolic order;
- The bilinear terms have been disregarded;
- Motivations for incomplete parabolic short characteristics:

1) Lowering the number of regions, while keeping high accuracy;
2) In 3D problems, $N_c = 4 \longrightarrow 7$, thus $N_{r/cell}$ has to be reduced by 50%;
3) Reducing users' work → The HCCs inner grid can be greatly simplified.

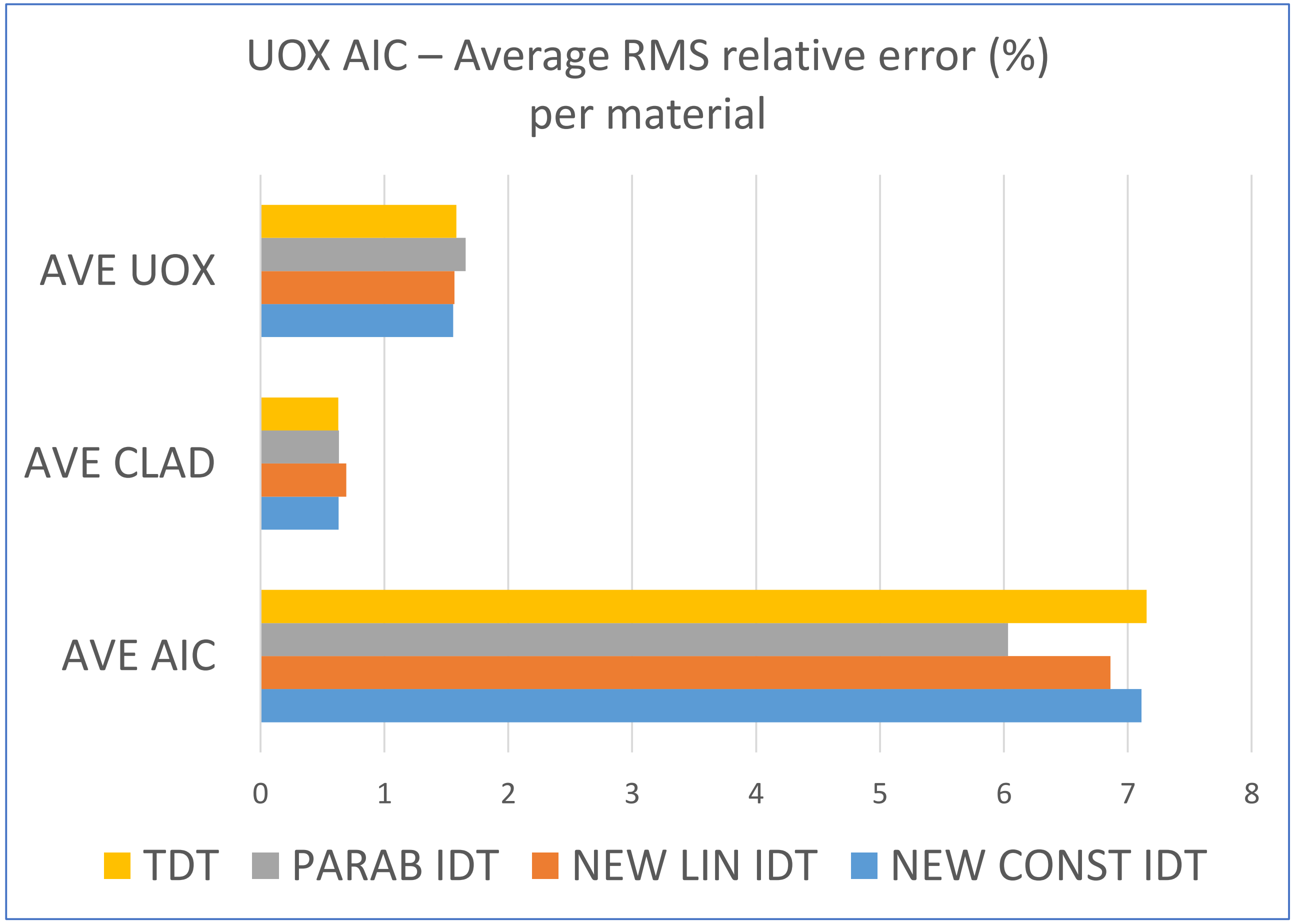
3x3 2D UOX/MOX Benchmarks

(Motif3x3_UOX_AIC_Valid_Autop.py - V&V APOLLO3®)

- Nuclear data: 281 g-P3 cross section library, LJ self-shielding model;
- Comparison of the flux distribution per energy group and material with APOLLO3® - TDT MOC and TRIPOLI4® (Standard deviation < 1%, almost everywhere).

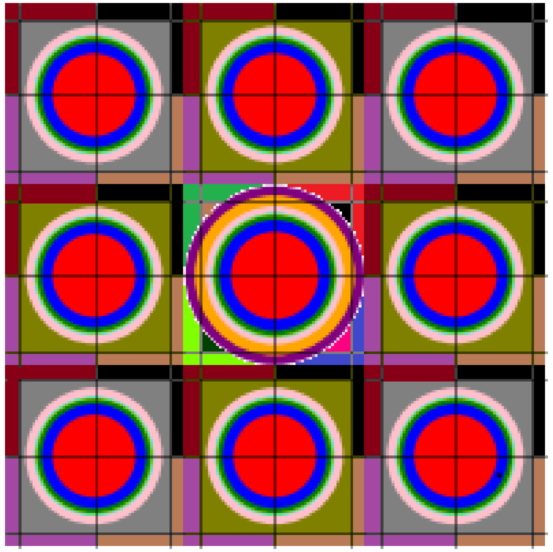


	UOX/MOX AIC			UOX/MOX Hf			UOX/MOX GT			UOX Gd			UOX/MOX B4C		
IDT	Const	Lin	Parab	Const	Lin	Parab	Const	Lin	Parab	Const	Lin	Parab	Const	Lin	Parab
Nb. Regions	387	128/161	65	401	128	65	472	164	59	358	109	70	383	128	65

