Recent and Future Improvements to MCNP6 for Isotope Production Applications

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Predictive Codes for Isotope Production

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Outline

- Overview of MCNP6®
- Isotope Production
- MCNP6 Modernization
- Future Improvements

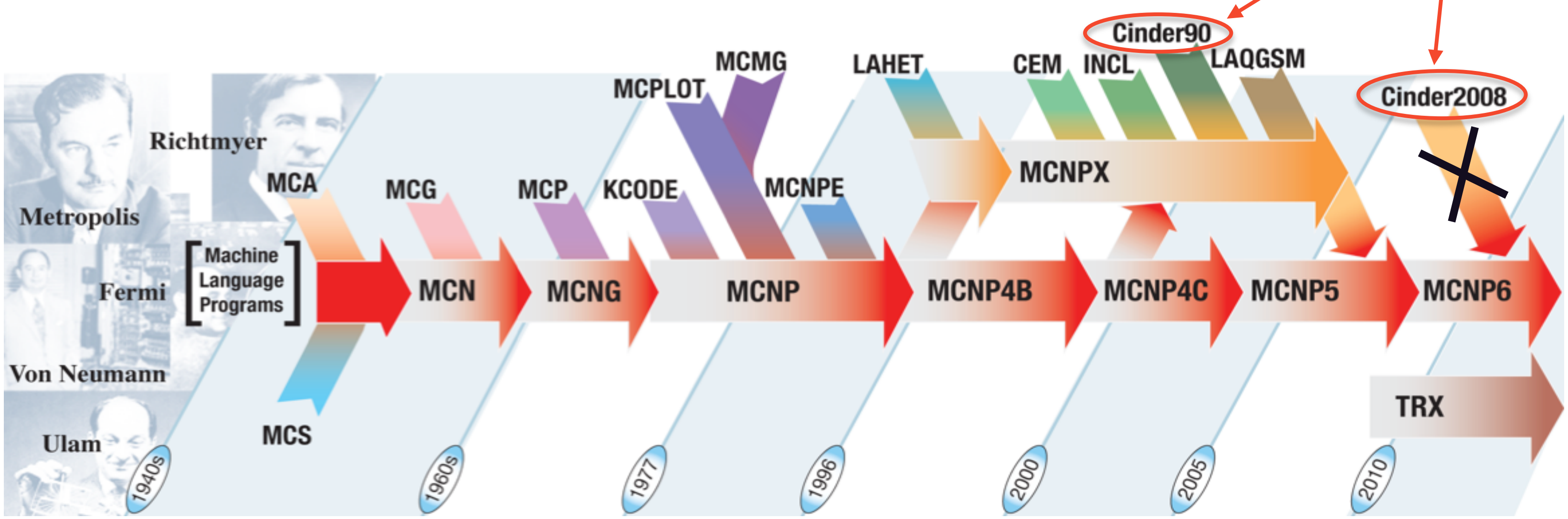
Overview of MCNP6®

Overview of MCNP6®

- MCNP6® is the LANL general purpose, continuous-energy Monte Carlo radiation transport code
- MCNP 6.1.0 released by RSICC in July 2013

  MCNP6.1 = MCNP5-1.60 + MCNPX-2.70
- MCNP 6.2.0 released by RSICC in April 2018
- MCNP5 & MCNPX are frozen – no future releases

CINDER'90 is the only version in all versions of MCNP6



RSICC distributions: 1,278 in FY19, 1,185 in FY20

Overview of MCNP6®

Focus of current developments within the MCNP code are driven primarily by three main long-term (decades) programs:

- **LANL Institutional Support**

Code Modernization, Maintenance, and User Support

- **NNSA Advanced Scientific Computing (ASC) program**

Unstructured Mesh, Neutron/Photon Physics, Advanced Variance Reduction, and High Performance Computing

- **DOE Nuclear Criticality Safety Program (NCSP)**

Criticality, Shielding/Dose, Parameter Studies, Verification and Validation, Upper Subcritical Limits

Many short term (years) projects drive new capability development Recent examples include:

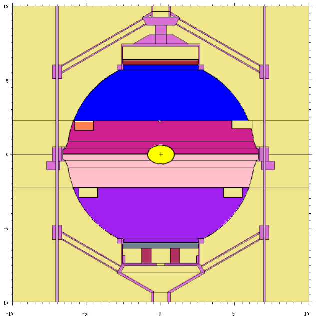
- **LANL LDRD (microreactor capabilities and unstructured mesh)**
- **NA-22 (fission model FREYA & CGMF integration, parallel PTRAC)**

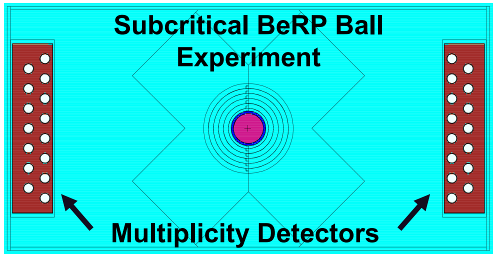
Overview of MCNP6®

Case Study in Nuclear Criticality: What Makes a Code Predictive?

