Computational neutronics analyses of deuteron interactions with lithium target in IFMIF-DONES for fusion applications

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- **Part II:** Application of the d-Li accelerator-based intense neutron source of IFMIF-DONES for fusion applications.

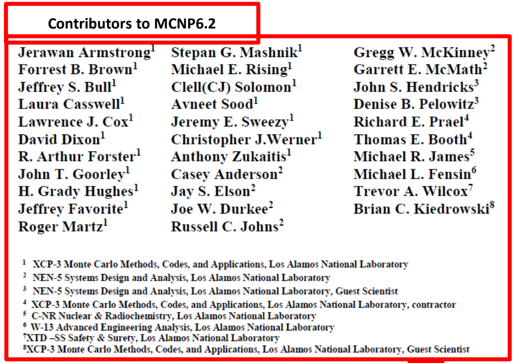
- **Conclusions**

- Backup slides:
  - McDeLicious code parallelization on Marconi-Fusion HPC
  - Use of On-The-Fly (OTF) Monte Carlo variance reduction technique

Radiation transport with the MCNP code

MCNP is a code for radiation transport calculations in 3D geometry. The abbreviation is translated as **M**onte **C**arlo **N**-**P**article.

Neutron, photon, electron, or coupled neutron/photon/electron transport can be performed by MCNP. The MCNP code was developed by X-5 Monte Carlo Team in Los Alamos National Lab. (LANL), USA.



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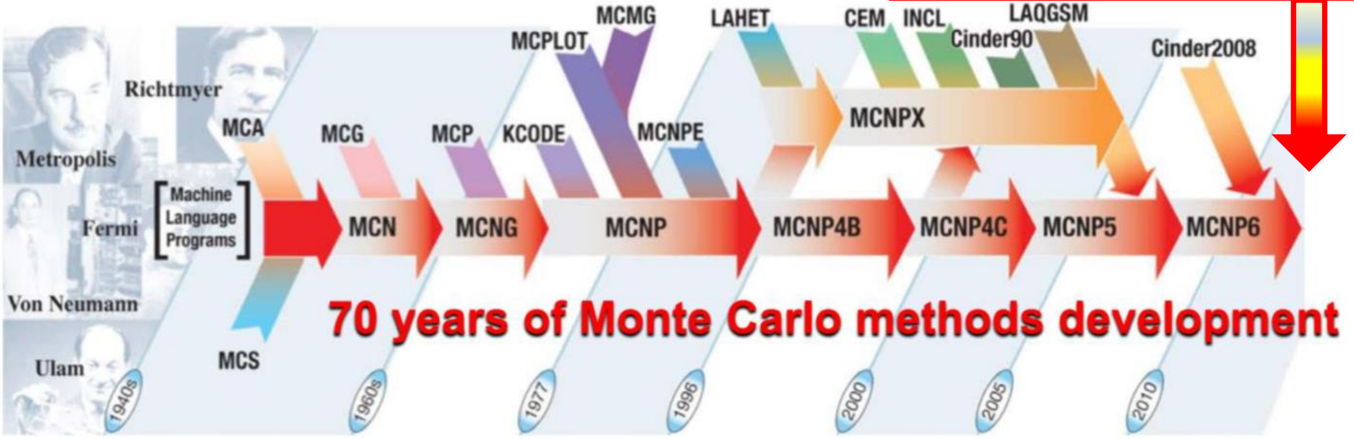
[7] XTD –SS Safety & Surety, Los Alamos National Laboratory
[8] XCP-3 Monte Carlo Methods, Codes, and Applications, Los Alamos National Laboratory, Guest Scientist

History of the MCNP code development [1]



Reference:
[1] Avneet Sood, 2017. The Monte Carlo Method and MCNP-A Brief Review of Our 40 Year History, Presentation to the International Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications Conference.

McDeLicious code development history

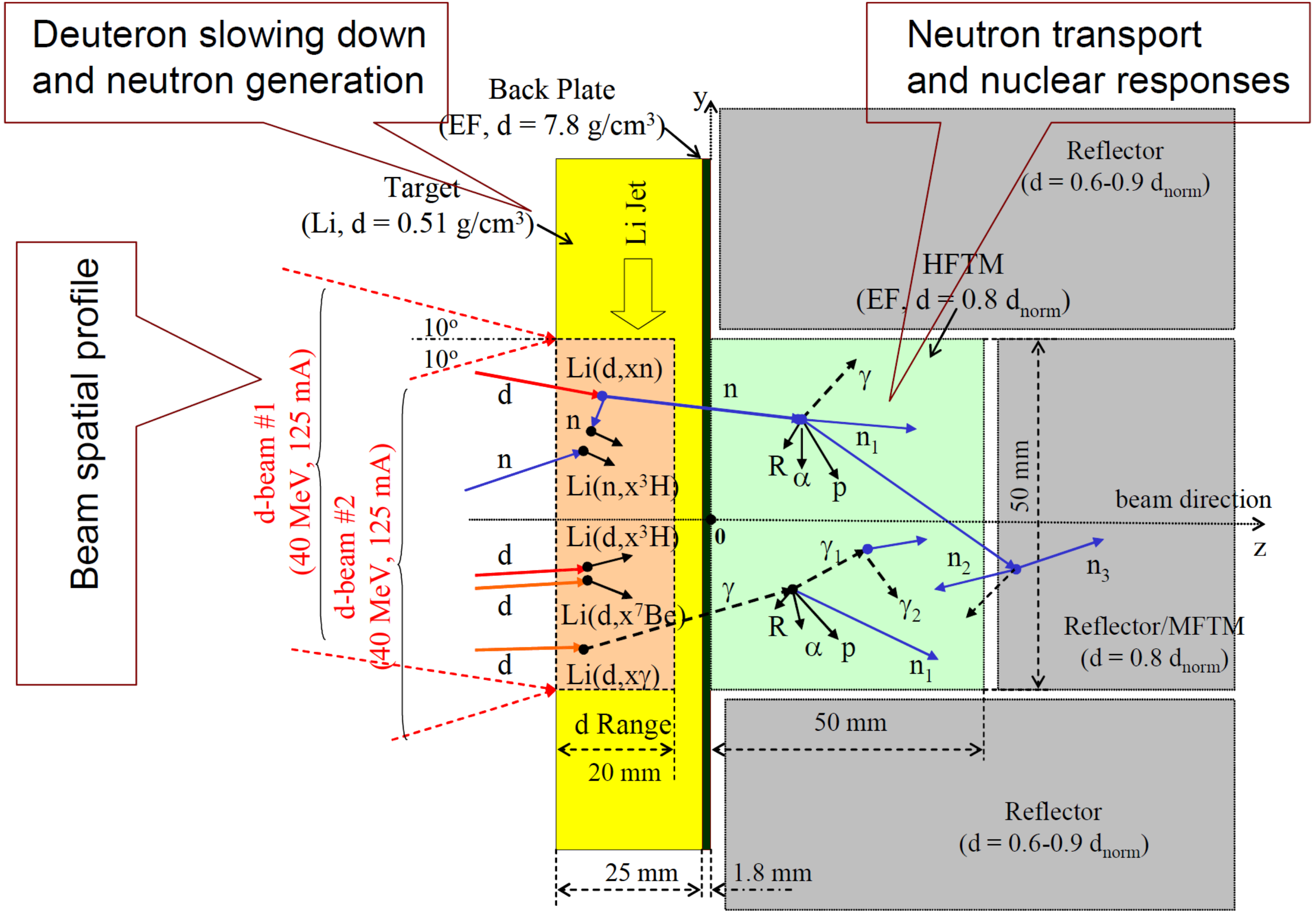
McDeLicious is an extension to the **MCNP Monte Carlo code** with the ability to simulate the generation of source neutrons based on deuteron - lithium (**D-Li**) interaction processes

- 1999: **McDeLi (***P. Wilson, Report FZKA 6218, 1999):*
  - An enhancement to MCNP-4a to sample the generation of d-Li source neutrons based on embedded analytical formulas representing direct deuteron striping (Serber model) and compound reactions.
- 2001: **McDeLicious** *(S.P.Simakov et al. J.Nucl.Mat.307-311(2002)1710, FZKA 6743)*
  - An enhancement to MCNP-4b,c to sample the d-Li source neutrons on the basis of tabulated double-differential d + 6,7Li cross-sections for deuteron energies up to 50 MeV (evaluated by *A. Konobeyev et al., NSE 139 (2001)1).*
- 2005: **McDeLicious-05** – compilation with MCNP-5 and use tabulated double-differential cross-sections from updated d + 6,7Li evaluation *(made by P. Pereslavtsev et al., J.Nucl.Mat.367-370(2007)1531).*
- 2011: **McDeLicious-11 -** a new approach is implemented to enable direct sampling from the tabulated deuteron beam distribution data without using fitting functions. In this approach, the beam entry position is sampled from tabulated data representing the intensity distribution of the impinging deuteron beam – (*S. P. Simakov et al., "Status of the McDeLicious approach for the D-Li neutron source term modeling in IFMIF neutronics calculations," Fusion Sci. Technol., 62 (2012), pp. 233-239*)
- 2017: **McDeLicious-17** – the actual version of McDeLicious upgraded to MCNP version 6.1.0, an extension of the MCNP Monte Carlo code with the capability to simulate the deuterium-lithium neutron source on the basis of evaluated d + 6,7Li cross-section data. This code has been tested and confirmed to generate identical source particle data as the previous version McDeLicious-11 – (Y. Qiu et al., "IFMIF-DONES HFTM neutronics modeling and nuclear response analyses," Nuclear Materials and Energy, 15 (2018), pp. 185-189)

Part I

Basic processes defined for (d-Li) atomic and nuclear interactions. Illustration on a simple model of cylindrical solid Li inside the aluminum capsule

Basic nuclear processes in IFMIF



Deuteron slowing down and neutron generation

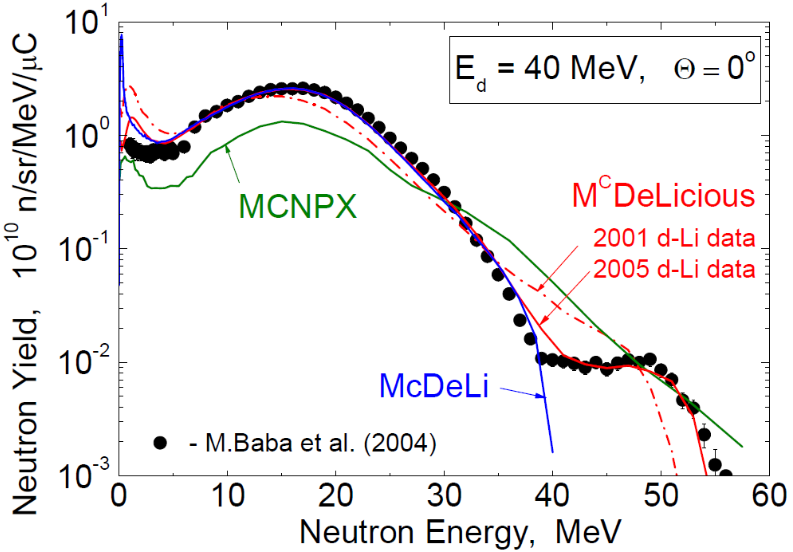
Neutron transport and nuclear responses

Beam spatial profile

Thick Li-target neutron source: Energy-Angular Yield

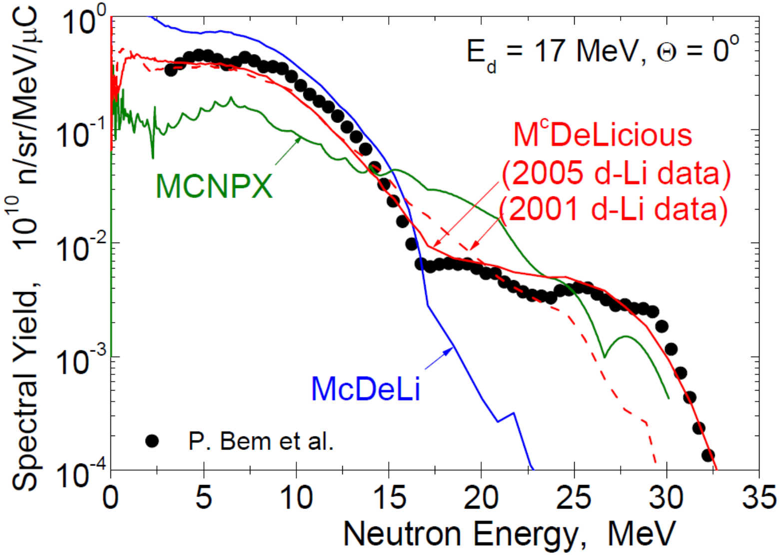
Ed = 40 MeV

Exp.: M. Hagiwara et al.