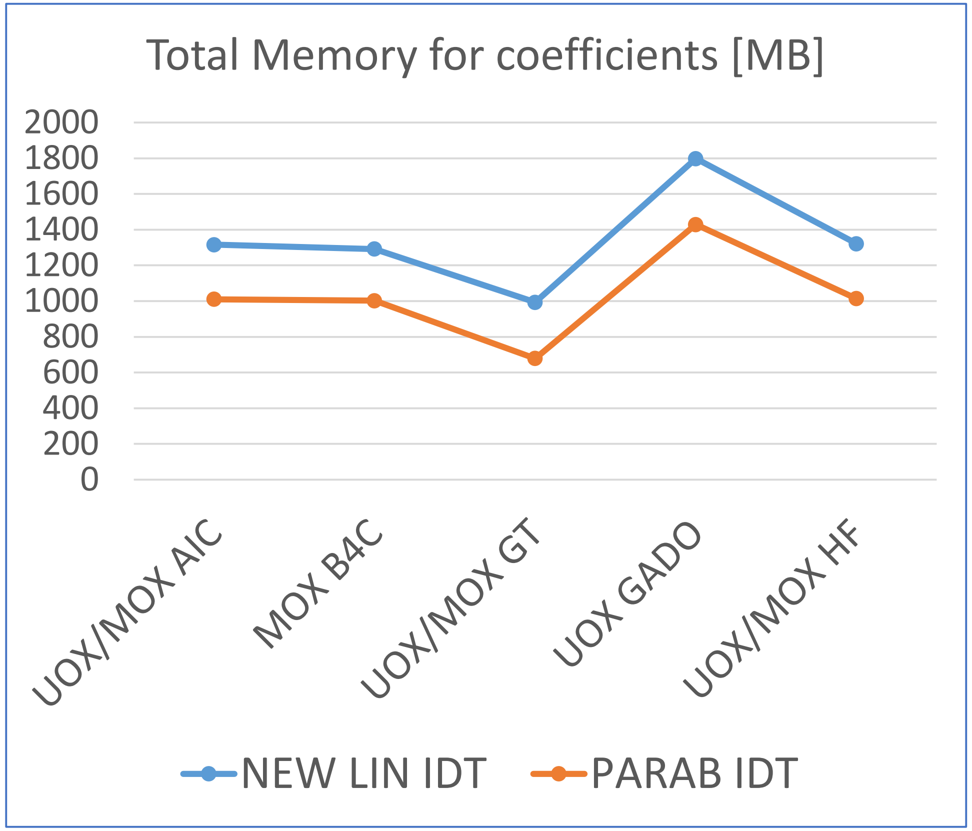


$$\overline{RMS} = \frac{1}{N_r}\sum_{r=1}^{N_r}(RMS)_r \;;$$

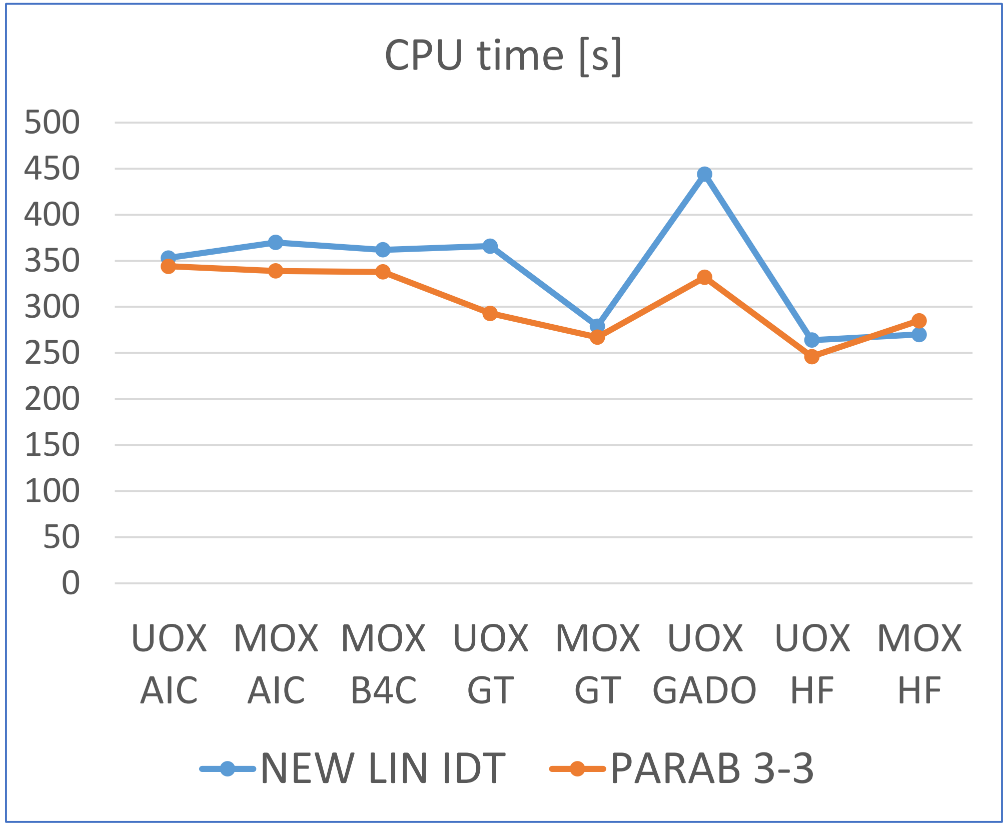
$$(RMS)_r = \sqrt{\frac{1}{N_g}\sum_{g=1}^{N_g}\left(1-\left(\frac{\varphi_r^{det}(\Delta E_g)}{\varphi_r^{MC}(\Delta E_g)}\right)\right)^2}$$



