MARS15(2019): Recent Developments and its DPA Model

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Outline

- MARS15 Improvements since NBI/RaDIATE 2017

- Geometry, ROOT-based Beamline Builder and MARS15-MADX-PTC

- Recent Benchmarking

- DPA Model

- Summary

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MARS15 Improvements since NBI/RaDIATE 2017

- Event generators: better matching at high energies and TENDL

- 3-body decays: matrix element of a **V-A** (vector minus axial vector) Lagrangian for weak interactions and polarization added to basic decay kinematics of kaons and muons

- Materials and newest low-energy neutron data libraries

- Geometry, tracking, RF cavities, dark current, variance reduction, histograming and GUI

- DPA and gas production

- Pre-release of MARS15(2019)

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High-Energy Nuclear Event Generator

- Projectile E_0 < 0.12 GeV down to 1 MeV (charged particles) and 14 MeV (neutrons): a combination of **extended** TENDL-2015 (inclusive, semi-inclusive or exclusive (coming) mode – user's choice) and LAQGSM; some issues with TENDL-2017

- 0.12 < E_0 < 0.5 GeV: a combination of CEM-2018 and LAQGSM-2018

- 0.5 < E_0 < 10 GeV: LAQGSM (also used if a projectile not in TENDL)

- 10 GeV < E_0 < 100 TeV: LAQGSM or inclusive (user's choice)
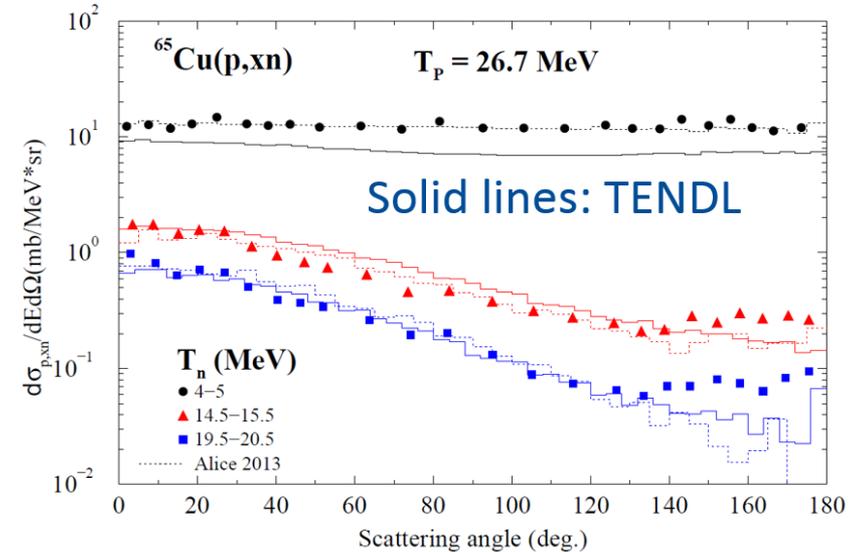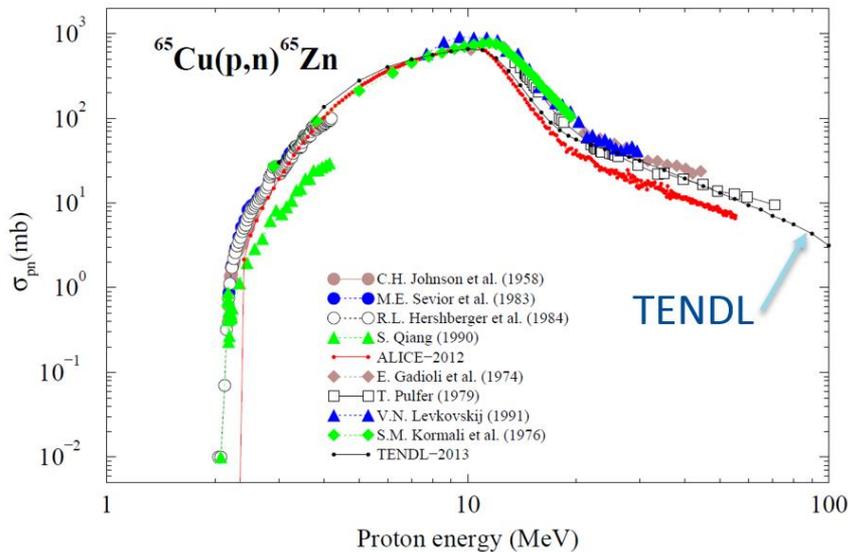
CEM Replaced with TENDL at 1 < E < 120 MeV
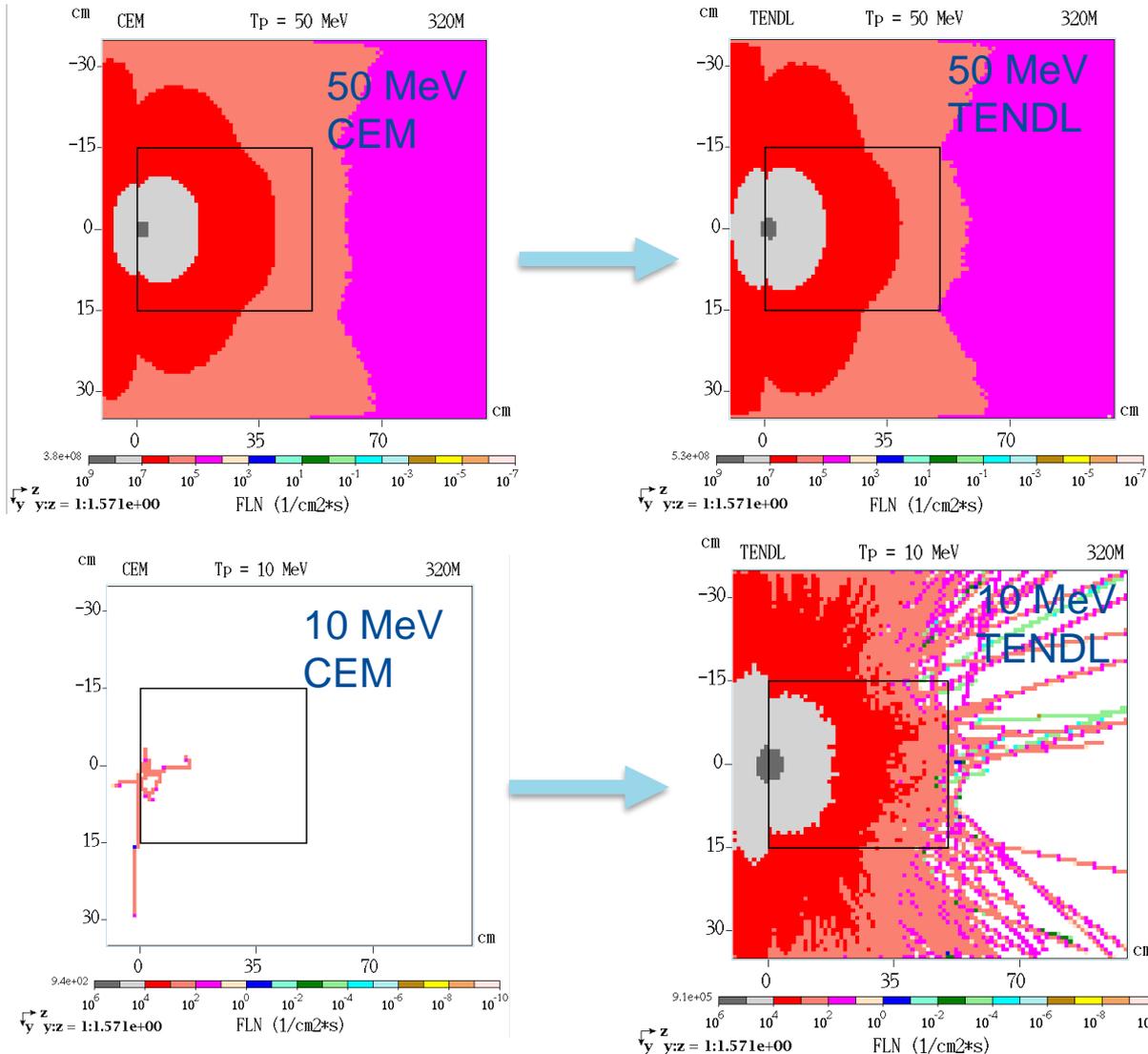
- Projectile list extended
- Drastic improvements for all materials at projectile energies 1 – 30 MeV, crucial for DPA and H/He gas production, especially in microstructures
- CPU performance is similar for CEM & TENDL

