Using MCNP and NJOY to Verify Charged Particle Data in CP2020

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Outline

- Introduction to CP transport in MCNP
  - Format of ACE data for Charged Particles
  - CP Energy Limits
  - Cut-Off Angles
  - nucleardata.lanl.gov for CP2020 and other data and documentation
- Broomstick Problems for Verification
- Conversion between Center of Mass and Lab Frames of Reference
- Comparison of Experimental Data, NJOY Processing, ACE file data, and the results from a pencil beam model in MCNP
  - Angular Distributions
  - Energy Distributions
- Comparison of Angle-Integrated Cross Sections from ACER and GROUPR
- Summary

Charged Particle Transport in MCNP

- MCNP has a hard coded lower E limit of 1 keV for Charged Particle energy
- There is also a default lower E limit of
  - 1 MeV for protons
  - 2 MeV for deuterons
  - 3 MeV for tritons and helium3
  - 4 MeV for alphas
- Default lower limits may be adjusted with a “cut” card down to 1 keV
- By convention, the evaluated CP data is given for lighter CP impinging onto the heavier CP. For a heavier CP impinging on a lighter CP -- we are working on that combination and expect to put more data into CP2020
  - There is some symmetry between the evaluated data of lighter onto heavier ions and heavier onto lighter ions
- Why is there no table data for transporting heavier CP’s? or heavier targets?
  - It hasn’t been done, yet
  - Heavier CP’s don’t travel very far (can use “local deposition” of energy)
  - Heavier targets don’t allow very much CP transport (can use “local deposition”)

Question: Which ACE Format is used for Charged Particle Data? (ACE Formats are selected based on the class suffix; c, y, t, p, m, …)

- 1. Neutron Continuous Energy
- 2. Dosimetry Data
- 3. Thermal Scattering Data
- 4. Photon Continuous Energy
- 5. Multi-group Neutron-Photon

- **Answer:** 1. Neutron Continuous Energy

Energy Limits for Table Data (like CP2020) for Charged Particle Transport in MCNP

- For each of the 25 reactions given in CP2020
  - There is a **lower** and an **upper** energy limit for the table
  - Any data below 1 keV is ignored by MCNP

- What happens when the particle goes below the default lower limit or below the table data or even below the hard-wired 1 keV limit?
  - The particle is terminated!, (*i.e., locally deposited*)

- What happens when the particle goes above the upper energy limit for the data given in CP2020 for the reaction in question?
  - MCNP supplies "model" data

MCNP Settings for Charged Particle Transport

Source Particle	Mode, Phys, Imp, Cut, and F (tally) cards	Target ZAID index ID (M card)
proton	h	h
deuteron	d	o
triton	t	r
helium3	s	s
alpha	a	a

o and r are used for the ZAID index ID for deuterons and tritons, because d (discrete) and t (thermal scattering) were already used for ZAID identification

Angular Data Used by MCNP in Charged Particle Transport

- For forward scattering cosine angles >0.96 (in the Center of Mass)
  - Use other data and or the CP transport algorithm
  - (For same particle scattering, this also applies to scattering cosine angles < -0.96)
- The 0.96 scattering cosine angle is the cut-off angle
  - also -0.96 for same particle scattering
- Use the tabular CP 2020 data in the ACE file for all scattering cosine angles in between the cut-off angles

- Experimental data, R matrix calculations, CP evaluation files, and NJOY produced ACE files usually use the center of mass for angular data of charged particles
- Pencil Beam problem angular results are in the lab frame of reference

Pencil Beam Problems (aka "broomstick")

- Fixed source problems with all source particles emitted in a particular direction – inside of and parallel to a very long length and very small radius cylinder of target material
  - The cylinder is surrounded by void with zero importance
  - Tallies are kept at the cylindrical radial surface – and will be in the LAB frame of reference

- The idea is for the source particle to have only 1 collision before it exits the cylinder and for the resultant particle to be tallied at the cylindrical surface on its way out.

- For Charged Particles, MCNP has a special option to facilitate such verification problems with charged particles:
  - "lca 7J -2 " -- causes all source particles to collide immediately and all of their progeny to transport without decay or interactions
  - Thus, no smearing of particles in space or energy due to very forward scattering
  - Thus, all particle histories interact with the data in the CP2020 files

Conversion of Center of Mass Angles to the Lab Frame of Reference

- It is somewhat easier to convert center of mass angles to the lab frame of reference, than vice-versa
- For CP elastic scattering, the formulas are very similar to neutron formulas we all know and love … ☺ (for elastic scattering)
  - The cosine of the lab angle (μ_l)
  - The cosine of the com angle (μ_c)
  - The ratio, A, of the heavier CP (target) to the lighter CP (projectile)
- Cut-off angle of 0.96 in the COM → ~0.99 in the LAB

$$\mu_1 = \frac{(1+A\mu_c)}{\sqrt{A^2+2A\mu_c+1}}$$

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Conversion of Center of Mass Cross Sections to the Lab Frame of Reference