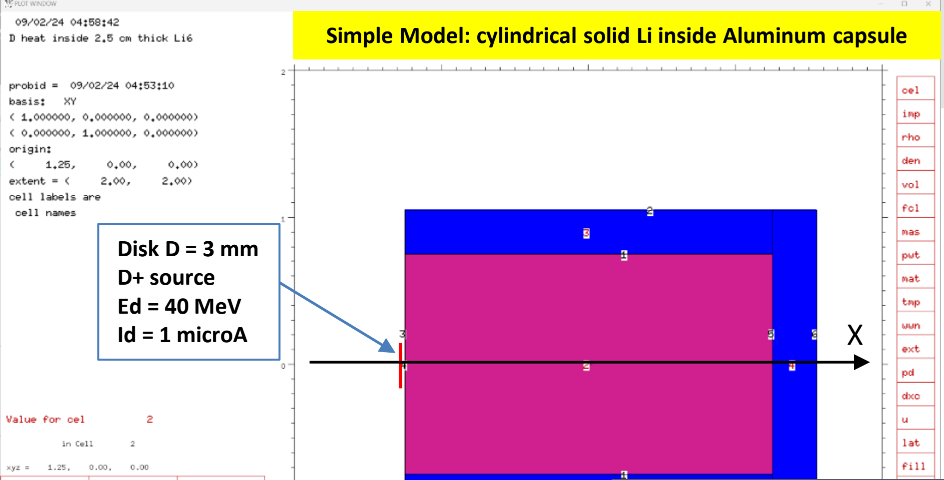
Ed = 17 MeV

Exp.: P. Bem et al.



Ref: S.P. Simakov, McDelicious Workshop, FZK/IRS, *Institut für Reaktorsicherheit, Forschungszentrum Karlsruhe, 13-14 March 2008*

Simple Model: cylindrical solid Li inside Aluminum capsule



```
 09/02/24 04:58:42
D heat inside 2.5 cm thick Li6


probid =  09/02/24 04:53:10
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( 0.000000, 1.000000, 0.000000)
origin:
(     1.25,     0.00,     0.00)
extent = (     2.00,     2.00)
cell labels are
 cell names


Value for cel          2

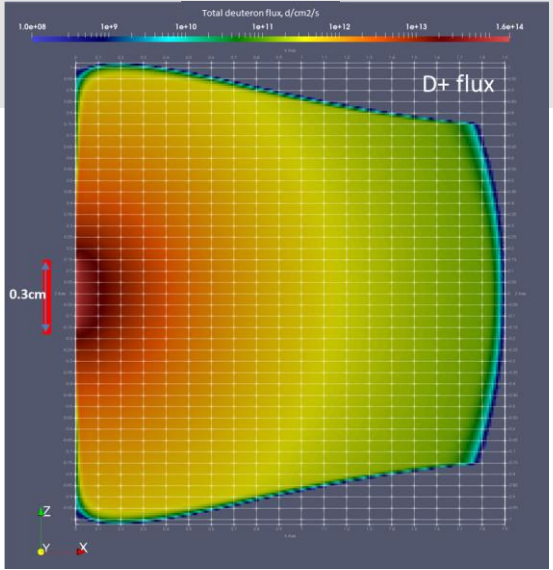
         in Cell        2

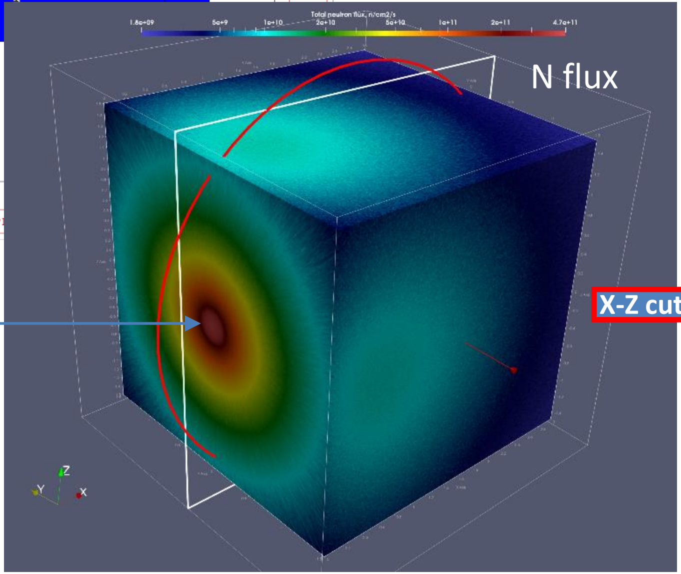
xyz =    1.25,    0.00,    0.00
```

Disk D = 3 mm
D+ source
Ed = 40 MeV
Id = 1 microA

MCNP model

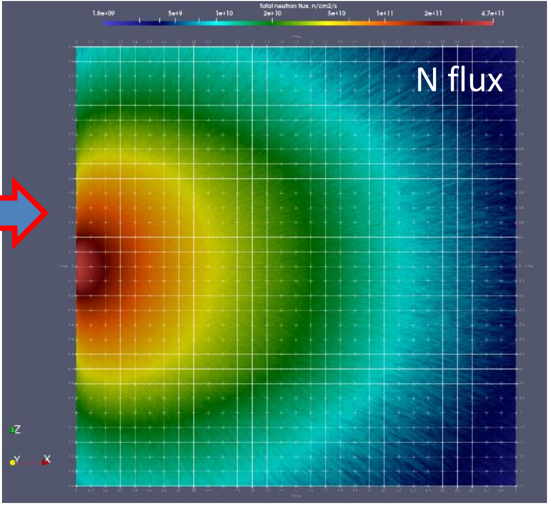
V1: Isotropic
uniformly distributed
disk D+ source