Left: TENDL *vs* CEM Neutron flux density for 50 and 10 MeV protons on Al cylindrical target in Air

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Material Description & Low-Energy Neutrons

- The code automatically unpacks the elemental distributions into isotope distributions for both user-defined and those from the 172 built-in material definitions for use in the 10^{-11} MeV < E < 100 TeV energy range

- For neutron interactions at 10^{-11} < E_n < 14 MeV, MARS15(2019) relies now on the heavily validated and recently released library of ACE files based on ENDF/B-VIII.0(2018) + NJOY-2016

- There is no need anymore to add material description in the MCNP format after the STOP card in MARS.INP files: the code does automatically all the required interface work for every single isotope found in the given run

- Accurate treatment of material state (solid, liquid and gaseous); He^3 treatment

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MARS15(2018): Other Improvements/Extensions

- Maximal energy 100 TeV is kept

- Minimal kinetic energy: 10^{-5} eV for neutrons and 1 keV for photons, charged particles and heavy ions

- Customized steppers (with 8th order Runge Kutta solver) for optimal particle tracking in SRF (with time-dependent electromagnetic fields and Dark Current production), quadrupole/dipole magnets and thick shielding

- Variance reduction techniques: multi-stage, splitting/Russian roulette, biasing, weight windows refined

- Set of flux-to-dose (FTD) conversion factors to calculate - in the course of Monte-Carlo - effective prompt dose distributions: ICRP103 + ICRP60 + Cossairt (2009) + Pellicioni (2000) + MARS generated for neutrinos

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Geometry Description and ROOT-based Beamline Builder

1. User-generated via MARS extended geometry input files

2. User-generated ROOT files

3. GDML files (two-way exchange with Geant4 teams)

4. G4beamline's BruitDeFond can generate MARS's input files MARS.INP, GEOM.INP and FIELD.INP

5. STEP files from project CAD models used to generate ROOT geometry modules

6. Lattice and beamline components such as dipole and quadrupole magnets, correctors, accelerating cavities, cryomodules and tunnel with all the details available on geometry, materials and electromagnetic fields by means of the advanced ROOT-based Beamline Builder

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MARS15-MADX-PTC Integration for Beam Loss and Collimation Modelling

A library containing functions and C++ classes which interfaces MARS with MADX is now packed with the MARS15 distribution. The library allows to

- Create a 3-D TGeo ROOT geometry model for the sequence described in a MADX-PTC input file. Alignment of elements is performed by means of the MAD-X survey table.

- Define transformation for each point in the phase space used in the PTC module to the phase space used in MARS15 and vice-versa.

- Inject particles transported by MARS15 to MADX-PTC module using a formulated acceptance for the accelerator code model.

- For particles transported in PTC, perform check of boundary crossing against the ROOT geometry in MARS15; the particle is forwarded to the MARS15 stack.

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Examples: Fermilab Recycler and ILC

Fermilab 8-GeV Recycler
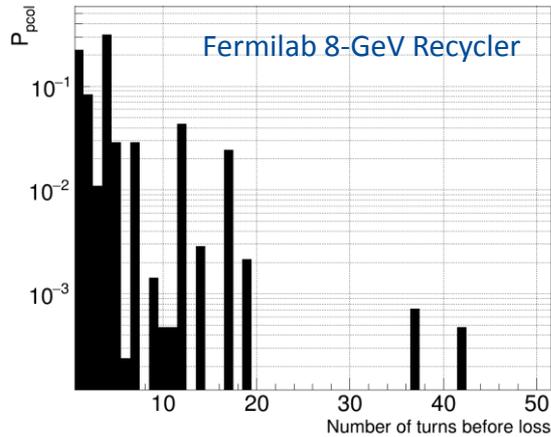
Probability to be lost for beam halo protons passed through the primary collimator vs #turns
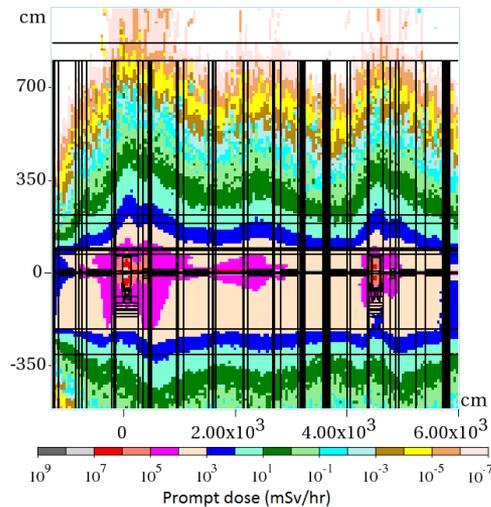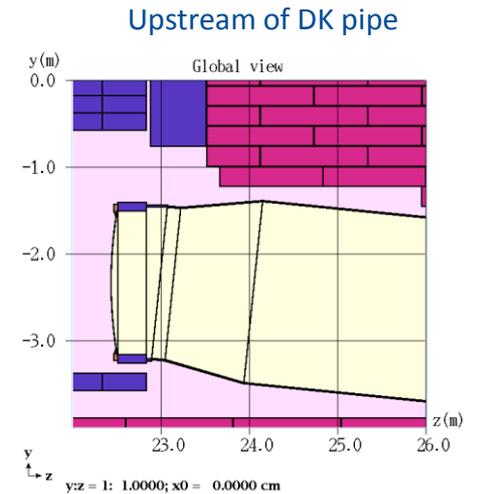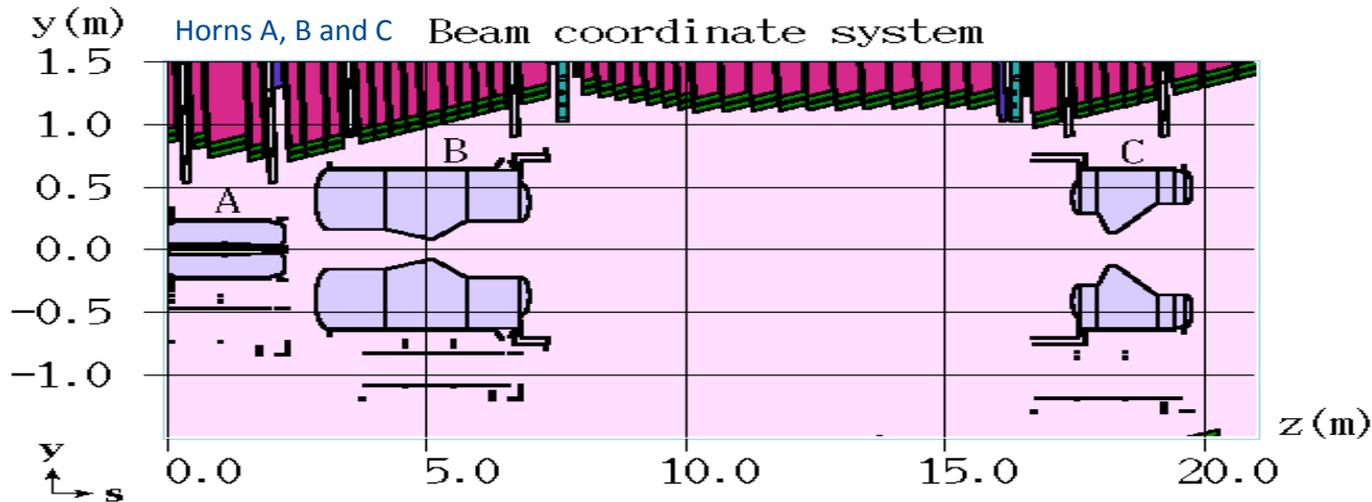

