MCNP Status

Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

David Wootan
Pacific Northwest National Laboratory

February 18, 2015

MCNP – What Is It?

- Monte Carlo particle transport code merging MCNP (<20 MeV for neutrons) and LAHET tracking high energy particles
- Significant simulation tool for accelerator and other physics work: target design, isotope production, isotope destruction, accelerator driven energy systems proton and neutron therapy, imaging technology, shielding design, detection technology, neutrino experiment design, charged particle tracking in plasmas, single-event upsets in semiconductors, nuclear reactor analysis
- Provides geometry-independent mesh tallies for visualization of flux, dose, energy deposition over continuous space volume without complicating particle transport through the geometry

MCNP Nuclear Data/Models

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

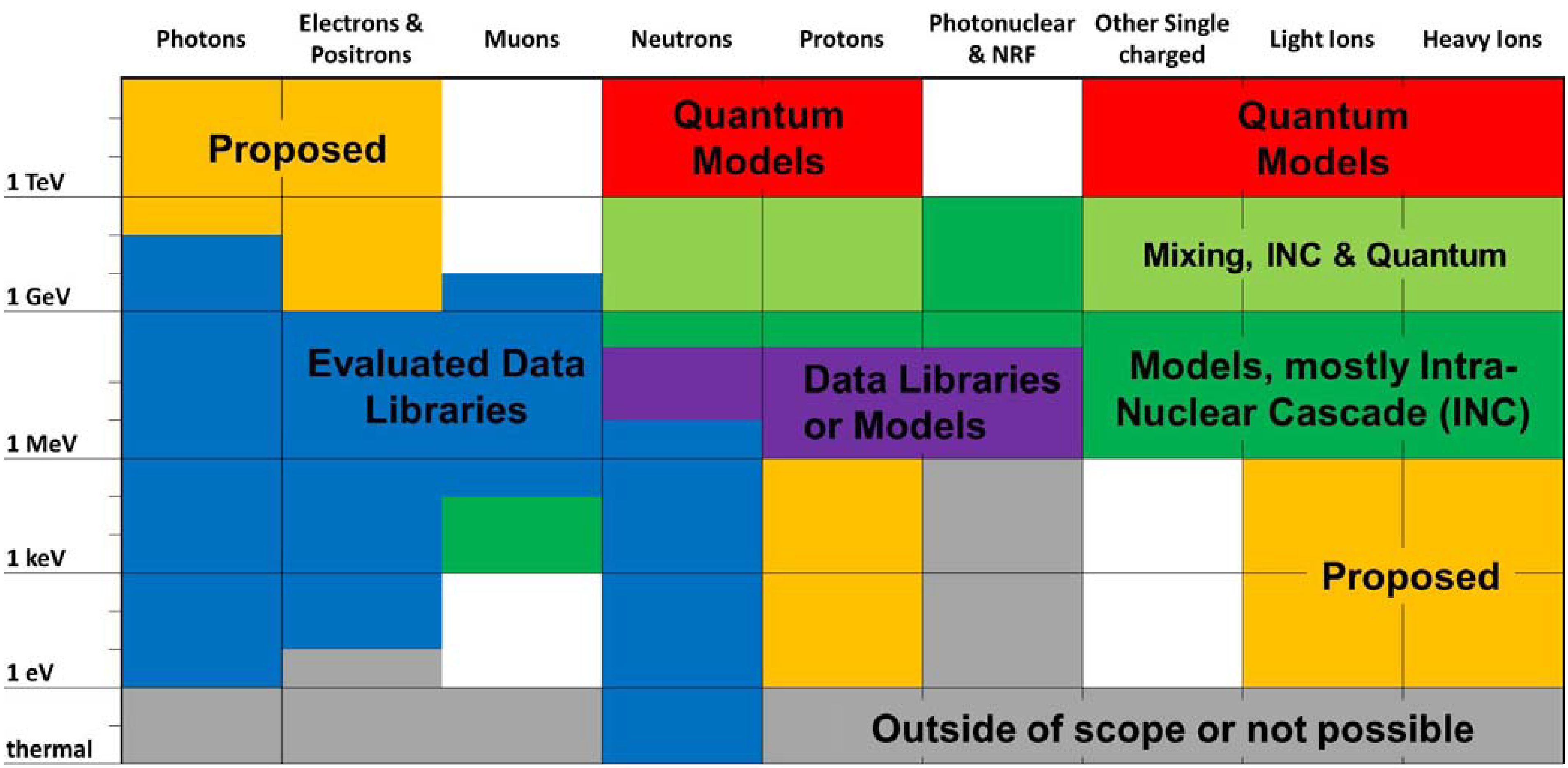
- Tabulated nuclear data
  - < 20 MeV neutrons for most isotopes
  - < 150 MeV LA150 proton library cross sections: H, C, N, O, Al, Si, K, Ca, Cr, Fe, Ni, Cu, Nb, W, Hg, Pb, Bi
  - <150 MeV ENDF/B-VII proton: H, D, T, 3He, Li, Be, B, C, N, O, Al, Ca, Si, Cr, Fe, Ni, Cu, Nb, W, Au, Pb, Bi
  - For incident neutrons and protons,secondary reaction product cross sections and angle energy correlated spectra have generally been provided for neutrons, photons, protons, deuterons, tritons, 3He, and alphas
- Intranuclear cascade/pre-equilibrium/evaporation models up to few GeV
  - BERTINI
  - ISABEL
  - CEM03.03
  - INCL
  - LAQGSM03.03