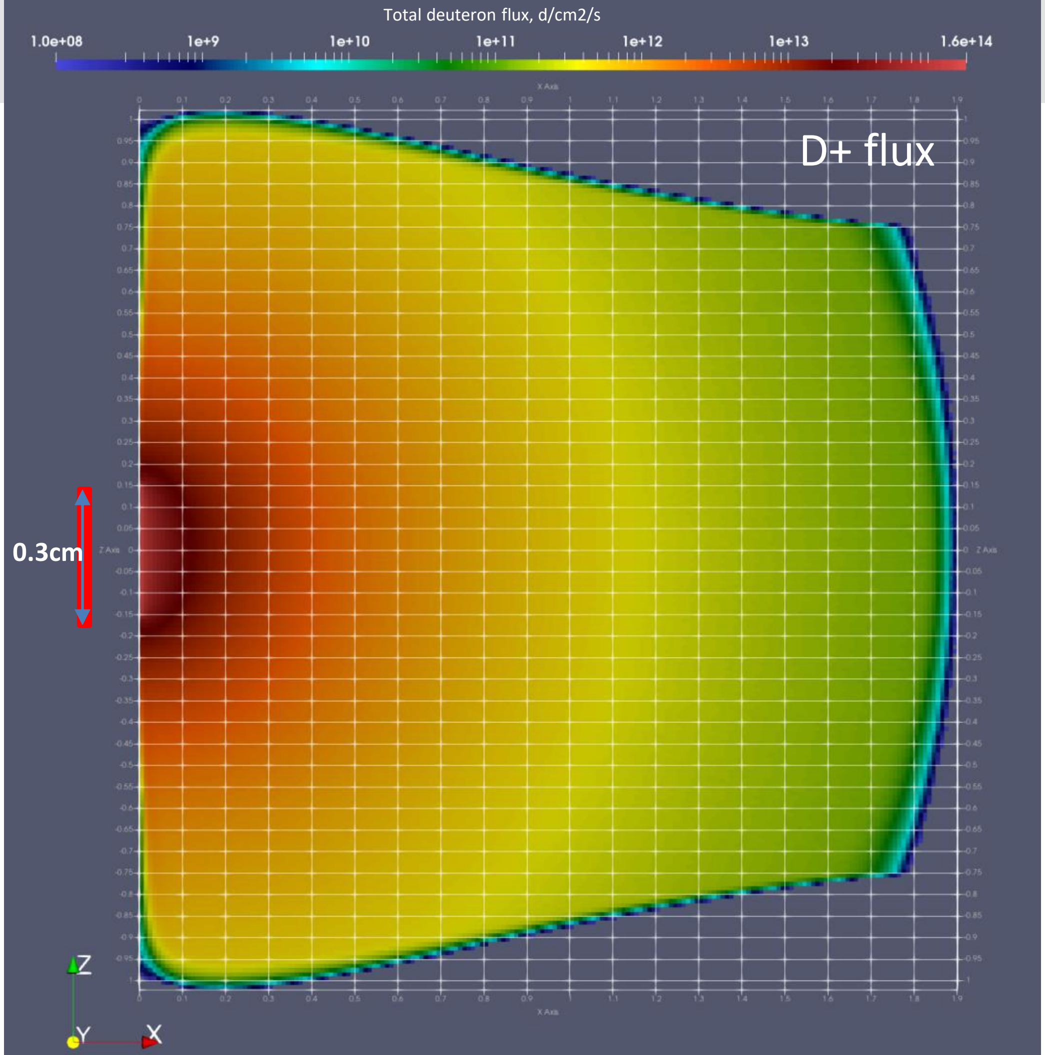


Disk D = 3 mm
D+ source
Ed = 40 MeV
Id = 1 microA

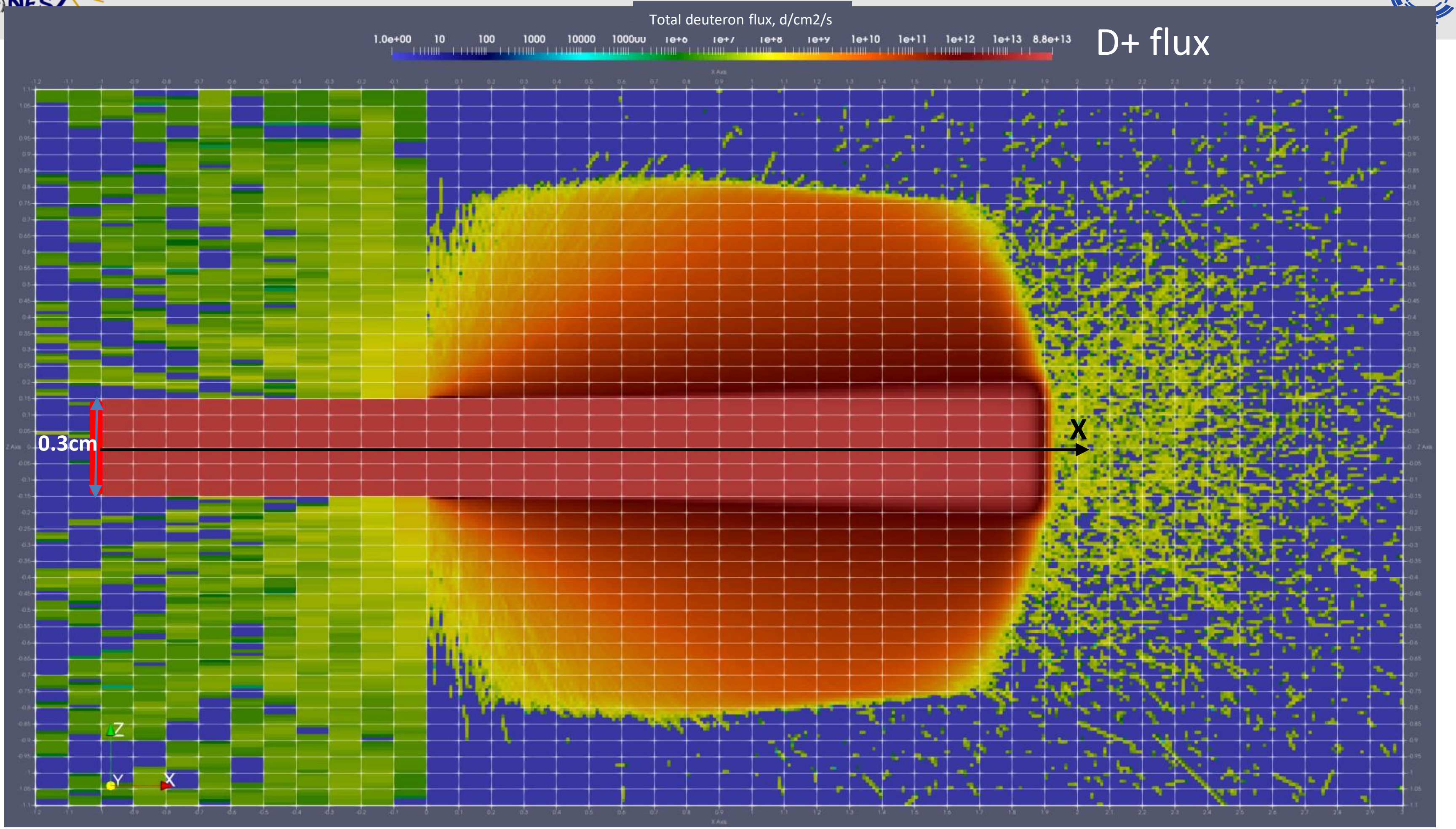
X-Z cut



V1: Isotropic
uniformly distributed
disk D+ source



V2: Monodirectional along X-axis disk D+ source, Ed = 40 MeV, Id = 1 microA

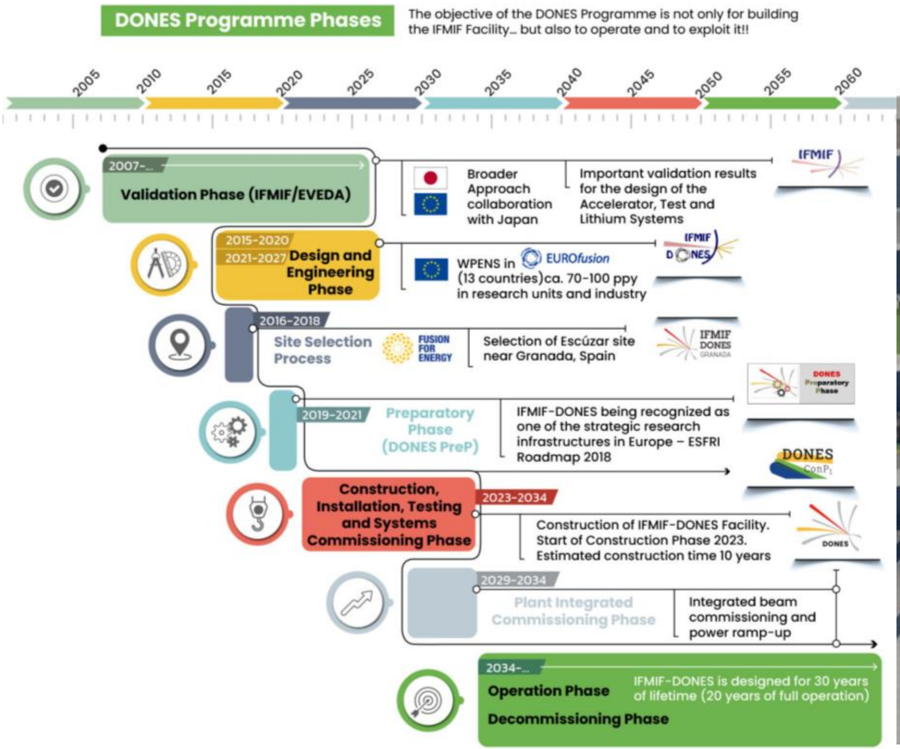


Part II

Application of the d-Li accelerator-based intense neutron source of IFMIF-DONES for fusion applications

DONES Programme, IFMIF-DONES España to build the DONES facility

The International Fusion Materials Irradiation Facility—DEMO Oriented NEutron Source (IFMIF-DONES) aims to evaluate and validate the structural and functional materials for developing DEMO-type reactors. To achieve this ambitious goal, several projects have been promoted in recent years, which together form the DONES Programme.



DONES Programme Phases

The objective of the DONES Programme is not only for building the IFMIF Facility... but also to operate and to exploit it!!

2007-... **Validation Phase (IFMIF/EVEDA)**
Broader Approach collaboration with Japan
Important validation results for the design of the Accelerator, Test and Lithium Systems

2015-2020 2021-2027 **Design and Engineering Phase**
WPENS in EUROfusion (13 countries)ca. 70-100 ppy in research units and industry

2016-2018 **Site Selection Process**
FUSION FOR ENERGY
Selection of Escúzar site near Granada, Spain

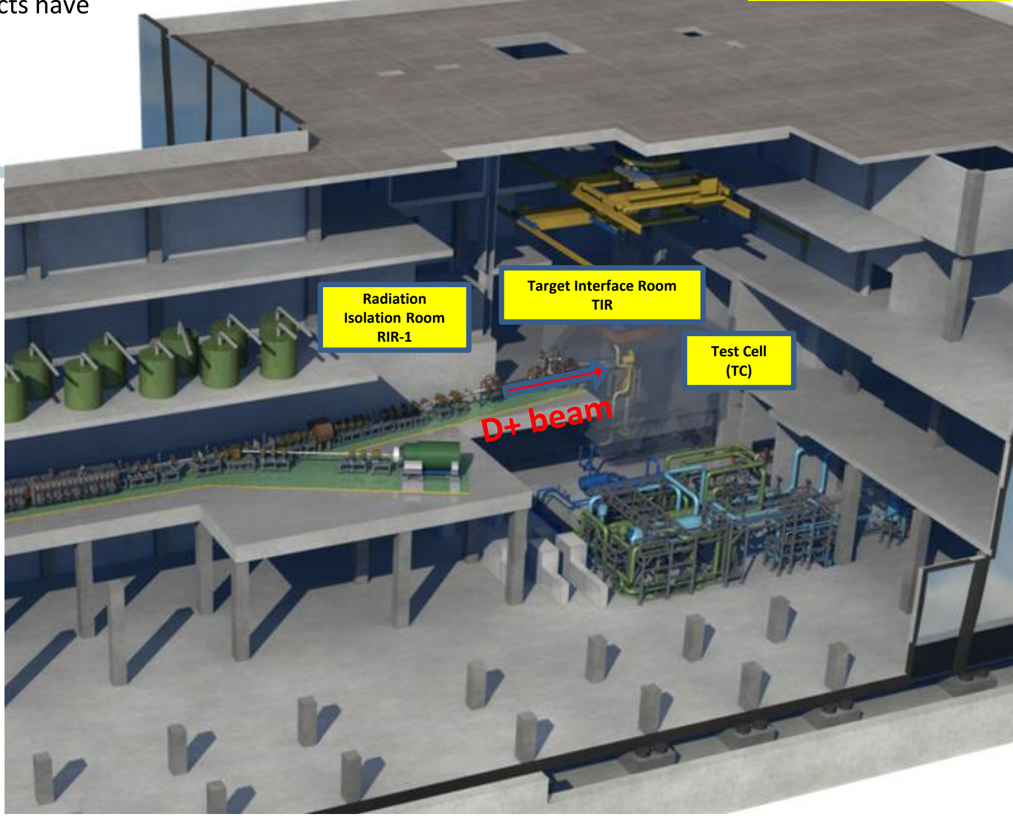
2019-2021 **Preparatory Phase (DONES PreP)**
IFMIF-DONES being recognized as one of the strategic research infrastructures in Europe – ESFRI Roadmap 2018

Construction, Installation, Testing and Systems Commissioning Phase 2023-2034
Construction of IFMIF-DONES Facility. Start of Construction Phase 2023. Estimated construction time 10 years

2029-2034 **Plant Integrated Commissioning Phase**
Integrated beam commissioning and power ramp-up

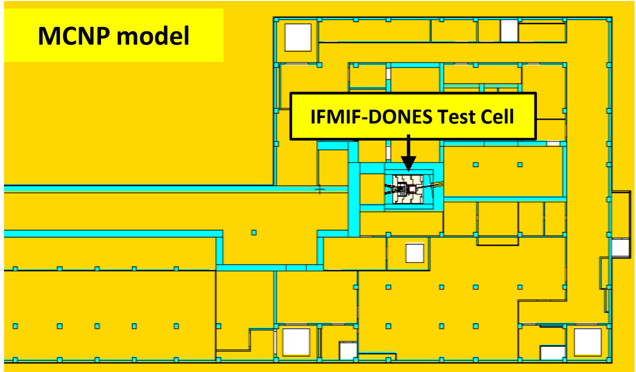
2034-... **Operation Phase**
Decommissioning Phase
IFMIF-DONES is designed for 30 years of lifetime (20 years of full operation)

DONES building CAD model

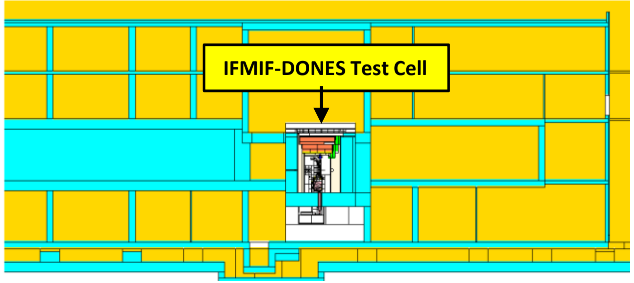


IFMIF-DONES neutronics simulations

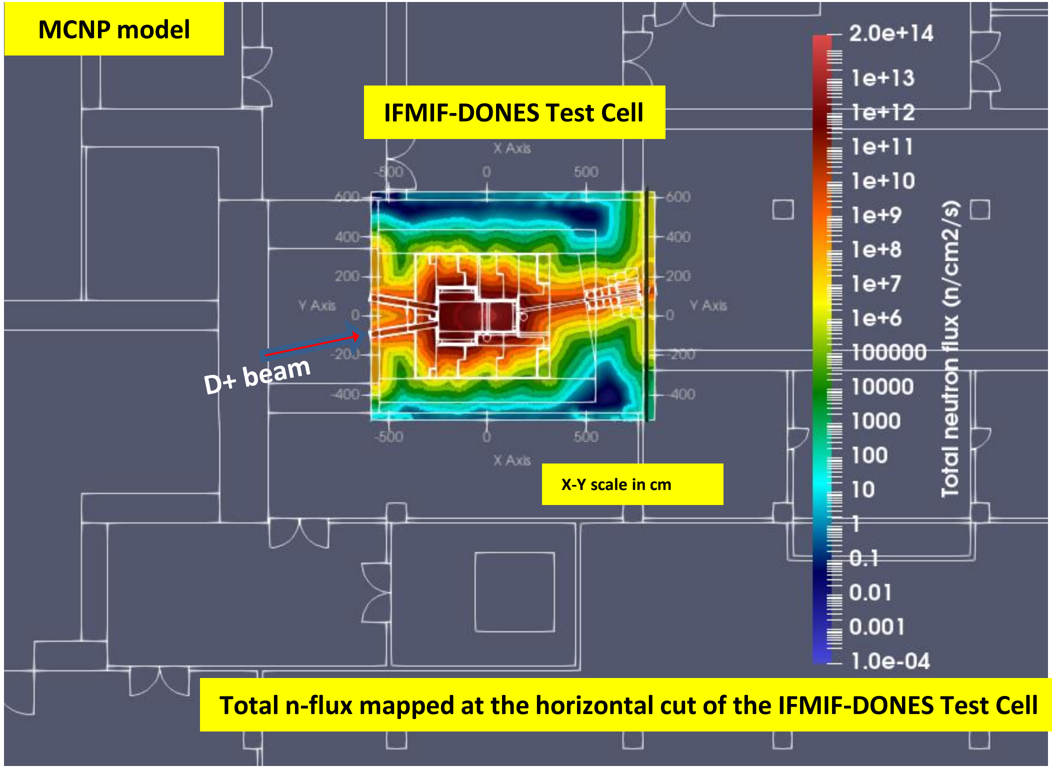
- The CAD model of IFMIF-DONES building is prepared (simplified and decomposed) for the CAD-to-MCNP conversion using the codes: **McCad (INR-KIT developed) or SuperMC (developed by FDS-team, China)**
- **McDeLicious-17 code package developed at INR-KIT** – an MCNP6 code modification for deuteron-lithium (d-Li) nuclear reactions in Li of IFMIF-DONES Test Cell. The beam of deuteron ions accelerated up to 40 MeV with current of 125 mA impinges the liquid Li target delivering 5 MW power. The Li target volume is 5×20×2.5 cm^3



DONES building model horizontal cut at the beam level.

