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Los Alamos NATIONAL LABORATORY

Progress Report on Charged Particle Transport in MCNP6

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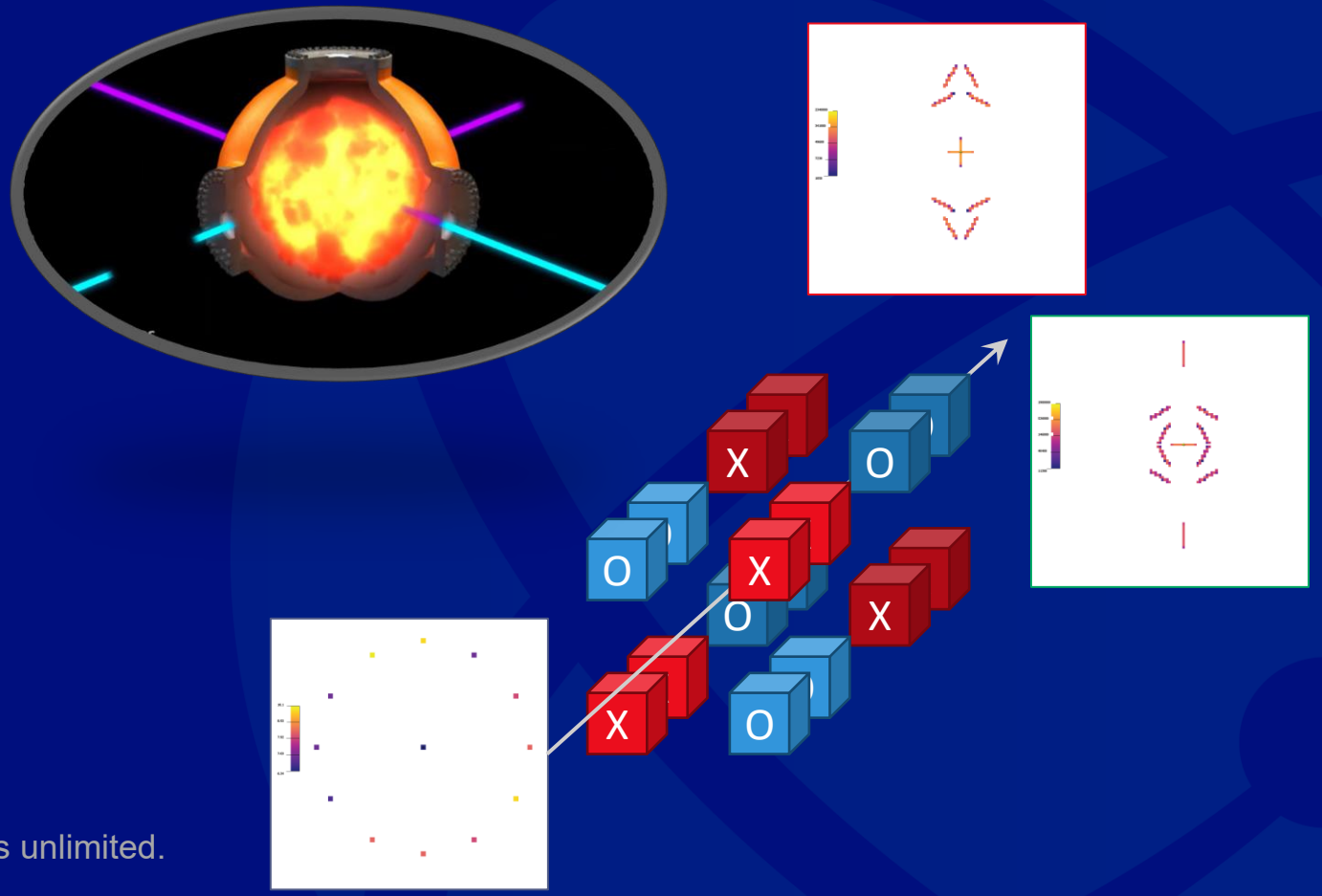
Monte Carlo Codes Group (XCP-3)

2025 MCNP® User Symposium
9 July 2025 14:10–14:35



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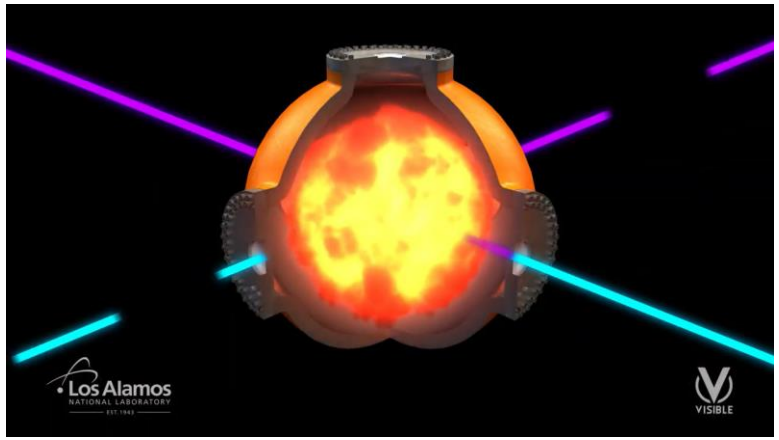
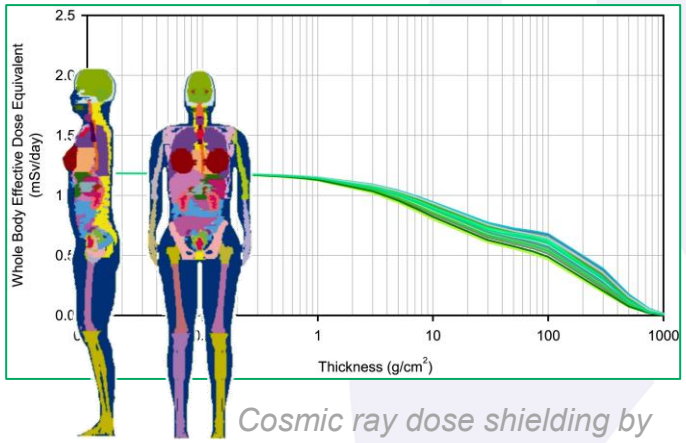
Charged particle applications of the MCNP® code