- It is somewhat easier to convert center of mass cross sections to the lab frame of reference, than vice-versa
- For CP elastic scattering, the formulas are very similar to neutron formulas we all know and love …
- The cross section, $\sigma_l(\mu_l)$, as a function of the cosine of the lab angle (μ_l)
- The cross section, $\sigma_c(\mu_c)$, as a function of the cosine of the com angle (μ_c)
- Note the derivative term (*and see the next slide*)

$$\sigma_1(\mu_1) = \sigma_c(\mu_c)\frac{d(\mu_c)}{d(\mu_1)}$$

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The Angle Derivative Term Needed for Cross Section Conversion

- A centered difference can be used as a 2nd order approximation to the desired derivative, or just …
- Differentiate the Angle conversion equation from 2 slides ago (and apply to the cross section equation shown below)

$$\sigma_1(\mu_1) = \sigma_c(\mu_c)\,\frac{d(\mu_c)}{d(\mu_1)}$$

$$\frac{d(\mu_1)}{d(\mu_c)} = \frac{-A(1+A\mu_c)}{\sqrt[3/2]{(A^2+2A\mu_c+1)}} + \frac{A}{\sqrt{(A^2+2A\mu_c+1)}}$$

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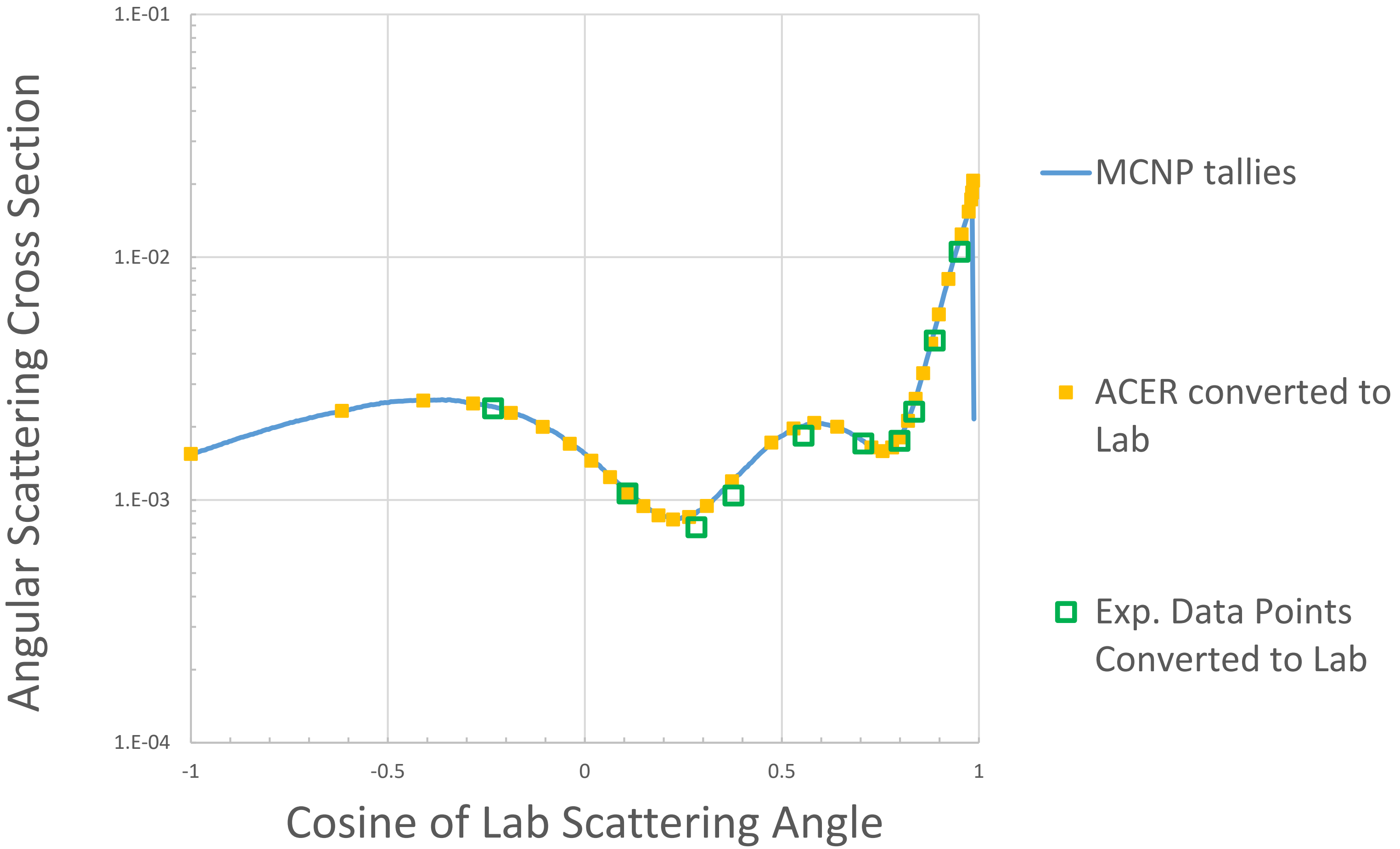
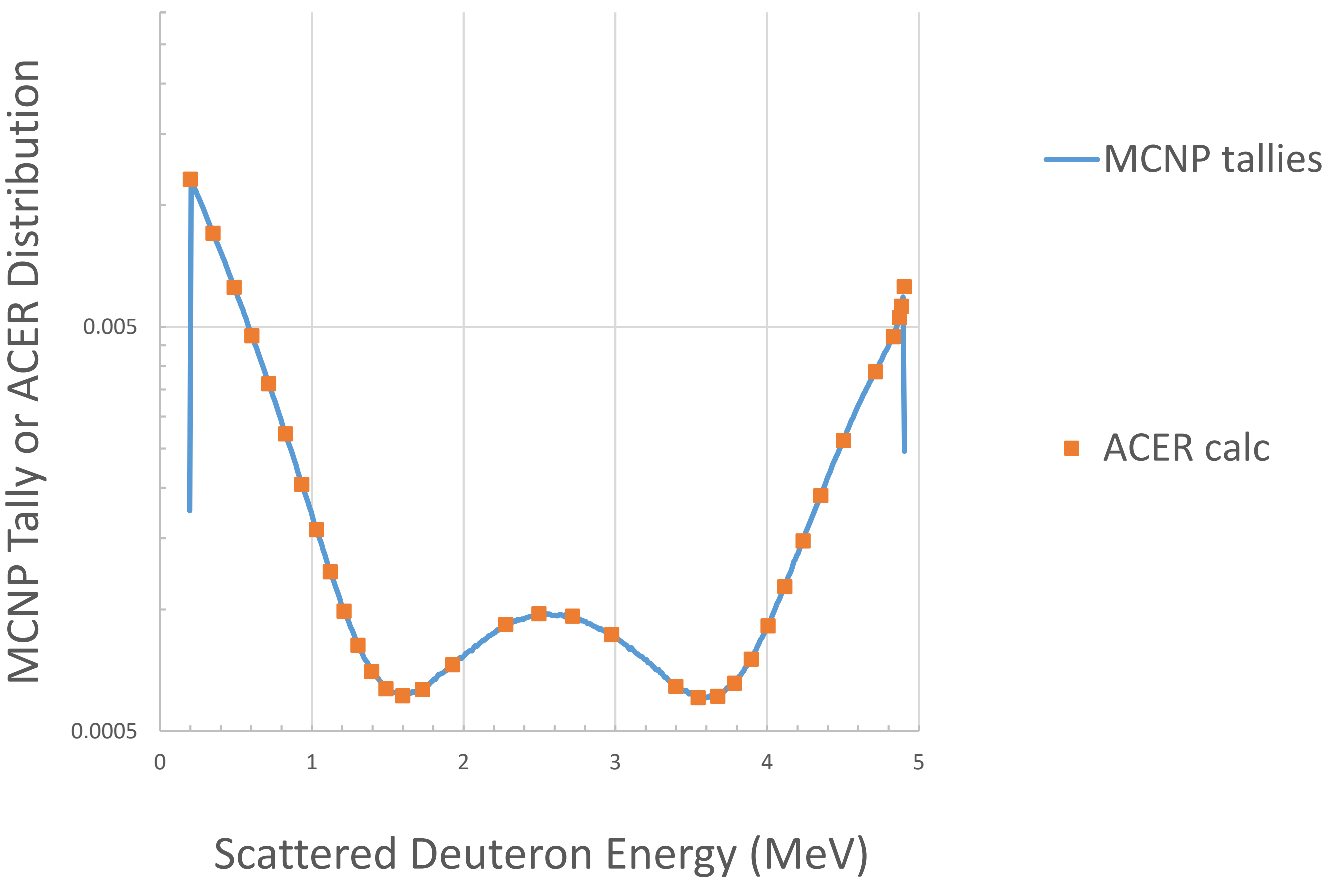
Lab Angular Scattering of 5 MeV Deuterons onto Tritium



Energy Distribution of the Scattered Deuterons (5 MeV Deuterons onto Tritons)



