MCNP Fusion Modeling of Electron-Screened Ions

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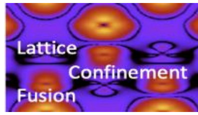


MCNP Modeling of Lattice Confinement Fusion (LCF)

NASA Glenn Research Center (GRC)

Advanced Energy Conversion Project

- Introduction
- Current MCNP Fusion Modeling Capabilities
- LCF Related Modeling Accomplished with MCNP
- LCF Calculations After MCNP Modeling
- Nuclear Reaction Modeling Limitations
- Proposed MCNP Enhancements
- Summary

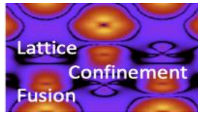
Introduction

- **NASA GRC and DoE LBNL discovered novel means of driving nuclear fusion reactions in deuterated lattices, *Lattice Confinement Fusion (LCF)***
  - Novel nuclear reactions observed in bremsstrahlung-irradiated deuterated metals, B. Steinetz, et. al., *Phys Rev C*, **101**, (2020) 044610 .
  - Investigation of light ion fusion reactions with plasma discharges, T. Schenkel, et. al. *J. Appl. Phys*., **126**, (2019) 203302.
- **Lattices provide Coulomb Barrier reduction through lattice, plasma, conduction and shell electron screening**
  - Nuclear Fusion Reactions in Deuterated Metals, V. Pines, et. al., *Phys Rev C*, **101**, 044609 (2020).
- **Weak and strong (degenerate) electron screening increase the fusion rate**
  - Electron Screening and Thermonuclear Reactions, Salpeter, E.E., *Australian Journal of Physics*, **7** (1954) 373
- **Lattice fusion rates increase by orders of magnitude over bare nuclei fusion**
  - Experimental and theoretical screening energies for the 2H(d,p)3H reaction in metallic environments, K. Czerski, *et al*., *Eur. Physics J. A,* **27**, (2006) 83-88.
- **NASA GRC used MCNP to guide electron screened, deuterated lattice, nuclear fusion research**
  - Model detector responses (MCNPX-PoliMi)
    - Validation of Geant4 and MCNPX-PoliMI Simulations of fast neutron detection with the EJ-309 liquid scintillator, S.F. Naeem, S.D. Clarke, S.A. Pozzi, *Nuc. Inst. and Meth. In Phys. Res. A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **714**, (21June2013) 98-104.
  - Model γ irradiated deuterated metals, activation, fission and shielding (MCNP-6.1 with Vised)
- **However, neither NASA nor LBNL were able to model LCF nuclear reactions with MCNP (or GEANT-4).**

Lattice Confinement Fusion

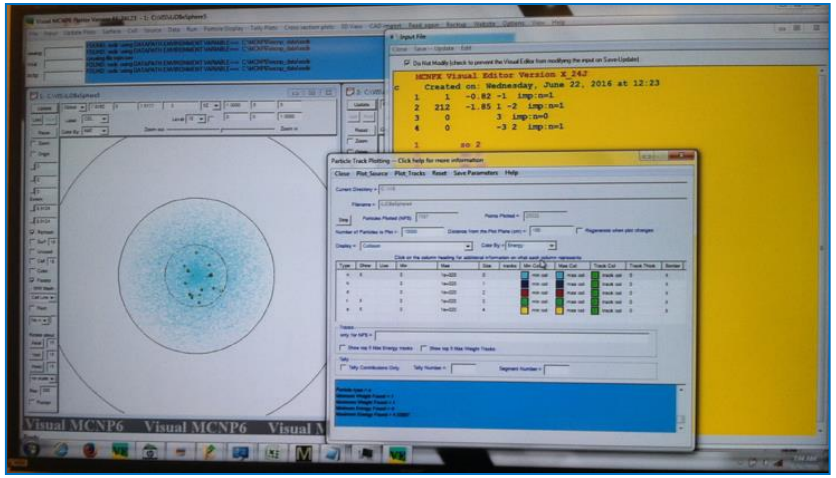
Current MCNP Fusion Modeling Capabilities