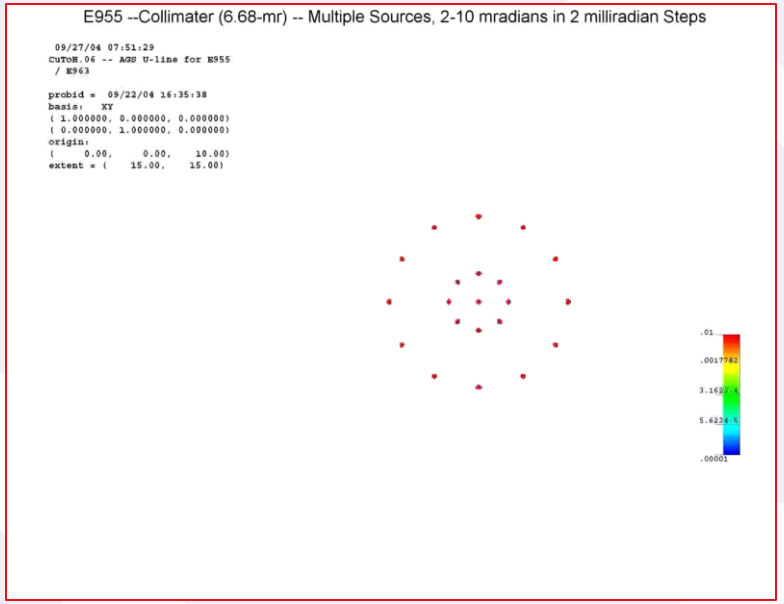
Charged particle transport is crucial for many applications of the MCNP® code.



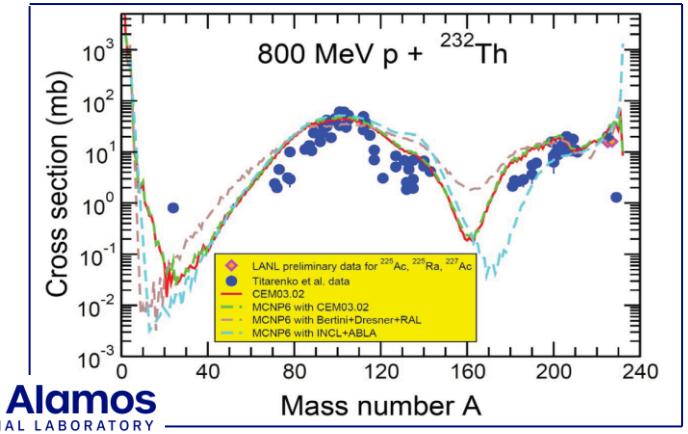
Dual-axis radiographic hydrodynamic test facility at Los Alamos (DAHRT) [LA-UR-19-30233].



Cosmic ray dose shielding by polymers and composite materials [D. Bond, Acta Astro. (2019)]. Inset: FAX phantom [R. Kramer, Phys. Med. Biol. (2004)].



Proton fluxes through a set of quadrupole focusing magnets (courtesy of Jeff Bull).

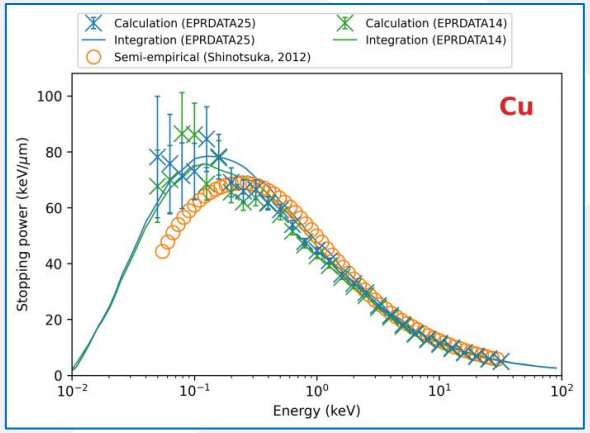


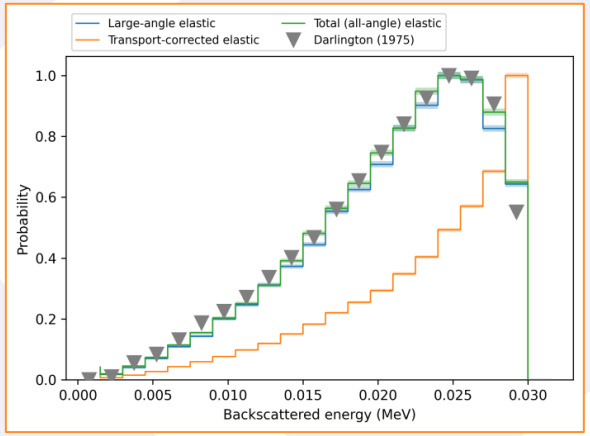
800 MeV proton-induced isotope production in ^{232}Th foils [S.G. Mashnik, LA-UR-11-00083].

