Methods for processing and use of thermal neutron scattering data in OpenMC

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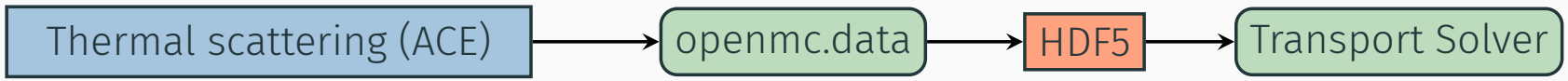
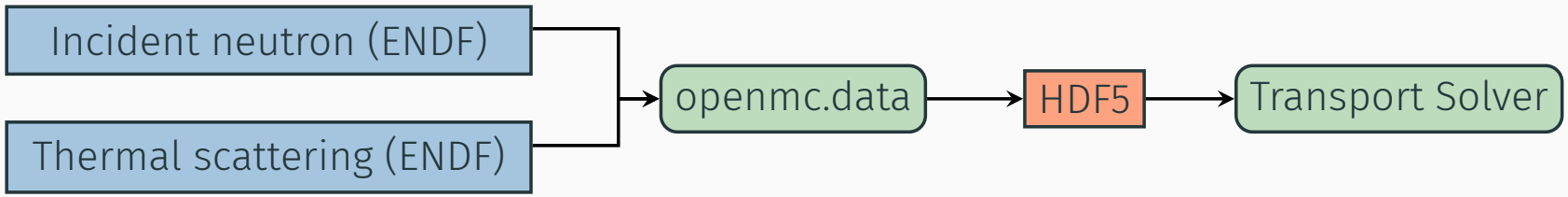
OpenMC

- OpenMC is a community developed, open-source Monte Carlo neutron/photon transport code
  - **Code:** https://github.com/openmc-dev/openmc
  - **Docs:** https://docs.openmc.org
  - **Forum:** https://openmc.discourse.group
- Relies on its own HDF5-based nuclear data format
  - Cross-platform binaries
  - Easy to extend format to accommodate new features
  - Significant data savings for multiple temperatures
- ENDF/ACE files need to be processed or converted to HDF5

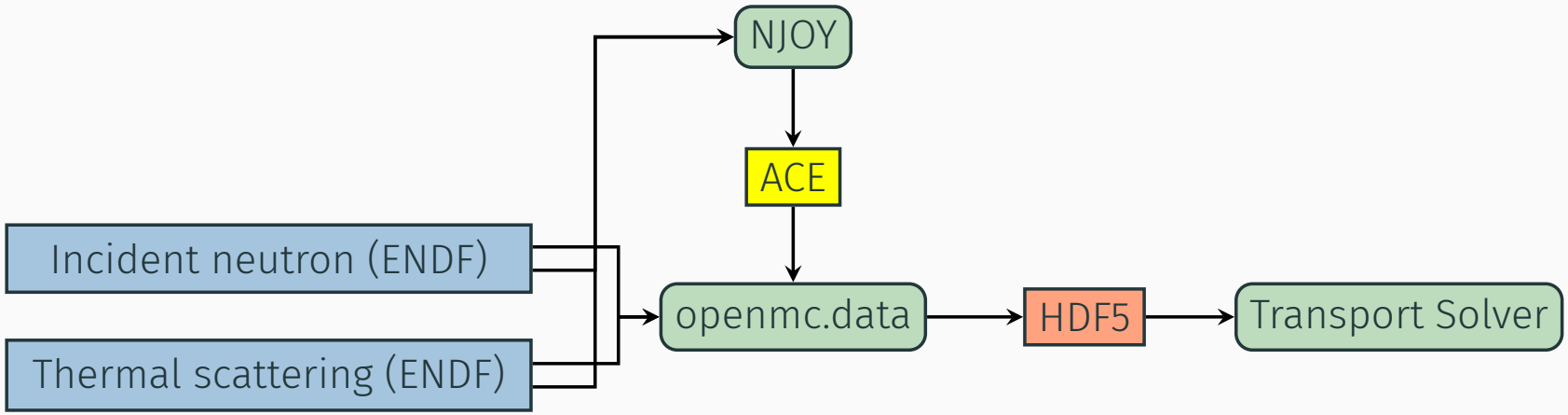
Processing pipeline (ACE-based)