NEW LIN IDT – Spatial mesh



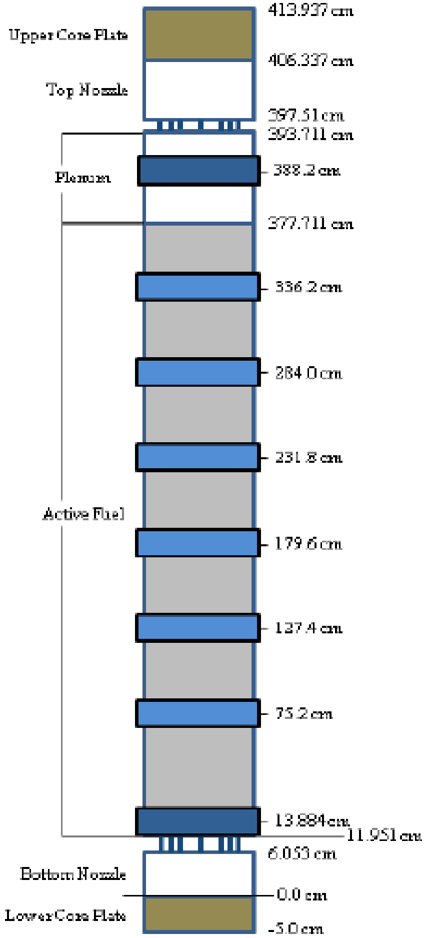
Total Memory for coefficients [MB]
2000
1800
1600
1400
1200
1000
800
600
400
200
0
UOX/MOX AIC
MOX B4C
UOX/MOX GT
UOX GADO
UOX/MOX HF
NEW LIN IDT
PARAB IDT



CPU time [s]
500
450
400
350
300
250
200
150
100
50
0
UOX AIC
MOX AIC
MOX B4C
UOX GT
MOX GT
UOX GADO
UOX HF
MOX HF
NEW LIN IDT
PARAB 3-3

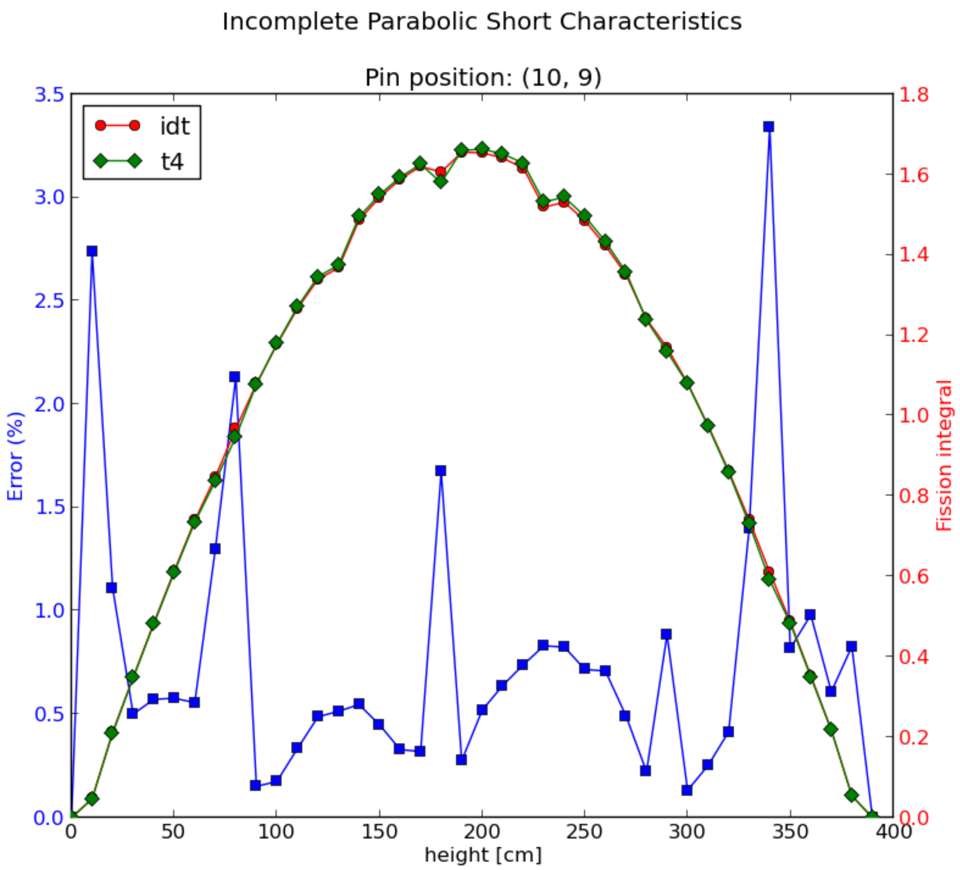
3D Watts Bar benchmark

- 17x17 3D UOX-Pyrex + water blades;
- 281g-P1 cross sections library;
- Fine-Structure self-shielding model;
- Reference: TRIPOLI4® continuous energy Monte Carlo;
- Response → Fission integral, on a 17x17x40 output grid (Standard deviation < 1%)



									lc
								c5	lv
							c3	c4	lv
						p2	c3	c4	lv
					py	p1	c3	c4	lv
				p2	p1	p1	p2	c4	lv
			py	p1	p1	py	p1	c4	lv
		p2	p1	p2	p2	p1	p2	c4	lv
	c2	p2	p1	p2	p2	p1	p2	c4	lv
tg	c1	p1	py	p1	p1	py	p1	c4	lv

3D Watts Bar benchmark – Comparison between LSC and PSC



Common parameters:

- 28.880 cells;
- 3x3x2 cell boundary mesh;
- S8 Level-Symmetric angular quadrature formula.

