Memorandum

idm@F4E Ref:	F4E_D_2JFFDN v.1.1	Date	2019-10-14

Subject: **iWW-GVR: A tool to manipulate MCNP weight window (WW) and to generate Global Variance Reduction (GVR) parameters**

From: **M. Fabbri, Á. Cubí**

Department: A&C / Engineering Unit / ITER Department

Contact alvaro.cubi@ext.f4e.europa.eu, marco.fabbri@f4e.europa.eu

To: **Everybody interested**

In order to keep F4E nuclear analysis capabilities up-to-date with the latest, state-of-the-art method and post-processing tools, a new practical tool called iWW-GVR to manipulate MCNP weight window and to generate global variance reductions has been developed.
The tool is a python 3.6 based script able to generate global variance reductions weight window (WW) importing any mesh format in meshtally by D1SUNED, MCNP5 or MCNP6. Mesh format includes usual MCNP column or matrix format and also specific D1SUNED format including cell or isotope contribution binning and source mesh importance format. Both Cartesian and Cylindrical coordinates are allowed. The tool incorporates also simple functions to operate with weight windows (e.g., analyse, add and remove WW set, write, plot).
The tool is used through a text based interactive menu, and it can be run under Windows system. To conclude, the tool has been verified and recorded in this document.

What iWW-GVR does

Capabilities of iWW-GVR are divided in four categories:

- WW information
- WW analysis
- Operation on WW
- Generation of GVR WW

WW information:
Display a summary of the WW sets contained and the correspondent detailed information (No. sets, dimensions, No. bins, No. Voxel).

WW analysis:
Analysis of the WW sets providing to the user the minimum and maximum value, the maximum ratio between nearby voxels and the corresponded histogram, the per cent No. of bins with value bigger that zero, reports the negative values (if present), the voxel average dimensions and volume (only for Cartesian coordinates).

Operation on WW
Operation on WW allows performing various operations as[1]:

- Add: to add a WW set copying the first one with the possibility to normalize and soften it according to the parameters inserted. In addition, there is the capability to fill automatically "all the holes" present within the domain using the closest value different from zero[2].
- Remove: to remove the first or the second WW set[3].
- Soft: to modify the WW values by applying a normalization factor and a softening factor.
- Mitigate: to decrease the ratio between nearby voxels which are bigger than the threshold inserted by the user. The single WW_{value} is computed as follow:

$$WW_{value} = \frac{\max|WW_{nearby}}{\max|WW_{ratio}*0.9}$$

  Where:

  - $\max|WW_{nearby}$ is the maximum value of the nearby cells
  - $\max|WW_{ratio}$ is the maximum ratio with the nearby cells imposed by the user

- Plot: to plot in an external JPEG file a user defined plane with a specific particle and energy (only for Cartesian coordinates).
- Write: to export the modified WW in the MCNP ASCII format or to VTK one which can be further analyzed/manipulated in dedicated readers (e.g., Paraview)

Generation of GVR WW:
To generate GVR WW employing a meshtally file given by the user[4] [1-2-3]. Taking advantage of the mesh2vtk libraries [4], the meshtal is loaded, selected and hence processed as follow:

$$WW_{GVR_i} = \left(\frac{\Phi_i}{\max|\,\Phi_{\text{value}}} * \frac{2}{\beta + 1}\right)^{softening_{factor}}$$

where:

- Φ_i is the mesh tally voxel value at the generic position i
- $\max|\,\Phi_{\text{value}}$ is the maximum value of the meshtal selected
- β is the maximum splitting ratio
- $softening_{factor}$ is a factor between]0,1] to mitigate the splitting/russian roulette [5]

The WW-GVR generated has a single energy bin and the dimension/discretization of the meshtally selected. If necessary, the WW can be further manipulated by the iWW-GVR routine.

[1] WW headers are updated if necessary according to the user selections.
[2] This operation can be done if only one WW set is present.
[3] This operation can be done if only two WW sets are present.
[4] The meshtally selected shall have only one energy bin.

How to install it

The iWW-GVR is distributed in a preassembled python wheel. Going to the dist folder and typing the following command line, the tool and all the related modules (i.e., dependencies), if not already present in the python environment, are installed:

```
$ pip install iww_gvr-<<version>> --user
```

It is recommended to create a dedicated python virtual environment or a conda env to avoid any possible conflict with different packaging versions.