MCNP Data Treatment

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

- All standard MCNP neutron libraries over their stated ranges (~0-20 MeV).
- Neutrons in the ENDF70x libraries from 0.0 - 150.0 MeV in tabular range.
- Neutrons from 1.0 MeV in the physics model regime.
- Photons from 1 keV - 100 GeV.
- Photonuclear interactions from 1.0 to 150.0 MeV in tabular range.
- Photonuclear interactions from 1.0 MeV in the CEM physics model.
- Electrons from 1 keV - 1 GeV.
- Protons from 1.0 to 150.0 MeV in tabular range for 47 isotopes.
- Protons from 1.0 MeV in the physics model regime.
- Pions, muons, and kaons are treated only by physics models.
- Light ions from 1 MeV/nucleon in the physics model regime.
- Heavy ions from 3 MeV/nucleon in the LAQGSM physics model.

MCNP6 Particle Types and Ranges



MCNP Advantages

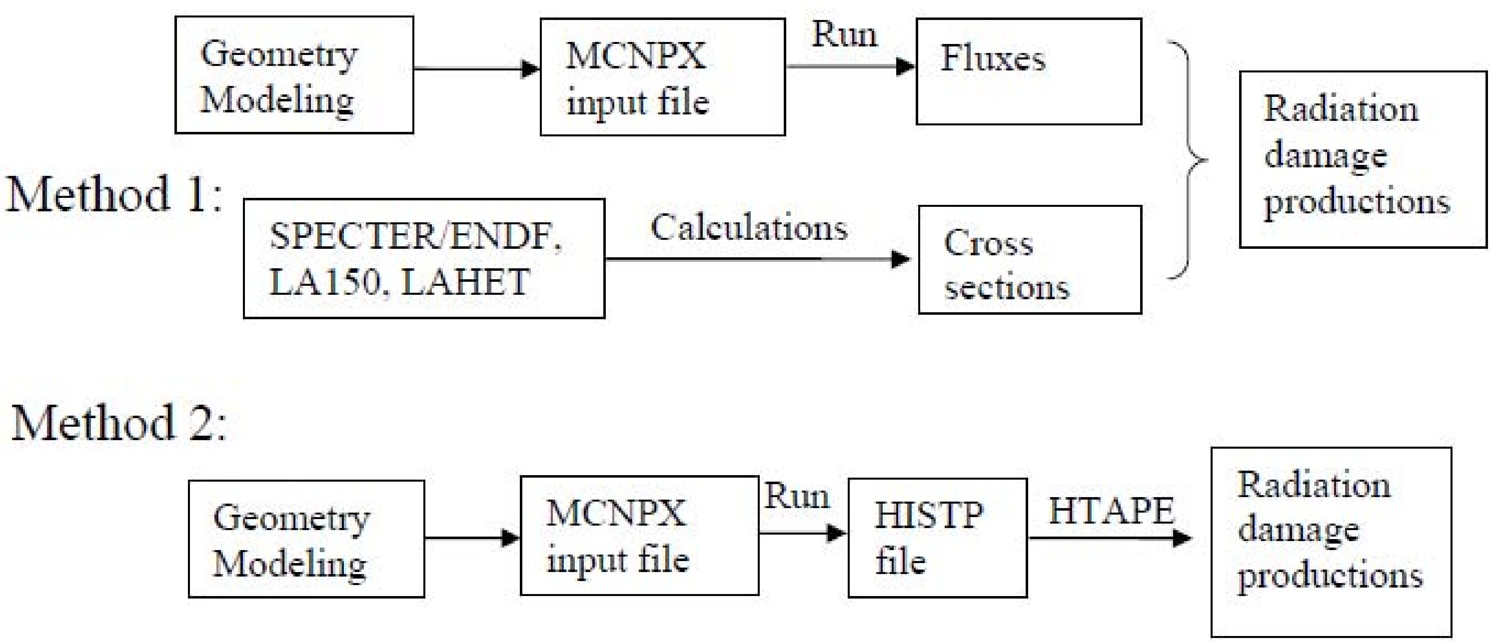
- Advantages
  - Explicit modeling of complicated geometries
  - Can select physics treatment from available options
  - Monte Carlo tracking of particle interactions
  - Extensive cross section library for low energy reactions <20 MeV
  - Physics treatment for when cross sections are not available
  - Calculates statistical uncertainties
  - Widely used for reactor analysis
  - Same model can be used for shielding, activation studies
  - Can calculate damage energy directly
  - Mesh tally can provide spatial distributions independent of problem model
  - Can add more XSs using NJOY

MCNP Disadvantages

- Disadvantages
  - Calculations can take time to obtain adequate statistics on small regions