Overview

This talk will review recent, current, and future work on charged particle transport in the MCNP® code.

- Data and V&V updates for electron transport:
  - New electron validation suites in 6.3.1 and 6.4.
  - **`eprdata25`** release and validation.
  - Documentation updates.
- Code improvements (for 6.4 unless noted):
  - Consistent handling of tabular light ion transport.
  - Other bug fixes and improvements.
  - Known issues.
- Current and future development…

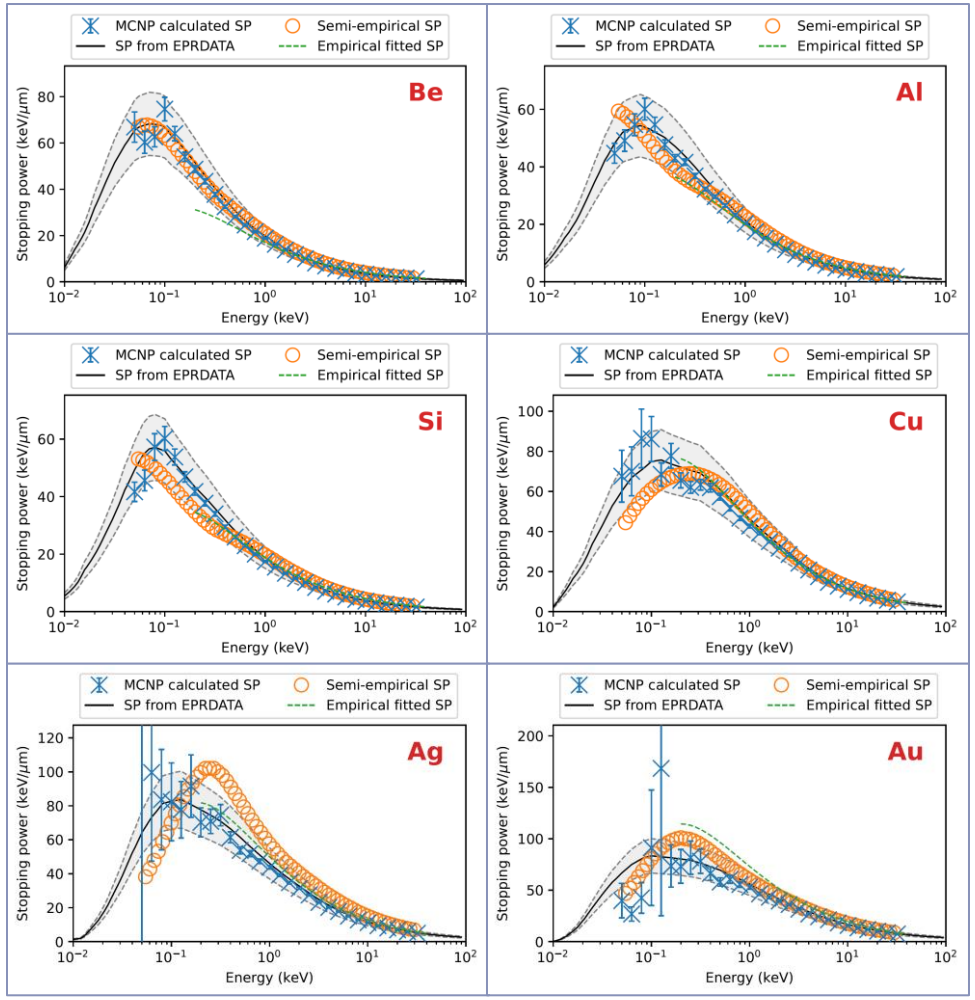




Data and V&V updates for electron transport

- We have implemented new MCNP® verification and validation (V&V) suites for electron transport:
  - Electron stopping power validation suite (released with 6.3.1).
  - Electron backscattering validation suite (will release with 6.4).
  - Additional validation suites are planned, including for heavier charged particles.
- These new capabilities are timely, enabling V&V to support the release of new **`eprdata25`** ACE files.
- This work is supported by documentation updates:
  - Electron stopping power references available in the Reference Collection.
  - Electron backscattering references are a TODO item.
  - ACE format description update for **`eprdata14`** and later (LA-UR-24-30590).