How to create a new package

1. Install proper tools, from command line execute:

```
$ python -m pip install --user --upgrade setuptools wheel
```

2. Go to iww_gvr/iww_gvr: add new scripts and modify main.py accordingly if necessary
3. Go to iww_gvr parent folder
4. Open '__version__.py'.
5. Modify the version number in the variable 'version' and save.
6. Go to iww_gvr parent folder
7. Go to the same folder where setup.py is located and from command line execute:

```
$ python setup.py sdist bdist_wheel clean --all install clean --all
```

8. A new version ready for installation has been built and stored in the "dist" folder.

How to use it

The iWW-GVR tool operates through an interactive text menu interface. To be launched the user has to type the command:

```
$ python -m iww_gvr.py
```

The principal menu has seven options (plus "Exit" option), see Fig.1. The keywords between parentheses displayed in the menu are to be used to select the operation described hereinafter.

```
************************************************
      Weight window manipulator and GVR
************************************************

* Open weight window file    (open)
* Display ww information     (info)
* Write                      (write)
* Analyse                    (analyse)
* Plot                       (plot)
* Weight window operation    (operate)
* GVR generation             (gvr)
* Exit                       (end)
```

Figure 1: main menu of iWW-GVR

- **open:** to append weight window files to be processed. This action is carried out with the keyword "*open*" hence followed by the "filename" of the WW once requested. The user can monitor the status of the operation by means of the progressing bar which provides information as the estimated time to complete the operation and the overall time passed.

```
************************************************
      Weight window manipulator and GVR
************************************************

* Open weight window file    (open)
* Display ww information     (info)
* Write                      (write)
* Analyse                    (analyse)
* Plot                       (plot)
* Weight window operation    (operate)
* GVR generation             (gvr)
* Exit                       (end)

enter action :open
enter ww file name:wwinp_V001
Reading: 100%|@@@@@@@@@@@| 277208/277208 [00:01<00:00, 174436.92 lines read/s]
enter action :
```

Figure 2: "end" selection

- **info:** to display basic information about the WW selected[5]. Data as axis ranges and discretization, No. of voxel, No. of particle contained and maximum energy are printed in screen.

```
************************************************
       Weight window manipulator and GVR
************************************************

* Open weight window file   (open)
* Display ww information    (info)
* Write                     (write)
* Analyse                   (analyse)
* Plot                      (plot)
* Weight window operation   (operate)
* GVR generation            (gvr)
* Exit                      (end)


Input files present:
- [1] wwinp_V001
- [2] wwinp_V007
enter ww index:1

The following WW file has been analysed:  wwinp_V001

               ------From----- -------To------ ----No. Bins---
    X -->          500.00         1700.00           120
    Y -->         -420.00          420.00           84
    Z -->         -700.00          950.00           165

The file contain 1 particle/s and 1663200 voxels!

***** Particle No.1 ****
Energy[1]: [50.0]
```

Figure 3: “info” operation

- **write:** to export the modified WW in the MCNP ASCII format or to VTK one which can be further analyzed/manipulated in dedicated readers (e.g., Paraview)

```
Input files present:
- [1] wwinp_V001
- [2] wwinp_V007
enter ww index:1

* Write to wwinp           (wwinp)
* Write to VTK             (vtk)
* Exit                     (end)

enter action :vtk
VTK... written!
```

Figure 4: “write” selection

The exported MCNP ASCII file is named as “filename_2write” whereas the vtk as “filename.vtr”.

[5] If only one WW is appended the selection step is skipped to improve the user experience.

- **analyse:** to precisely analyze the WW providing to the user parameters as the minimum and maximum value, the maximum ratio between nearby voxels and the corresponded histogram, the per cent No. of bins with value bigger that zero, reports the negative values (if present), the voxel average dimensions and volume. In addition, it exports the distribution of the ratio between nearby voxels per energy bin and particle in a dedicated histograms in a file named as "filenameWW+ParNo+E=ENERGYMeV+Ratio_Analysis.jpeg", Fig. 5.

```
Input files present:
- [1] wwinp_V001
- [2] wwinp_V007
enter ww index:1
Insert the toroidal coverage of the model [degree, all, auto]: 40
Ratios: 100%|████████████████████████| 165/165 [00:05<00:00, 31.29 Z slices/s]

The following WW file has been analysed:  wwinp_V001

----------------Par.No 1----------------

Min Value        : [0.0]
Max Value        : [0.333333]
Max Ratio        : [4521.467125180551]
No.Bins>0 [%]    : 177.65
Neg.Value        : NO
Voxel Dim[X,Y,Z]: [10.0, 10.0, 10.0] cm
Voxel Vol[cm3]   : 1.0000e+03

----------------------------------------
```

