Monte Carlo radiation transport parallel computations on Marconi-Fusion HPC for the IFMIF-DONES radiation shielding tasks



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Part I

Monte Carlo radiation transport massively parallel computations in the framework of the **MCHIFI** (Monte Carlo High Fidelity) project:

2012 – 2016: MCHIFI project foundation with the HPC resources of the F4E Broader Approach (BA) IFERC-CSC Helios supercomputer;
2016 – 2023: MCHIFI project continuation on the EUROfusion Marconi-Fusion HPC



Monte Carlo radiation transport parallel computations



Monte Carlo (MC) radiation transport runs on supercomputers

- ⇒ Simulation of <u>independent</u> random pathways on microscopic level, i. e. tracking of individual particle histories from "birth" to "death"
- \Rightarrow Simulation can be computed on <u>parallel</u> multiprocessor systems



<u>Monte Carlo method</u> is most suitable computational technique for nuclear fusion applications. That is because of the following reasons:

- <u>Geometry</u>: complex fusion devices can be modelled in 3D geometry without major geometry approximations
- <u>Data:</u> continuous energy representation as stored on evaluated data files in ENDF format
- <u>Calculation accuracy:</u> only limited by statistics and data uncertainties (no numerical approximations)

Used supercomputers:

- Europe HPC-FF system at JSC (Germany);
- CampusGrid OpusIB, SCC-KIT (Germany);
- Europe HC3 at SCC-KIT (Germany);
- Europe BWGrid (Germany)
- IFERC-CSC Helios (Japan)
- EUROfusion HPC Marconi-Fusion (Italy)

The maximum speed-up was found on **EUROfusion HPC Marconi-Fusion** supercomputer with **OpenMP / MPI parallelization** for non-biased MCNP5 run equalled <u>2500 on 4096 cores</u> (or ~850 on 1024 cores, and ~450 on 512 cores) – because dependence of speed-up to number of cores is not linear due to overhead time spent for communications between computing nodes.

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



- MCHIFI (Monte Carlo High Fidelity) 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 Sandybridge 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.

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• 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 deeppenetration 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]



Radiation transport with the MCNP code



MCNP is a code for radiation transport calculations in 3D geometry. The abbreviation is translated as Monte Carlo N-Particle.

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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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.



MCNP6 Versatility and Flexibility



- MCNP6 performs continuous-energy transport of 36 different particle types plus heavy-ion, fuel burnup, and high-fidelity delayed gamma emission. MCNP is written in Fortran 90, has been parallelized (OpenMP and MPI), and works on platforms including PCs, workstations, Linux clusters, and supercomputers.
- MCNP6 has thousands of MCNP users worldwide.

Examples of the MCNP6.2 applications:

- Neutronics and nuclear reactor design
- Nuclear criticality safety
- Fusion neutronics
- Transmutation, activation, and burnup in reactor and other systems
- Nuclear safeguards
- Medical physics, especially proton and neutron therapy
- Design of accelerator spallation targets, particularly for neutron scattering facilities
- Investigations for accelerator isotope production and destruction programs, including the transmutation of nuclear waste
- Research into accelerator-driven energy sources
- Accelerator based imaging technology such as neutron and proton radiography
- Detection technology using charged particles via active interrogation
- Design of shielding in accelerator facilities
- Activation of accelerator components and surrounding groundwater and air
- High-energy dosimetry and neutron detection
- Investigations of cosmic-ray radiation backgrounds and shielding for high altitude aircraft and spacecraft
- Single-event upset in semiconductors from cosmic rays in spacecraft or from the neutron component on the earth's surface
- Analysis of cosmo-chemistry experiments, such as Mars Odyssey
- Charged-particle propulsion concepts for spaceflight
- Investigation of fully coupled neutron and charged-particle transport for lower-energy applications
- Nuclear material detection
- Design of neutrino experiments



Particles transported by MCNP6. As listed in Chapter 2 of the MCNP® 6.2 USER'S MANUAL, October 27, 2017