  - Damage energy calculations do not include tabular XS contributions
  - May need separate calculations of low energy (<20 MeV) and medium to high energy contributions

MCNP Methods for Calculating DPA

- Two methods for calculating DPA with model of specific geometry
  - Method 1 - Calculate flux and fold with DPA XS
  - Method 2 - Calculate DPA directly with MCNP (HISTP/HTAPE)



MCNP Calculation of DPA Method 1

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

- Calculation of neutron, proton spectrum at specific locations or for regular spatial mesh
- Fold neutron and proton DPA XS with neutron and proton flux spectrum
- Advantages
  - Straightforward, like other MCNP tallies, provides spatial distributions
- Disadvantages
  - Limited to energy range and materials in libraries
    - ENDF XS < 20MeV
    - SPECTER limited to neutrons < 20 MeV
    - LA150 neutron and proton XS < 150 MeV
    - DXS DPA cross sections for neutrons, protons, H production, He production <3 GeV
  - Limited materials
  - Average DPA for cell or material or spatial distributions

MCNP Calculation of DPA Method 1

- Neutron DPA
  - Tally neutron flux spectrum in MCNP as function of energy
  - Multiply by neutron DPA cross section for each material (spreadsheet)
- Proton DPA
  - Tally proton flux spectrum in MCNP as function of energy
  - Multiply by proton DPA cross section for each material (spreadsheet)

MCNPX Calculation of DPA Method 1

$$DPA = \int \sigma_{disp}(E)\frac{d\emptyset(E)}{dE}dE$$

$\emptyset(E)$: fluence (particles/cm^2)

$\sigma_{disp}(E)$: displacement cross section (barns)