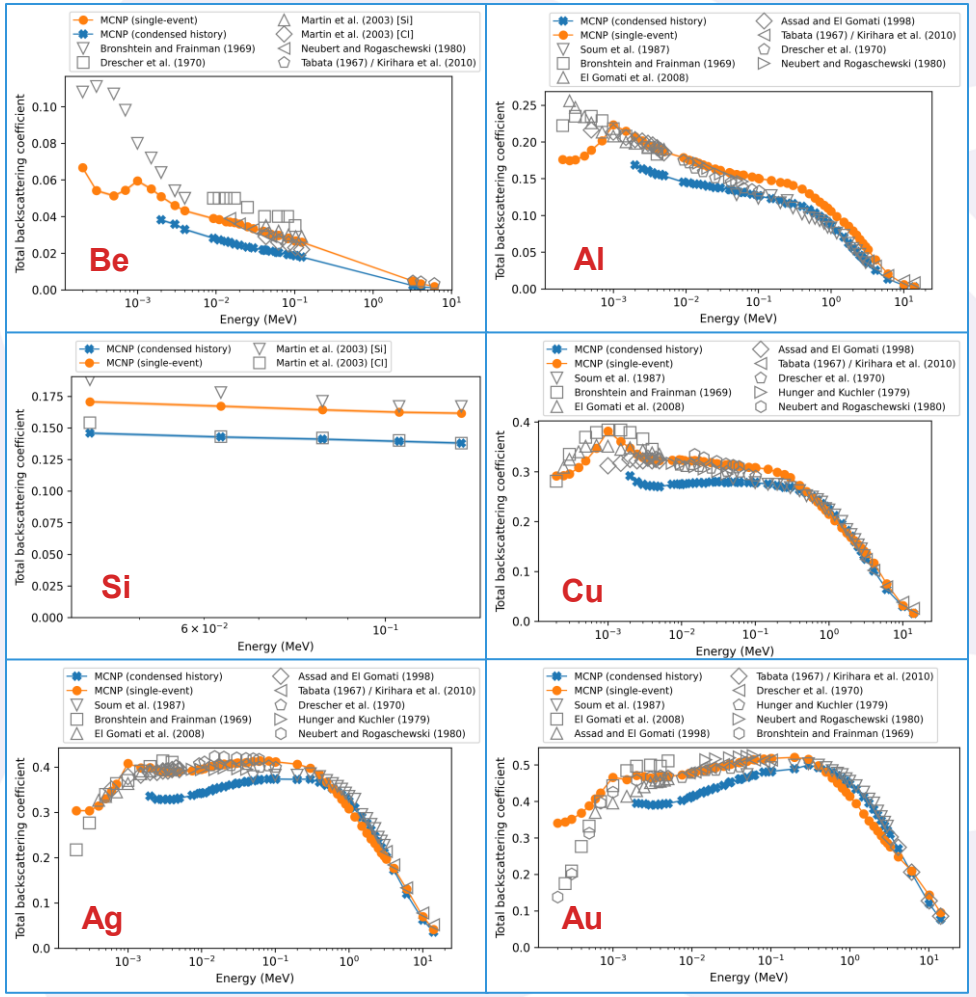
Electron stopping power validation suite



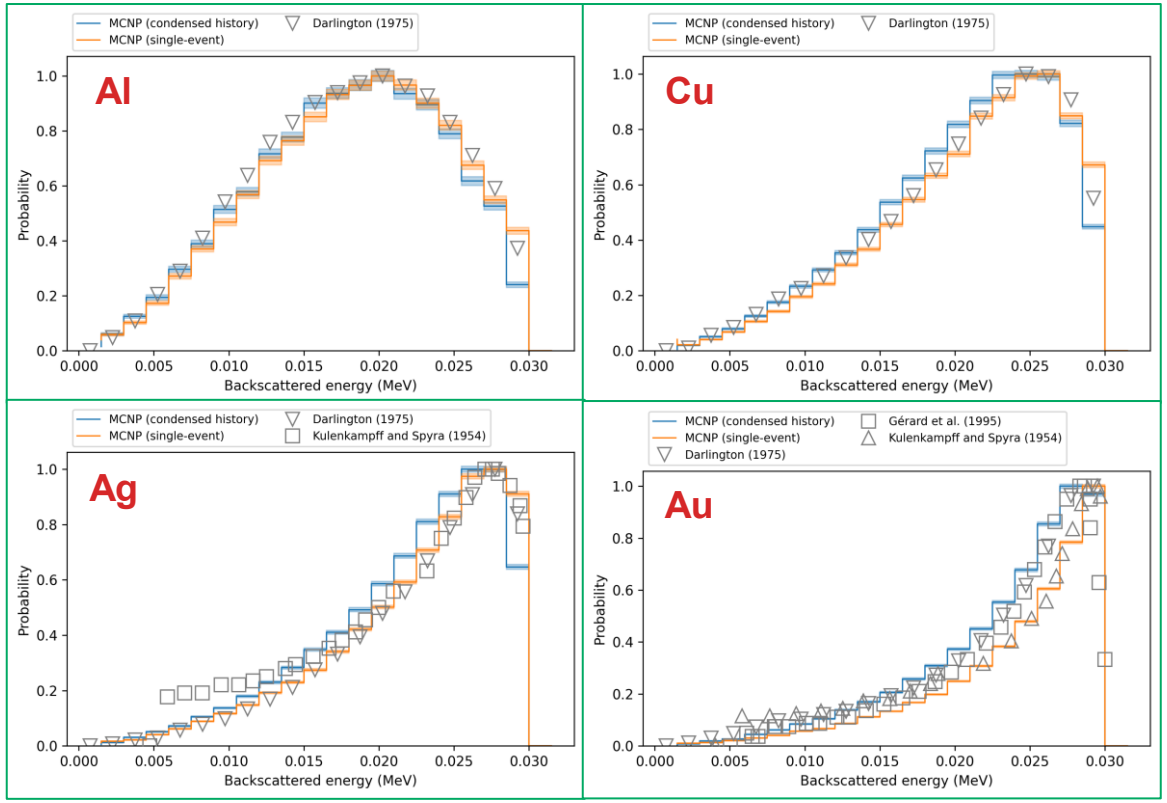
- Objective: calculate electron stopping powers in single-event mode and compare against (semi-)empirical measurements.
- Method: compute displacements between energy-loss events to estimate $R(E)$ and stopping power as $S(E) = (dR/dE)^{-1}$.
  - Excitation, ionization, and bremsstrahlung.
  - Also integrate $S(E) = N \int_0^{T_m} T(\partial\sigma/\partial T)\, dT$ from **`eprdata`** ACE files as verification.
- References: Lively et al., *Rad. Phys. Chem.* **216** (2024) 111483 and LA-UR-23-30022; MCNP6.3.1 V&V Report (LA-UR-25-22398).

