ASC program particle transport codes at LANL and LLNL

Presenter: Jon Dahl (LANL)
Contributors: Teresa Bailey (LLNL), Patrick Brantley (LLNL), Scott McKinley (LLNL), Steve Nolen (LANL), Michael Rising (LANL), Travis Trahan (LANL), Steve Wilson (LANL)

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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

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

Brown, Chadwick, ENDF/B-VIII.0

Neudecker, Taddeucci, PFNS evaluation

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
ASC Platforms and Facilities Timeline

- **Advanced Technology Systems (ATS):**
  - **ATS-1: Trinity (LANL/SNL) 41 PF**
  - **ATS-2: Sierra (LLNL) 125 PF**
  - **ATS-3 Facility Prep: EC3E (LANL)**
  - **ATS-4: El Capitan (LLNL) 1.5 EF**
  - **ATS-3: Crossroads (LANL/SNL)**
  - **ATS-4 Facility Prep: ECFM (LLNL)**

- **Commodity Technology Systems (CTS):**
  - **CTS-1**
  - **CTS-2**

- **Advanced Arch Prototype System (AAPS):**
  - **Astra (SNL) – 2.3 PF**

**Timeline:**
- **Fiscal Year:** '17 '18 '19 '20 '21 '22 '23 '24 '25 '26 '27
- **August 2019**

**Legend:**
- Yellow: Procure & Deploy
- Orange: Use
- Red: Retire
- Green: Acceptance