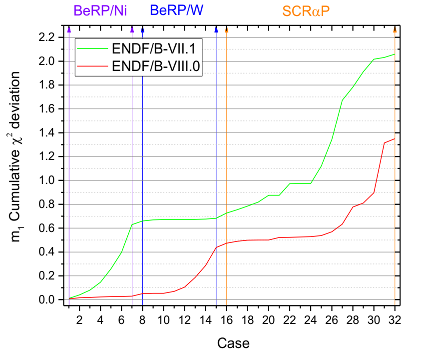
- **Ongoing method development**
  - Quick updates to methods when **nuclear data changes:** recent example with ENDF/B-VIII.0 S(α,β)
  - Ongoing research in critical and subcritical systems
- **Code verification**
  - Assume data is perfect, how does the code perform?
  - Routine use of **analytic** criticality (k_{eff}) problems to test algorithms/methods is necessary
- **Code and nuclear data validation**
  - Compare the predictions (code+data) to reality
  - Routine use of a variety of criticality benchmark simulations in **comparison to experiment** is essential
    - Criticality (k_{eff}), reactor kinetics (β_{eff}, Rossi-α), subcritical multiplication (singles, doubles, leakage multiplication)

Jezebel Critical Experiment





Hutchinson, et al., subcritical studies



Isotope Production

Isotope Production

MCNP6 is used in a broad set of accelerator applications

- Spallation source calculation
- Transmutation of radioactive materials
- Shielding design (not discussed here)

Other accelerator-specific features

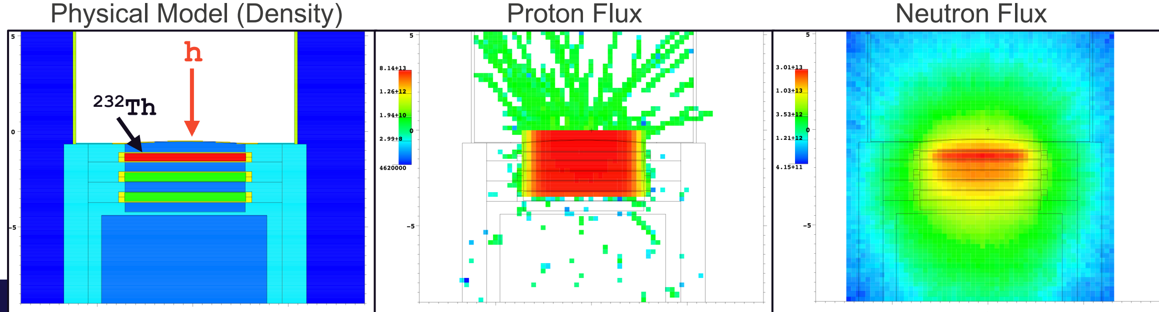
- Magnetic fields
- Source options, i.e., beam shape

For **spallation source** simulation or similar, need charged particle transport and data and/or models for collision physics

For **transmutation** of radioactive materials, need both reaction rate information from transport simulation and production/depletion capability and decay sub-library data/physics

100 MeV proton source impinging on ^{232}Th target

Physical Model (Density) | Proton Flux | Neutron Flux



MCNP Model courtesy of Ellen O'Brien

Isotope Production

MCNP6 includes some proton cross section data tables

- LA150h library – 41 isotopes – extension .24h
  - ^{1}H, ^{2}H, ^{12}C, ^{14}N, ^{16}O, ^{27}Al, ^{28}Si, ^{29}Si, ^{30}Si, ^{31}P, ^{40}Ca, ^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr, ^{54}Fe, ^{56}Fe, ^{57}Fe, ^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni, ^{63}Cu, ^{65}Cu, ^{93}Nb, ^{182}W, ^{183}W, ^{184}W, ^{186}W, ^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{209}Bi

- ENDF70PROT – 47 isotopes – extension .70h
  - ^{1}H, ^{2}H, ^{3}H, ^{3}He, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{12}C, ^{14}N, ^{16}O, ^{27}Al, ^{28}Si, ^{29}Si, ^{30}Si, ^{31}P, ^{40}Ca, ^{50}Cr, ^{52}Cr, ^{53}Cr, ^{54}Cr, ^{54}Fe, ^{56}Fe, ^{57}Fe , ^{58}Fe, ^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni, ^{63}Cu, ^{65}Cu, ^{93}Nb, ^{182}W, ^{183}W, ^{184}W, ^{186}W, ^{196}Hg, ^{198}Hg, ^{199}Hg, ^{200}Hg, ^{201}Hg, ^{202}Hg, ^{204}Hg, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{209}Bi

