

# TXT<sub>2</sub>NTAB

## Generating NEMTAB cross-section libraries from SCALE

C. Mesado, A. Labarile, R. Miró, **A. Bernal**

University Research Institute for Industrial, Radiophysical and Environmental Safety (ISIRYM)

Universitat Politècnica València (UPV)

---

**SCALE USERS GROUP WORKSHOP**

**September 26-28 - ORNL**



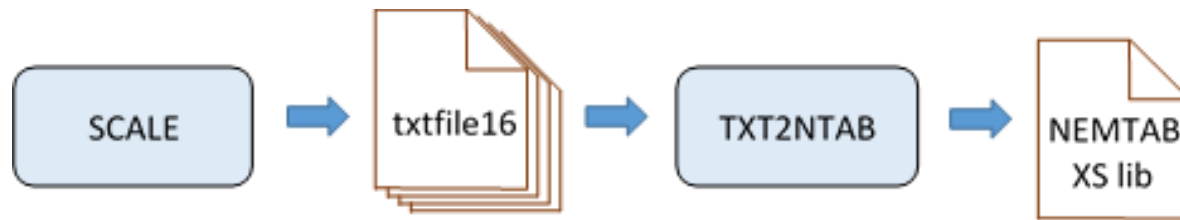
## INDEX

1. INTRODUCTION
2. GUIDE
3. EXAMPLE CASE
4. CONCLUSIONS
5. ONGOING WORK



# 1. INTRODUCTION

**TXT2NTAB** is a set of **MATLAB** scripts developed to **convert** cross sections predicted by **SCALE** (**txtfile16** format) into **NEMTAB** formatted cross section libraries (to use with PARCS for example).

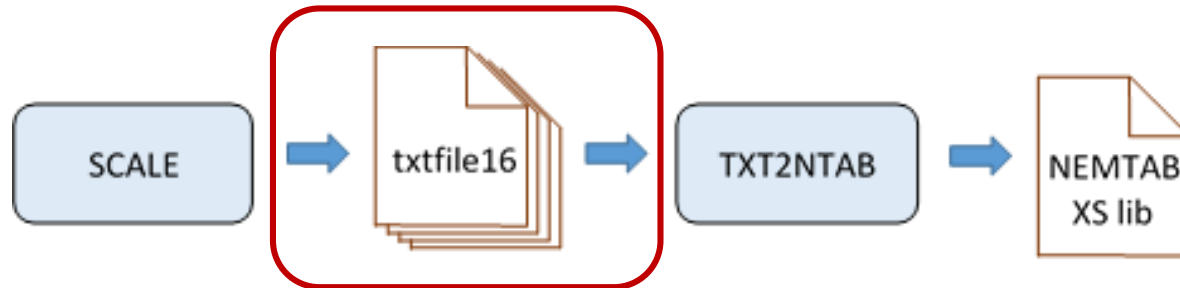


The methodology has been **tested** with a **BWR** GE6 within the author's **PhD** thesis and was also **verified** for a fresh fuel simulation with a **code-to-code** comparison with **CASMO**.



# 1. INTRODUCTION

TXT2NTAB is a set of MATLAB scripts developed to convert cross sections predicted by SCALE (txtfile16 format) into NEMTAB formatted cross section libraries (to use with PARCS for example).



**Each** reactor **segment** must be run in **SCALE** to provide all *txtfile16* needed for a complete core representation.



- ❑ TXT2NTAB was requested by the **UAM-LWR benchmark** organizers.
- ❑ They use it to generate NEMTAB to **distribute** among benchmark participants.
- ❑ Developed within the author's **PhD thesis** (UPV).
- ❑ It handles **TRITON-NEWT** and **Polaris** modules.
- ❑ **Burn-up** dependence feature.
- ❑ It is provided with a friendly **user interface** in ASCII format.
- ❑ A friendly **manual** is also provided with examples.
- ❑ Optionally, it also generates **GEOM** auxiliary file for PARCS.



## Feedback parameters...

- ❑ It is the user **responsibility** to introduce proper feedback parameters.
- ❑ These are set using **branches** in SCALE.
- ❑ There are three important things to consider.
  - Feedback **parameters** to be included: Tfuel, Dmod, Crod (this is fixed in the NEMTAB format).
  - Number of **points** for each parameter. More accurate library, but more computational time.
  - The **range** for the feedback parameters should cover the range of all possible operational conditions.