	Nb of regions	Mean nb of regions per cell	Time [h]	Relative error on k-eff (pcm)	Max error (%)	Average RMS (%)
LSC	571073	19,78	6	83	3,51	0,73
PSC	298699	10,35	24	94	3,36	1

Asymptotic method - Introduction

- Novel approach to reduce the memory imprint of the angular probability matrices;
- Fixed source problem, $\boldsymbol{L}\varphi = q$, where $\boldsymbol{L} = \hat{\Omega} \cdot \nabla + \Sigma$;
- Memory imprint of the angular coefficients $\propto N(HCCs)$;
- Idea: $\boldsymbol{L} = \boldsymbol{L}_0 - \boldsymbol{\delta L}$, where $\boldsymbol{\delta L} = \Sigma_0(\vec{r}) - \Sigma(\vec{r})$, and explicitly invert $\boldsymbol{L}_0$;
- Criteria to define $\boldsymbol{L}_0 = \hat{\Omega} \cdot \nabla + \Sigma_0$?

Asymptotic method – How to define $\boldsymbol{L}_0$

- Two heterogeneous cells share the same set of coefficients if

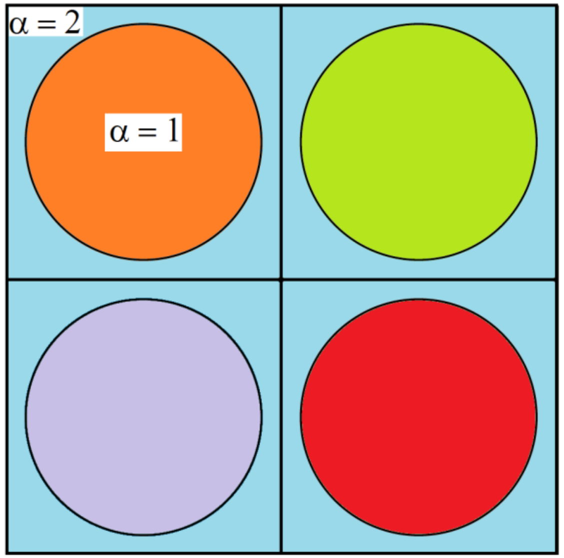
1) They share the same geometry;

2) The group-by-group distance of the total Σ is less then a user's tolerance,

$$\left|\Sigma_{i,\alpha}^{g} - \Sigma_{j,\alpha}^{g}\right| < \varepsilon,\ \ \alpha = 1, \dots, N_R\ ,\ \ g = 1, \dots, N_g\ ,\ \ i \neq j$$

- Reference cross section in region α and group g:

$$\Sigma_{0,\alpha}^{g} \equiv max_{i=1,\dots,4}\left(\Sigma_{i,\alpha}^{g}\right), \alpha = 1, \dots, N_R\ , g = 1, \dots, N_g$$



$i = 1,\dots,4$ heterogeneous cell index

Asymptotic method – Recap and solution

- The original problem has been transformed as follows:

$$\boldsymbol{L}\varphi = q \rightarrow (\boldsymbol{L}_0 - \ \boldsymbol{\delta L})\,\varphi = q$$

- The reference operator $\boldsymbol{L}_0$ is inverted:

$$(\boldsymbol{I} - \boldsymbol{L}_0^{-1}\boldsymbol{\delta L})\varphi = \boldsymbol{L}_0^{-1}q$$

- If $\left\|\boldsymbol{L}_0^{-1}\boldsymbol{\delta L}\right\| < 1$, the solution is given by a Von Neumann expansion :

$$\varphi = \sum_{n=0}^{\infty}\left(\boldsymbol{L}_0^{-1}\boldsymbol{\delta L}\right)^n \boldsymbol{L}_0^{-1}q$$

Asymptotic method – Algorithm

Iteration 0 : $\varphi_{(0)} = \boldsymbol{L}_0^{-1} q$

Check : if $\|\delta \boldsymbol{L}\| < \varepsilon_{\delta L}$, then RETURN

Source update : $q = q + \delta \boldsymbol{L} \varphi_{(0)}$

For $i = 1, 100$:

$\varphi_{(n)} = \boldsymbol{L}_0^{-1} q$ # new iterate

$\delta\, \varphi = \varphi_{(n)} - \varphi_{(n-1)}$ # residual update

if $(\delta\, \varphi < \varepsilon_{\delta\varphi})$, then EXIT

$q = q + \delta \boldsymbol{L}\, \delta\, \varphi$ # source update

Factors causing variation of total macroscopic cross sections

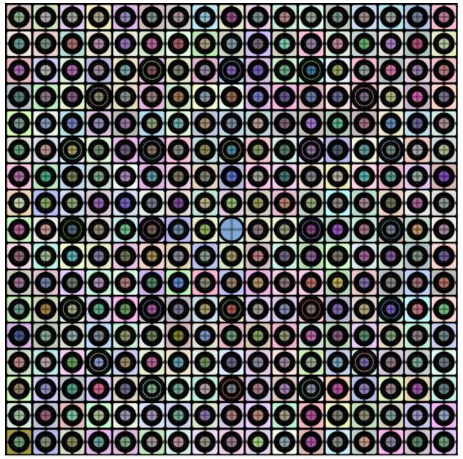
- The flux → Self-shielding;
- Temperature → TH feedback;
- Concentrations → fuel depletion, water density, boron concentration.

In the following, a 17x17 2D UOX-Pyrex benchmark will be considered.

Objective: comparison between standard and asymptotic approach for a depletion calculation.

Validation: depletion effect

- Full assembly, 1473 regions;
- 281-g P3 XS library, fine-structure self-shielding model;
- S(16,8) Chebyshev-Legendre, 128 directions.



Assembly depleted from 0 up to 70 GWd/ton
(50 BU steps).

