ASC program particle transport codes at LANL and LLNL

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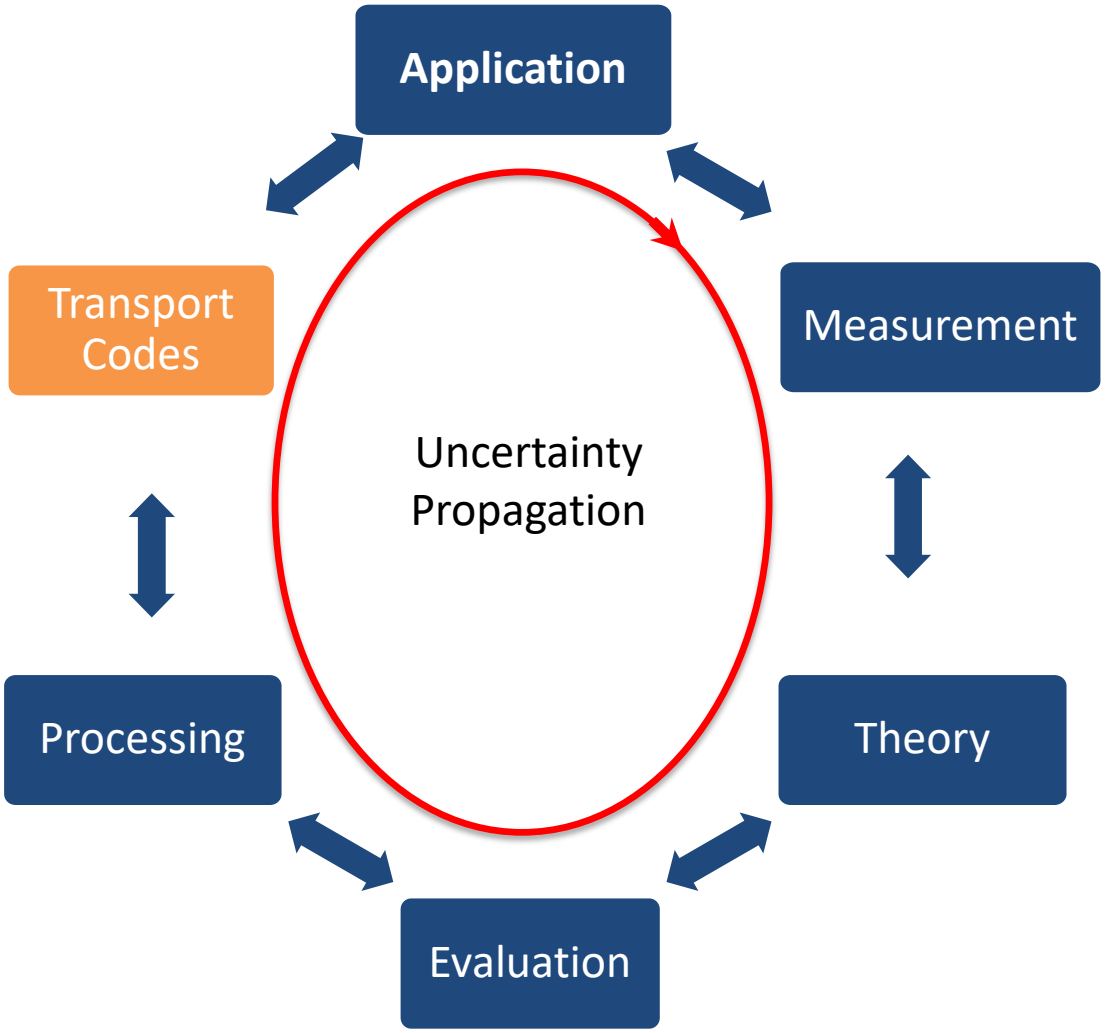
Transport is key for the nuclear data pipeline

- Transport code developers:
  - Often the first customer of nuclear data
  - Often develop a strong interest in nuclear data
  - Develop a deep understanding about need for high quality data
- Goals of this talk:
  - Provide a high-level overview of ASC transport code and research goals
  - Build a stronger bridge between the transport community and the nuclear data community
- We are all interested in improving predictive science



The ASC program supports general transport code development

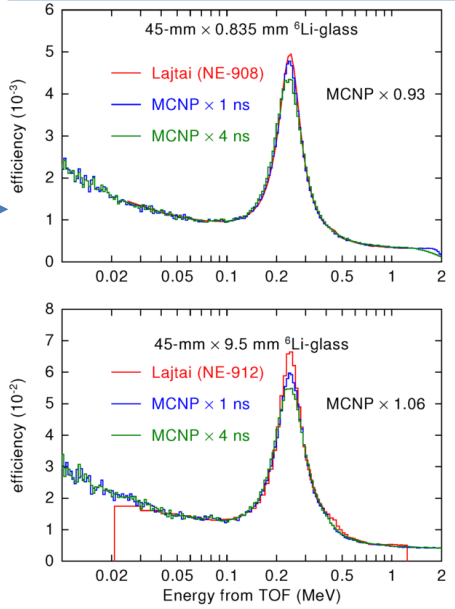
Code	Description	Lab	POC
PARTISN	Particle Transport, Multigroup, Deterministic SN	LANL	Jon Dahl
Ardra	Particle Transport, Multigroup, Deterministic SN	LLNL	Teresa Bailey
MCATK	Monte Carlo, Combinatorial Geometry, Continuous Energy	LANL	Travis Trahan
Mercury	Monte Carlo, Combinatorial Geometry, Multigroup (hybrid) and Continuous Energy	LLNL	Patrick Brantley
MCNP	Monte Carlo, Combinatorial Geometry, Continuous Energy and Multigroup	LANL	Michael Rising