Figure 5: "analyse" selection

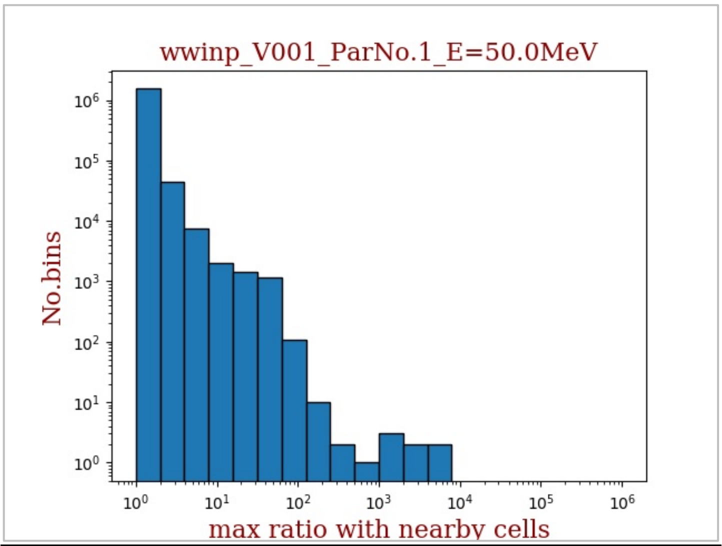

Figure 6: "ratio" histogram distribution selection

To properly compute the analyzed parameters in Cartesian coordinates, the user shall define the toroidal coverage of the model by one of the three options provided[6]:

- *all*: the WW is completed contained within the MCNP model domain
- *No.degree*: insert the toroidal coverage of the model assuming that the torus is developed in the XY plane having the middle plane over X.
- *auto*: the script automatically computes the coverage of the model assuming the domain is composed by any XY points which have at least a voxel different from zero along the Z direction.

In the case of cylindrical coordinates there is two coverage options:

- *all*: the WW is completed contained within the MCNP model domain

[6] The routine considers one a XY plane which is representative for all the Z planes.

- *auto*: the script automatically computes the coverage of the model assuming the domain is composed by a section of an axial slice of the cylinder. The section is defined as all the positions that have a value different than zero in at least one axial slice.

As for the "open" function, the status of the operation can be evaluated by means of the progressing bar which provides information as the estimated time to finish the operation and the overall time passed.

- **plot:** to export a logarithmic plot of a specific plane which is defined under the guidance of the iWW-GVR tool. The file is named as "filenameWW+Plane +Pos+ParNo+E=ENERGYMeV.jpeg", Fig.7. Fields are requested only if more than one option is present. This capability is not present for cylindrical WWs.

```
Input files present:
- [1] wwinp_V001
- [2] wwinp_V007
- [3] test2
enter ww index:3
Select the plane[X,Y,Z] :Y
Select the quote [Y-->-50.0, 5.0 cm]:0
Select the energy [MeV]:10
Plot...Done!
```

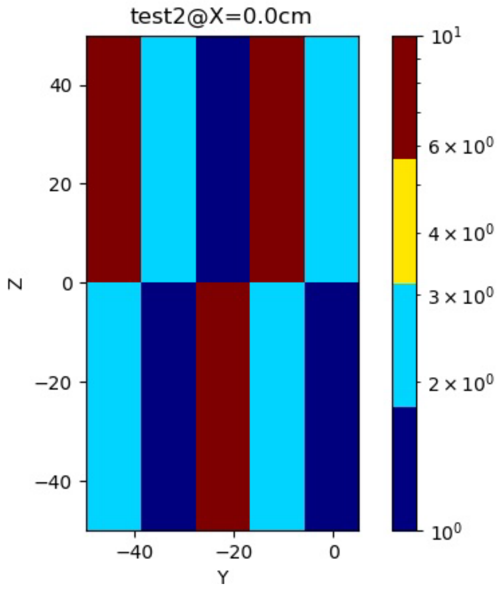

Figure 7: "plot" option: command line vs plot

- **operate:** to perform operation and manipulation on meshes. The operate menu is shown in Fig.8.

```
* Softening and normalize      (soft)
* Mitigate long histories      (mit)
* Add                          (add)
* Remove                       (rem)
* Flipping                     (flip) >> To be completed
* Exit                         (end)
```