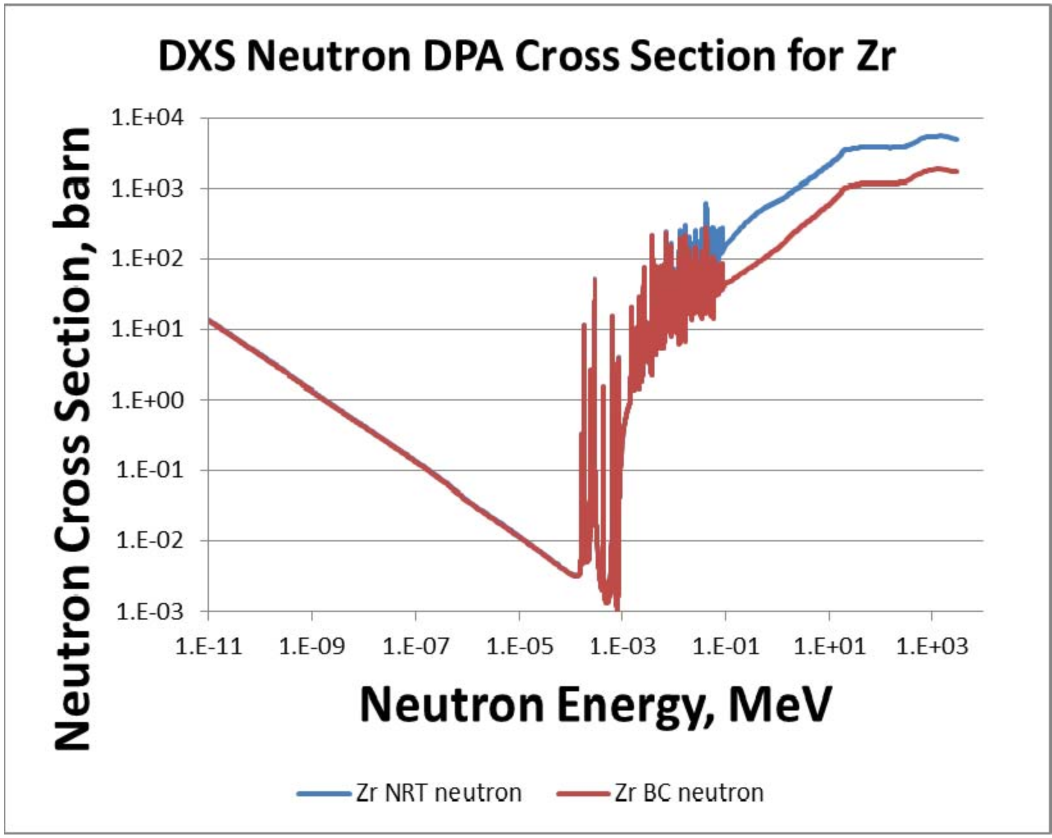
- DPA is calculated by folding displacement cross section with particle spectrum
  - Energy dependent particle spectrum (neutron, proton) calculated with transport model (MCNP)
  - Neutron spectrum folded with neutron DPA cross section,
  - Proton spectrum folded with proton DPA cross section
  - Main difference between proton and neutron displacement cross section is Coulomb interaction of charged particle at low energies