Prompt dose in collimation region

MARS15 SRF model
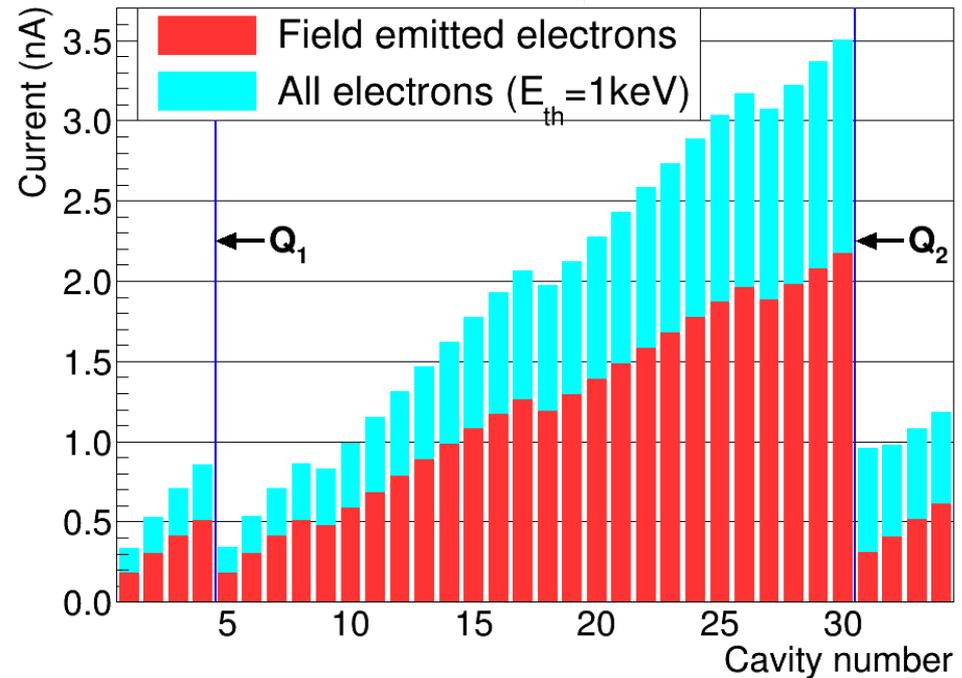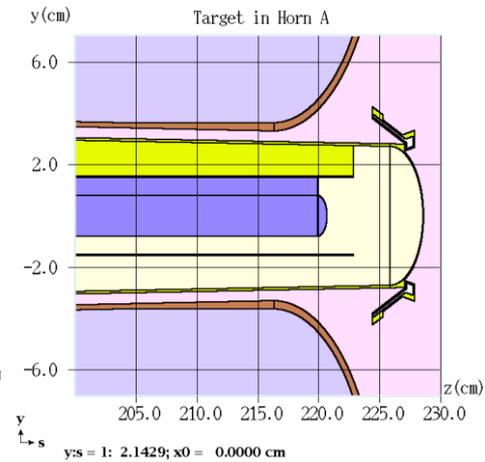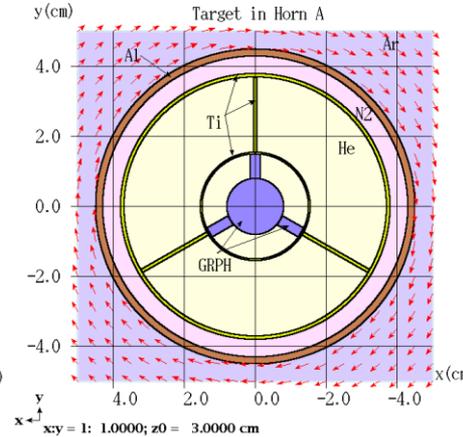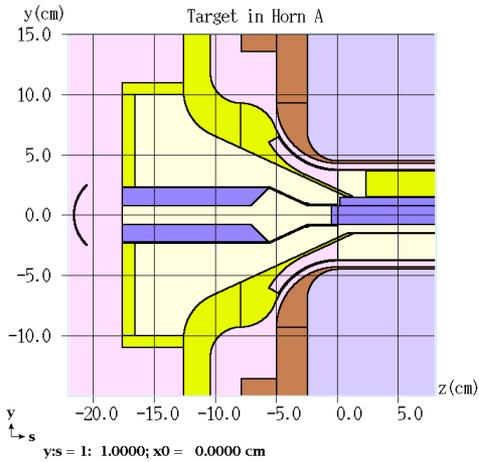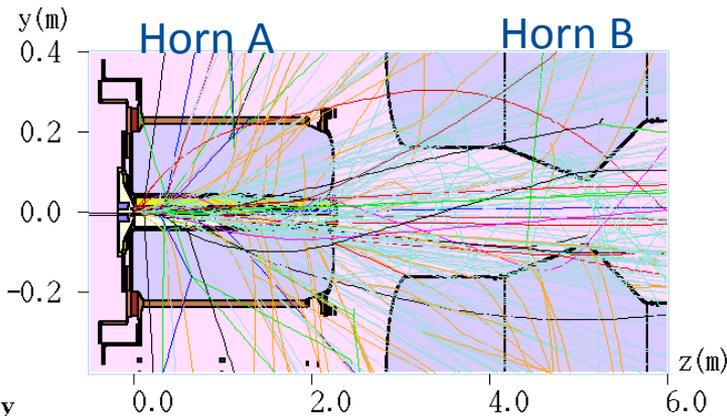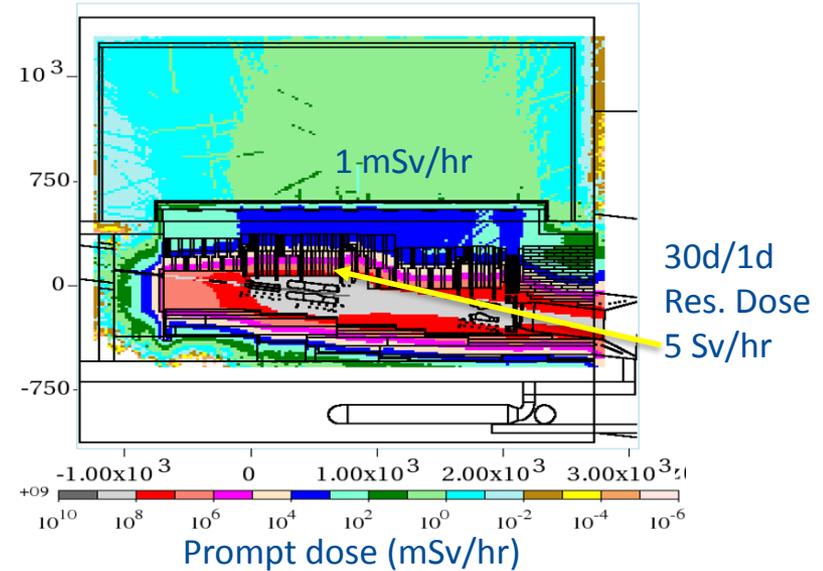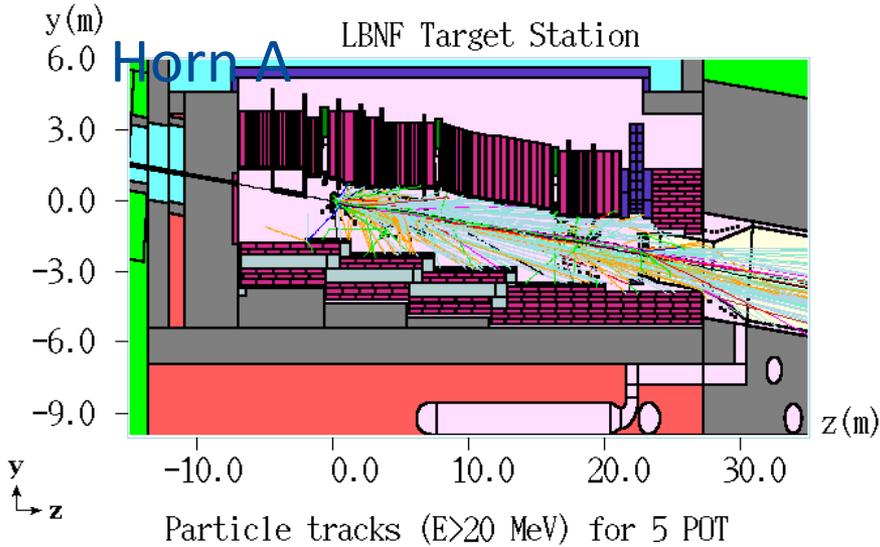