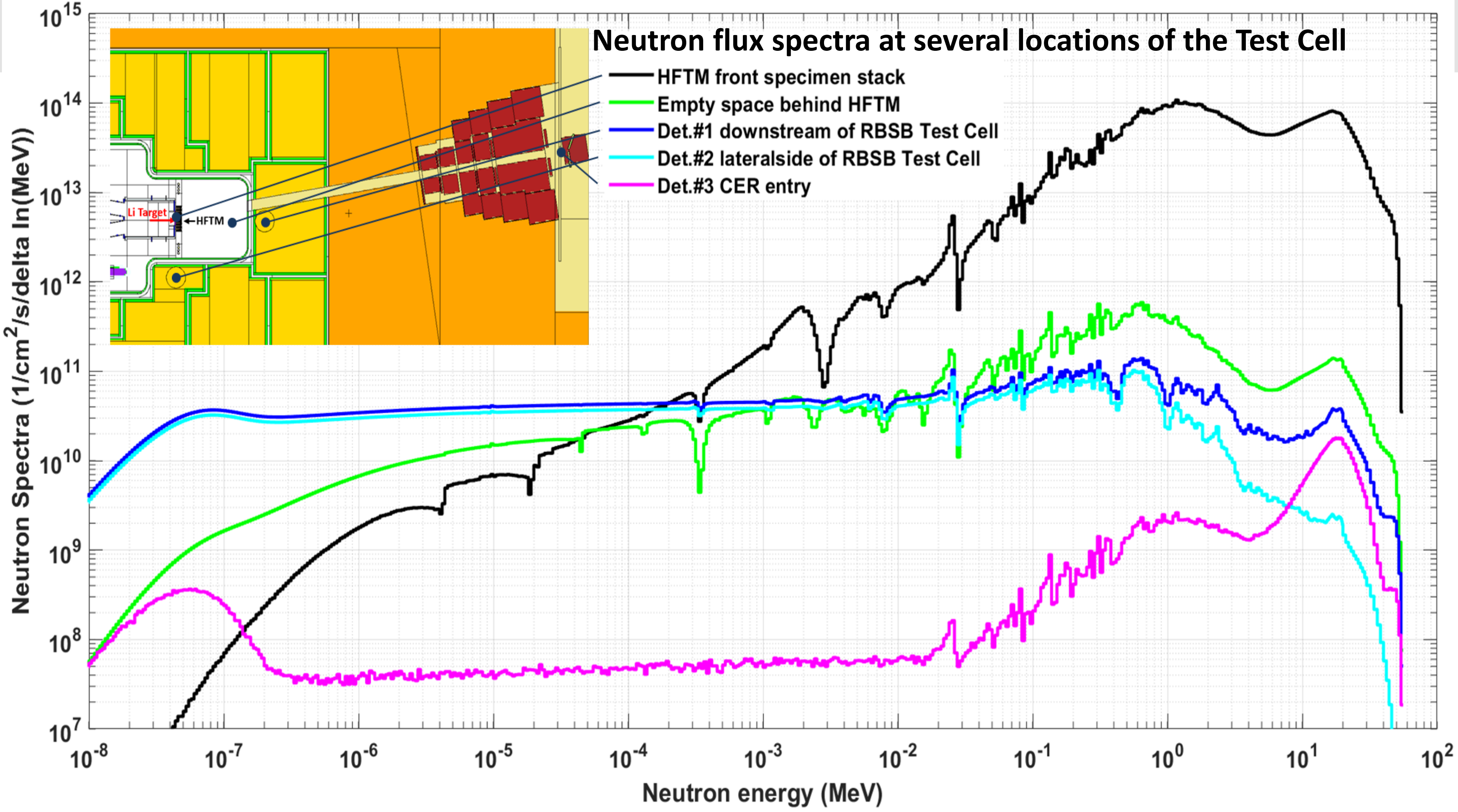


DONES building model vertical cut at the target center

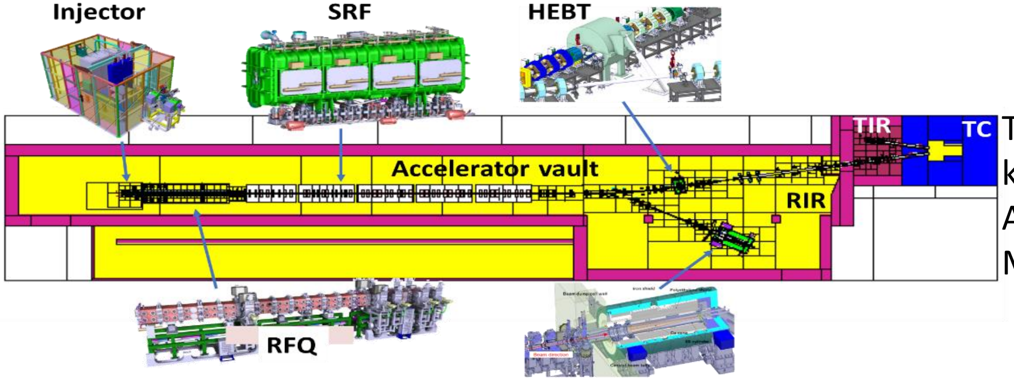


Total n-flux mapped at the horizontal cut of the IFMIF-DONES Test Cell

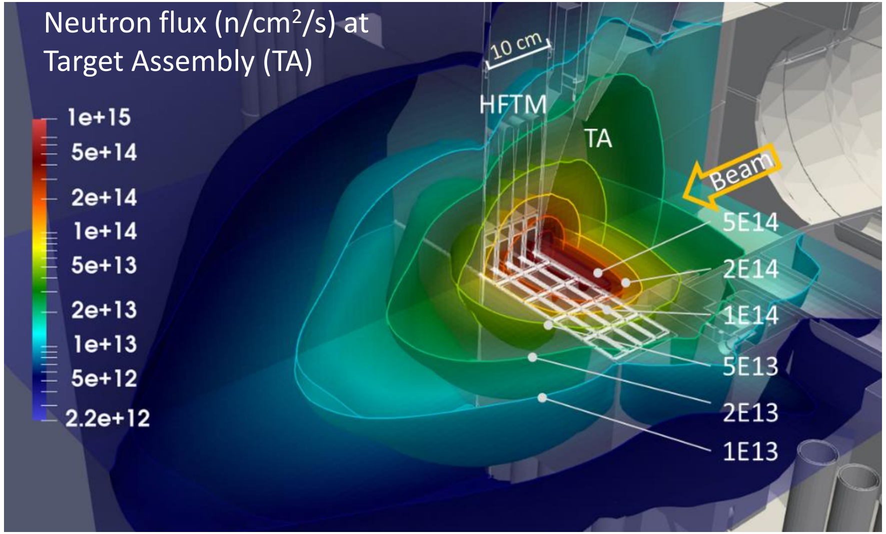
Neutron flux spectra at several locations of the Test Cell

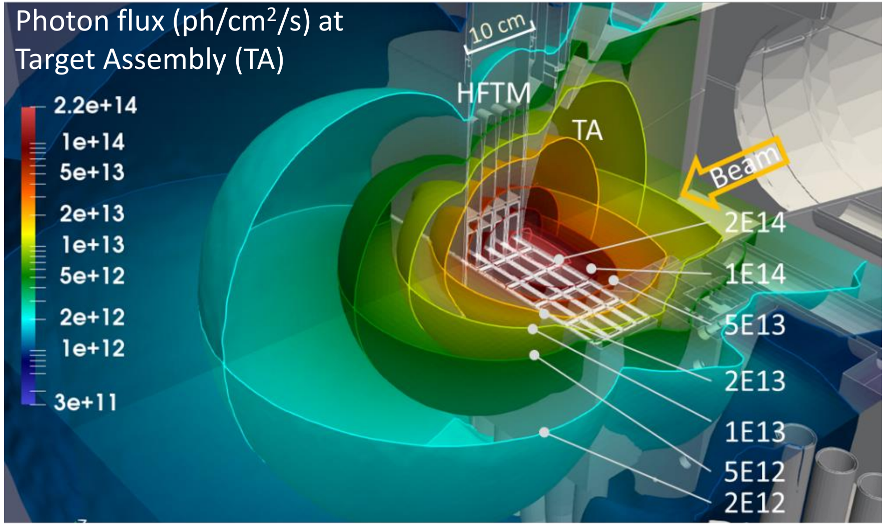


Neutronics geometry of the accelerator systems



The test cell (TC), which houses the key components of the Target Assembly (TA) and the High Flux Test Module (HFTM)

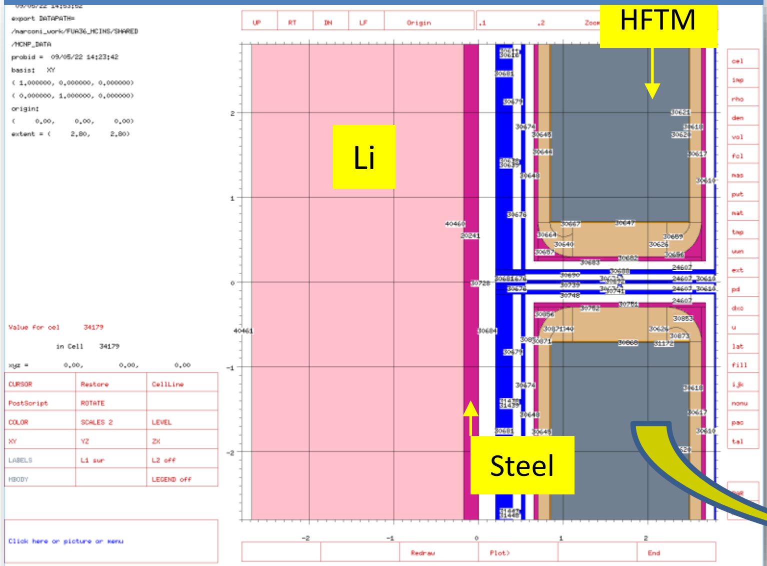

Neutron flux (n/cm^2/s) at Target Assembly (TA)


Photon flux (ph/cm^2/s) at Target Assembly (TA)

Deuteron beam energy deposition in the Li jet at the TA d-Li footprint area

- D+ ion beam stops in the lithium jet delivering a total power of 5 MW on a volume of 5×20×2.5 cm^3, with d-Li footprint area of 5x20 cm^2.
- Deuterons lose their energy in Li by interactions with Li electron clouds and nuclei – all the processes have been taken into account in the MCNP6 energy deposition calculations with the TMESH card.
- For calculation of deuteron beam energy deposition in Li at the d-Li footprint area, **transport of neutrons, photons, deuterons, and protons** – 4 particles have been transported with the MCNP6 mode **n p d h**