Table 2-2. MCNP6 Particles

IPT*	Name of Particle	Symbol	Mass ¹ (MeV)	Low Kinetic Energy Cutoff / Default Cutoff (MeV)	Mean Lifetime ¹ (seconds)						Low Kinetic Energy	Mean Lifetime ¹ (seconds)	
					As treated by MCNP6	Actual (if different)	IPT*	Name of Particle	Symbol	Mass ¹ (MeV)	Cutoff / Default Cutoff (MeV)	As treated by MCNP6	Actual (if different)
1	neutron (n)	Ν	939.56563	0.0 / 0.0	no decay	887.0	20	positive pion (π +)	/	139.56995	1.e-3 /	2.603×10-8	
2	photon (γ)	Р	0.0	1.e-6 / 1.e-3	1×1029		21	nontrol nion (=0)	7	124.0764	0.14875	8 4×10 17	
3	electron (e)	E	0.511008	1.e-5 / 1.e-3	1×1029		21	neutral pion (<i>n</i> 0)		134.9704	1 2 2 /	8.4×10-17	
4	negative muon (μ)		105.658389	1.e-3 / 0.11261	2.19703×10-6			positive kaon (K+)	K	493.077	0.52614	1.23/1^10-8	
5	anti neutron ()	Q	939.56563	0.0 / 0.0	no decay	887.0	23	kaon, short (K0S)	%	497.672	0.0 / 0.0	0.8926×10-10	
6	electron neutrino (ve)	U	0.0	0.0 / 0.0	1×1029		24	kaon, long (K0L)	^	497.672	0.0 / 0.0	5.17×10-8	
7	muon neutrino (vm)	V	0.0	0.0 / 0.0	no decay		25	anti lambda baryon ($\overline{\sqrt{2}}$)	В	1115.684	1.e-3 / 1.0	DOP^\dagger	2.632×10 ⁻¹⁰
8	positron (e ⁺) (See Note 1)	F	0.511008	1.e-3 / 1.e-3	1×10 ²⁹		26	anti positive sigma		1189.37	1.e-3 /	DOP [†]	7.99×10 ⁻¹¹
9	proton (p+)	Н	938.27231	1.e-3 / 1.0	1×1029			baryon (Σ^+)			1.26760		
10	lambda baryon ($\Lambda 0$)	L	1115.684	1.e-3 / 1.0	DOP†	2.632×10-10	27	anti negative sigma baryon $(\overline{\Sigma}^{-})$	~	1197.436	1.e-3 / 1.26760	DOP^\dagger	1.479×10 ⁻¹⁰
11	positive sigma baryon (Σ+)	+	1189.37	1.e-3 / 1.26760	DOP†	7.99×10-11	20	anti cascade; anti	C	1314.9	1.e-3 / 1.0	DOP [†]	2.9×10 ⁻¹⁰
12	negative sigma baryon(Σ)	-	1197.436	1.e-3 / 1.26760	DOP†	1.479×10-10	28	$\overline{\Xi}^0$)	C				
13	cascade; xi baryon (Ξ0)	Х	1314.9	1.e-3 / 1.0	DOP†	2.9×10-10	29	positive cascade; positive xi baryon (Ξ ⁺)	W	1321.32	1.e-3 / 1.40820	DOP^\dagger	1.639×10 ⁻¹⁰
14	negative cascade; negative xi baryon (Ξ)	Y	1321.32	1.e-3 / 1.40820	DOP†	1.639×10-10	30	anti omega ($\overline{\Omega}^-$)	0	1672.45	1e-3 / 1.78250	DOP^\dagger	8.22×10 ⁻¹¹
15	omega baryon (Ω)	0	1672.45	1e-3 /	DOP†	8.22×10-11	31	deuteron (d)	D	1875.627	1.e-3 / 2.0	1×1029	
				1.78250	1		32	triton (t)	Т	2808.951	1.e-3 / 3.0	12.3 years	
16	positive muon (μ^+)	!	105.658389	1.e-3 /	2.19703×10-6		33	helion (3He)	S	2808.421	1.e-3 / 3.0	1×1029	
	anti alaatran nautrina			0.11201			34	alpha particle (α)	А	3727.418	1.e-3 / 4.0	1×1029	
17	(\overline{v}_{e})	<	0.0	0.0 / 0.0	1×10 ²⁹		35	negative pion (π^{-})	*	139.56995	1.e-3 / 0.14875	2.603×10-8	
18	anti muon neutrino (\overline{v}_{m})	>	0.0	0.0 / 0.0	no decay		36	negative kaon (K ⁻)	?	493.677	1.e-3 / 0.52614	1.2371×10 ⁻⁸	
19	anti proton (\overline{p})	G	938.27231	1.e-3 / 1.0	1×10 ²⁹		37	heavy ions [‡]	#	varies	1.e-3 / 5.0	1×10 ²⁹	

[†] DOP=Decayed on production

[†] The "#" symbol represents all possible heavy-ion types—in other words, any ion that is not one of the four light ions available in MCNP6.