Figure 8: "operate" menu

The "soft" function creates a copy a previously appended WW which is modified by with the normalization, the softening and the hole-filling if requested.

```
enter action :soft
Name of the result file:WW_SOFT
Hole Filling approach [Yes, No]: No
Insert the softening factor: 0.5
Insert the normalization factor: 1
Softening done!
```

Figure 9: "soft" options

The "mit" option modifies the voxel values in which the ratio between nearby voxels overpasses the threshold inserted by the user. To give an idea of the modification performed, the number of voxel impacted is reported in screen. An example of the effect on a typical WW for C-Model with a maximum value of 100 is reported next.

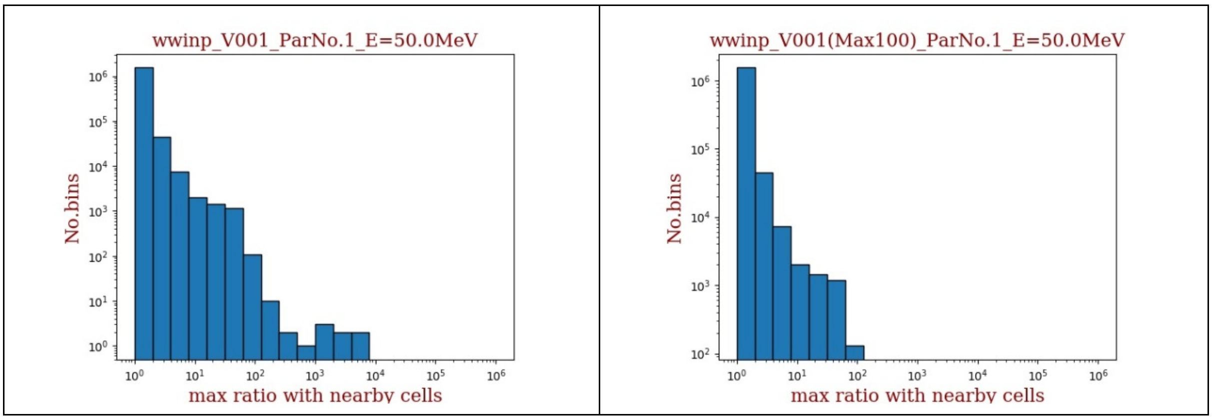

Figure 10: "mit" options effect

To conclude, the "add"/"remove" options are very useful in adding or removing WW set from the file to prepare the simulation for instance for coupled transport giving the user also the possibility to soften, normalize or hole-fill the WW set.

- **gvr:** to generate GVR WW by means of the global variance reduction techniques importing the flux directly from a MCNP meshtal file which is used as a skeleton (i.e., dimension, discretization, which are also printed in screen). The user has also the possibility to select the tally to use, normalize it, soften and hole-fill the mesh if necessary.
-

```
Please write the name of the resulting GVR: GVR2WW
Insert the maximum splitting ratio (beta): 5
Insert the softening factor: 0.5
Enter the meshtally file to load:V000_MODE-0_PLASMA_5e9.mesh
The following tallies have been found:

 14

Choose the mesh tally to use for the GVR: 14

The following WW file has been analysed:  GVR2WW

                -------From----- --------To------ ----No. Bins---
    X -->             0.00          1700.00          85
    Y -->          -580.00           580.00          58
    Z -->         -1310.00          1690.00          150

The file contain 1 particle/s and 739500 voxels!

***** Particle No.1 ****
Energy[1]: [100]


 Insert the toroidal coverage of the model [degree, all, auto] for Hole Filling
approach or [No]: No
 GVR: 100%|############################| 150/150 [00:03<00:00, 44.97 Z slices/s]
```