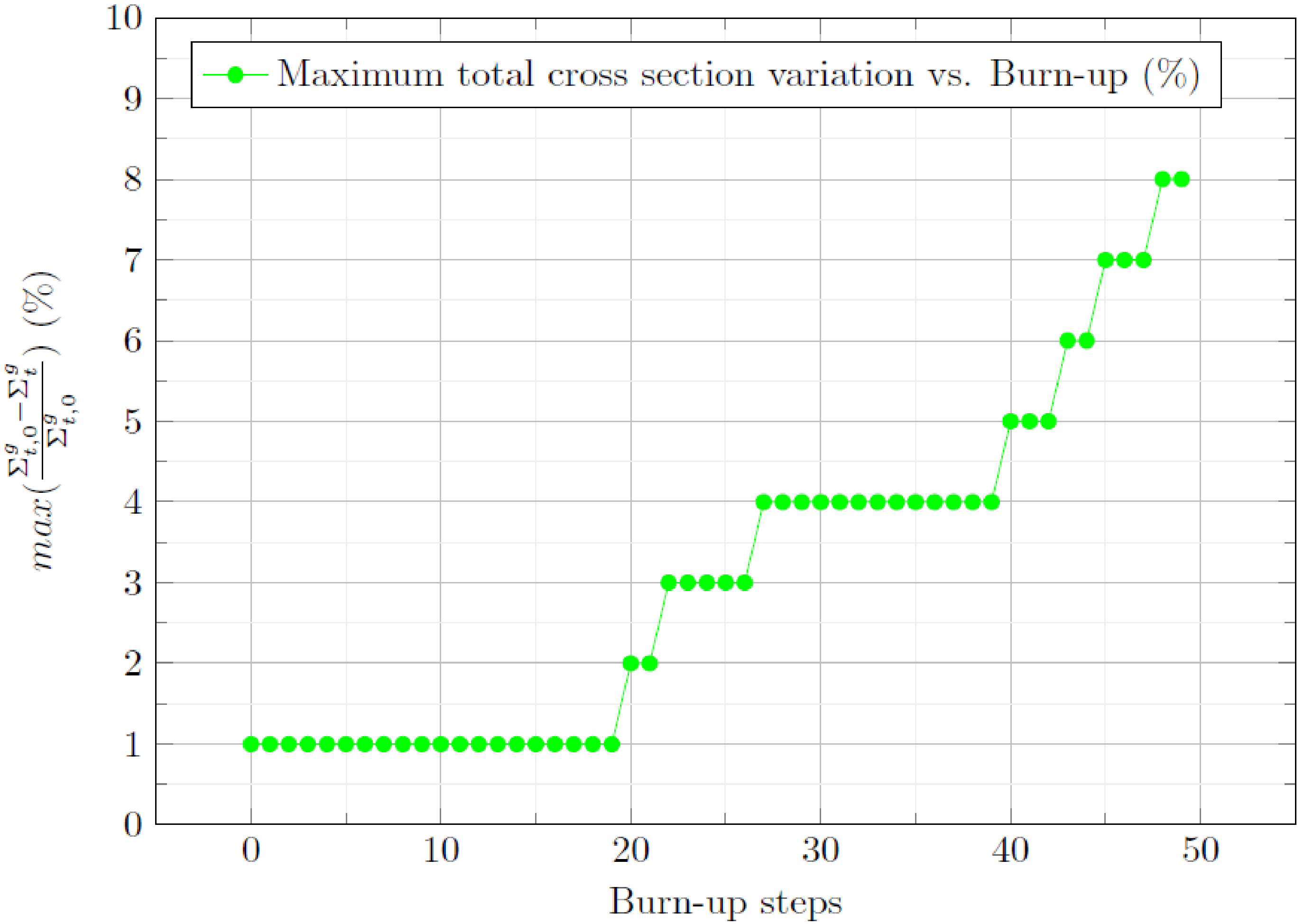
Reference (Standard IDT): 51 cells

- 45 depleted cells (40 for fuel, 5 for PYREX);
- 5 water gap cells, 1 cell for the instrumentation.

Asymptotic IDT : 6 cells

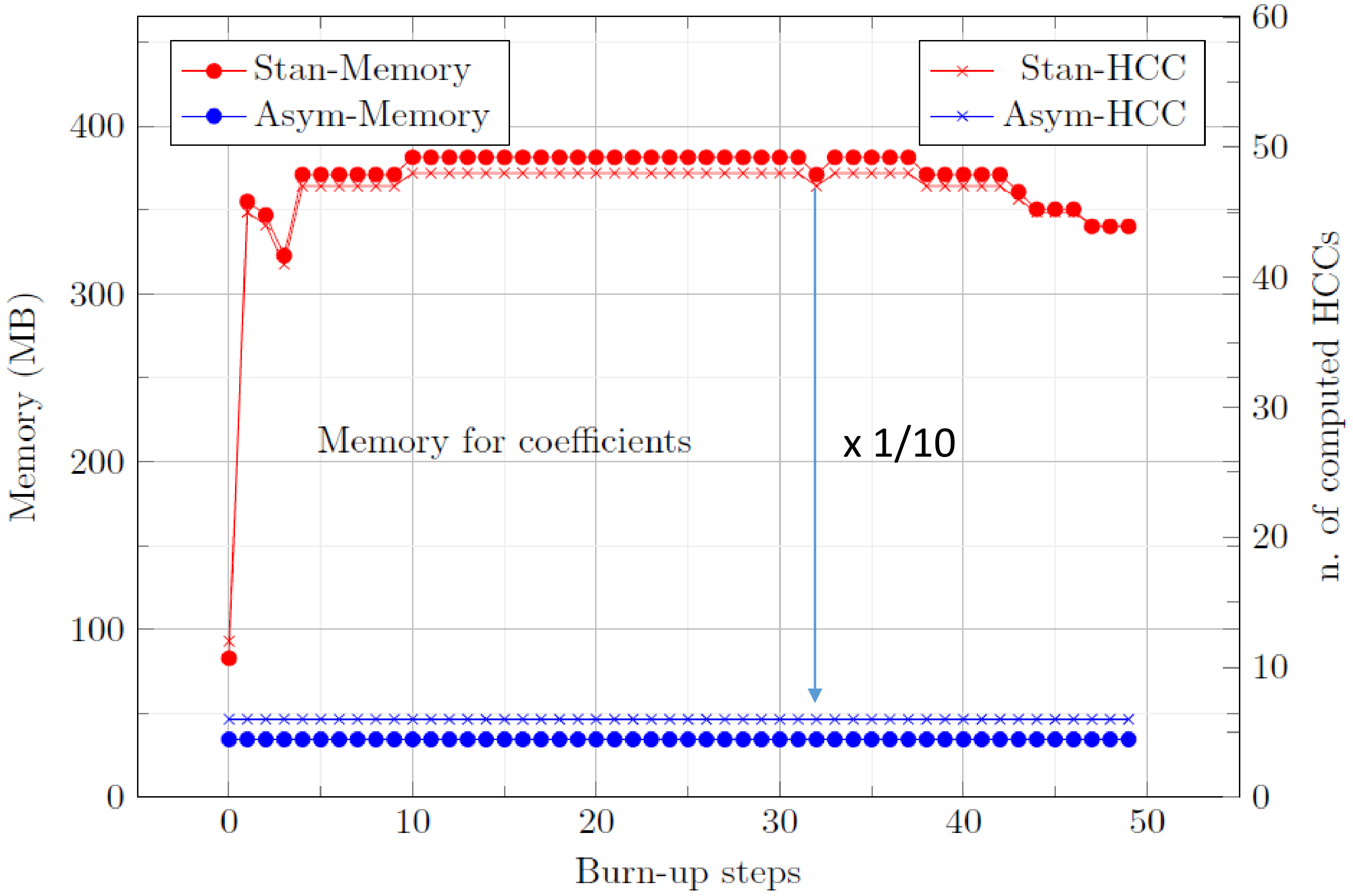
- 2 “unperturbed” cells (1 for the fuel, 1 for the PYREX);
- 3 water gap cells, 1 cell for the instrumentation.