### TRITON-NEWT

There are:

$i$  moderator density points

$j$  fuel temperature points

one *boron* concentration point

two control rod states (*in/out*)

The reactor history is constant for all branches (nominal state).

Branch index	Feedback parameters	Comment
0	hdm, htm, htf, hbo, hcr=0	Nominal branch.
1	dm1, tm1, tf1, cb1, cr0	
2	dm2, tm2, tf1, cb1, cr0	
...		
$i$	dmi, tmi, tf1, cb1, cr0	$i$ branches with dm, tm points.
...		
$i \cdot j - i + 1$	dm1, tm1, tfj, cb1, cr0	Repeat same branches $j$ times with different tf points.
$i \cdot j - i + 2$	dm2, tm2, tfj, cb1, cr0	
...		
$i \cdot j$	dmi, tmi, tfj, cb1, cr0	
$i \cdot j + 1$	dm1, tm1, tf1, cb1, cr1	Repeat $i \cdot j$ branches with control rod inserted.
$i \cdot j + 2$	dm2, tm2, tf1, cb1, cr1	
...		
$i \cdot j + i$	dmi, tmi, tf1, cb1, cr1	
...		
$2 \cdot i \cdot j - i + 1$	dm1, tm1, tfj, cb1, cr1	
$2 \cdot i \cdot j - i + 2$	dm2, tm2, tfj, cb1, cr1	
...		
$2 \cdot i \cdot j$	dmi, tmi, tfj, cb1, cr1	Total number of branches $2 \cdot i \cdot j + 1$



### POLARIS

In order to maintain the analogy with txtfile16 generated by TRITON-NEWT, the first branch specified in Polaris must define the nominal state (or reactor history).

```

state FUEL : temp=htf
state COOL : temp=htm
state COOL : dens=hdm
state COOL : boron=hbo
state BANK : in=false

'branch - instantaneous change
read branch
'
  BRANCH:      NOM| Branch 1| Branch i| Branch ij | Branch ij+i CR| ...
  add FUEL : temp=htf      tf1 ... tf1 ... tfj ... ... tf1 ... ...
                        tm1 ... tmi ... tmi ... ... tmi ... ...
  COOL : temp=htm      tm1 ... tmi ... tmi ... ... tmi ... ...
  COOL : dens=hdm      dm1 ... dmi ... dmi ... ... dmi ... ...
                        ... ..
  BANK : in=false      ... .. .. .. .. .. .. .. true ... ..
end branch

```





## POLARIS

- File txtfile16 generated by Polaris has some **discrepancies** compared to the **txtfile16** generated by TRITON.
  
- User must **complete** some information for a couple of data blocks:
  - Block 3: Polaris does not write this block only for fresh fuel conditions.
  - Block 4: user must complete the feedback parameter information.
  
- This will be **automatized** in a future release of TXT2NTAB.
  
- More information can be found in the user **guide**.



### Input files and data.

- ❑ **fueltype.dat** contains the **fuel** type **distribution** for the particular reactor (radial mapping).
- ❑ **burnup.dat** only provided for burn-up conditions (no fresh fuel), contains the **burn-up distribution** as a 3D map.
- ❑ **input.dat** is the input data provided by the **user** to define the reactor dimensions, segment information, parameters, feedback parameters...
  - Define as many fuel assemblies and segments as needed.
  - Option for cross section extrapolation for low moderator densities.
  - Three neutronic composition options.
  - NEMTAB generation for a specific burn-up point.
  - Optionally, generate GEOM auxiliary file for PARCS.

More information can be found in the user **guide**.