Electron backscattering validation suite (1/2)

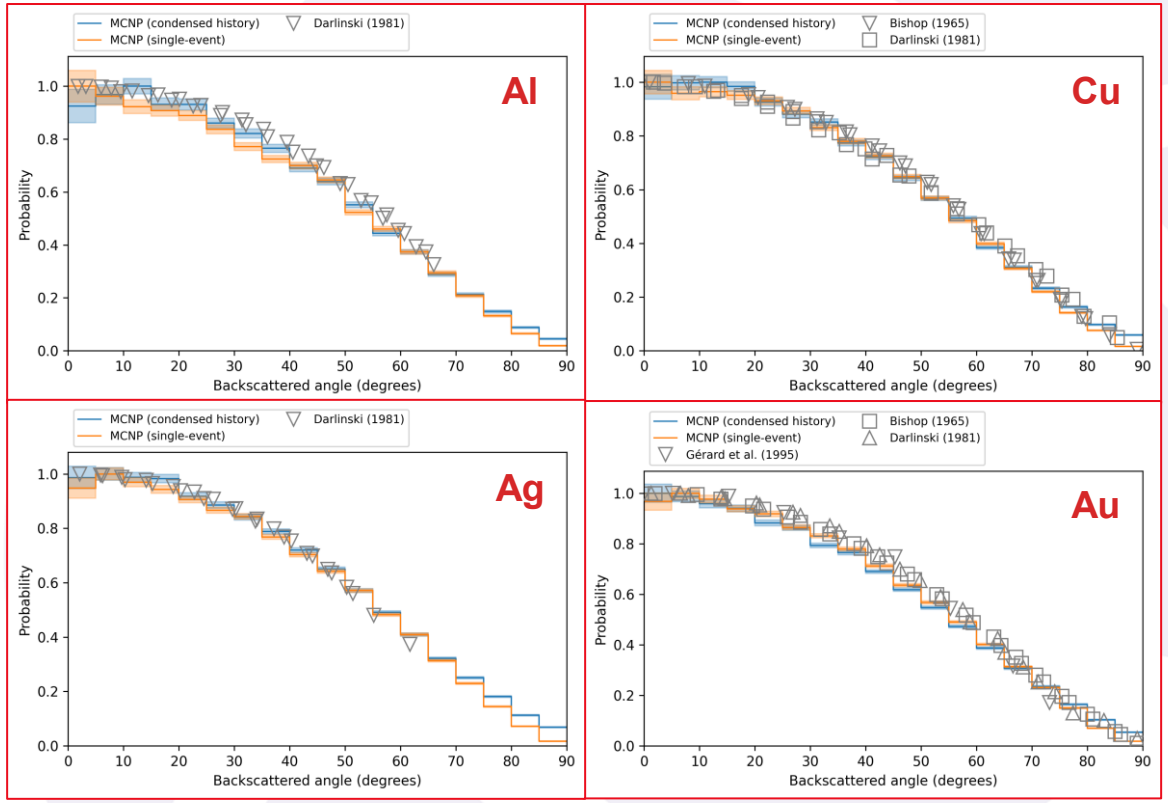
- Objective: Calculate electron backscattering yields and distributions and compare against a wide range of experimental datasets.
- Methods: Compute with both traditional condensed history (**`e103`**) and single-event (**`eprdata14`**) algorithms.
  - CH only for electron energies above 2 keV.
- Results: Generally, Yield(SE) > Yield(CH) due to single large scattering events.
  - Approximate “accuracy threshold” at 100 keV.
- References: Work in progress…



Electron backscattering validation suite (2/2)



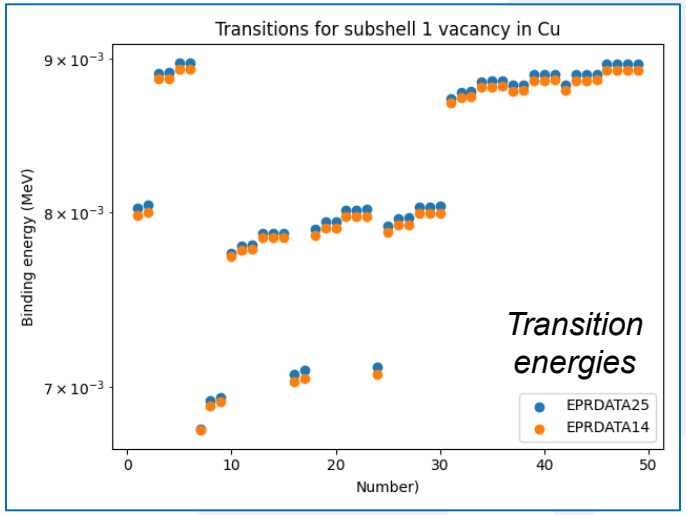
Backscattered electron energy distributions at 30 keV.