Dark current electrons and EMS electrons in ILC aperture with their loss responsible for radiation load to components and radiation field in ILC tunnel
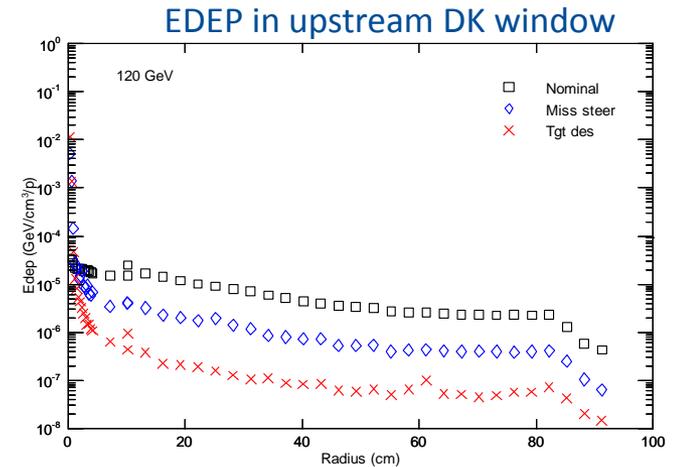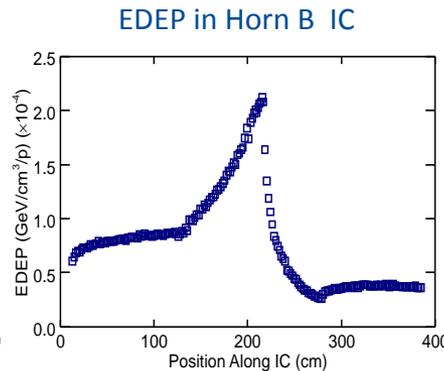
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Details of the LBNF-MARS TS Model

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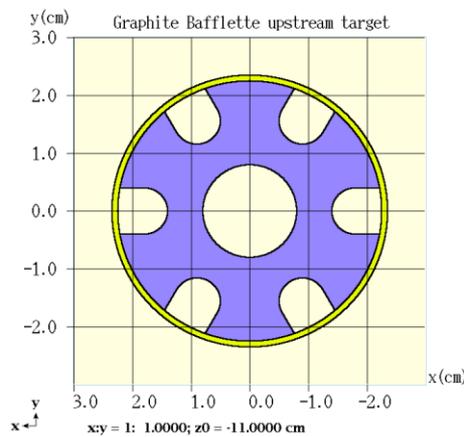
Target Station Simulations

Horn A

LBNF Target Station

y(m)
Particle tracks (E>20 MeV) for 5 POT

1 mSv/hr

30d/1d
Res. Dose
5 Sv/hr

Prompt dose (mSv/hr)

Horn A   Horn B

Particle tracks (E>20 MeV) for 5 POT

Note stretched y-axis and squished s-axis

EDEP in Horn B IC

EDEP in upstream DK window

120 GeV

Nominal
Miss steer
Tgt des

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Air Activation at NuMI Neutrino Production Facility

To get more confidence in the MARS15-based LBNF target station design, a benchmarking campaign on air activation has been recently undertaken at the Fermilab NuMI target station for 120-GeV beam on target

NIM **B414** (2018) 4-10

Measured and calculated production rate density (cm^{-3} POT^{-1} s^{-1}) for the most important radionuclides generated in the air in the beam enclosure of the NuMI target chase.

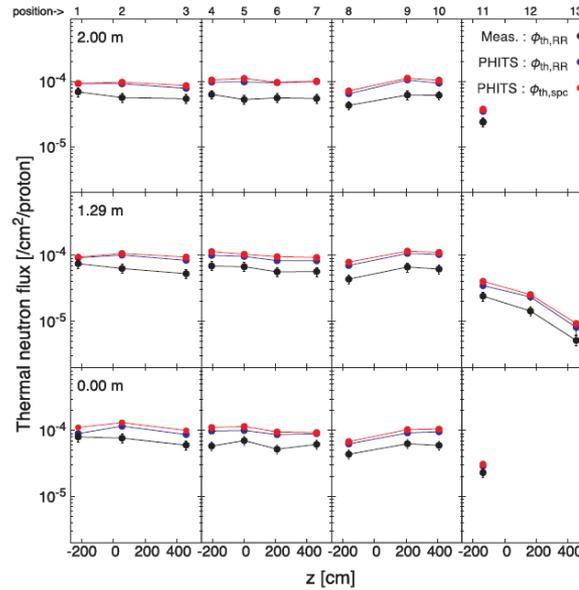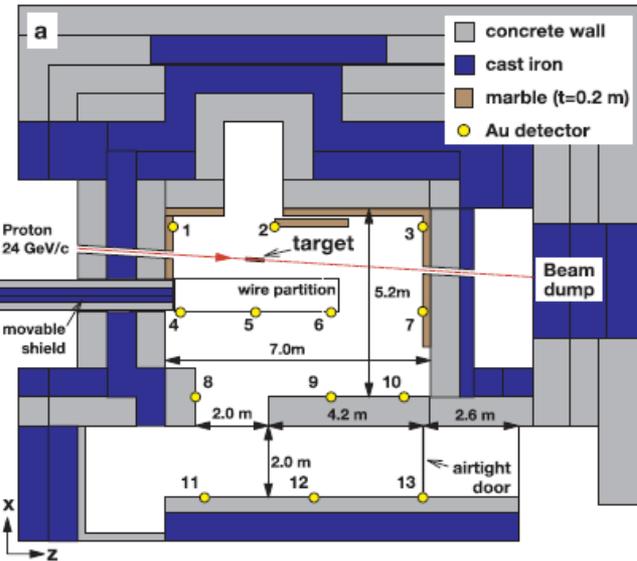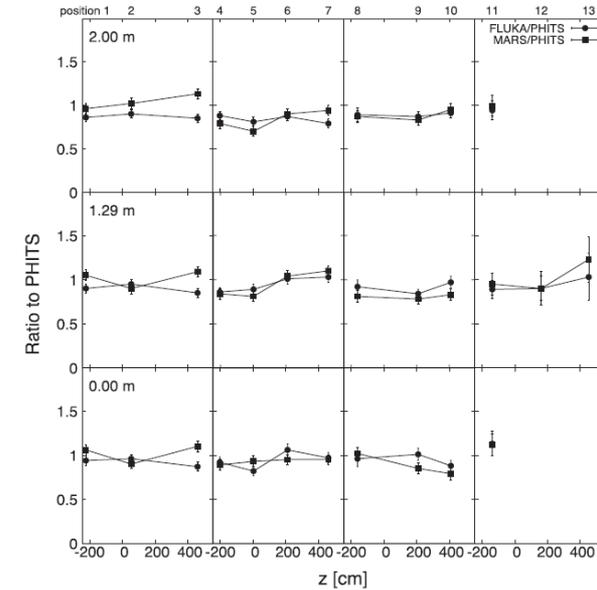| Production rate	^{41}Ar	^{11}C	^{13}N	^{15}O
Measurement	1.98×10^{-12}	6.38×10^{-11}	4.07×10^{-11}	3.50×10^{-11}
Standard methodology	6.85×10^{-12}	2.22×10^{-10}	5.22×10^{-11}	9.16×10^{-11}
MARS15	1.08×10^{-12}	4.44×10^{-11}	3.71×10^{-11}	4.16×10^{-11}
MARS15/data	0.55	0.70	0.91	1.19