## Input.dat example

- **Structured** with variables and cards.
- **Comments** are available with % symbol.
- In-code **checks** to reduce bugs.
- Whole description in user **guide**.
- And more ...

```
%radial reflector
ftyp 1                                %fuel type for this assembly
segm 1 1 1                            %segment number for this assembly
fuel 0 0 0                            %1 for fuel segments, 0 for reflector segments, nsegm
absz -15.00 0.00 375.00 390.00       %absolute segment height, nsegm+1

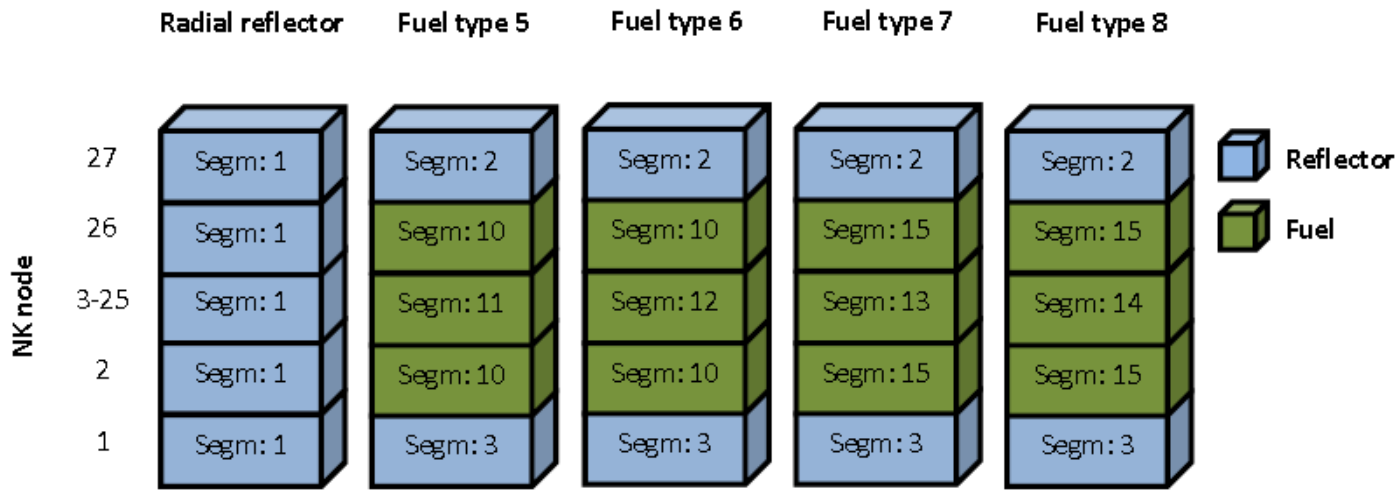
%CALCULATION PARAMETERS
pola 1                                %optional, 1 if txtfile16 were obtained with Polaris module, 0 otherwise, default is 0 ('
nobu 1                                %optional, 1 for fresh fuel, variable burn is then omitted, default is 1
intp linear                          %optional, interpolation method accepted by MATLAB: linear or spline, default and recommu
extp 0                                %optional, 1 for cross section extrapolation for low moderator densities, default is 0 (:
dlim 0.17075;                        %limit for extrapolation, omitted if variable extp is 0
geop 0                                %optional, 1 to create GEOM file to be used with PARCS, default is 0
nkop 0                                %optional, options are 0, 1 or 2. Option to compute number of neutronic composition, the:

%FEEDBACK PARAMETERS
%to look up in txtfile16
dm16 0.03814 0.17753 0.45632 0.73511 0.84034 0.94281 0.99829 %moderator density, increasing order
tm16 561.4 561.4 561.4 561.4 493 393 293 %moderator temperature for each moderator den.
tf16 293 660.8 879.5 1028.6 1396.5 1764.3 2132.2 %fuel temperature, increasing order
cb16 1935 %scalar only (no variation with boron concentration yet)
```