- **end:** it is used to terminate the usage of the iWW-GVR which, by the way, can be abnormally interrupted by Ctrl+C at any time.

```
************************************************
       Weight window manipulator and GVR
************************************************

* Open weight window file    (open)
* Display ww information     (info)
* Write                      (write)
* Analyse                    (analyse)
* Plot                       (plot)
* Weight window operation    (operate)
* GVR generation             (gvr)
* Exit                       (end)

enter action :end

Thanks for using iWW-GVR! See you soon!
```

Figure 11: "end" selection

iWW-GVR verification process

The script has been verified in a first step employing simple weight window meshes and verifying each single function. The WW values were manually input to easily check the results from typical operations. The reader and the plot function was endorsed double checking all possible sections. In the same way, the info, analyse, soft and mitigate functions operated as expected once WW values were manually changed. As these files are relatively small, the complete WW were double checked visually, parameter by parameter.

In a second verification step, the code was tested against more complex sets as for instance a Cartesian ww mesh (120x84x165) previously employed for a C-Model simulation and a cylindrical one obtained from E-lite. As this mesh is too large to be verified manually, the analyse and plot functions were employed to confirm the validity of the manipulation performed. The correct orientations of the cross section were endorsed by the position of components and their orientations. Operations like hole-filling, soft and mitigate were also validated, Fig.12-13-14-15. Moreover, the write function was also verified importing in Paraview and MCNP the WW modified files validating the correctness of the values as well as of the formats.

Moreover, several WW were specifically created by dummy MNCP simulation to double check each single feature of the iWW-GVR nonetheless they are not reported here for sake of simplicity.

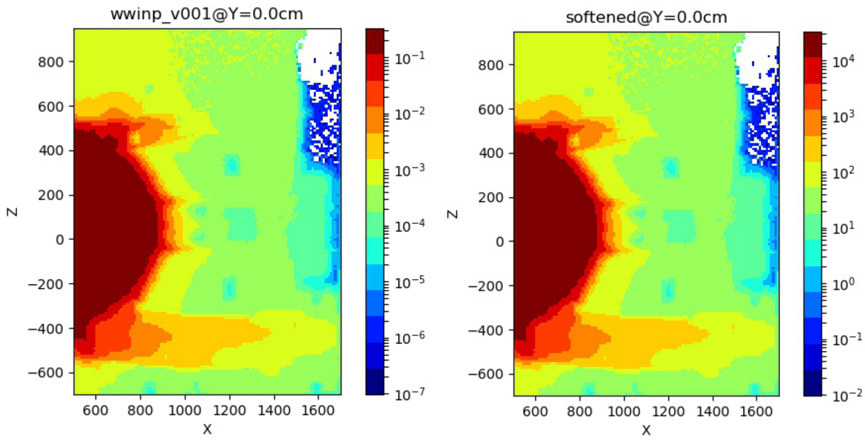

Figure 12 : C-Model WW before and after normalization (x100000)

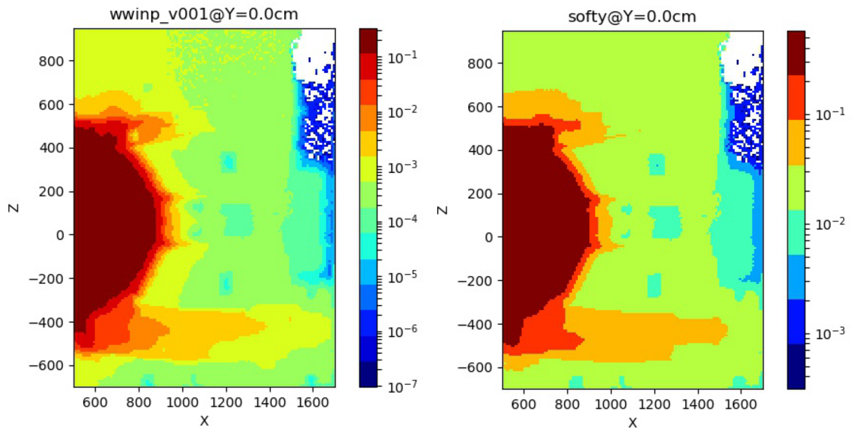

Figure 13 : C-Model WW before and after softening (factor=0.5)