Variation of the total cross section vs Burn-Up



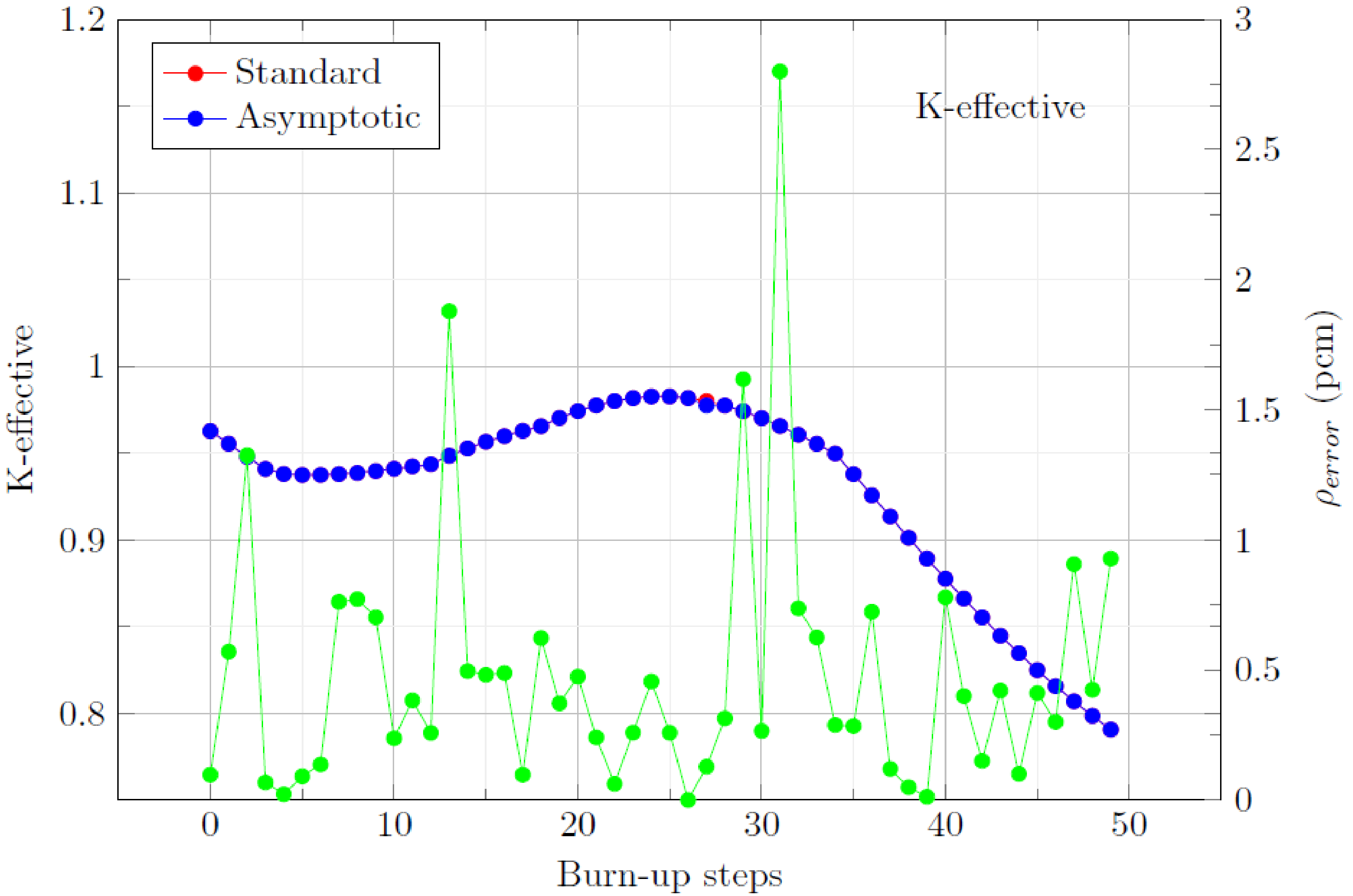
The variation of the total XS does not exceed 8%

Reduction of memory for the angular coefficients



The memory is reduced almost by a factor 10.