Horizontal cut of the MCNP6 geometry at d-Li footprint



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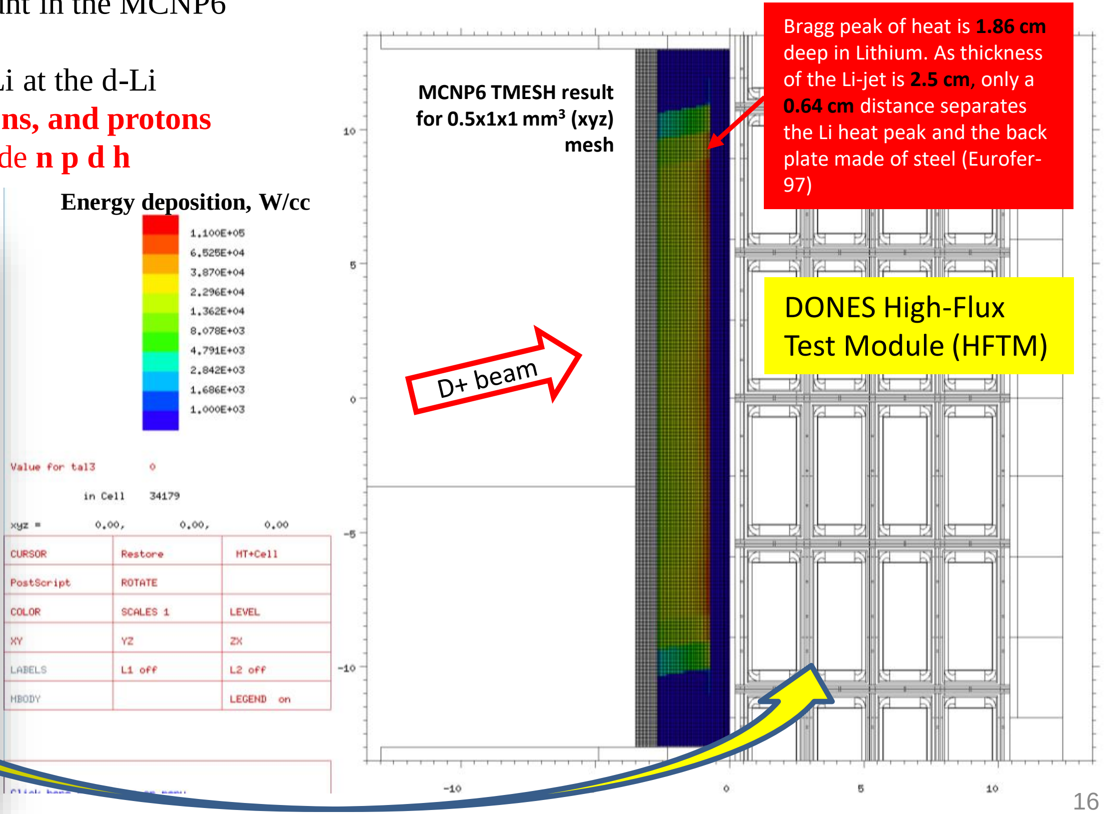
MCNP6 horizontal cut of the D+ beam energy deposition at the d-Li footprint area with heat peak of 110 kW/cc



Energy deposition, W/cc

🟥	1.100E+05
🟧	6.525E+04
🟧	3.870E+04
🟨	2.296E+04
🟩	1.362E+04
🟩	8.078E+03
🟩	4.791E+03
🟦	2.842E+03
🟦	1.686E+03
🟦	1.000E+03

```
Value for tal3         0

          in Cell    34179

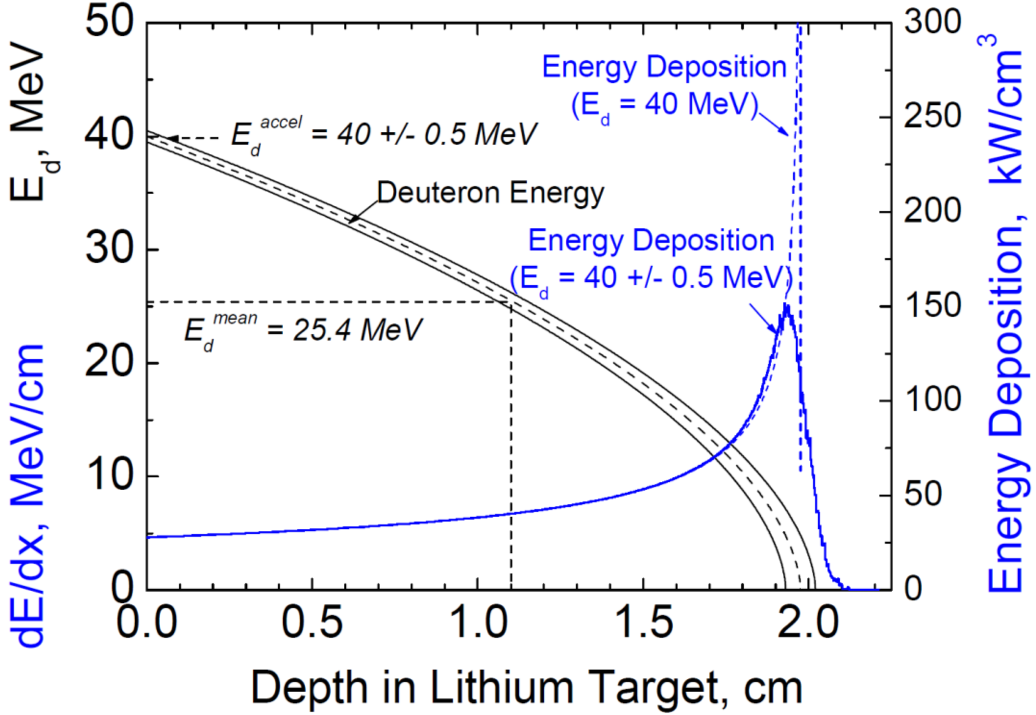
xyz =        0.00,        0.00,        0.00
```

MCNP6 TMESH result for 0.5x1x1 mm^3 (xyz) mesh

Bragg peak of heat is **1.86 cm** deep in Lithium. As thickness of the Li-jet is **2.5 cm**, only a **0.64 cm** distance separates the Li heat peak and the back plate made of steel (Eurofer-97)

DONES High-Flux Test Module (HFTM)

Deuteron slowing down and energy deposition in Li-jet

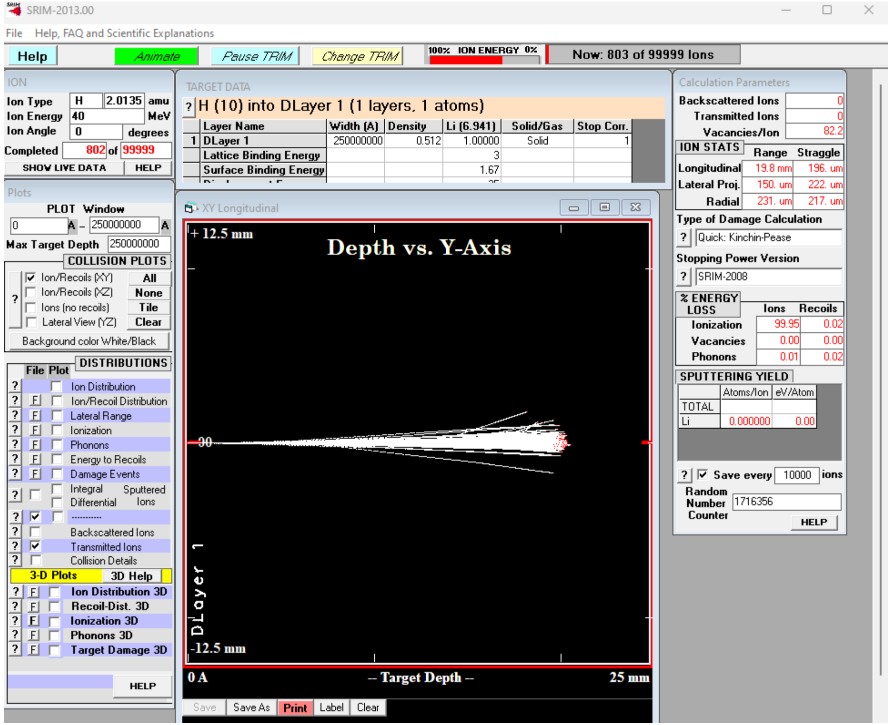


- *Deuteron track length reach 2.1 cm;*
- *Peak Energy Deposition is 150 kW/cc at the depth of 2.0 cm (at the end of d-track)*
- *Average energy deposition in Li jet = (40 MeV x 250 mA=10,000 kW)/(20x5x2 cc) =50 kW/cc*

Ref: S.P. Simakov, McDelicious Workshop, FZK/IRS, *Institut für Reaktorsicherheit, Forschungszentrum Karlsruhe, 13-14 March 2008*

Deuteron track depth (longitudinal, Ld) dependence on the D+ energy (Ed)

Ld=19.8 mm for Ed=40.0 MeV



SRIM-2013.00

Now: 803 of 99999 Ions

Ion Type: H 2.0135 amu
Ion Energy: 40 MeV
Ion Angle: 0 degrees
Completed: 802 of 99999

H (10) into DLayer 1 (1 layers, 1 atoms)

	Layer Name	Width (A)	Density	Li (6.941)	Solid/Gas	Stop Corr.
1	DLayer 1	250000000	0.512	1.00000	Solid	1
	Lattice Binding Energy			3		
	Surface Binding Energy			1.67		

PLOT Window: 0 A – 250000000 A
Max Target Depth: 250000000

Backscattered Ions: 0
Transmitted Ions: 0
Vacancies/Ion: 82.2

ION STATS	Range	Straggle
Longitudinal	19.8 mm	196. um
Lateral Proj.	150. um	222. um
Radial	231. um	217. um

Type of Damage Calculation: Quick: Kinchin-Pease
Stopping Power Version: SRIM-2008

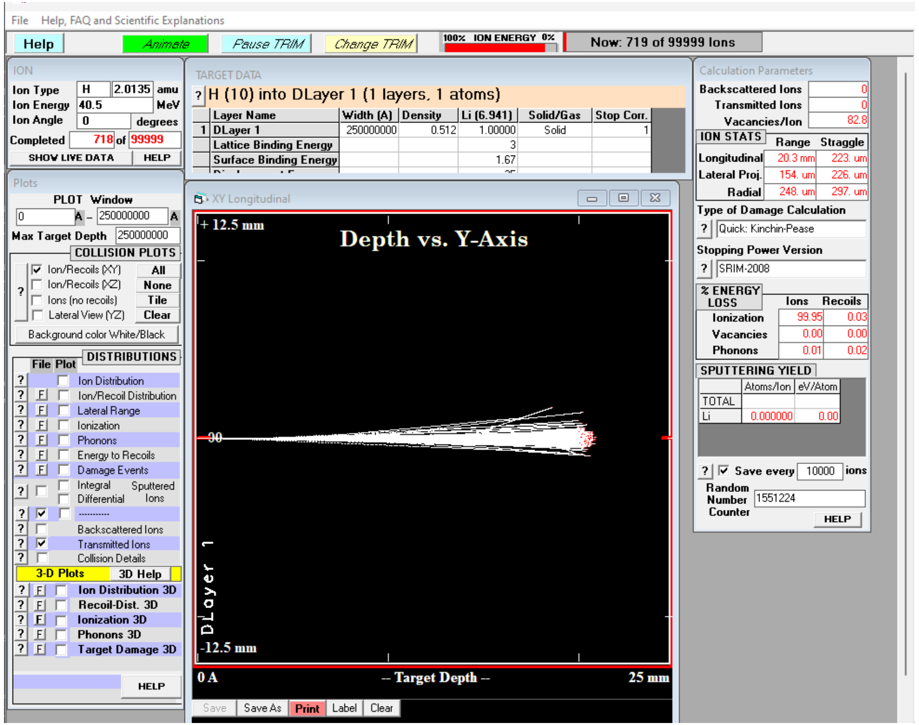
% ENERGY LOSS	Ions	Recoils
Ionization	99.95	0.02
Vacancies	0.00	0.00
Phonons	0.01	0.02