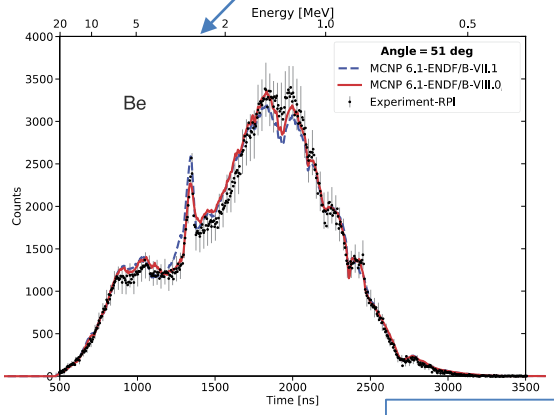
A big driver for all ASC transport codes is performance portability and emerging computer architectures

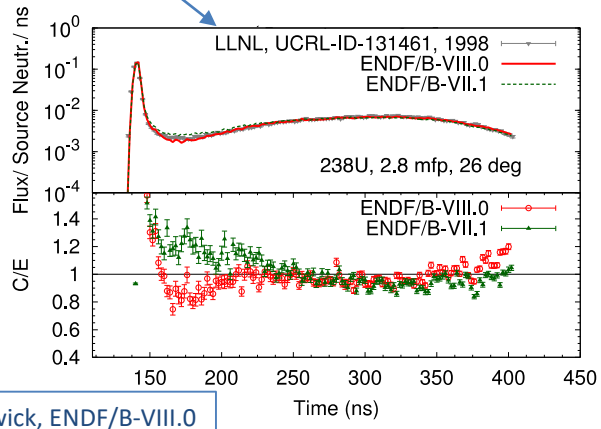
The MCNP transport code is used to vet national nuclear data

- MCNP® has a long-standing reputation as the ”gold-standard” Monte Carlo radiation transport code
- In the nuclear data pipeline, MCNP® also plays a role in supporting the evaluations and verifying the processing
- Nuclear data testing and validation starts (beta-releases) and ends (final production data) with MCNP® simulations
  - k-eigenvalue, delayed neutrons, critical masses, reaction rate ratios, subcritical multiplication
  - Quasi-differential, pulsed spheres

Neudecker, Taddeucci, PFNS evaluation

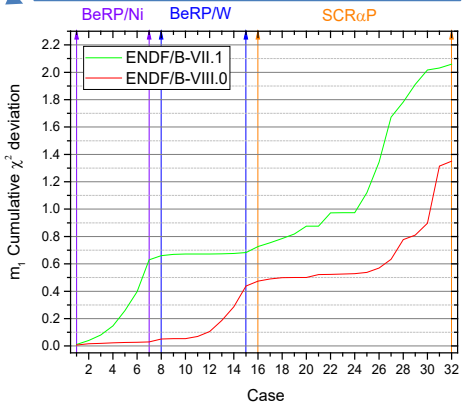






Brown, Chadwick, ENDF/B-VIII.0

Hutchinson, recent subcritical studies



Common drivers for transport all codes

- Performance portability for ASC HPC platforms
- Large emphasis on V&V to enable predictive science through computational physics
  - Hierarchical testing is essential to finding bugs
    - Evaluations
    - Processed data libraries
    - Transport numerical methods
    - Both Monte Carlo and deterministic methods together help narrow down bugs
- Propagation of uncertainties using Covariance information and criticality benchmarks when available
- Updated/modern gamma cross section data for shielding and detector response

Deterministic specific needs, with emphasis on nuclear data

- Faster solutions and better physics rely on next generation methodologies for multigroup data
  - Software tools to support problem specific data generation capabilities
  - Machine learning for
    - generalized flux weighting methods
    - alternate group structures
  - “On-the-fly” multigroup processing
    - Doppler broadening
    - Self shielding factors
    - Flux re-weighting
    - Compressed storage of fission and scattering matrices
  - Multiband processing extensions
    - Optimal band structures over several isotopes
    - Correlations of bands between isotopes
    - Research into tradeoffs of band resolution vs group resolution

Monte Carlo specific needs, with emphasis on nuclear data

- Faster Solutions:
  - Efficient Monte Carlo transport on GPUs is an ongoing research challenge
  - Nuclear data collision physics software libraries must run on GPUs
  - Multipole data representations for Continuous Energy (CE)
    - Significant memory savings (orders of magnitude)
      - Allows “nearby” memory storage on compute unit providing faster access
    - Multi-temperature data treatments with zero additional memory cost
    - Will require extensive V&V
- Better Physics:
  - Research into thermalization models incorporating increased physics fidelity
  - Research into on-the-fly Doppler broadening/thermalization models possibly enabled by advanced architectures
  - Interested in outcomes of research into next generation multigroup algorithms

Transport code developers are partners with the nuclear data community

- The goal of this talk was to provide a high-level perspective about issues that transport code developers are currently facing within the ASC program
- The ASC program supports a variety of transport codes, with both Monte Carlo and Deterministic methods
- The ASC program invests in technology to improve predictive science
  - Transport code compute performance and portability enables more calculations to be run faster and at larger scale
  - Tighter integration with nuclear data enables higher physics fidelity simulations
- Transport code developers recognize the need for:
  - High-quality, well-tested nuclear data
  - New physics included in the nuclear data
  - New algorithms shared between the transport codes and other parts of the data pipeline
  - Stronger partnerships with the nuclear data community

Backup

ASC Platforms and Facilities Timeline