50%   10-30%

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PHITS, FLUKA & MARS *vs* CHARM 24 GeV/c Data

24-GeV/c p + 50cm Cu target

$^{197}Au(n, g)^{198}Au$: Thermal neutron flux at 3 heights
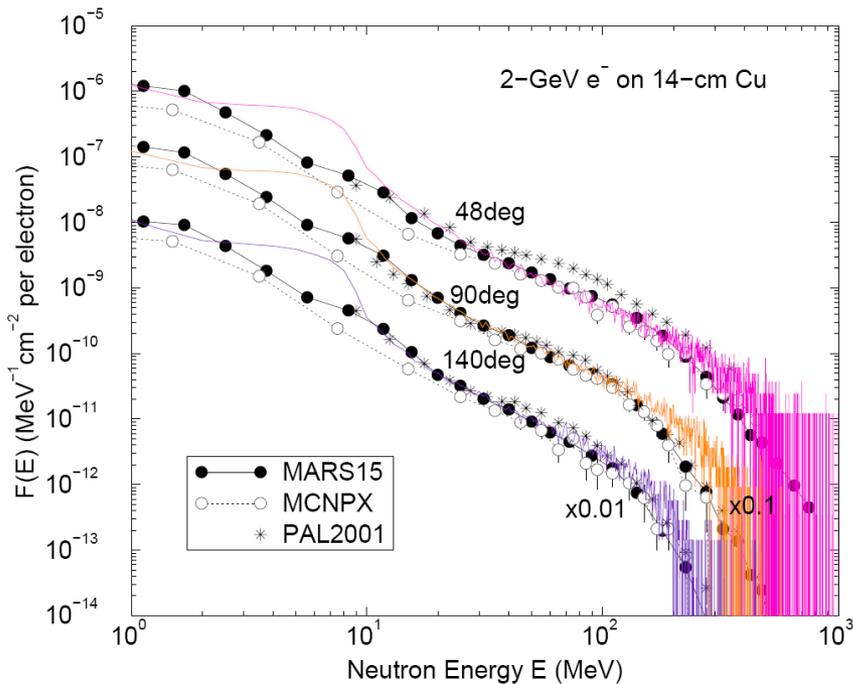

PHITS & Exp within 50%   FLUKA, PHITS & MARS within 30%

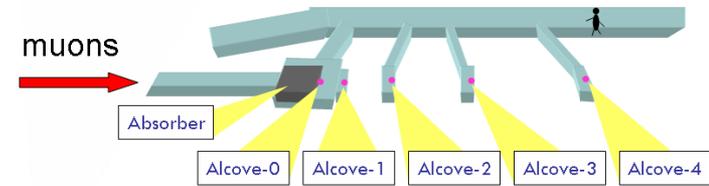T. Oyama et al., NIM, **B434** (2018) 29-36

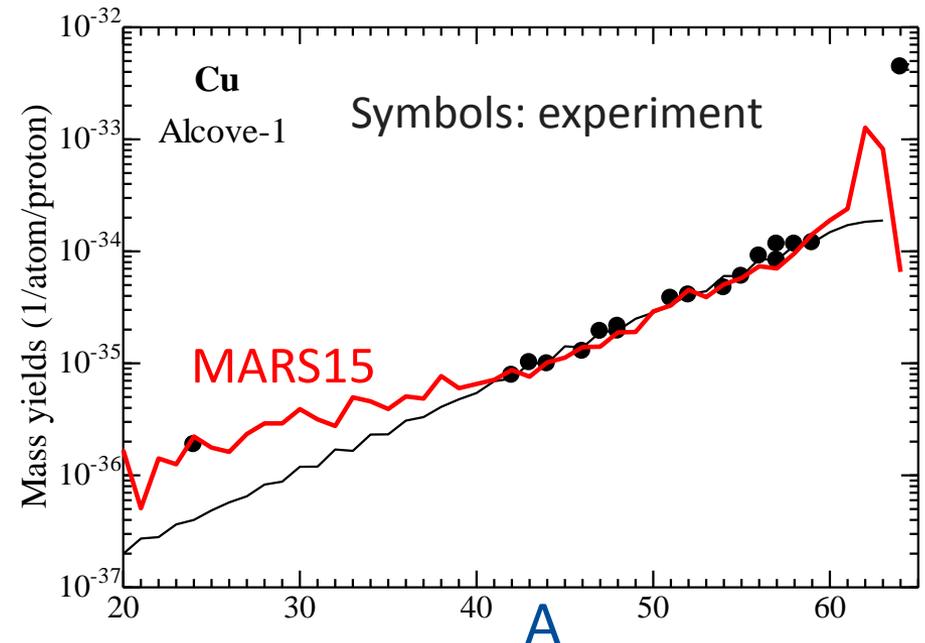🔷 **Fermilab**

Benchmarking with PAL and JASMIN Data

Photo-Neutron Yield:
MARS15 and MCNPX *vs* PAL data

JASMIN NuMI at FNAL

Nuclides in muon-induced nuclear interactions

DPA in MARS15(2019)

- Energy of recoil fragments and new charge particles in (elastic and inelastic) nuclear interactions is used to calculate atomic displacement cross sections σ_{DPA} for the NRT model – with and w/o damage efficiency $\xi(T)$ for a number of stable defects

- Atomic screening parameters are calculated using the Hartree-Fock form-factors and recently suggested corrections to the Born approximation

- NJOY2016+ENDF/B-VIII.0(2018) was used to generate a NRT/Nordlund/Stoller database for 490 nuclides for neutrons from 10^{-5} eV to 150 MeV; DPA in neutron-nuclear interactions above 150 MeV are treated the same way as described in the first bullet

- In the same run/output, atomic displacement x-sections and resulting DPA in regions of interest are calculated in three ways: pure NRT and those for surviving defects with Nordlund and Stoller efficiency functions $\xi(T)$
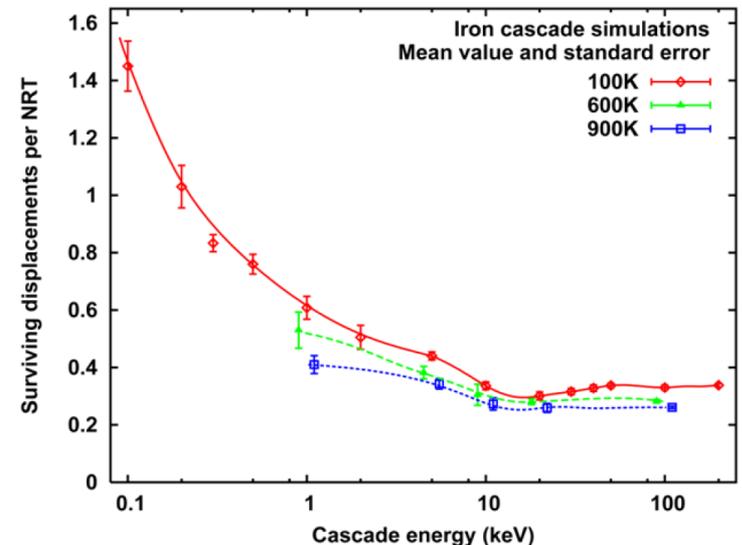
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NRT "Standard" Model to Calculate a Number of Frenkel Pairs and Damage Energy and Corrections