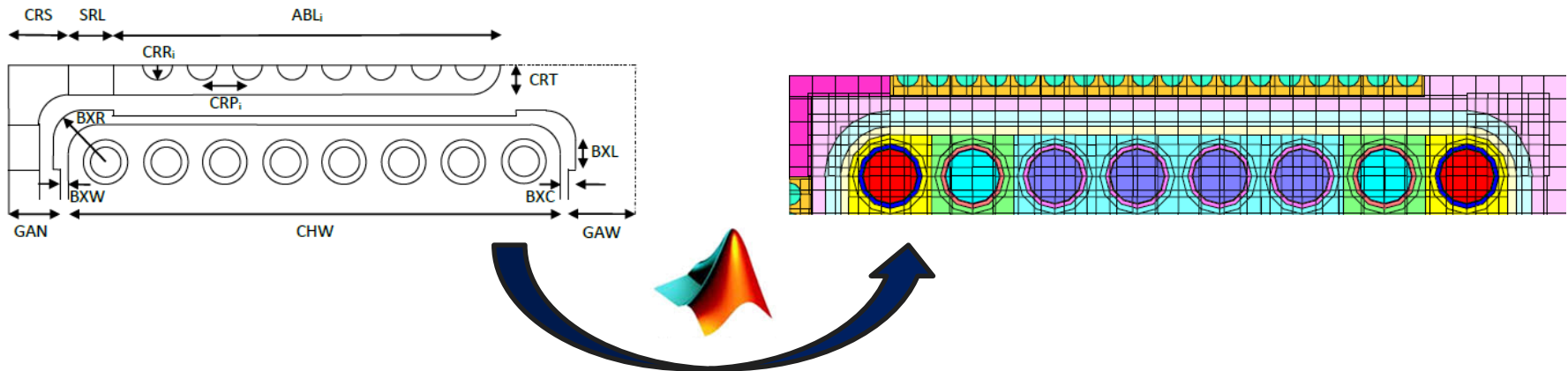
### 3. EXAMPLE CASE

- ❑ **Segment information** is given by IBERINCO.
- ❑ **Simplified** case to **test** the methodology.
- ❑ **Fresh** fuel **conditions** (computational resources).
- ❑ 6 fuel segments and 3 reflector segments.
- ❑ **Burn-up** conditions **implemented** (interpolation).



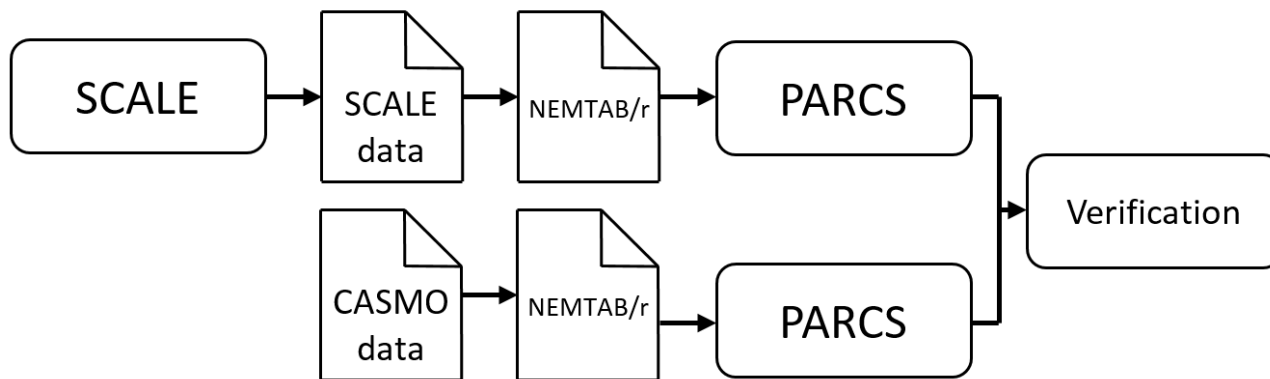
### 3. EXAMPLE CASE

- ❑ **Verification** with a code-to-code comparison with **CASMO**.
- ❑ CASMO outputs are given by **IBERINCO**.
- ❑ A **MATLAB** tool was developed to **translate CASMO** inputs into **SCALE** models.