- CP2011 – 7 isotopes – extension .71h
  - ^{1}H, ^{2}H, ^{3}H, ^{3}He, ^{4}He, ^{6}Li, ^{7}Li

If no tabular data is available then MCNP6 will use model physics

Upper energy limits may vary (150 MeV is typical)

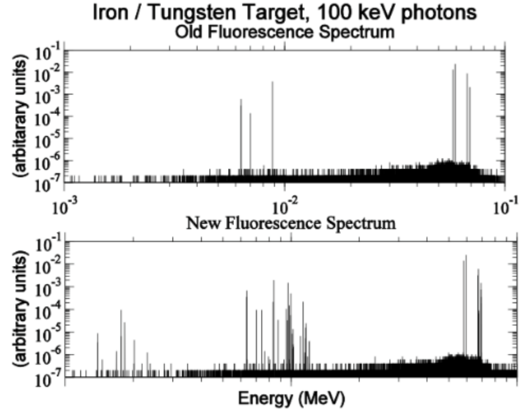
Production cross sections and emission spectra also vary

Isotope Production

- "Newer" electron physics options
  - Single Event Electron physics
  - EPRDATA
    - Improved atomic relaxation →
  - Likely too computationally expensive and unnecessary for isotope production

Old

New



- Heavy ion and other "spallation" physics options
  - Specify heavy ions as source particle (`SDEF par=ZA`)
  - Model Physics →
- Routine **validation** of the model physics options is extremely sparse

Variable	Bertini	ISABEL	CEM (default)	INCL	LAQGSM
Lower Energy	20-150 MeV	20-150 MeV	~ 10 MeV	~ 100 MeV (not in MCNP: ~ 5 MeV/A)	~ 100 MeV/A (not in MCNP: ~a few MeV/A)
Upper Energy	3.5 GeV (nuc-nuc) 2.5 GeV (pion-nuc)	1 GeV	5 GeV	2 GeV (not in MCNP: ~ 15 GeV)	~ 1 TeV/A (not in MCNP: ~ 20-100 TeV)
Target Nuclei	All	All	$A \geq 4$	All	All
Incident particles	h, n, pions	h, n, $A \leq 4$, (not in MCNP: also A>4)	h, n, pions, γ	h, n, $A \leq 4$ (not in MCNP: ~ A<16)	Almost all particles & ions

Isotope Production

MCNP6 includes an embedded version of CINDER'90

Integrated into the reactor physics burn-up/depletion feature

- `BURN` card
- k-eigenvalue calculation only

Material activation and transport of delayed-particles

- `ACT` card
- fixed-source calculation

Spontaneous source options

- Particle-type options on `SDEF` card
- fixed-source calculation

Code coupling efforts:

- MCNP + CINDER
- MONTEBURNS
- MCNP + ORIGEN
- MCNP + FISPACT
- and more

In practice, isotope production calculations are not done with inline transport + production/depletion physics – coupled simulations are used, i.e. 1) MCNP6, then 2) CINDER'90

MCNP6 Modernization

MCNP6 Modernization

Modernization via modularization

Modular components

- Improved testing ⟶ provable correctness of the code
- Easier maintainability
- Cleaner code
- Component reuse
- New features more efficiently developed and integrated
- Early career staff excited to work on a more modern code

MCNP6 Modernization

Recent and ongoing efforts relevant to isotope production applications

Event Record

Event Record

- New `PTRAC` replacement is done
  - HDF5-formatted output
  - Parallel threading and MPI

Collision Physics

Collision Physics

- Just beginning a nuclear data interface project
  - Handle sampling/access to tabulated nuclear data
  - Provide consistent interface to model physics

Production Depletion

Production / Depletion

- Some planning, but this has been a low priority so far
  - Disentangle MCNP/CINDER dependencies (modularize)
  - Develop interface so alternatives can be used inline

Future Improvements

Future Improvements

Thoughts on potential future efforts relevant to isotope production applications

Event Record

Event Record

- `HISTP/HTAPE`
  - Patch MCNP6.2 to fix this broken capability (short term)
  - Deprecate in favor of `PTRAC`-based capability (long term)

Collision Physics

Collision Physics

- Proton data and model physics
  - New interface will help with verification of data/model
  - Updates to proton data/models

Production Depletion

Production / Depletion

- First steps to make CINDER a callable library
  - Flexibility to use inline in MCNP6 and in coupled calculation
  - The future of CINDER is not clearly defined

Future Improvements

How to make isotope production applications more predictive…

- **Ongoing method developments**
  - Code improvements relevant to charged-particle transport
  - Data and model physics updates as necessary
- **Method verification (comparisons to analytic results)**
  - Charged-particle / condensed history algorithm verification
  - Production / depletion method verification
- **Validation, validation, validation!**
  - Need benchmark experiments and models that integrate collision physics data and models, residual nuclide calculations, and production/depletion physics

Questions?

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