M.J. Norgett, M.T. Robinson, I.M. Torrens Nucl. Eng. Des 33, 50 (1975). Based on 40-year old binary collision model. *De facto*, international standard to quantify atomic displacement level in irradiated materials

$$N_d = \frac{0.8}{2E_d} T_d \qquad T_d = \frac{T_r}{1 + k(Z_t, A_t, Z_r, A_r) g(T_r, Z_t, A_t, Z_r, A_r)}$$

At the very beginning of this century, it was realized that NRT-DPA overestimates the number of stable defects. R. Stoller (2000) proposed corrections to NRT to account for atom recombination in elastic cascading, based on his MD simulation for iron at 100-900K. Its parametrization for efficiency function $\xi(T) = N_d/N_{NRT}$ is used in MARS15 and FLUKA. We use $\xi(T) = 1$ if it becomes > 1. It is in a very good agreement with σ_{DPA} derived by Jung (J. Nucl. Mater. 117 (1983) 70) from low-temperature experiments.

Iron cascade simulations
Mean value and standard error
100K
600K
900K

Surviving displacements per NRT vs Cascade energy (keV)

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ARC-DPA Efficiency Function

The ARC-DPA concept (athermal recombination-corrected DPA), was introduced by K. Nordlund in 2012 and supported by OECD/NEA working group. Its parametrization ξ(T) is based on MD simulations for copper. It is in MARS15 since 2016.

"The recombination process does not require any thermally activated defect migration (atom motion is caused primarily by the high kinetic energy introduced by the recoil atom), this recombination is called "athermal" (i.e. it would also happen if the ambient temperature of the sample would be 0 K)."
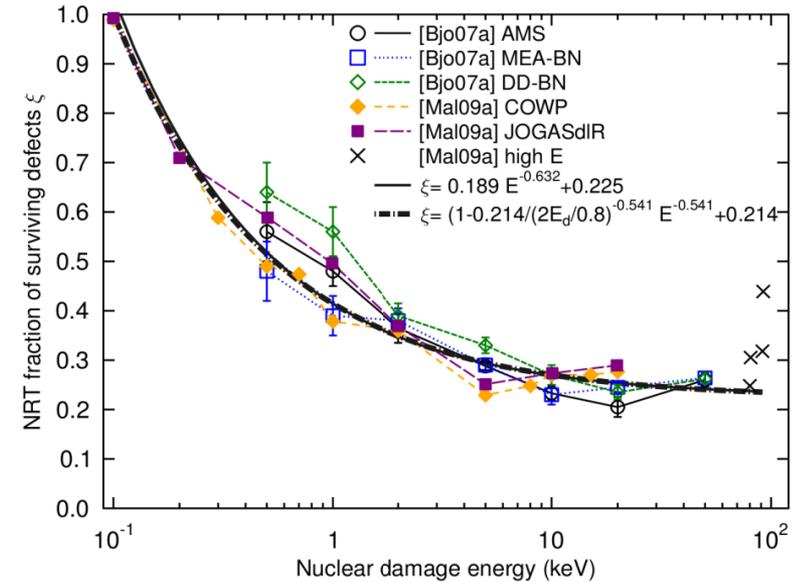
Modified NRT

$$N_d = \begin{cases} 0 & T_d < E_d \\ 1 & E_d < T_d < 2.5E_d \\ \dfrac{T_d}{2.5E_d}\,\xi(T_d) & 2.5E_d < T_d \end{cases}$$

with 2012's efficiency function

$$\xi(T) = 0.214 + 0.786 \times (2.5E_d / T)^{0.541}$$

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ARC-DPA Developments and Verification