### 3. EXAMPLE CASE

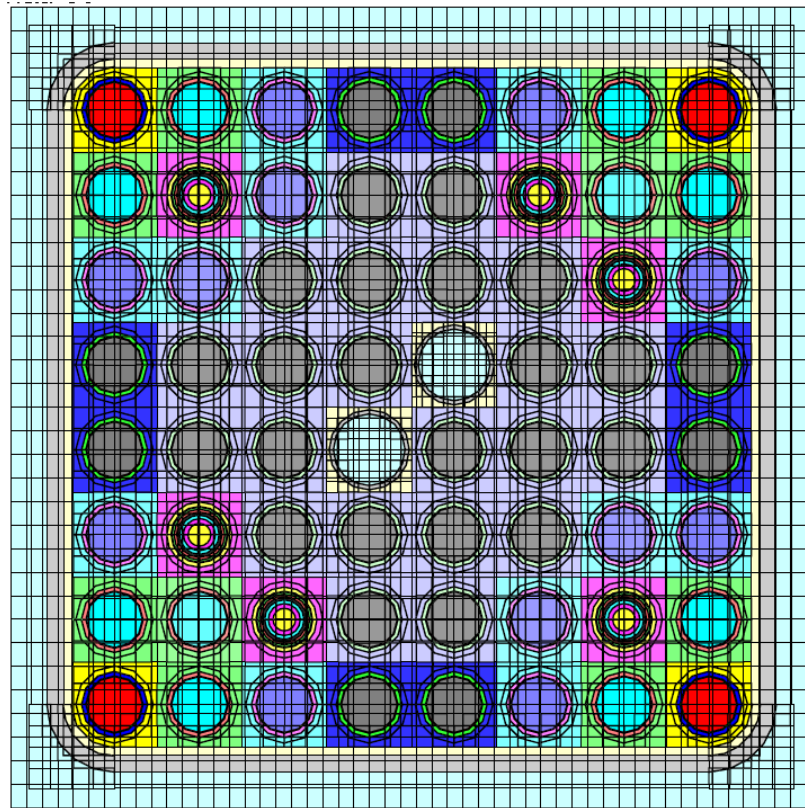
- ❑ **Verification** with a code-to-code comparison with **CASMO**.
- ❑ CASMO outputs are given by **IBERINCO**.
- ❑ A **MATLAB** tool was developed to **translate CASMO** inputs into **SCALE** models.
- ❑ **NEMTABs** can be **obtained** out of CASMO results and out of SCALE results.
- ❑ The same **PARCS model** can be run with both NEMTAB sets.
- ❑ Results comparison is used to **verify** the process.



### 3. EXAMPLE CASE

- ❑ Example of lattice model translated from CASMO and obtained with MATLAB tool.
- ❑ Represents only one segment of the core.

- ❑ TRITON-NEWT is used.
- ❑ 5 different  $\text{UO}_2$  pin types.
- ❑ 1 Gd pin type.
- ❑ Two water rods.



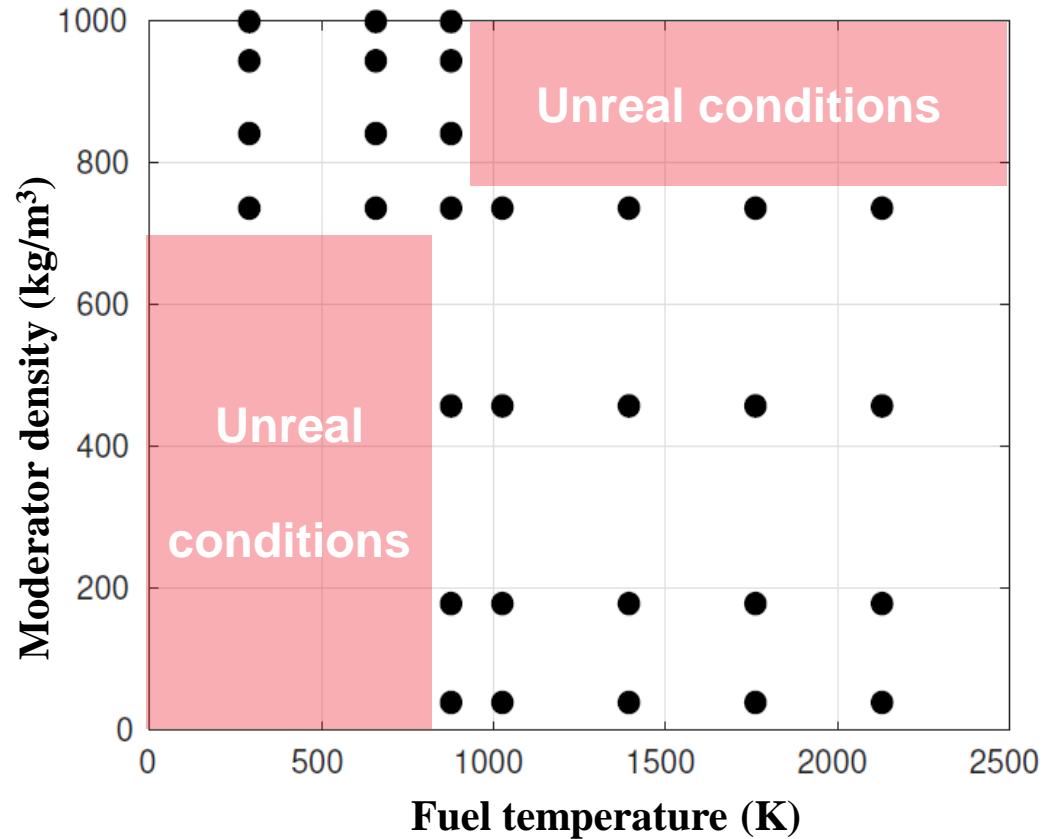


### 3. EXAMPLE CASE

User must decide what **feedback parameters** (branches) to include for each segment.