SPUTTERING YIELD

	Atoms/Ion	eV/Atom
TOTAL		
Li	0.000000	0.00

☑ Save every 10000 ions
Random Number Counter: 1716356

Ld=20.3 mm for Ed=40.5 MeV



Now: 719 of 99999 Ions

Ion Type: H 2.0135 amu
Ion Energy: 40.5 MeV
Ion Angle: 0 degrees
Completed: 718 of 99999

H (10) into DLayer 1 (1 layers, 1 atoms)

	Layer Name	Width (A)	Density	Li (6.941)	Solid/Gas	Stop Corr.
1	DLayer 1	250000000	0.512	1.00000	Solid	1
	Lattice Binding Energy			3		
	Surface Binding Energy			1.67		

PLOT Window: 0 A – 250000000 A
Max Target Depth: 250000000

Backscattered Ions: 0
Transmitted Ions: 0
Vacancies/Ion: 82.8

ION STATS	Range	Straggle
Longitudinal	20.3 mm	223. um
Lateral Proj.	154. um	226. um
Radial	248. um	297. um

Type of Damage Calculation: Quick: Kinchin-Pease
Stopping Power Version: SRIM-2008

% ENERGY LOSS	Ions	Recoils
Ionization	99.95	0.03
Vacancies	0.00	0.00
Phonons	0.01	0.02

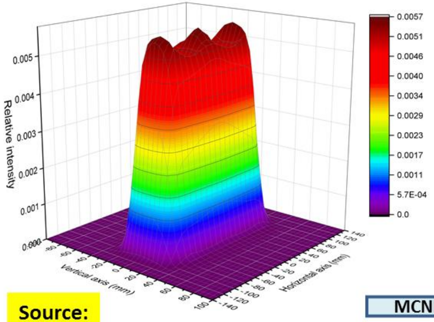
SPUTTERING YIELD

	Atoms/Ion	eV/Atom
TOTAL		
Li	0.000000	0.00

☑ Save every 10000 ions
Random Number Counter: 1551224

D+ ion beam energy deposition in Li target with Li(d, xn) neutron source in IFMIF-DONES

D+ beam profile (IFMIF/EVEDA)

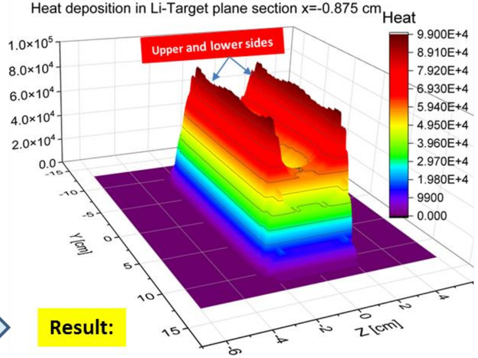


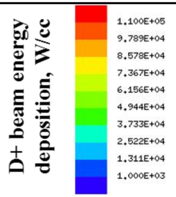
Source:

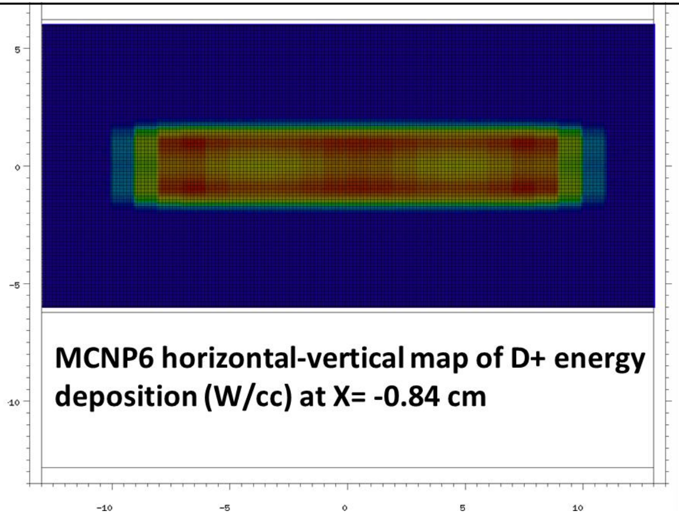
MCNP6 transport

Result:

Heat deposition in Li-Target plane section x=-0.875 cm



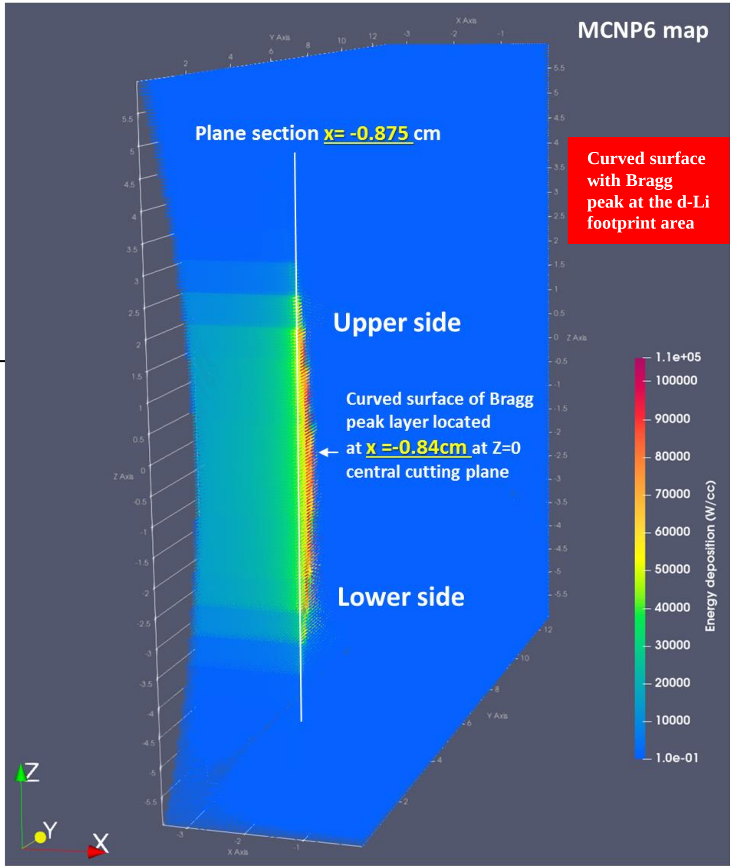




MCNP6 horizontal-vertical map of D+ energy deposition (W/cc) at X= -0.84 cm

Heat at peak is 110 kW/cc
Integral D+ heat 4.8 MW

Notice: Bragg peak at Lithium thickness of **1.86 cm** corresponds to **-0.84 cm** coordinate in the MCNP model geometry with X=0 at the TA back plate and X=-2.7cm is the front point of Li at Z=0 central plane: **1.86cm - 2.7cm = -0.84cm**



MCNP6 map

Plane section x= -0.875 cm

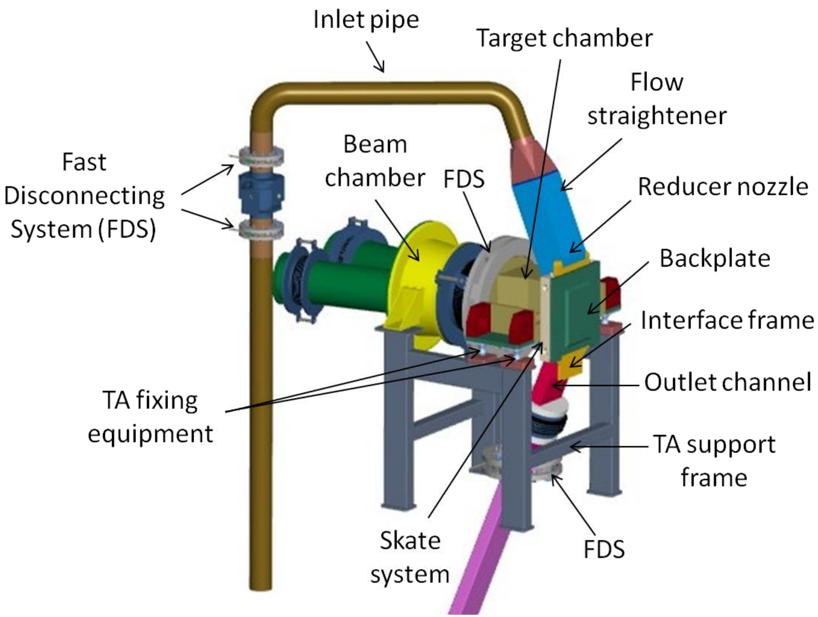
Upper side

Curved surface of Bragg peak layer located at x =-0.84cm at Z=0 central cutting plane

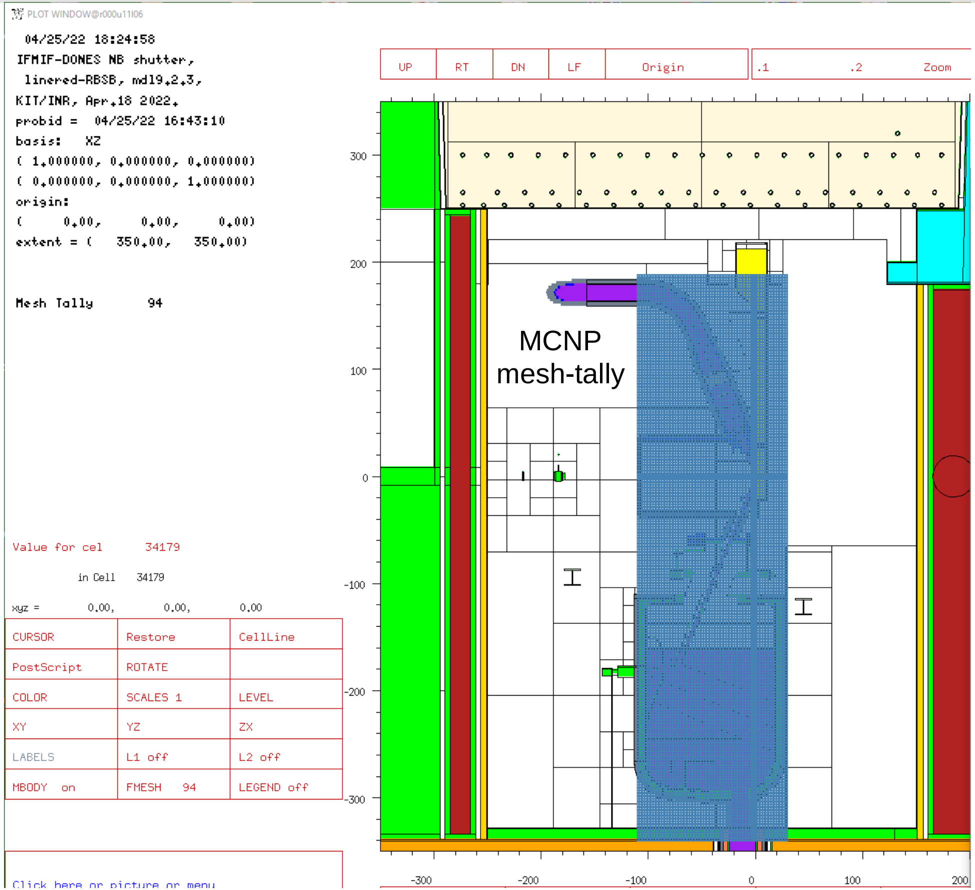
Lower side

Curved surface with Bragg peak at the d-Li footprint area

MCNP modeling of the d-Li source Target Assembly (TA) in DONES



DONES Target Assembly (TA) components



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KIT/INR, Apr.18 2022.
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basis:   XZ
( 1.000000, 0.000000, 0.000000)
( 0.000000, 0.000000, 1.000000)
origin:
(      0.00,      0.00,      0.00)
extent = (   350.00,   350.00)