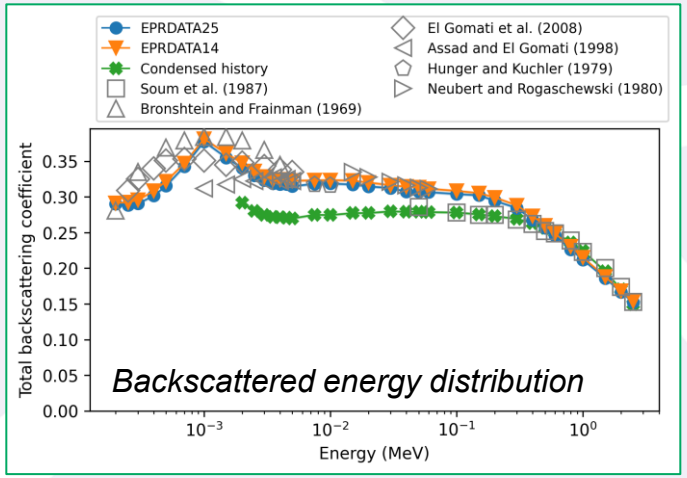


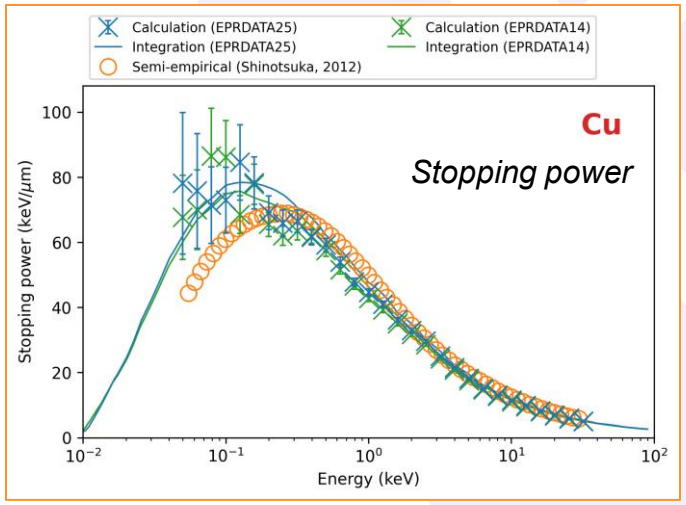
Backscattered electron angular distributions at 30 keV.

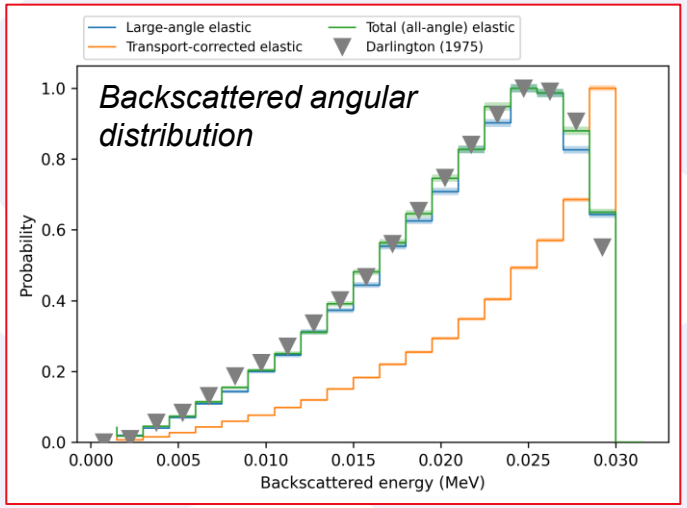
Validation of the `eprdata25` ACE library release

- **`eprdata25`** includes data updates from EPICS2017 and EPICS2023.
  - No data changes in EPICS2025.
  - See talk by Wim Haeck.
- Validated by electron stopping power + backscattering suites.
  - Stopping power generally ~20% improvement vs measurements due to subshell energies.
  - Backscattering: no clear trends.
  - Also compare between different elastic scattering modes.









Code improvements for charged particle transport

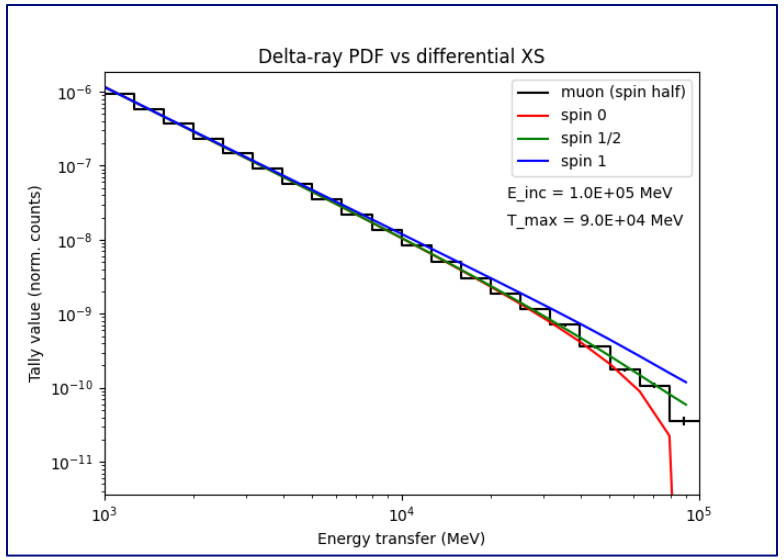
- We have invested significant time and effort into bug fixes, improvements, and consistency/quality upgrades for charged particle code.
  - In large part, this has laid the groundwork for major improvements in coming FYs.
  - “New feature” development is constrained by the scope of our site support mission, but many critical needs fall within this scope.
- Significant updates:
  - Tabular light handling consistency.
  - Delta-ray production (i.e., heavy-charged-particle ionization) high-energy fixes.
  - Magnetic field transport improvements connected to the above.
- And many smaller improvements which may be of interest to users…

Consistent handling of tabular light ion transport

- The MCNP® code can use tabular nuclear data for non-proton light ions.
  - Deuterons (**`dlib=80o,00o`**)
  - Tritons (**`tlib=80r,00r`**)
  - Helions (**`slib=80s,00s`**)
  - Alpha particles (**`alib=80a,00a`**)
- These should be handled identically to protons, but this was not always true.
- These inconsistencies have been rectified. Notable impacts include:
  - D/T/S/A particle tallies may now use reaction-rate tally multipliers.
  - D/T/S/A particle F6 tallies now use tabulated heating numbers.
  - D/T/S/A particles now score in source-type mesh tallies (e.g., **`fmesh type=source`**).
  - D/T/S/A cross section tables use the same logic as neutron and proton tables.
    - Previously, these used photonuclear logic for some reason, leading to odd artifacts.
  - Mixing tabular and model physics for D/T/S/A no longer double-counts collisions.
  - Additional impacts on code layout and quality which most users will not notice.