Some **branches** can be **discarded** to save computational time.

However, there is no problem if the user wants to simulate **all branches**.





### 3. EXAMPLE CASE

Data shown hereafter are full core results obtained with **PARCSv3.2**, either with NEMTABs out of SCALE (with TXT2NTAB) or with NEMTABs out of CASMO.

ARO	CASMO	SCALE v7-56		SCALE v7-252	
		Default	MCDANCOFF	Default	MCDANCOFF
$k_{\text{eff}}$	1.03171	1.03601	1.03417	1.03533	1.03416
<b>Error (pcm)</b>	-	429.5	246.0	362.1	<b>244.9</b>

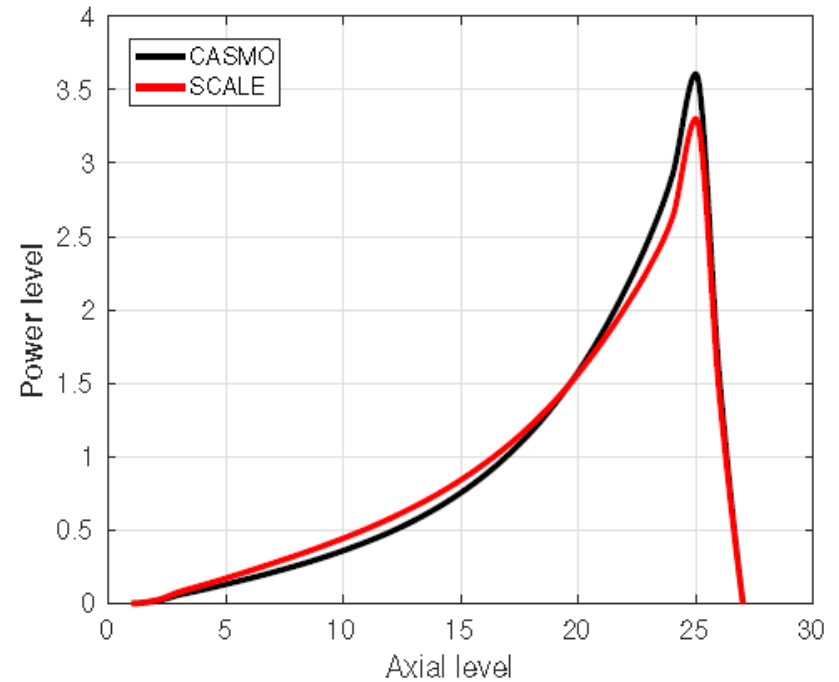
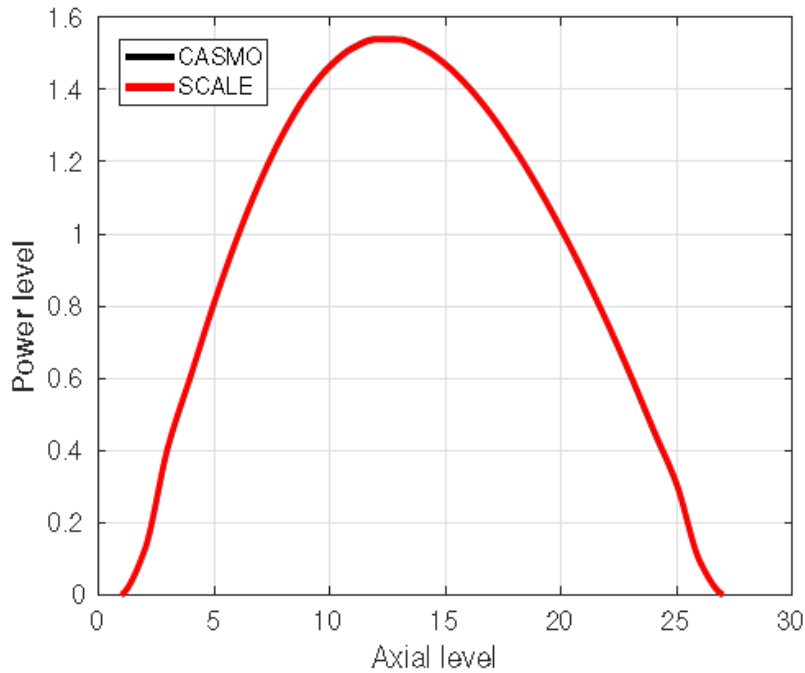
ARI	CASMO	SCALE v7-56		SCALE v7-252	
		Default	MCDANCOFF	Default	MCDANCOFF
$k_{\text{eff}}$	0.79702	0.80023	0.79893	0.80011	0.79925
<b>Error (pcm)</b>	-	321.1	<b>191.5</b>	308.9	223.3