** A list of heavy ions available for transport is provided in Appendix G.

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.
- OTF performs "on-the-fly" iterations to get a global flux map and a weight-window mesh (WWM).
- OTF uses novel dynamic WW upper bound method to solve the neutron streaming and "long-history" particles
- Compared with ADVANTG, the Figure-of-Merit in OTF is raised by a factor of 20

OTF-GVR:

Definition of "c" to avoid "long-history" by limiting the n, p particles splitting in the OTF run in Ref. Yu Zheng, Yuefeng Qiu, et al.,



On-the-fly Global weight window mesh generation



"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, <u>https://doi.org/10.1016/j.fusengdes.2019.06.011</u>]







Part II

Application of the EUROfusion Marconi-Fusion HPC **MCHIFI** project for solving the IFMIF-DONES radiation shielding tasks



DONES Working Group, IFMIF-DONES España to build the DONES facility



The International Fusion Materials Irradiation Facility – DEMO Oriented NEutron Source (IFMIF-DONES). DEMO is a demonstration fusion reactor prototype. In relation to this international project, in Dec. 2017, Fusion for Energy (F4E) evaluated positively the joint Spain-Croatia proposal to site the IFMIF-DONES in Granada, Spain.

Countries and Organizations
involved in the DONES
Working Group
Hungary
Croatia
Italy
Spain
Germany
Slovenia
Denmark
Greece
Finland
Sweden
Lithuania
Estonia
France
F4E - Support
EUROfusion - Observer
DG-ENER - Lead
DG-RTD - Observer

EURATOM (DG-ENER) organized a Working Group with Spain, Croatia and other EU countries supported by F4E to initiate the IFMIF-DONES project. Updates of the IFMIF-DONES: https://ifmif-dones.es/

In 2021 the **IFMIF-DONES España** consortium of the Spain General State Administration and the Autonomous Community of Andalusia established to provide the IFMIF-DONES facility design, construction, and operation.

The IFMIF-DONES facility **construction began in 2022**, its commissioning is planned for 2029, and the first results are expected to be obtained in 2035.









IFMIF-DONES geometry CAD-to-MCNP conversion



The CAD model of IFMIF-DONES building is properly prepared to be used with the MCNP code. The geometry of
each component of the building was simplified and decomposed into a number of simple primitive blocks. Then the
CAD model is converted into MCNP model and fill into the separate envelope using the MCNP universe card. The
CAD-to-MCNP conversion is performed using McCad and SuperMC programs.



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 DONES Test Cell

Neutronics modeling of the IFMIF-DONES



The neutron and photon radiation transport was performed by the **McDeLicious** code package – an **MCNP** source extension that simulates the deuteron-lithium (d-Li) nuclear reactions in Li of Test Cell. The neutron cross-sections library FENDL-3.1d used in calculations. The neutronics results were normalized to a 125 mA deuteron beam of 40 MeV deuterons impinging the Li target.



MCNP model horizontal cut at the center of the Li target and two TWBD beam ducts.

MCNP model vertical cut throught the center of the Li target. The spacial dimension of the model is given in the length scale [cm].



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





Click here or picture or menu

DONES Target Assembly (TA) components

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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







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



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

- D+ ion beam stops in the lithium jet delivering a total power of 5 MW on a volume of $5 \times 20 \times 2.5$ cm³, with d-Li footprint area of 5×20 cm².
- 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



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

MCNP6 TMESH result for

0.5x1x1 mm³ (xyz) mesh

IFMIF Deuteron beam energy deposition in the Lithium jet at the d-Li 20×5 cm² footprint area D ()NES

9.900E+4

8.910E+4

7.920E+4

6.930E+4

5.940E+4

4.950E+4

3.960E+4

2.970E+4

1.980E+4

9900

10

0.000

Heat deposition in Li-Target plane section x=-0.875 cm D+ beam profile (IFMIF/EVEDA) 0.005 1.0×10 Upper and lower side 0.0051 8.0×10⁴ - 0.0046 0.00 6.0×104 0.0040 z 0.004 0.0034 4.0×10⁴ - 0.0029 2.0×104 \$ 0.003 - 0.0023 0.0 - 0.0017 0.002 0.0011 5.7E-04 Ylom **Result:** MCNP6 transport Source: 1.100E+05 deposition, W/cc D+ beam energy 9,789E+04 5 8.578E+04 7.367E+04 6.156E+04 4.944E+04 3.733E+04 2.522E+04 1.311E+04 1.000E+03 Heat at peak is 110 kW/cc Integral D+ heat 4.8 MW Notice: Bragg peak at Lithium thickness of **1.86 cm** corresponds MCNP6 horizontal-vertical map of D+ energy to -0.84 cm coordinate in the deposition (W/cc) at X= -0.84 cm MCNP model geometry with X=0 at 4 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





MCNP model mesh-tally for TIR and adjacent rooms





- In distributed memory MPI-jobs, simple MCNP models must fit in 4 GB RAM memory per each Marconi core: 4 GB/core * 48 cores/node = 192 GB/node of A3-SKL (Skylake) conventional partition.
- The reduced numbers of cores per node (~20 cores/node) must be set in the MPI MCNP runs due to the high memory consumption of the complex models with large mesh-tallies.