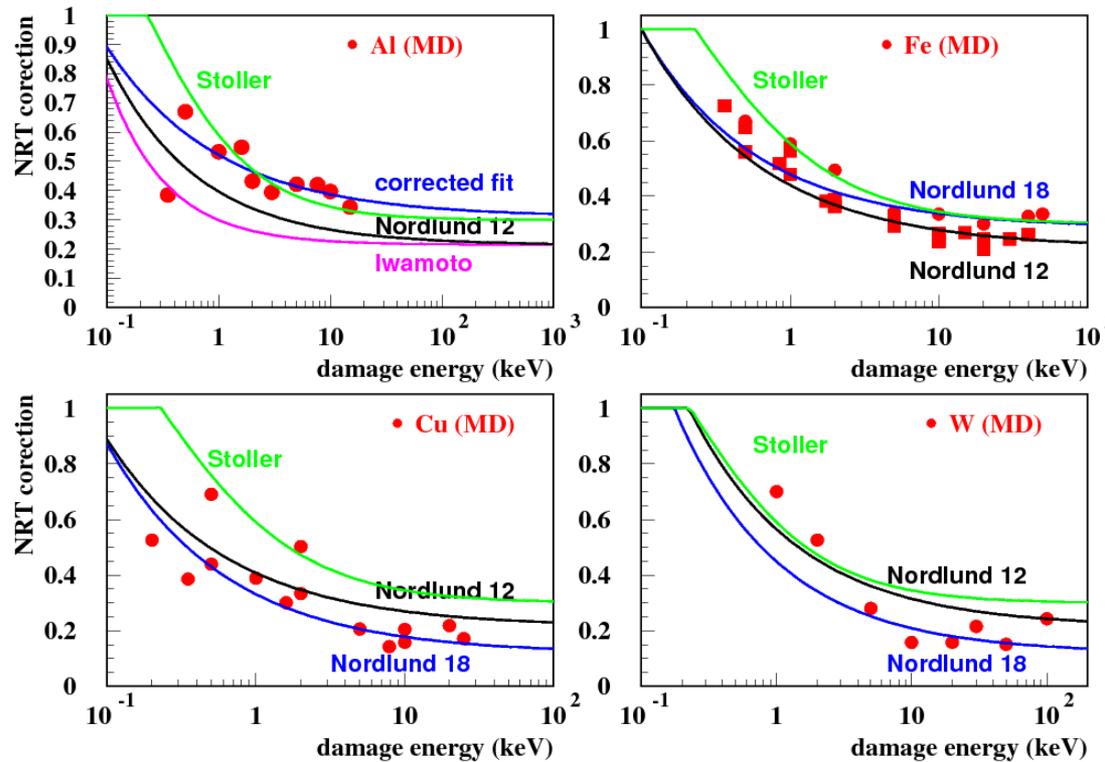**2018's developments:**

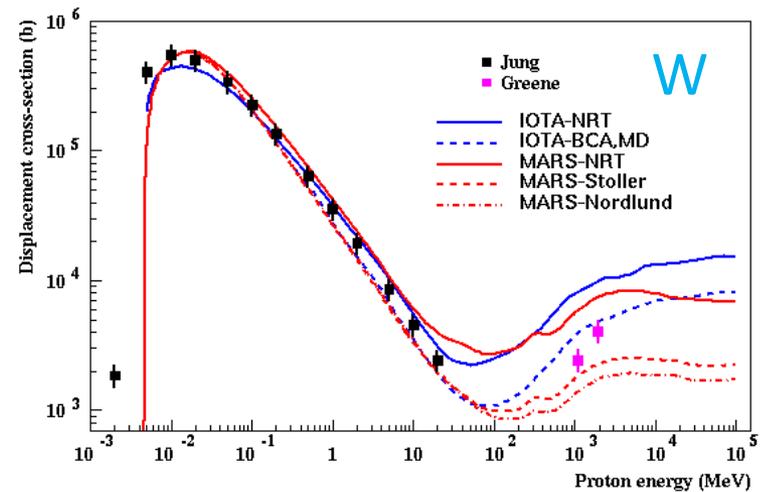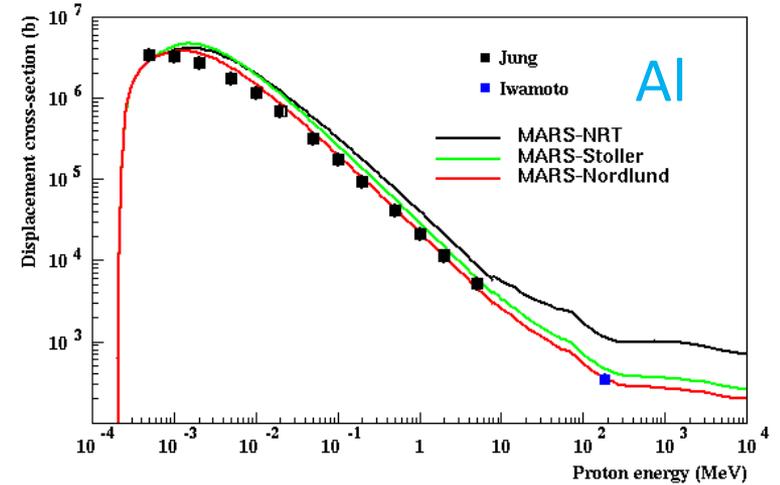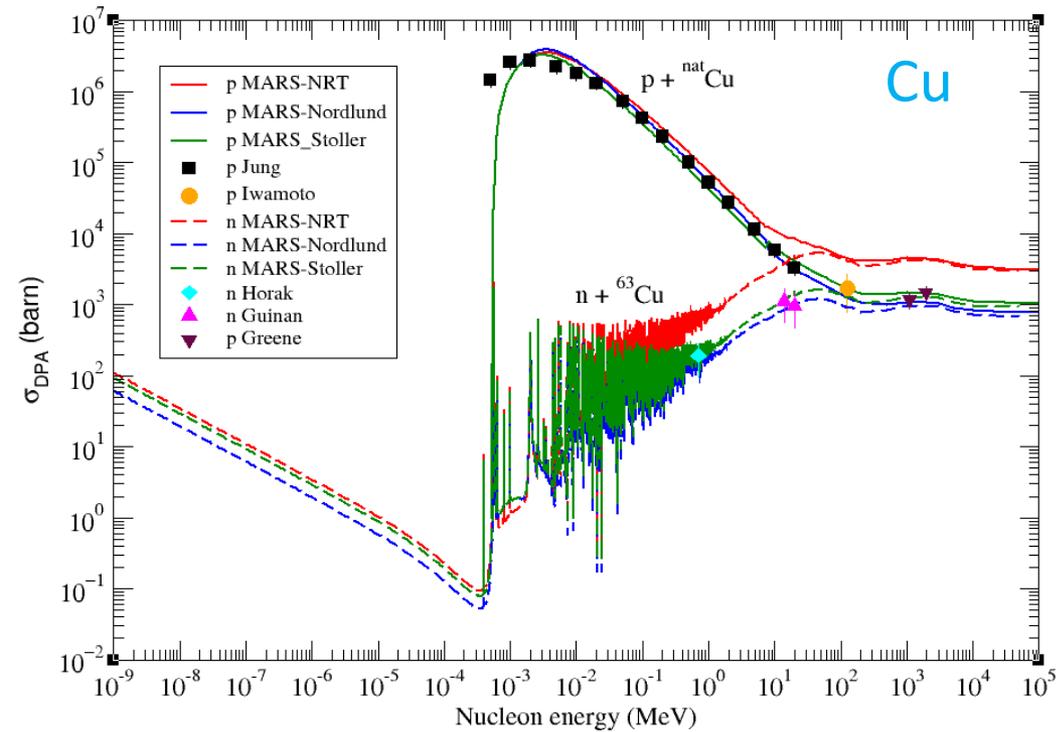K. Nordlund et al: arc-dpa ξ(T) parametrization for Fe, Ni, Pd, Cu, W, Pt.

Y. Iwamoto et al. – arc-dpa ξ(T) parametrization for Al (should be reconsidered).

S. Striganov – new fit of arc-dpa ξ(T) for Al.

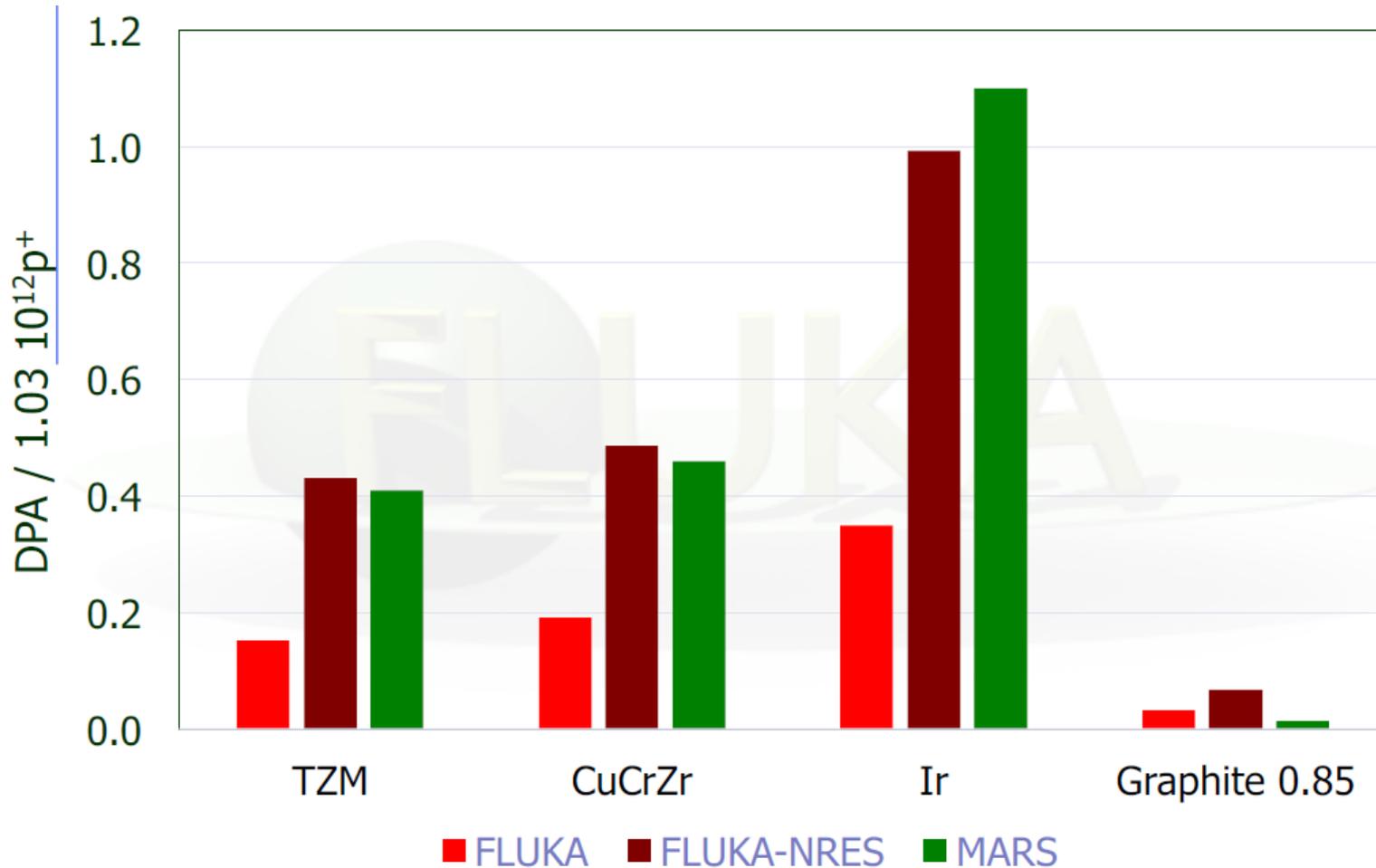Xin Yang et al. – arc-dpa ξ(T) parametrization for Zr.