### 3. EXAMPLE CASE

ARO	RMS <sub>axial</sub> (%)	
	V7-56	V7-252
Default	0.24	<b>0.21</b>
MCDANCOFF	0.24	<b>0.21</b>

ARI	RMS <sub>axial</sub> (%)	
	V7-56	V7-252
Default	11.98	<b>11.53</b>
MCDANCOFF	12.09	11.56

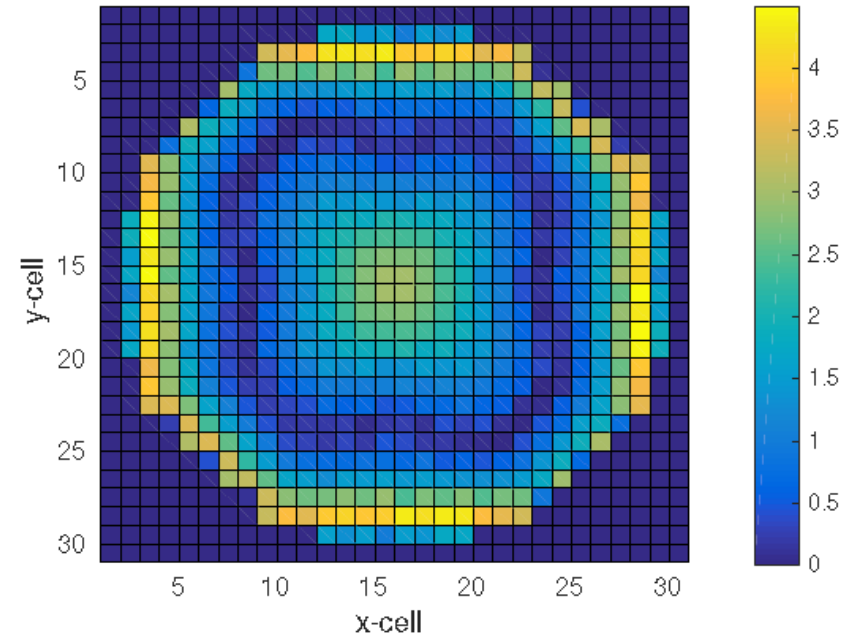
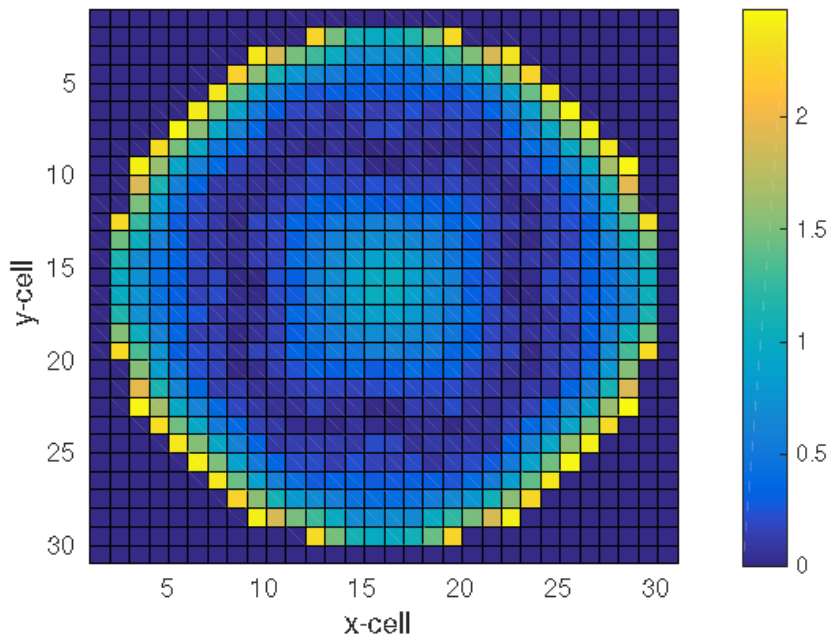