- **MCNP6.2 Overview:** ***Electron screening for fast ions, only > 100 keV ion support***
  - Review of heavy charged particle transport in MCNP6.2 K. Zieb, H.G. Hughes, M.R. James, X.G. Xu, *Nuclear Inst. and Methods in Physics Research, A* **886**, (2018)
- **MCNP6-McDeLicious:** ***40 MeV accelerated deuteron, ^{6,7}Li(d,n) neutron source***
  - Benchmarking and verification of the OpenMC code for accelerator-based neutron source analyses, Y. Hu, et al, *Fusion Engineering and Design*, **170**, (September 2021) 112512.
- **ITER Tokamak Models:** ***Only neutron propagation and interaction***
  - Using MCNP for Fusion Neutronics, Dissertation by Frej Wasastjerna at Helsinski University of Technology, (Dec 2008).
  - A Full and Heterogeneous Model of the ITER Tokamak for Comprehensive Nuclear Analyses, R. Juarez et. al., *Nature Energy Journal*, (Jan 2021). "… let us assume a point-wise isotropic 14.1 MeV neutron source…"
  - Integration of the Full Tokamak Reference Model with the Complex Model for ITER Neutronic Analysis. J. Yang, et. al., (ORNL), *Fusion Science and Technology*, (Nov 2018).
- **Laser Inertial Fusion-Fission Model:** ***Hybrid Fusion neutron source for a Fission Reactor***
  - Laser Inertial Fusion-based Energy: Neutronic Design Aspects of a Hybrid Fusion-Fission Nuclear Energy System, dissertation by Kevin James Kramer, University of California at Berkeley, (May 2010).
- **Nuclear Fusion Data Modeling:** ***NJOY data conversion of ENDF, FENDL for MCNP neutron transport/activation***
  - Nuclear data for fusion: Validation of typical pre-processing methods for radiation transport calculations, T. Hutton, et. al., *Fusion Engineering and Design*, (Nov 2015). "The interaction of the 14.1 MeV neutrons from D-T fusion with the reactor components cause radiation damage, activation and heating."

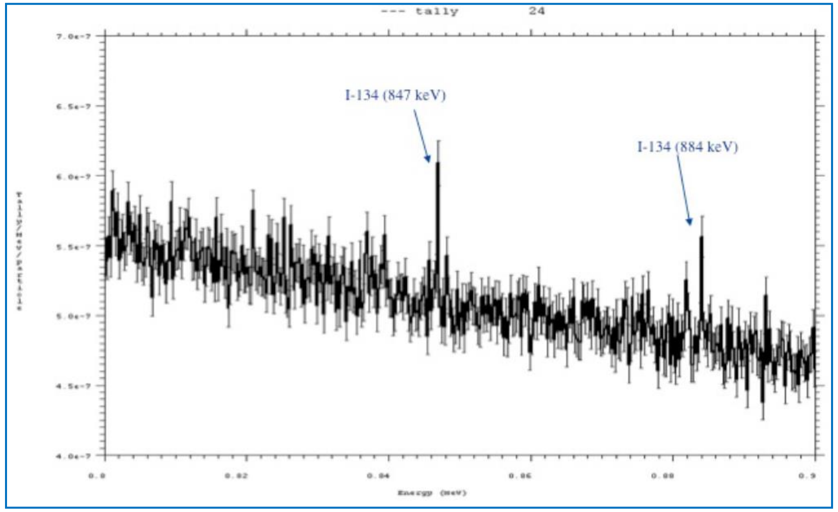


LCF Related Modeling Accomplished in MCNP

- **Model 1 eV - 15 MeV photons and 10 eV- 15 MeV electrons**
  - *Bremsstrahlung photo-neutron triggered Lattice Confinement Fusion*
- **Model thermal, epithermal and fast neutrons**
  - *LCF lattice activation and momentum transfer for reaction gain*
  - *LCF neutron scattering and capture*
  - *LCF fast neutron momentum transfer (recoil)*
- **Model actinide fission**
  - *Synthetic HPGe detector*
- **Model neutron spectrometer response functions**
  - *Scintillator response functions with CVT PoliMi under MCNPX*
  - *U2D using moderated planes of ^{6}Li neutron capture electronics*[1]
- ***Only track* > 100 keV charged fusion products**
- ***Only model* ≥ 1 MeV charged fusion products**



Vised & MCNP-6.1 LCF Neutron Propagation



MCNP-6.1 Synthetic DU Fission γ Spectra

[1] C.B. Hoshor, et al., “Real-time neutron source localization and identification with a hand-held, volumetrically-sensitive, moderating-type neutron spectrometer” *Nuclear Instrumentation and Methods In Physics Research, A*, **866** (2017) 252-264.