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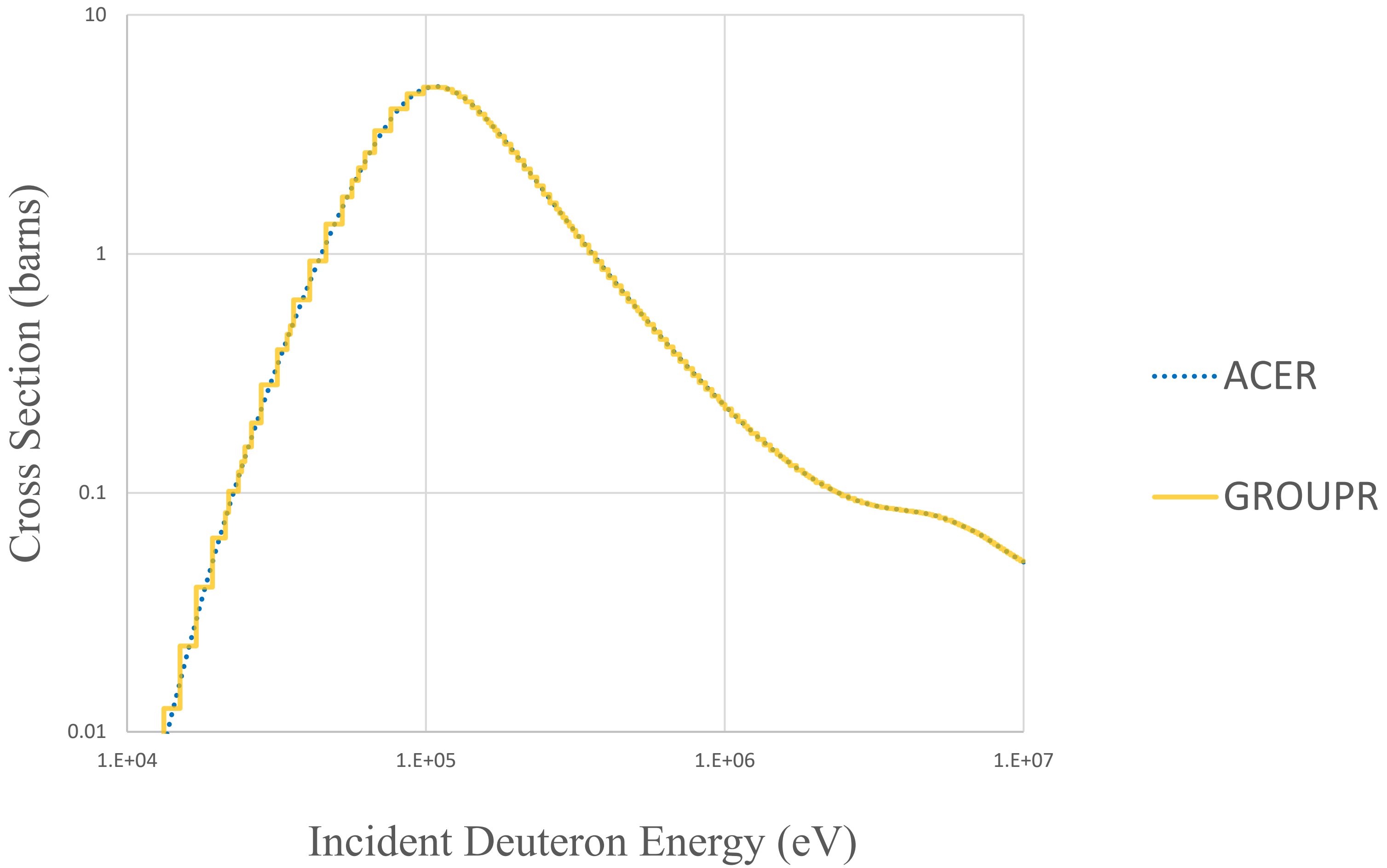
Comparison of ACER and GROUPR Processing of Angle-Integrated CP Cross Sections as a Function of Energy

- Use the same evaluated CP data for both ACER and GROUPR

- Thus, independent code modules within NJOY are used to calculate the same quantity of interest – a CP cross section
  - ACER results (for Monte Carlo codes like MCNP) come out as continuous (i.e., pointwise) values
  - GROUPR results (for deterministic codes like Partisn) come out as histograms corresponding to the energy group structure

- Looking for consistency!

ACER versus GROUPR for DT Reaction MT 50



Summary

- CP2020 data has been released for use with MCNP
  - 5 projectiles (H, D, T, He3, He4)
  - 7 targets (H, D, T, He3, He4, Li6, Li7)
  - Lighter ions onto heavier ions
- The CP2020 Library has been verified on 25 test problems with the "lca 7J -2" option of MCNP
  - Broomstick Problems with conversion of the COM data to the LAB frame for comparisons with MCNP results
    - Angular Scattering
    - Outgoing Energy Distribution
  - Cross Comparisons of ACER and GROUP Results
    - Angle-Integrated Cross Sections.
  - More CP2020 data coming in the near future
    - Heavier ions onto lighter ions are coming …