Mesh Tally        94
```

```
Value for cel       34179

          in Cell    34179

xyz =         0.00,          0.00,          0.00
```

MCNP model vertical cut of the DONES TA covered with mesh-tally

Nuclear heat density (W/cc) in the TA materials of the MCNP model

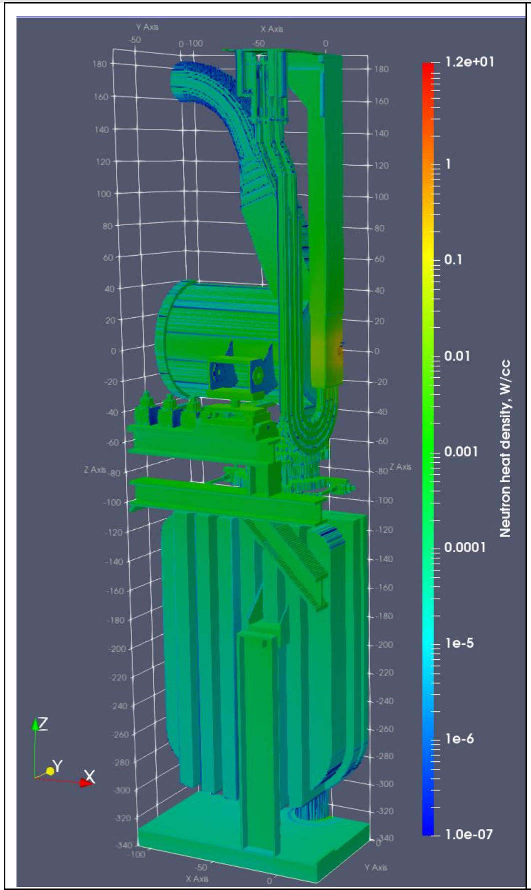


Fig. 1. Neutron heat density (W/cc) in actual materials of the MCNP model – look from the outside.

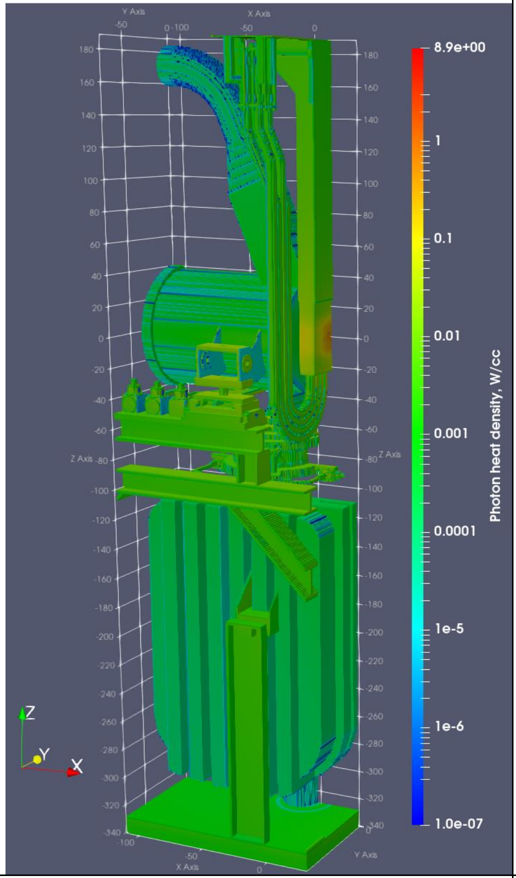


Fig. 2. Photon heat density (W/cc) in actual materials of the MCNP model – look from the outside.

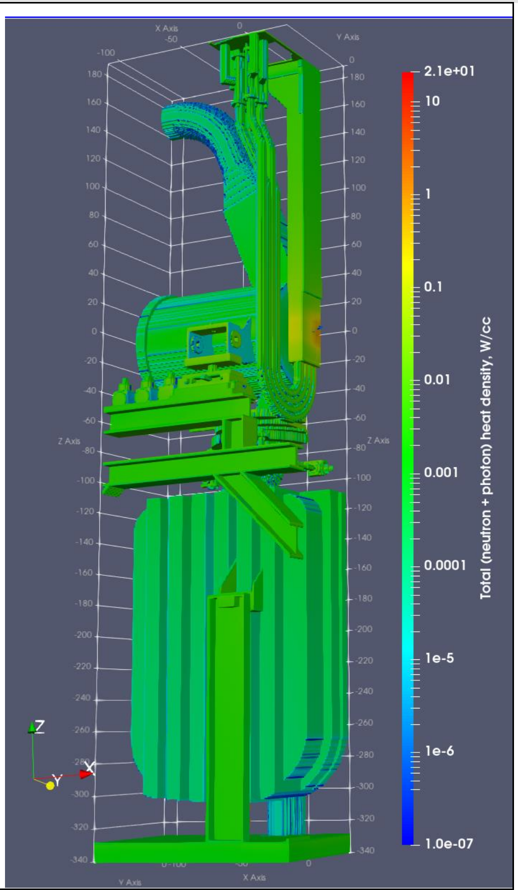


Fig. 3. Total (neutron + photon) heat density (W/cc) in actual materials of the model – look from the outside.

TA materials:

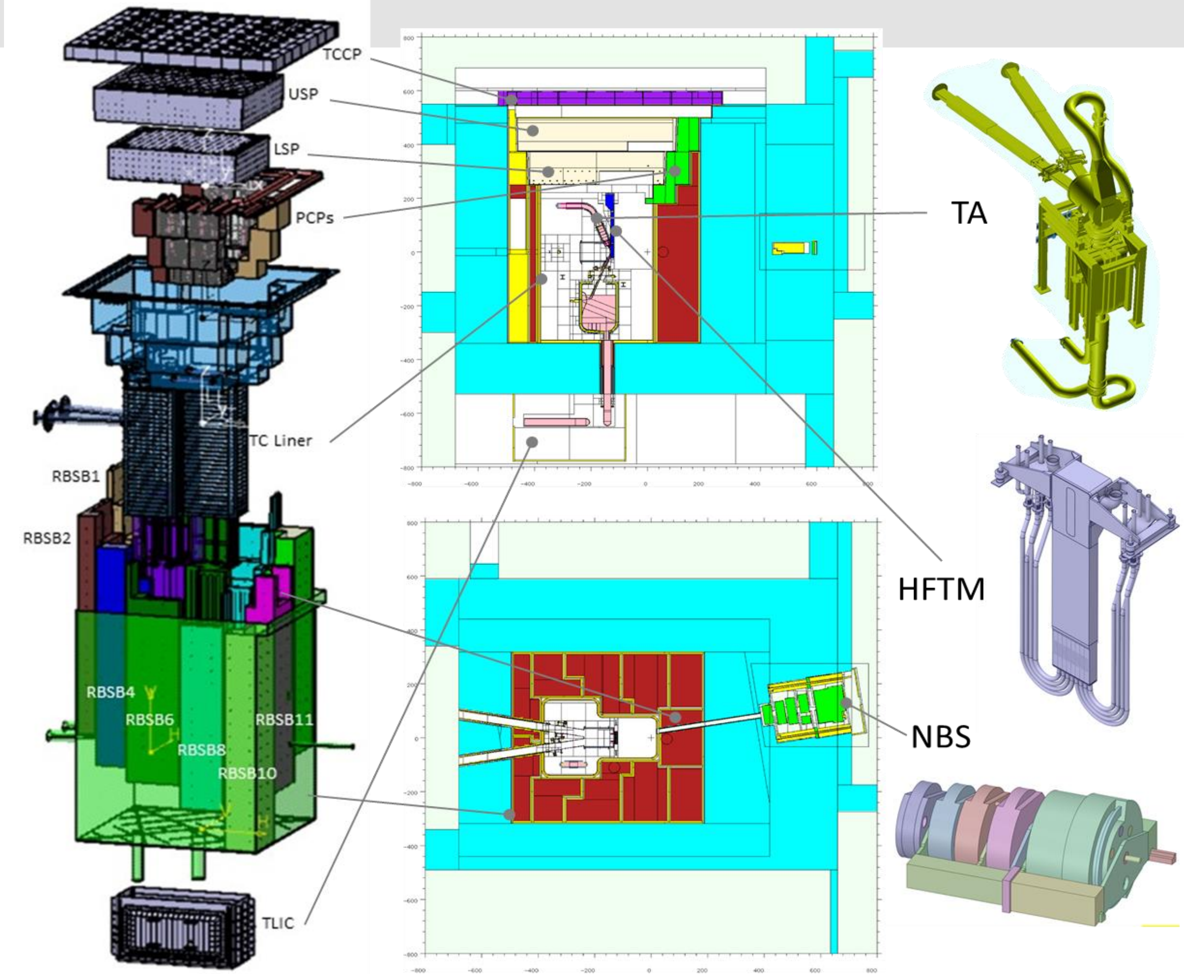
Steel SS316L material density 7.93 g/cc

EUROFER steel with density 7.87 g/cc

Lithium (Li) with impurities, its density is 0.512 g/cc.

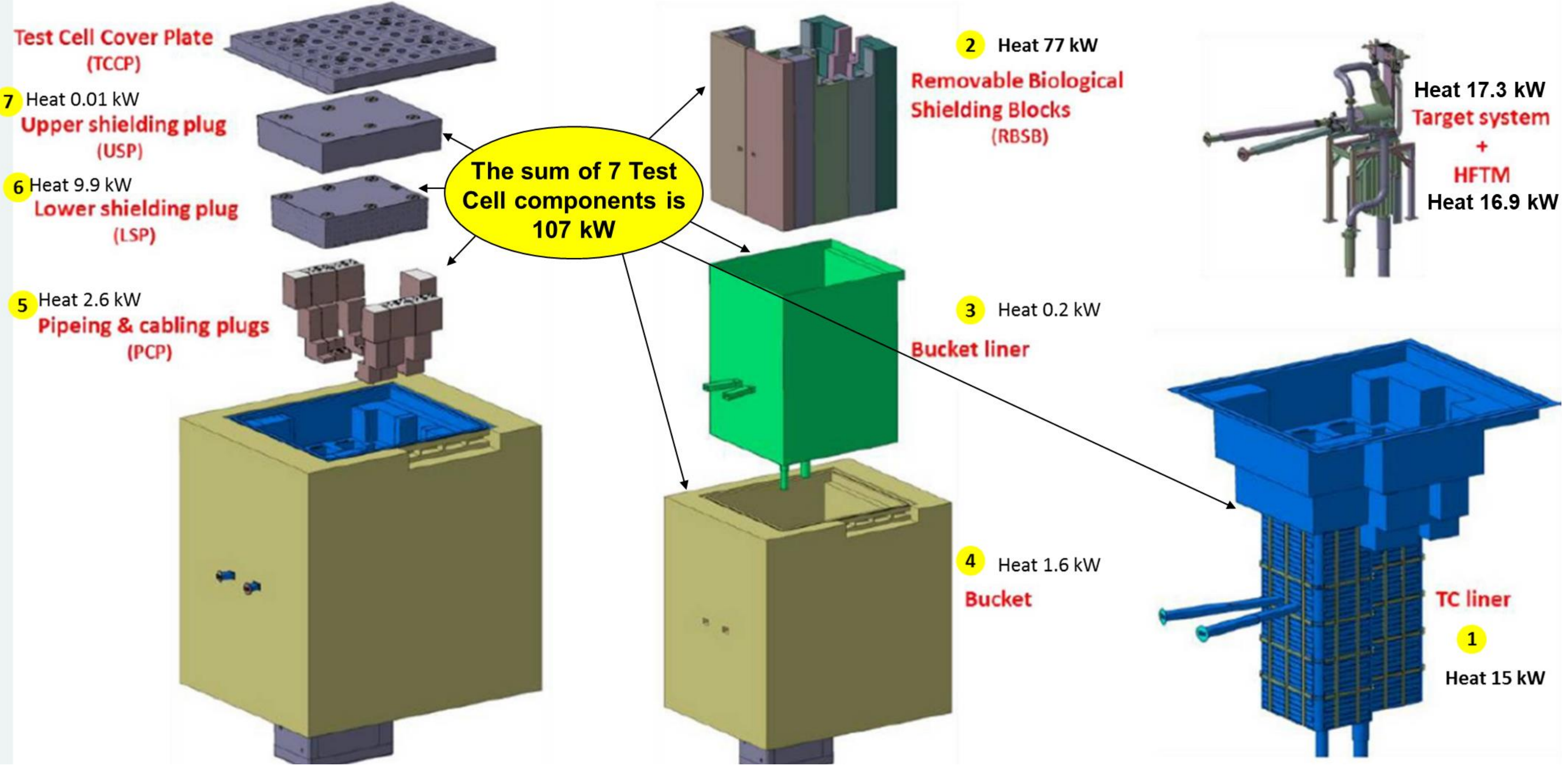
Heating in Li jet at the area of deuteron footprint requires inclusion of the heat contributions of charged particles.

Power balance for the D+ beam energy released in Test Cell (TC) and internal components



Type of heat power	Heat, kW
Input heat power of D+ beam delivered by the IFMIF-DONES one accelerator beam current of I=125 mA	**5000**
D+ heat released in Li Target	**4858.8**
Neutron + Photon heat released in the TC components (numbered and displayed in the next slide):	
1) TC liner	**15.2**
2) Removable Biological Shielding Blocks	**77.3**
3) Bucket liner	**0.2**
4) Bucket	**1.6**
5) Piping and Cabling Plugs (PCP)	**2.6**
6) Lower Shielding Plug (LSP)	**9.9**
7) Upper Shielding Plug (USP)	**0.01**
The sum of 7 TC components:	**107**
Target Assembly (TA) structural parts	**17.3**
High Flux Test Module (HFTM)	**16.9**
Integral neutron and photon heat in all considered TC components	**~141.2**
Output: total integral heat released by D+, neutrons, and photons:	**4858.8+141.2 = 5000**

Integral nuclear (neutron + photon) heating in the Test Cell (TC) components



The sum of 7 Test Cell components is 107 kW

Test Cell Cover Plate (TCCP)

7 Heat 0.01 kW
Upper shielding plug (USP)

6 Heat 9.9 kW
Lower shielding plug (LSP)

5 Heat 2.6 kW
Pipeing & cabling plugs (PCP)

2 Heat 77 kW
Removable Biological Shielding Blocks (RBSB)

Heat 17.3 kW
Target system + HFTM
Heat 16.9 kW

3 Heat 0.2 kW
Bucket liner

4 Heat 1.6 kW
Bucket

TC liner
1
Heat 15 kW

Conclusions

- **The interactions of deuterons with lithium target** for the energies relevant to fusion applications, particularly Ed=40 MeV in IFMIF-DONES facility, are most accurately described with the McDeLicious code in its actual version McDeLicious-17, as an extension of the MCNP6.1 Monte Carlo radiation transport code. The McDeLicious code has been validated & verified in experimental and computational benchmarks.
- Using the D+ beam settings, McDeLicious samples neutrons and photons using evaluated d+ ^{6,7}Li data.

- The simple model of D+ interactions with cylindrical solid Li inside Aluminum capsule allows to investigate the D+ flux attenuation, track length, Ed attenuation, and D+ energy deposition. This work presented simple model with two settings of the D+ sources:
  - V1: Isotropic uniformly distributed disk
  - V2: Monodirectional directed source defined at a disk

- The (d-Li) reactions defined in McDeLicious-17 have been studied for the IFMIF-DONES facility. The beam of deuteron ions accelerated up to 40 MeV with current of 125 mA impinges the liquid Li target delivering 5 MW power. The presented results include distributions of D+ energy deposition, neutron and photon fluxes and heating.

- The integral heating calculations in IFMIF-DONES Test Cell (TC) components reveals that D+ energy deposition in liquid Li at thin Bragg peak with a D+ beam footprint area of 20x5 cm^2 contributes 97% of total heating in the whole Test Cell volume. The 5 MW heat power of D+ beam delivered by the IFMIF-DONES is released by 97% in liquid lithium.