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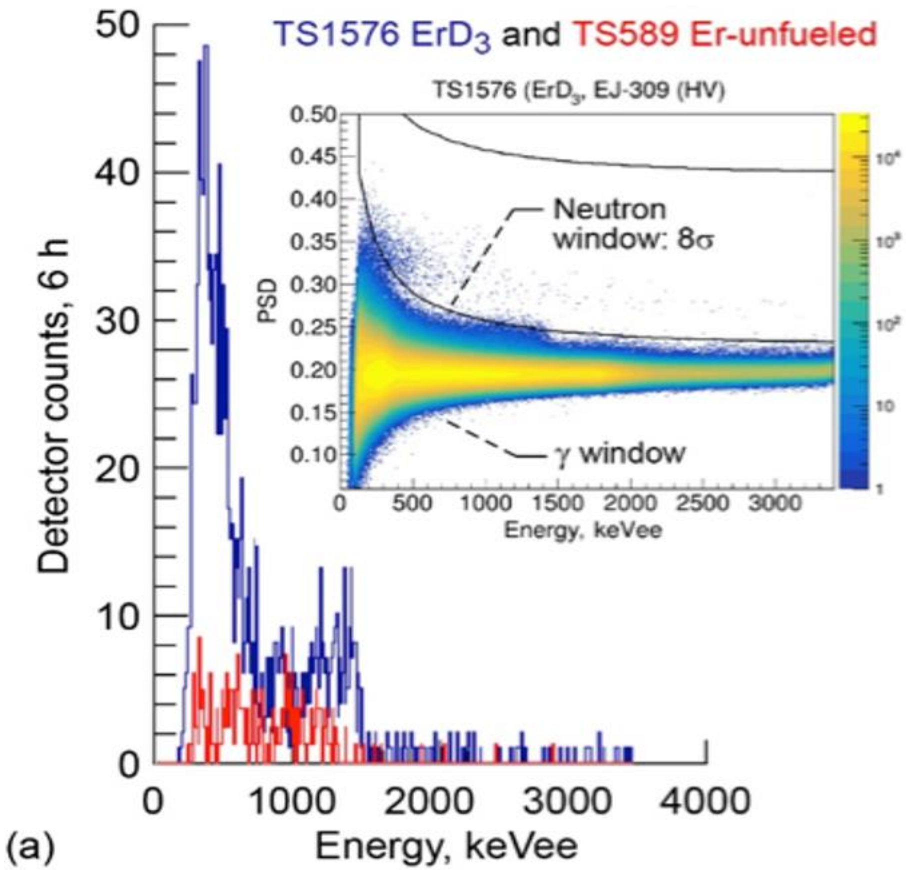
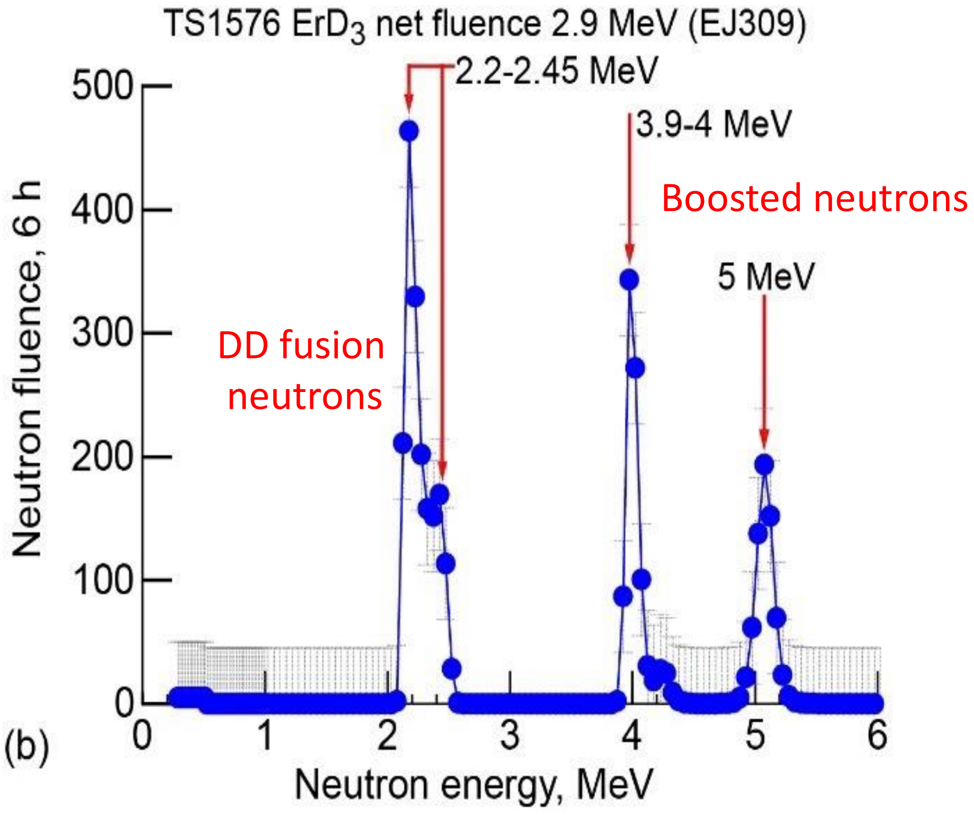
LCF Calculations After MCNP Modeling[1]