 For the results production we assumed middle-size MCNP model with averaged use of 10 nodes with 48 cores/node equalled to 480 cores of A3-SKL.

Total n-flux distribution in TC and empty TIR thresholded scale



RIR behind concrete wall 1 TWBD-2 TWBD-1 **TIR – TC concrete wall** TC TIR AY I Total neutron flux, n/cm2/s 7 X 1.0e+06 1e+7 1e+8 1e+9 1e+10 1e+11 1.0e+12

Total n-flux calculated with d-Li source on scale from 1e6 to 1e12, with flux threshold at 1e6 n/cm2/s







IFMIF Total n-flux distribution in TC and TIR – proposed shielding box D (ONES



Total n-flux calculated with d-Li source on scale from 1e6 to 1e12, with flux threshold at 1e6 n/cm2/s





Neutron and photon heating contributors to nuclear heat density (W/cc)







<u>Comparison of two BDs:</u> Shielded BD2 vs. Empty BD1: View from the top on the map of biological dose rate (microSv/h) from neutrons







Neutron flux computations in TC-CER using the MCNP mesh-tallies





Mapping of neutrons streaming from Test Cell (TC) through the Neutron Beam Tube and Shutter (NBT & S) system to CER. The collimated neutrons will be supplied to conduct variety neutronics experiments inside CER.



Total neutron flux, n/cm2/s 1.0e+00 10 100 1000 10000 10000 1e+6 1e+7 1e+8 1e+9 1e+10 1e+11 1e+12 1e+13 1e+14 5.8e+14 _____

Total neutron flux horizontal central cut at entrance to CER from TC with installed HCPB Model Blanket Module (MBM) behind HFTM





1e5

1e5-

1e5

1e3

10

3

0.5



Position #1: Open NB shutter



CER is Red (forbidden) radiation zone: DR>1e5 microSv/h

CER is Yellow (limited regulated) rad. zone: (10<DR<1e3) microSv/h



Ultimate proof of solving the IFMIF-DONES radiation shielding task: Biological dose rate (microSv/h) from neutrons, with 15 orders of magnitude dose attenuation along the Y-line distribution

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Conclusions



- Serving most demanded Monte Carlo radiation transport computations for fusion large facilities, the MCHIFI (Monte Carlo High Fidelity) HPC project has been established in 2012 to use the IFERC-CSC Helios supercomputer in the framework of the F4E Broader Approach (BA) for ITER neutronics tasks.
- Since 2016, MCHIFI project was deployed on the computational resources of the Marconi-Fusion HPC facility offered by EUROfusion and operated by ENEA/CINECA. At this moment, MCHIFI is running on 7th cycle of Marconi-Fusion HPC. In our application for the 8th cycle, we have justified the number of core-hours requested to fulfill not only the IFMIF-DONES shielding tasks, but also numerous Shutdown Dose Rate (SDR) calculations for the JET NEXP SDR experiment of the C38 2019-2020 DD and the C41 2021 DT2 campaigns of JET, and using the data of JET DT3 campaign to be available at the end of 2023.
- A large number of the Marconi-Fusion HPC nodes are needed in the for the IFMIF-DONES large-scale complicated models to run the Monte Carlo (MC) radiation transport parallel computations with the MCNP and McDeLicious codes.
- The methodology improvement is demonstrated in the recent development of the On-The-Fly (OTF) modification of the MCNP code. The OTF Global Variance Reduction (OTF-GVR) is the state-of-the-art code for the IFMIF-DONES radiation shielding tasks characterized by neutrons deep penetration. We have used OTF-GVR for radiation transport through the 6.4 m shielding between the IFMIF-DONES Test Cell and its Complementary Experiments Room (CER).
- Developed at KIT Monte Carlo radiation transport CAD-based methodology can reproduce the d-Li neutron & photon source at the Li target and extremely strong radiation attenuation in heterogeneous IFMIF-DONES geometry:
 - Neutron flux attenuation by 18 orders of magnitude (from 2e14 to 2e-4 n/cm²/s inside Tritium room);
 - Biological dose rate from neutrons attenuation by 15 orders of magnitude (from 2e14 to 0.3 microSv/h inside Tritium room);
 - Radiation energy deposition attenuation by 11 orders of magnitude (heat at peak of 110 kW/cc in d-Li footprint to ~ 1 microW/cc inside steel of the IVVS shielding box inside the Target Interface Room -TIR).
 - The MCNP mesh-tally reveled the dominancy of fast neutrons in the total neutron flux at the exit from Neutron Beam (NB) shutter to CER.