Reactivity error vs Burn-Up



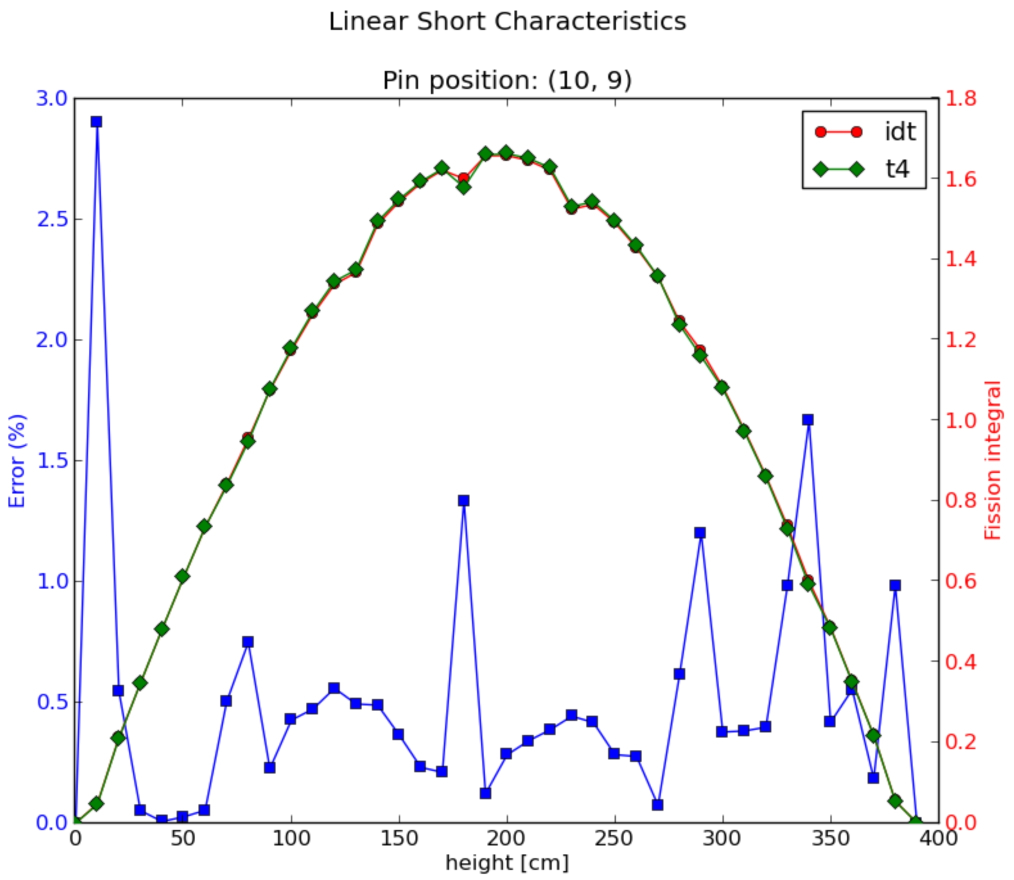
Maximum reactivity error < 3 pcm

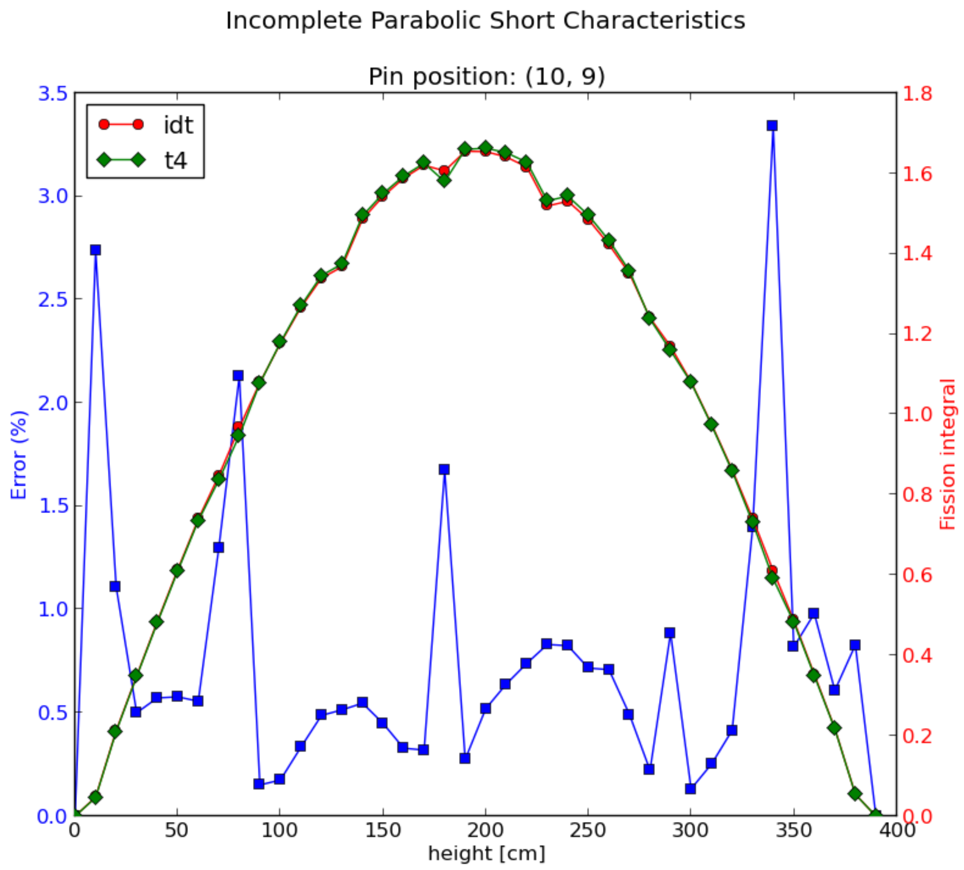
Conclusions and future developments

- Incomplete PSC is able to reduce the memory imprint, while retaining high accuracy;
- Novel approach based on a Von Neumann expansion to lower the number of computed nodes;
- Mixed-order short characteristics $\longrightarrow$ Future work;
- N-Th coupling $\longrightarrow$ Future work.