Pulse Shape Discrimination (PSD) to Remove γ & Unfold Neutron Spectra

Detector Counts: Fueled & Unfueled



Neutron Spectra, Net: Fueled minus Unfueled



Note: Unfolding uncertainty bars 2-sigma.

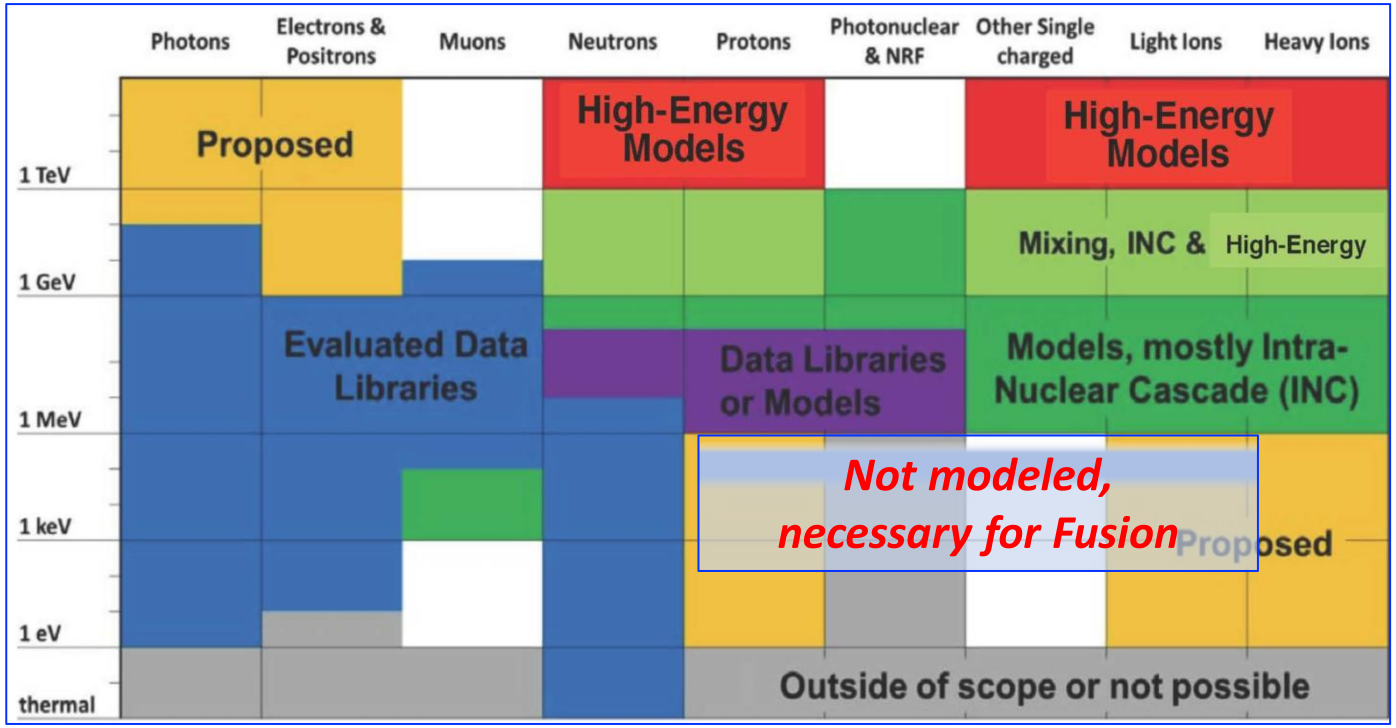
Dynamitron 2.9 MeV Bremsstrahlung with triggered ErD_3, DD fusion with boosted energy neutrons.