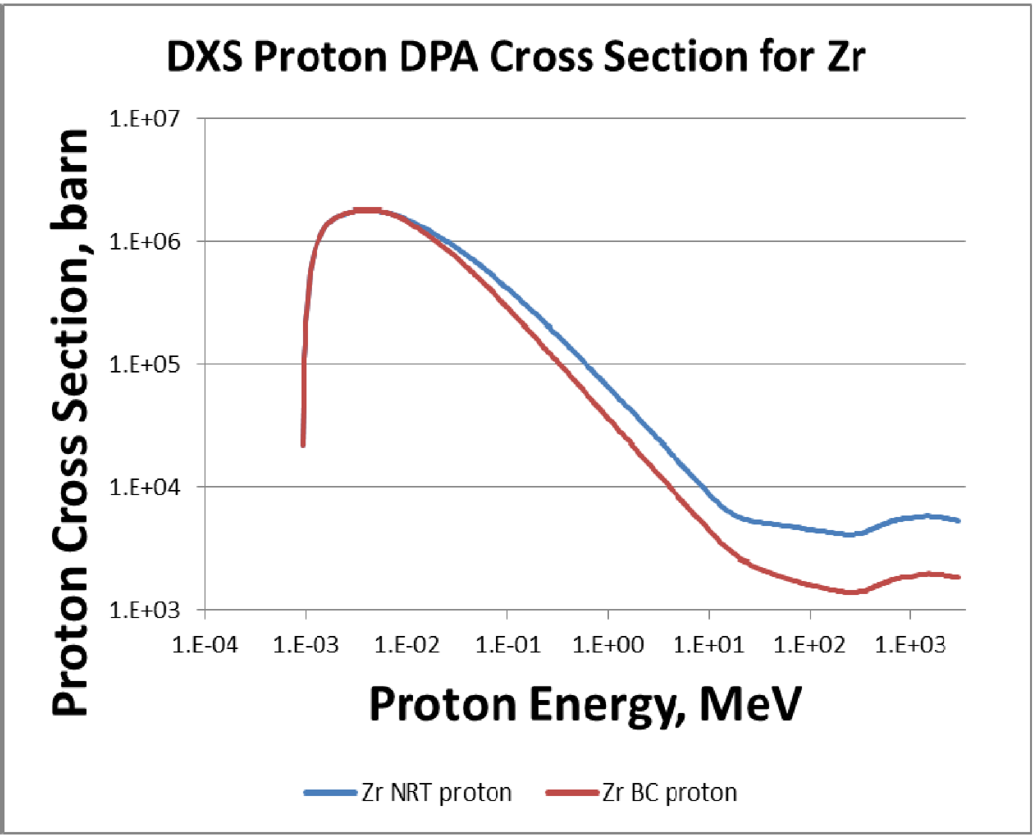
MCNP Calculation of DPA Method 1
DPA Cross Section

- Cross sections can be based on traditional NRT or new methods such as Molecular Dynamics (MD), Binary Collision Approximation (BCA) or other simulations
- IAEA Nuclear Data Section database DXS in ENDF/B format includes both NRT and MD-BCA DPA cross sections as well as gas production cross sections
  - Al, Ti, V, Cr, Fe, Ni, Cu, Zr neutron, proton < 3 GeV
  - ENDF/B-VII data processed with NJOY for neutrons <20 MeV
  - Model physics for >20 MeV
  - DPA cross section is sum of proton or neutron elastic scattering and nonelastic interactions
  - Gas (p,d,t,^{3}He,^{4}He) production in Cr, Fe, Ni, W neutron, proton < 3 GeV,

MCNP Calculation of DPA Method 1
DPA Cross Section

- IAEA Nuclear Data Section database DXS includes both NRT and MD-BCA DPA cross sections
- MD-BCA DPA are substantially lower than NRT





MCNP Calculation of DPA Method 1
DPA Cross Section

- Neutron damage cross sections that can be used in MCNP
  - ASTM E693 for up to 20 MeV in Fe, steel
  - ENDF/B Evaluations up to 20 MeV for most isotopes
  - Neutron dosimetry file IRDF-2002 contains neutron damage cross sections up to 20 MeV for Si, GaAs, ASTM E722 electronic, Cr, Fe, Ni,

MCNP DPA Calculation Method 2

- HISTP card included in input file produces history file of medium and high energy collision data
  - Low energy neutron and proton collisions utilizing the MCNPX libraries are not included
- HTAPE3X INT=myinput OUTT=myoutput HISTP=file1
  - IOPT=16 damage energy spectra
  - Provides tables as function of input energy grid by cell or material and total
    - total recoil, elastic recoil, total damage, elastic damage
  - Provides mean values of recoiling fragments and damage energy per history and mean energy per recoil
  - IOTP = -16 multiplies damage energy spectra by flux

MCNP Calculation of DPA Method 2

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle *Since 1965*

- Calculate neutron, proton transport at specific locations the same as method 1 but record histories on HTAPE file
- HTAPE3X included with MCNP (from LAHET) reads HTAPE histories and calculates damage energy spectrum, which is converted to DPA
- Advantages
  - Doesn’t require separate DPA XS
  - Includes most reaction mechanisms
- Disadvantages
  - Only includes contributions from physics models
  - Tabulated XS contributions are not included
  - Can underestimate damage if <20 MeV contributions are significant
  - Interactions using tabulated cross sections are not recorded in HISTP file, only those based on physics models