### 3. EXAMPLE CASE

ARO	RMS <sub>radial</sub> (%)	
	V7-56	V7-252
Default	0.53	0.53
MCDANCOFF	0.53	0.53

ARI	RMS <sub>radial</sub> (%)	
	V7-56	V7-252
Default	1.75	1.73
MCDANCOFF	1.74	<b>1.72</b>

#### Absolute radial error (%)



### 3. EXAMPLE CASE

- ❑ With **accurate Dancoff** factors the  $k_{\text{eff}}$  difference is **reduced** almost 50%.
- ❑ Their influence over the axial and radial **power** profiles is **negligible**.
- ❑ It was found that when accurate Dancoff factors are used, an unexpected **increase** in **memory** was required by **SCALE**.

ARO	$k_{\text{eff}}$ (pcm)		RMS <sub>axial</sub> (%)		RMS <sub>radial</sub> (%)	
	V7-56	V7-252	V7-56	V7-252	V7-56	V7-252
Default	429.5	362.1	0.24	0.21	0.53	0.53
MCDANCOFF	246.0	244.9	0.24	0.21	0.53	0.53

ARI	$k_{\text{eff}}$ (pcm)		RMS <sub>axial</sub> (%)		RMS <sub>radial</sub> (%)	
	V7-56	V7-252	V7-56	V7-252	V7-56	V7-252
Default	321.1	308.9	11.98	11.53	1.75	1.73
MCDANCOFF	191.5	223.3	12.09	11.56	1.74	1.72



### 3. EXAMPLE CASE

- ❑ The **master library** has an effect over the  $k_{\text{eff}}$  (20 – 70 pcm).
- ❑ But it is almost **irrelevant** to the power **profiles**.
- ❑ In general, the  $k_{\text{eff}}$  difference is smaller when the **v7-252** is used.

ARO	$k_{\text{eff}}$ (pcm)		RMS <sub>axial</sub> (%)		RMS <sub>radial</sub> (%)	
	V7-56	V7-252	V7-56	V7-252	V7-56	V7-252
Default	429.5	362.1	0.24	0.21	0.53	0.53
MCDANCOFF	246.0	244.9	0.24	0.21	0.53	0.53

ARI	$k_{\text{eff}}$ (pcm)		RMS <sub>axial</sub> (%)		RMS <sub>radial</sub> (%)	
	V7-56	V7-252	V7-56	V7-252	V7-56	V7-252
Default	321.1	308.9	11.98	11.53	1.75	1.73
MCDANCOFF	191.5	223.3	12.09	11.56	1.74	1.72



## 4. CONCLUSIONS

- ✓ TXT2NTAB program is developed to fill the **gap** between SCALE and a core simulator.
- ✓ Problem-dependent cross section libraries in NEMTAB format can be obtained from **TRITON** or **Polaris**.
- ✓ The choice of **feedback parameters** is the user responsibility.
- ✓ Significant **computational time** could be needed with TRITON models (use of Polaris).
- ✓ A **friendly** ASCII user **interface** is used to introduce the data with ease.
- ✓ A user **guide** is provided.



TXT2NTAB is actively being updated...

- ✓ For **U&S** analysis. Process **SAMPLER** perturbed txtfile16 to generate...
  - One set of NEMTAB/r with the **average** response.
  - One set of NEMTAB/r with their **standard deviation**.
- ✓ Handle **branches** of **Polaris** without the user intervention.
- ✓ Generate NEMTABs for different **reactor histories**.



You can forward any **question** or **comment** to ...

[cmesado@iqn.upv.es](mailto:cmesado@iqn.upv.es)

Besides you can download **TXT2NTAB User Guide**

and the author PhD Thesis here ...

[goo.gl/nbmxNp](https://goo.gl/nbmxNp)

**C. Mesado (2017).** *“Uncertainty Quantification and Sensitivity Analysis for Cross Sections and Thermohydraulic Parameters in Lattice and Core Physics Codes. Methodology for Cross Section Library Generation and Application to PWR and BWR.”* PhD thesis, Universitat Politècnica de València (UPV).