[1] Fast Neutron Spectroscopy with Organic Scintillation Detectors in a High Radiation Field, B. Baramsai, et. al., *NASA*/**TM-20205008493** (2020)

Nuclear Reaction Modeling Limitations

MCNP, GEANT-4 and SRIM/TRIM

MCNP Particle Interaction Modeling Domains[1]



- ***No model for DD, DT and D^3He fusion reactions at peak cross-sections < 100 keV.***[2]
  - *LCF gain is from large-angle scattering of electron screened fusion alpha, proton and neutron products causing deuteron recoils*
- ***No model for electron screened ions < 10 keV.***[3]
  - *Applicable as ions slow*
- ***SRIM/TRIM***[4] ***models ion scattering***
  - *But not nuclear reactions*
- ***No model for electron screened deuteron stripping reactions***
  - *Possible source of fast neutrons:* $^{A}M_{Z}(d,n)^{A+1}M_{Z+1}$ n_{KE} >> 4 MeV

[1] MCNP6 Class, H. Grady III and James, Michael R., *LANL, LA-UR-14-21281* (2014)
[2] Review of heavy charged particle transport in MCNP6.2, K. Zieb, *et al.*, *Nuclear Instruments and Methods in Physics Research, A.*, **886**, (2018) 78.
[3] Radiation correction to astrophysical fusion reactions and the electron screening problem, K. Hagino and Balantekin, A.B., *Physical Review C*, **66**, (2002) 055801.
[4] SRIM - The stopping and range of ions in matter, J.F. Ziegler, M.D.,Ziegler & J.P. Biersack, *Nuclear Instruments and Methods in Physics Research, B*, **268**, (11-12), (2010)

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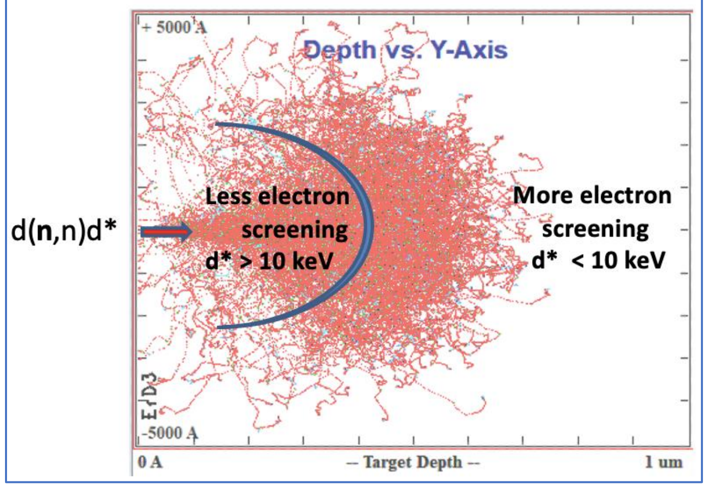
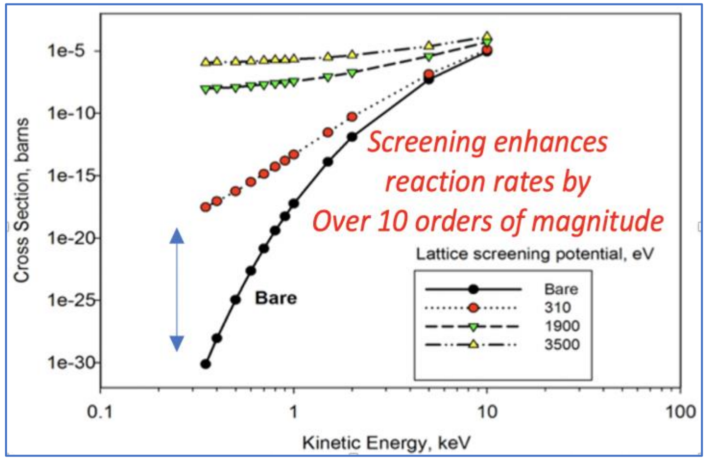
Proposed MCNP Enhancements