Extension of MCNP 6.1 Cross Sections

- Need to include gas-production and DPA dosimetry cross sections for a number of nuclides (Fe, Ti, W, C, Be, and others)
- Current evaluations of ENDF/B do not contain this type of information
- Evaluated files in ENDF format exist and are available

Current Effort

- Obtained gas production and DPA dosimetry cross section files
- Converted ENDF files to ACE format suitable for MCNP with NJOY 99.396 (latest update)
- Reactions MT=203 to 207 represent gas production reactions
- Currently working on modifying MCNP 6.1 and/or NJOY 99.396 to accommodate these new dosimetry cross sections
- Neutron cross sections appear to work, but proton cross sections do not

Status

- Main hurdles are represented by a potential non-compatible format produced by NJOY for these cross sections
- Work is in progress to adapt the codes

Radiation Damage

- Radiation damage in materials results from nuclear collisions and reactions which produce energetic recoil atoms of the host material or reaction products
- These recoiling atoms generate electronic excitations in host material that displace additional host atoms – this is displacement damage
- In metals this is the main process that leads to permanent damage, but generated He and H also contribute to radiation damage
- Displacements per atom is routinely used to characterize irradiations
- Only initial displacements of atoms from lattice sites are calculated
- Many displaced atoms recombine with holes in the lattice, especially at elevated temperatures
- Measure of total damage energy deposited in a material, and changes in physical and mechanical properties are fundamentally related to the available energy

NRT-DPA

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

- In 1975 Norget, Torrens and Robinson proposed the NRT-DPA standard. Number of displacements = $0.8T_d/2E_d$
  - 0.8 factor was determined from binary collision models to account for realistic scattering
  - E_d is the minimum energy required to create a stable Frankel pair
- NRT DPA has been widely used and has proven useful for correlating radiation damage phenomena
  - Comparing thermal and fast spectrum neutron irradiations
  - Comparing charged particle with neutron irradiation
  - While did not predict actual number of Frenkel pairs, provided means of correlation for steels and other mid-atomic weight metals