Backup slides:

Additional information about

1) McDeLicious code parallelization on Marconi-Fusion HPC
2) Use of On-The-Fly (OTF) Monte Carlo variance reduction technique

MCHIFI project: fusion neutronics computations on HPCs of F4E BA and EUROfusion

- **MCHIFI** (**M**onte **C**arlo **Hi**gh **Fi**delity) project has been organized for massively parallel computations on the EUROfusion Marconi-Fusion HPC for the most urgent and computationally demanded fusion neutronics tasks.
- The MCHIFI project was founded in 2012 to use the IFERC-CSC Helios supercomputer in the framework of the F4E Broader Approach (BA) to serve the ITER neutronics tasks.

- MCNP5 tested on the F4E Broader Approach IFERC-CSC Helios: 2x8 Intel Sandy-bridge EP processors with 2.7 Hz and 64 GB RAM per node:
  - Excellent scalability of MPI/OpenMP parallel runs of MCNP5 code up to 1024 cores in analogue runs, no variance reduction.
  - Speed-up equals ~450 on 512 cores, and ~850 of speed-up for 1024 cores.
  - OpenMP/MPI hybrid, the satisfactory speed-up of more than 2500 on 4096 cores was achieved for not-biased MCNP5 calculations, as it is illustrated in Figure 1

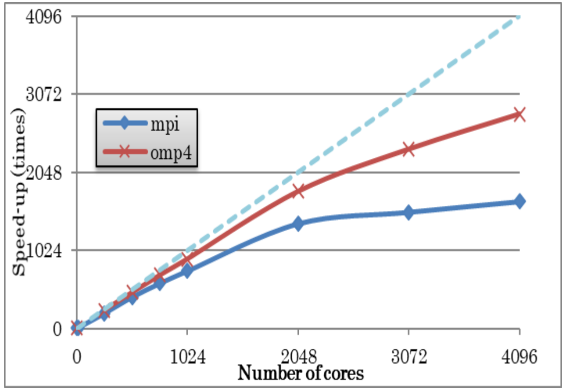


Figure 1. The MCNP5 speed-up on IFERC-CSC Helios supercomputer.

- McDeLicious tested on the EUROfusion HPC Marconi-Fusion with conventional partition (A3) based on INTEL Skylake with peak performance ~9.2 Pflops (2848 nodes). Each node is equipped with 2x24-cores Intel Xeon 8160 CPU (Skylake) at 2.10 GHz and 192 GB of RAM per node.
  - Speed-up MPI-parallel performance has been measured and presented in Figure 2 for the McDeLicious code for IFMIF-DONES radiation deep-penetration shielding tasks with variance reduction.

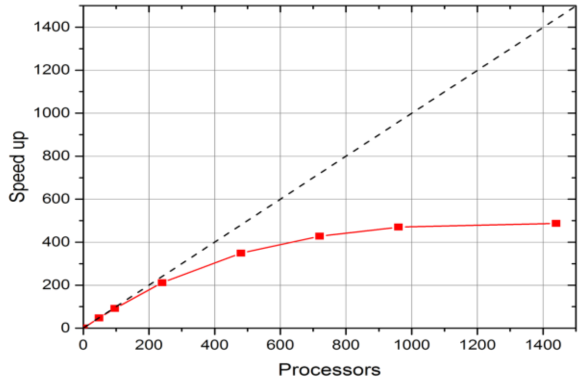
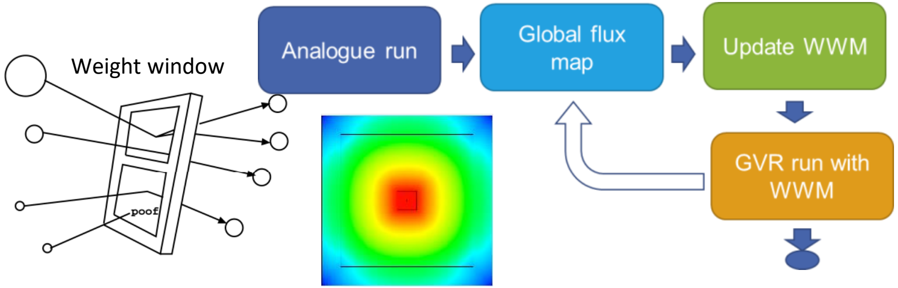


Figure 2. The speed-up of McDeLicious code on Marconi-Fusion HPC.

The optimal number of CPUs used in MCNP5/6 parallel calculations is dependent on complexity of the model. To improve the statistical errors of the MCNP5 results we are using the ADVANTG approach and the recently developed at KIT On-The-Fly (OTF) Monte Carlo variance reduction technique with dynamic Weight Window upper bounds, see Ref. [Yu Zheng, Y. Qiu, “Improvements of the on-the-fly MC variance reduction technique with dynamic WW upper bounds,” *Nuclear Fusion* **62** (2022) 086036, https://doi.org/10.1088/1741-4326/ac75fc]

MCHIFI: Development of the On-The-Fly (OTF) MC variance reduction technique

- **OTF-GVR**: On-The-Fly Global Variance Reduction
  - Weight windows mesh (WWM) is a common method used for MC shielding calculation.
  - Performs “on-the-fly” iterations to get a global flux map and a weight-window mesh.
  - Using novel dynamic WW upper bound method to solve the neutron streaming and “long-history” particles
  - Comparing with ADVANTG, OTF-GVR shows **enhancement by a factor of 20**



Analogue run

Global flux map

Update WWM

GVR run with WWM

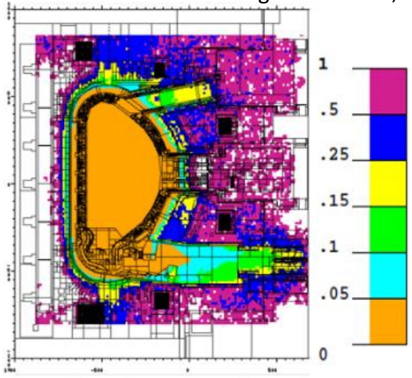
On-the-fly Global weight window mesh generation

OTF-GVR:

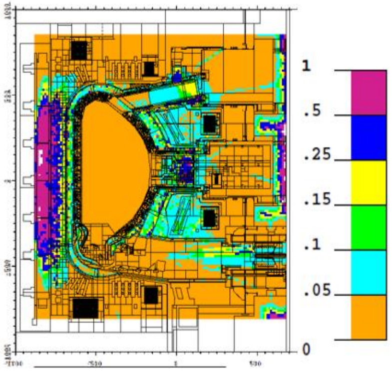
$$n(\vec{r}) \approx m(\vec{r})\bar{w}(\vec{r})$$

$$\bar{w}(\vec{r}) = \phi(\vec{r})/\max(\phi(\vec{r})) \Rightarrow \bar{w}(\vec{r}) = c \times \phi(\vec{r})/\max(\phi(\vec{r}))$$

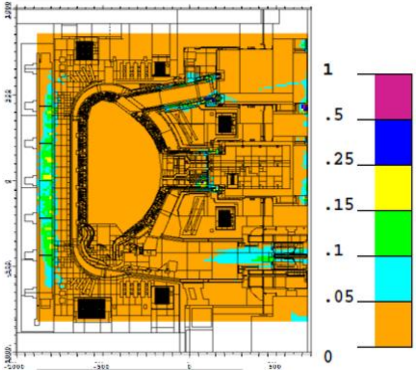
Definition of “c” to avoid “long-history” by limiting the splitting in the OTF run in Ref. [Yu Zheng, Yuefeng Qiu, et al., “An improved on-the-fly global variance reduction technique by automatically updating weight window values for Monte Carlo shielding calculation”, Fusion Eng. Des. 147 (2019) 111238, https://doi.org/10.1016/j.fusengdes.2019.06.011]



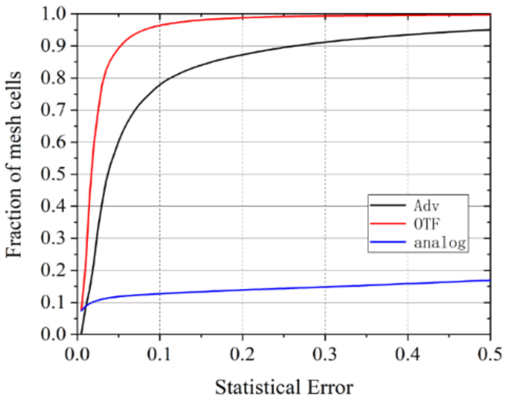
Analogue run



ADVANTG WWM run



OTF-GVR run



Percentage of mesh cells and rel. error

Ref.: [Yu Zheng et al 2022 Nucl. Fusion 62 086036, https://doi.org/10.1088/1741-4326/ac75fc]