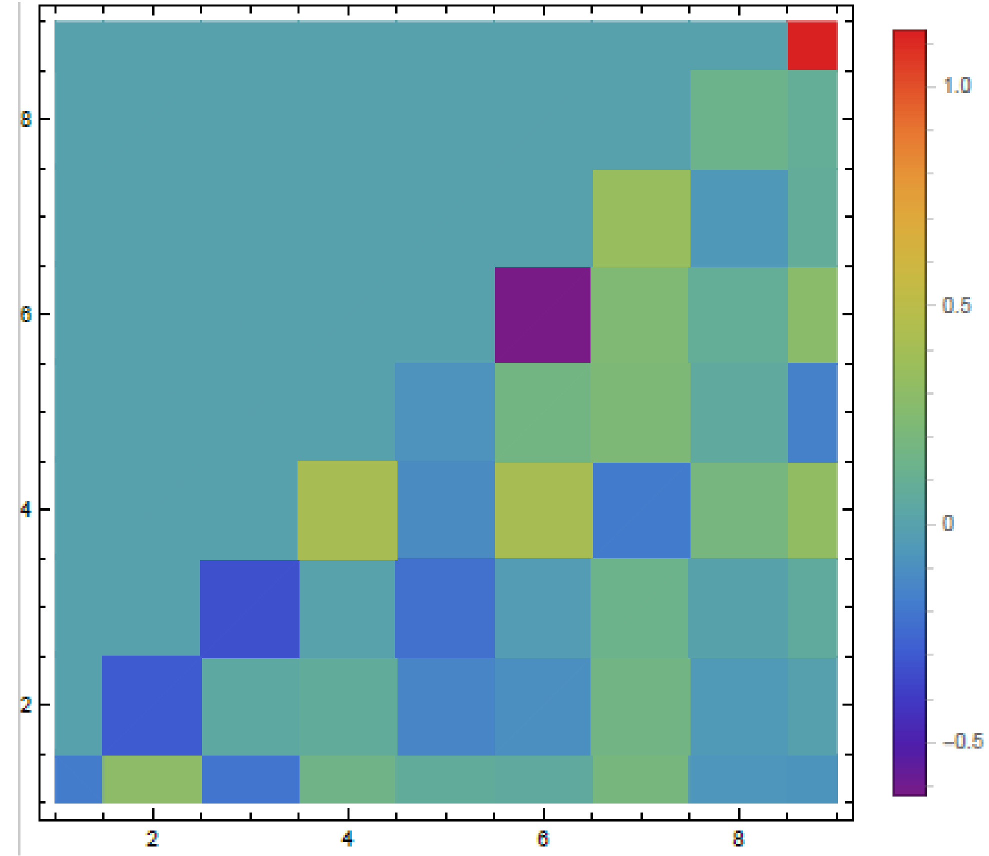
Thank you for your kind attention

3D Watts Bar benchmark – Comparison between LSC and PSC





Validation: self-shielding effect



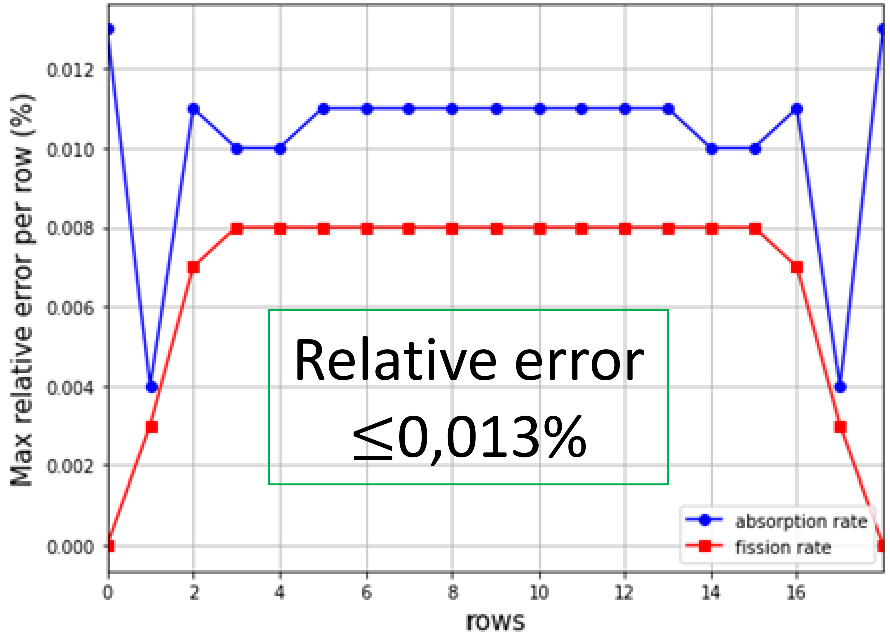
17x17 2D UOX/B4C benchmark

- The “Non-Asymptotic” IDT solution has been verified against TRIPOLI4®;
- The relative error on the absorption rate is at most 1%, as shown in the figure;
- The error on the fission rate is at most 0,4%;
- The relative error on the k-eff is 53 pcm (previous version of IDT → 393 pcm)

Asymptotic method – Numerical results

Comparison between standard and asymptotic approach

IDT	Approx order	Angular quadrature	Tot. nb. of reg.	Tot. nb of surf.	Memory saving (%)	Time [min]	Time (%) for coefficients
Reference	Linear	S(48,6) Cheby-Leg	7256	152	0	72,46	3,12
Asymptotic	Linear	S(48,6) Cheby-Leg	7256	152	57	127,12	0,72



k-eff (ref)	k-eff (pert)	rel. err. (pcm)
0,7963796	0,7963842	-0,58