δ-ray production fixes for high particle energies

- δ-ray production (i.e., ionization electrons from heavier charged particles) was added in code version 6.2. The implementation had several errors:
  - Spin correction for $s = 1/2$ implemented but only used for protons.
  - No spin correction for $s = 1$ was implemented, notably affecting deuterons.
  - An incorrect term was used in the denominator of this correction.



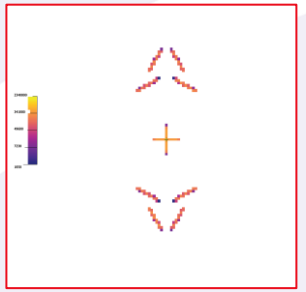
δ-ray energy distribution for 100 GeV μ.

- These errors have been corrected.
  - Documentation: LA-UR-25-23077.
- The impact is felt only at very high energies.
  - Few TeV for protons, ~100 TeV for alphas, etc.
  - Tens of GeV for muons (most accessible).
  - Relevant primarily for cosmic ray applications.

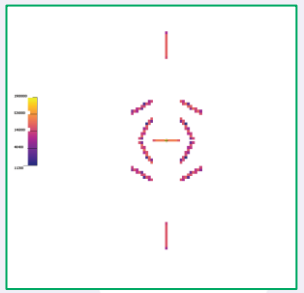
Related to these changes: removed 1 TeV/n energy hard limit.

Magnetic field transport fixes and improvements

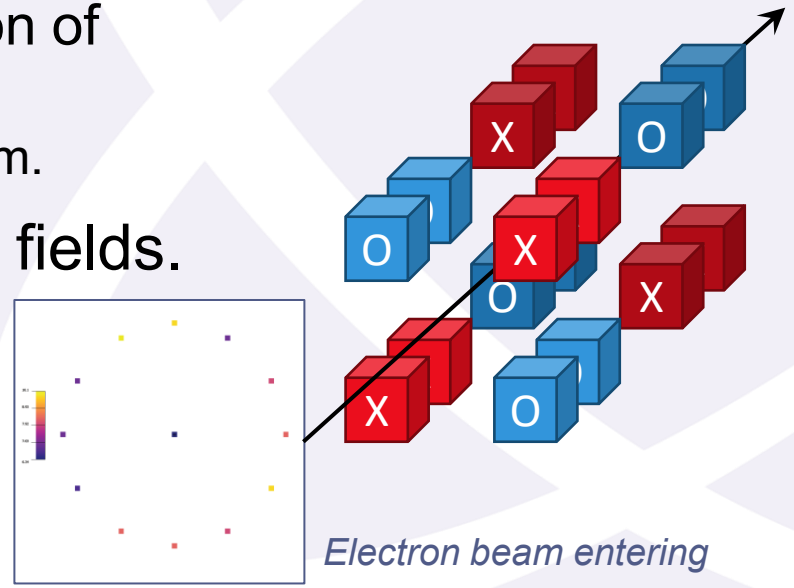
- Quadrupole fringe field (**`bfld type=quadff`**) kick improvements:
  - All charged particles now receive fringe field kicks (previously limited to protons only).
    - This includes electrons, improving modeling of electron beam lines.
  - Fringe field kick now uses the local magnetic field coordinate system.
    - Previously the fringe field was required to be aligned with the z-axis.
    - With this change, **`bfld type=quadff`** may now be used with arbitrary axes, allowing modeling of full quadrupole beam lines.
  - Corrected and expanded manual documentation of the fringe field kick.
    - N.B., only valid within ~2% of the design momentum.
- δ-ray production is now allowed in magnetic fields.
  - Position of knock-on electrons is now computed correctly, preventing cell errors.



Without FF kick



With FF kick



Electron beam entering

Other charged particle fixes and improvements in FY25

Electrons

- ★ Added collision events during single-event electron transport to `ptrac` output.
- ★ Added sections about single-event electron transport data and physics to the user manual.
- Fixed thread-unsafe behavior of the variable used to reference stopping powers for the `ft let` tally treatment and `de/df` cards.
  - Thanks to Scott O. Schwan (ORNL) for bringing our attention to this bug!
- Removed a warning that electron ACE tables were inappropriate for `mode e` problems.