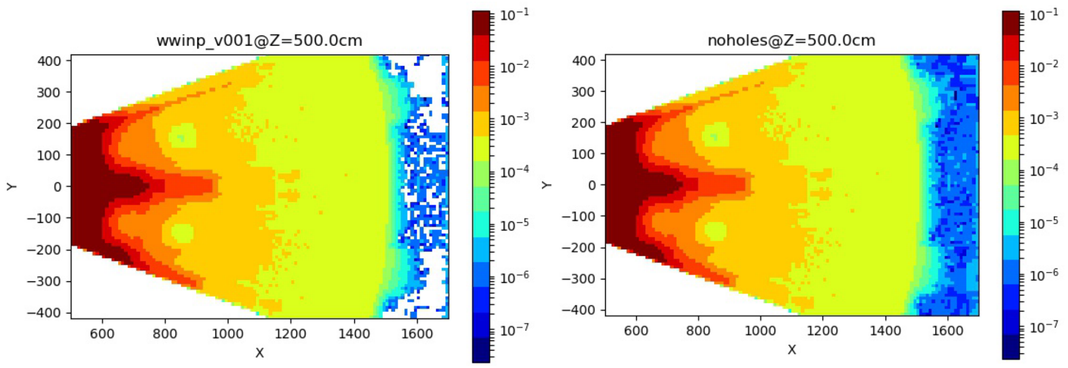

Figure 14: C-Model WW Before and after a Hole-filling operation

Internal

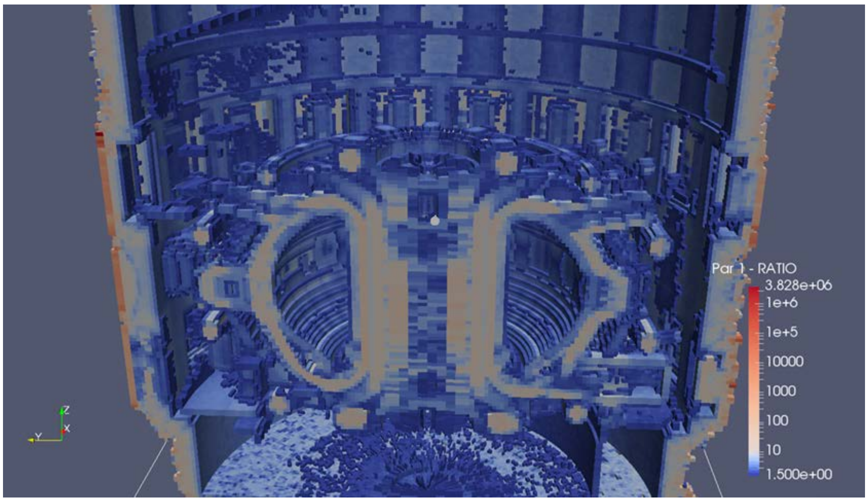

Figure 15: E-lite WW ratios values

Recommendations and warnings

- Testing only done over neutron/photon/neutron&photon WW sets
- The “voxel volume” parameter reported in the “analyse function” for Cartesian coordinates is averaged all over the domain
- The mitigate option may leave ratio cells values bigger than the imposed value as it is done not iteratively
- The GVR option cannot employ meshtal with more than one energy bins
- The Meshtal files produced with MCNP5 and D1SUNED do not provide information on the reference vector of the cylinder. The default VEC [1,0,0] will be applied in these cases.

Further developments

- Insert the flipping methodology as a further option of the WW manipulation
- Improve the assignments of values in the hole-fill options
- Improve the mitigate long history particle option

Reference

1. "MCNP Users Manual - Code Version 6.2", C.J. Werner (editor), LA-UR-17-29981, 2017
2. A.J. van Wijk, G. Van den Eynde, J.E. Hoogenboom, An easy to implement global variance reduction procedure for MCNP, Annals of Nuclear Energy, Volume 38, Issue 11, 2011, Pages 2496-2503, ISSN 0306-4549, https://doi.org/10.1016/j.anucene.2011.07.037.
3. Andrew Davis, Andrew Turner, Comparison of global variance reduction techniques for Monte Carlo radiation transport simulations of ITER, Fusion Engineering and Design, Volume 86, Issues 9–11, 2011, Pages 2698-2700, ISSN 0920-3796, https://doi.org/10.1016/j.fusengdes.2011.01.059.
4. mesh2vtk, https://idm.f4e.europa.eu/?uid=2BM86T
5. Practical experience using ADVANTG for ITER C-lite applications, A.Turner (CCFE), 2016, ADVANTG workshop at JET