NRT-DPA

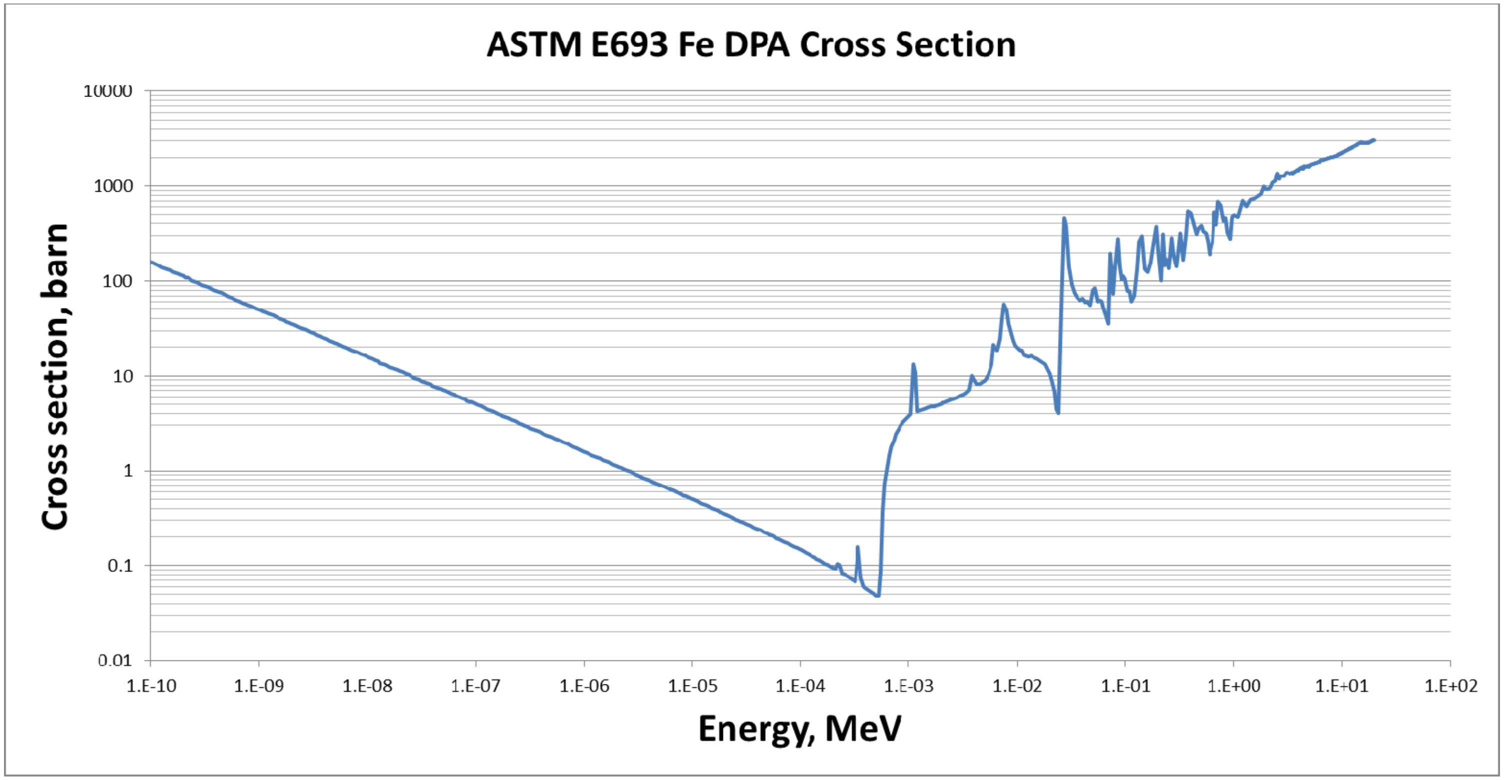
Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle *Since 1965*

- NRT-DPA has limitations
  - Some material property changes are sensitive to results of nuclear collisions
  - Others are more sensitive to ionization effects
  - Limited to metals, has been applied to compound materials like ceramics by mathematical weighting of separate elements
  - Does not account for recombination of atoms during cascade evolution
  - Cannot be directly measured or validated
  - Has no uncertainties/covariances
- NRT DPA methodology incorporated into
  - ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA)
  - ASTM E521 Standard Practice for Neutron Radiation Damage Simulation by Charged Particle Irradiation

ASTM E693 Standard for DPA for Neutron Exposures in Iron and Low Alloy Steels

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

- ASTM E693 Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom
- Specifies energy dependent neutron DPA cross section that is multiplied with neutron energy spectrum to calculate DPA



ASTM E521 Standard for Neutron Radiation Damage by Charged Particle Irradiation

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

- ASTM E521 Standard Practice for Neutron Radiation Damage Simulation by Charged Particle Irradiation
- Calculation of damage energy per atom per unit fluence for neutrons, light ions, heavy ions, and electrons
- All possible reactions that transfer energy to an atom of the medium to displace it must be considered
- Damage energy is converted to DPA using NRT model

$$N_d = 0 \qquad T < T_d$$

$$N_d = 1 \qquad T_d \le T < 2T_d/\beta$$

$$N_d = \beta T_{dam}/2T_d \qquad T \ge 2T_d/\beta$$

$\beta = 0.8$, $T_d = 40$ eV

SPECTER Code for Calculating Neutron Damage

- Simplified neutron damage calculations compared to MCNPX
- Instead of calculating DPA in MCNPX, user inputs MCNPX calculated energy-dependent neutron spectrum to SPECTER, which calculates spectral-averaged displacements, recoil spectra, gas production, and total damage energy for 41 isotopes at the same time
- Limited to neutron reactions
- Includes elastic scattering, multiple (n,xn) reactions, (n,d), (n,t), (n,^{3}He), (n,^{4}He), (n,γ), β-decay
- Limited to energy range from 10^{-10} to 20 MeV
- Limited to ENDF/B-V nuclear data