Heavier charged particles

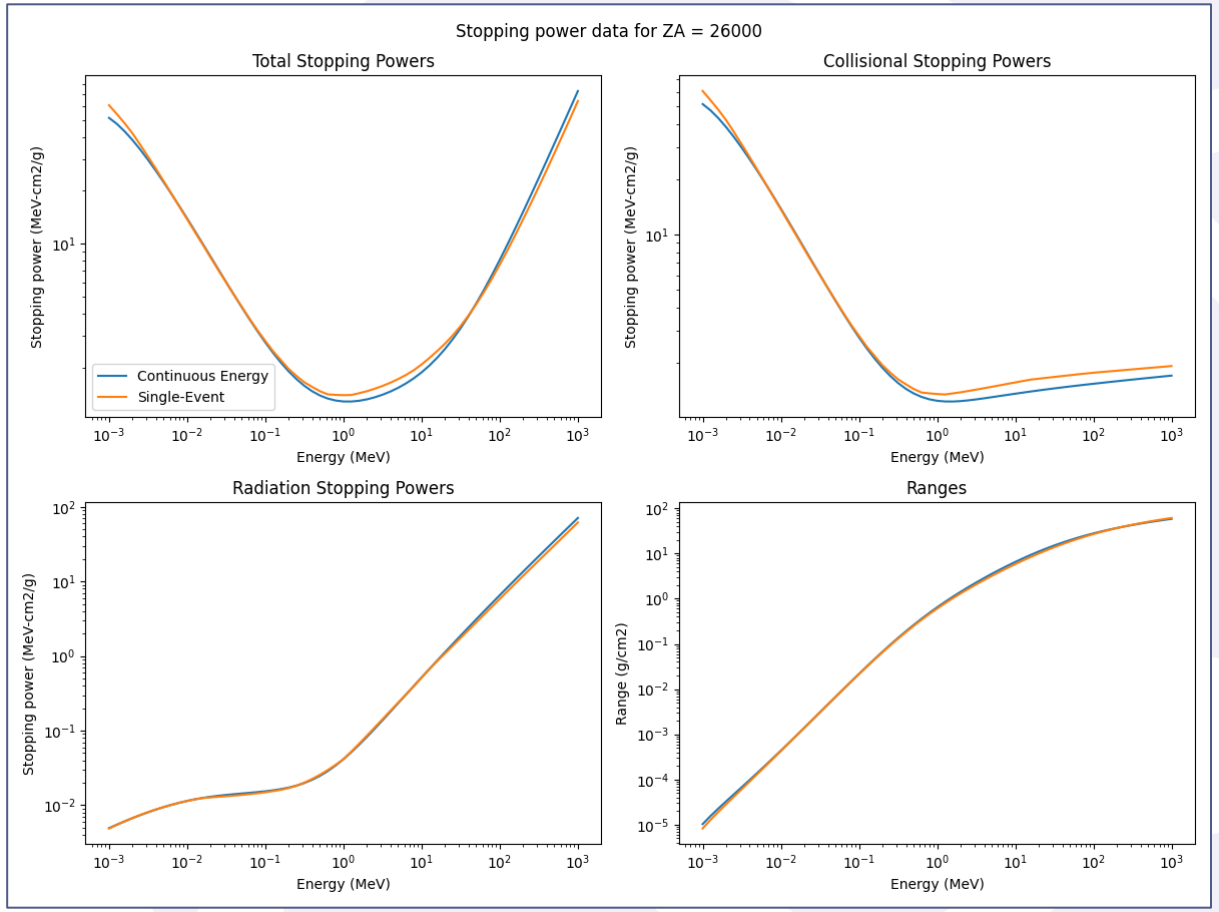
- ★ Fixed memory access error when accessing charged particle γ-ray production ACE data (**release 6.3.1!**).
- Added regression tests for Cerenkov radiation produced by heavy charged particles.
- Documented the `tabl` option on the `phys:d,t,s,a` cards in the user manual.
- Added references to the Reference Collection for charged particle transport and δ-ray production.

Current and future charged particle development

- Work done to this point has laid a foundation for major future efforts.
  - Both from a technical perspective and in terms of knowledge-building.
- The major current direction for charged particle transport is assessing and revamping stopping powers:
  - `stppwr` package in development as a diagnostic tool.
  - Heavy charged particle stopping powers rework.
- Many promising directions are open for future work:
  - Documentation of heavy charged particle physics.
  - Expanding charged particle V&V, especially for non-electron problems.
  - Synergistic/concurrent improvements to condensed-history and single-event electrons.
  - Particle-induced x-ray emission physics.

Development highlight: stppwr package

- Purpose: compute and plot various stopping powers which are used by the MCNP® code or can be derived from ACE data tables.
  - Currently handles continuous-energy (CH mode) and single-event (SE mode) electron stopping powers.
  - Next step: heavy charged particle stopping powers.
  - Future plans for neutral particles (neutrons and photons) as well.
- Intended for release as a component of PyMCNP.



Example plots of stopping power data calculated for continuous-energy and single-event electron transport modes.

Conclusions

- Charged particle transport is an essential component of the MCNP® code.
- We have made significant progress for both electrons and heavier charged particles in the past FY (and change).
  - Verification and validation for electron transport.
  - Release and validation of the new **`eprdata25`** ACE library.
  - Consistent treatment of tabular light ion transport.
  - High-energy δ-ray production fixes and improvements.
  - More robust charged particle transport in magnetic fields.
  - And many more…
- We are accelerating towards bigger and better things in the coming years.
- **WANTED:** User feedback and ideas on current and future development!

Contact and Acknowledgments

- Questions? Comments? Concerns? ~~Scathing insults?~~ Please contact:

  mcnp_help@lanl.gov

  (Or, if you really need that personal touch: livelym@lanl.gov)

- Thanks and acknowledgments to:
  - All MCNP Team members who have contributed to this work.
  - Joel Kulesza and Mike Rising for especially supporting the V&V efforts.
  - Wim Haeck for processing the **`eprdata25`** libraries, occasionally under duress.
  - Jeff Bull for helpful discussions and the video on Slide 3.
  - And a special thanks to our users for:
    - Sharing their applications and use cases.
    - Diligently seeking out and reporting arcane bugs of diverse kinds.
    - Sharing current needs and future ideas.