- Incorporate Frascati fusion neutron generator subroutines (10—50 keV deuterons) for ITER (International Thermonuclear Exp. Reactor).
- Test with NASA bremsstrahlung photoneutron-deuteron recoil 64 keV average (32 keV center-of-mass) kinetic energy.
- Add LCF Theory Paper enhancement factor, *f(E)*, for electron screening < 10 keV deuteron kinetic energy.
- Test with LBNL plasma/glow discharge 1.25 keV - 6 keV center-of-mass deuteron kinetic energy.
- Add DFT (Density Functional Theory) and DMFT (Dynamic Density Functional Theory) < 1 keV electron screening calculations to modify Gamow and Astrophysical factors.

Model 64 keV d* Ions in ErD_3 Lattice



Electron Screening Enhanced Fusion Rates



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Summary

- **Augment MCNP to model nuclear reactions**
  - Add ion scattering from 10 keV – 64+ keV
  - Add electron screening of ions from < 1 keV - 10 keV
- **NASA and DoE would benefit from this modeling**
  - Terrestrial and space-based fusion reactor technology
  - Astrophysics of warm dense matter (Jovian-like planets), stellar nucleosynthesis
  - Differentiate between boosted fusion and stripped neutrons
- **NASA is interested in partnering with LANL MCNP developers to fully incorporate these enhancements into MCNP.**
- **Consistent with NASA/DoE MOU on Space Nuclear Power**

Lattice Confinement Fusion

Slide 8 References

- **Incorporate Frascati fusion neutron generator subroutine supporting ITER (International Thermonuclear Experimental Reactor):**
  - D-D, D-T and D-^{3}He fusion from 10 keV - 50 keV
    - A Monte Carlo Model for Low Energy D-D Neutron Generators, A. Milocco, et. al., *Nuclear Instruments and Methods in Physics Research B*, **271**, (2012).
  - Charged particle scattering using SRIM/TRIM tables (10 keV – 100 keV)
    - SRIM - The stopping and range of ions in matter, Ziegler, J.F., Ziegler, M.D. and Biersack, J.P., *Nuclear Instruments and Methods in Physics Research Section B*, **268**, (11-12), (2010)
- **Test with NASA bremsstrahlung 64 keV average photoneutron-deuteron recoil KE (32 keV center-of-mass)**
  - Novel Nuclear Reactions Observed in Bremsstrahlung-Iradiated Deuterated Metals B. Steinetz, et. al., *Phys Rev C*, **101**, (2020).
- **Add LCF Theory Paper enhancement factor, *f(E)*, for electron screening < 10 keV deuteron kinetic energy.**
  - Nuclear Fusion Reactions in Deuterated Metals, V. Pines, et. al., *Phys Rev C*, **101**, 044609 (2020).
- **Test with LBNL plasma/glow discharge, 1.25 keV - 6 keV center-of-mass deuteron kinetic energy.**
  - Investigation of light ion fusion reactions with plasma discharges, T. Schenkel, et. al. *J. Appl. Phys.*, **126**, (2019)
- **Add DFT (Density Functional Theory) and DMFT (Dynamic Density Functional Theory) < 1 keV electron screening calculations to modify Gamow and Astrophysical factors.**
  - Strained Layer Ferromagnetism in Transition Metals and it Impact Upon Low Energy Nuclear Reactions, L.F. DeChiaro, L.P. Forsley and P.A. Mosier-Boss, *JCMNS,* **17** (2015) 1 – 26.