Proton and Neutron DPA Verification

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DPA at BLIP: FLUKA *vs* MARS15

σ_{DPA} at $E_n < 150$ MeV Implementation in MARS15(2019)

Features	DPA model 2012	DPA model 2018
No. of isotopes	395	485
Energy range (MeV)	0 – 20 MeV; 0-150 MeV	0 – 20 MeV; 0-150 MeV
Code used	NJOY 2012	NJOY 2016
keV*barn to barn conv.	applied at post-processing	embedded in NJOY calculation
x-section library	ENDF-VII (2012)	ENDF-VIII (2018)
Models	NRT + temperature correction	NRT; Nordlund; Stoller

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DPA X-sections at $10^{-11} < E_n < 150$ MeV in MARS15

ENDF/B-VIII.0(2018) + NJOY2016: ——NRT, ——Nordlund, —— Stoller

RaDIATE CM5, Dec. 17-21, 2018   MARS15 & DPA

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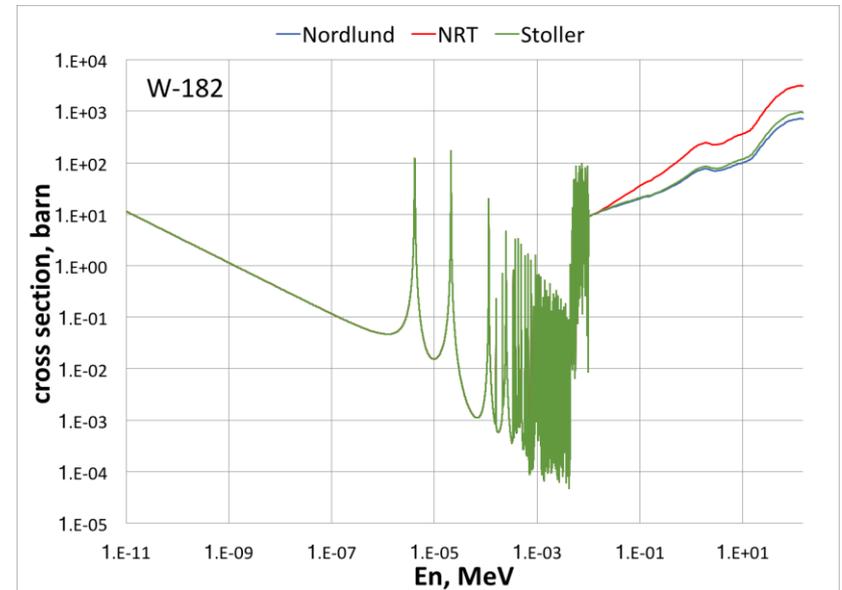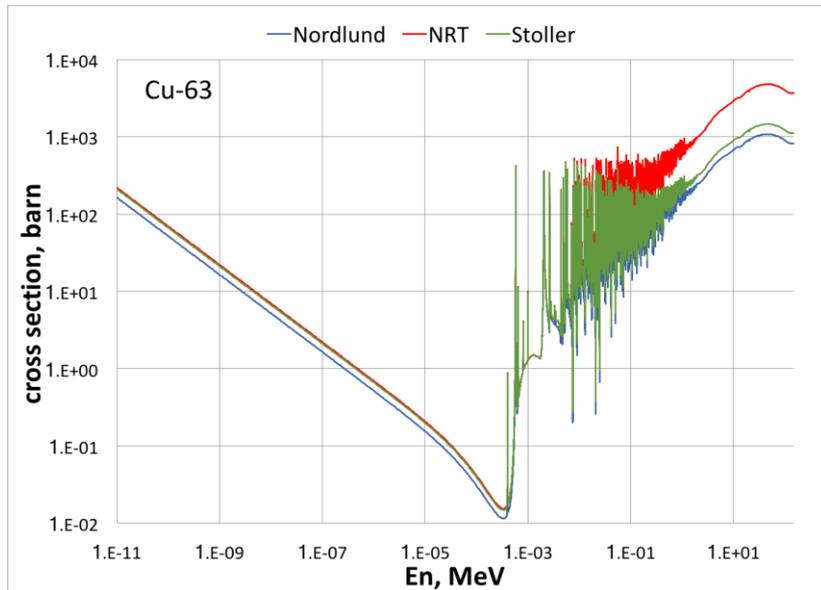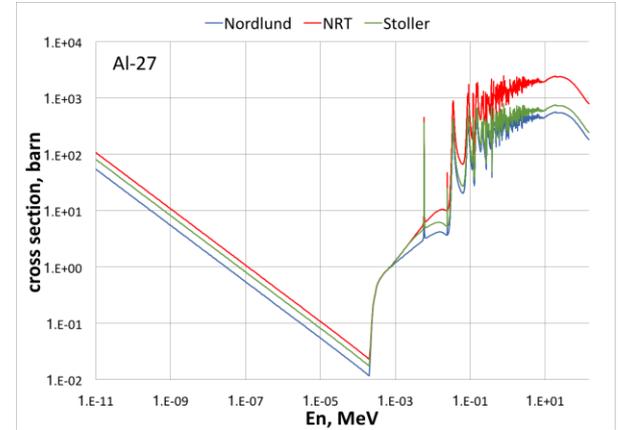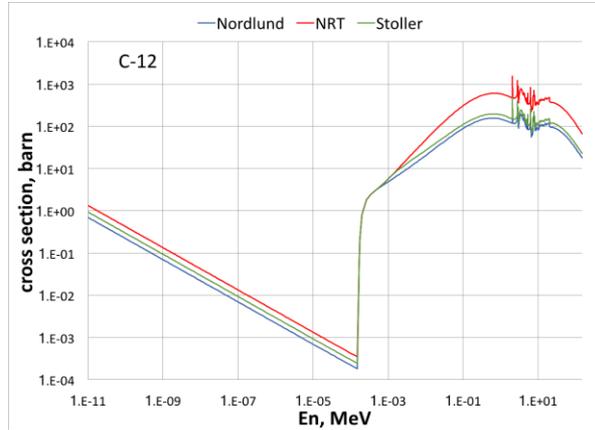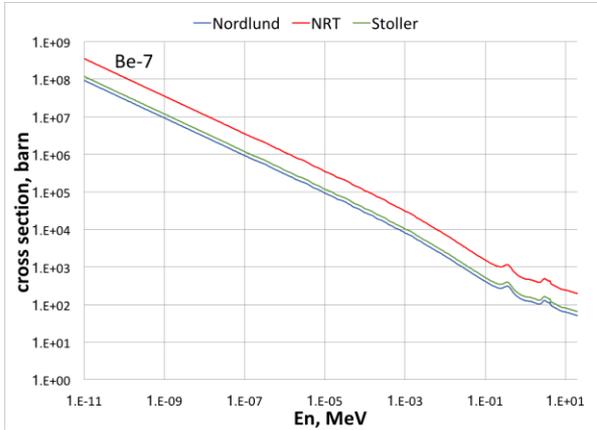
Summary

- Extensions and new features in MARS15(2019) – including substantial upgrade of the DPA model - improve the code performance, user friendliness and predictive power in accelerator applications

- Results of recent code benchmarking in complex applications are quite encouraging; neutrino-fluxes at the Far Detector (1300 km) calculated with MARS15 and Geant4 agree within 10%

- Justified in MARS15 simulations changes to the LBNF design improve its performance and provide substantial mitigation of energy deposition and radiological problems along with the muon monitor complexity in one of the two most critical systems, Hadron Absorber

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