Processing pipeline (ENDF-based)



Processing pipeline (ENDF-based)



NJOY Automation

- `openmc.data` module automatically generates NJOY input deck, executes NJOY, and collects data from resulting ACE files
- Most information needed for NJOY input can be determined from ENDF file, except for:
  - Associated isotopes (`iza`)
  - Number of atom types in mixed moderator (`nmix`)
- OpenMC maintains a list of recognized materials
  - `MAT` numbers are no longer unique in ENDF libraries
  - Use `ZSYMAM` to query list of recognized materials
  - When a new evaluation comes out, it requires manual intervention

Classes

- Thermal scattering integrated cross sections and angle/energy distributions fit into existing hierarchy of classes in OpenMC
- Cross sections are one-dimensional functions
  - `CoherentElasticXS` — evaluate cross section at energy E given Bragg edges and structure factors
  - `IncoherentElasticXS` — evaluate cross section at energy E given Debye-Waller integral
- Secondary angle/energy distributions follow similar concept, but have more variations due to different representations:
  - `CoherentElasticAE`
  - `IncoherentElasticAE`
  - `IncoherentElasticAEDiscrete`
  - `IncoherentInelasticAE`
  - `IncoherentInelasticAEDiscrete`

Incoherent elastic scattering

Double-differential cross section from ENDF is:

$$\frac{d^2\sigma}{dE'd\mu}(E \to E', \mu, T) = \frac{\sigma_b}{2} e^{-2EW'(T)(1-\mu)} \delta(E - E')$$

Integrate over E' and divide by total cross section to obtain probability density in μ:

$$p(\mu)d\mu = \frac{ce^{-c(1-\mu)}}{1 - e^{-2c}} d\mu$$

where $c = 2EW'(T)$. Integrate to get a cumulative distribution and then invert to generate a sampling scheme gives

$$\mu = \frac{1}{c} \log \left[1 + \xi(e^{2c} - 1)\right] - 1$$

where $\xi \sim U(0, 1)$.

Incoherent elastic scattering: H in ZrH

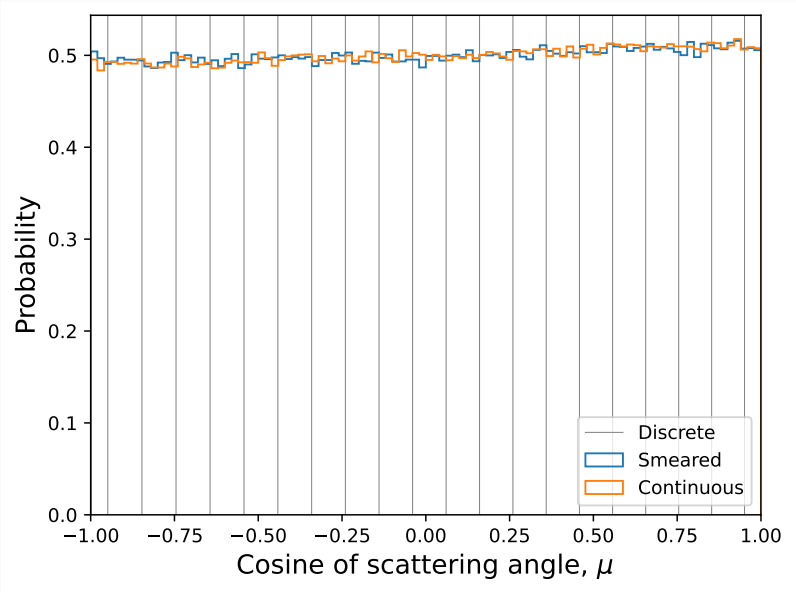


Figure 1: Samples at E=1.25 $\times$ 10^{-3} eV

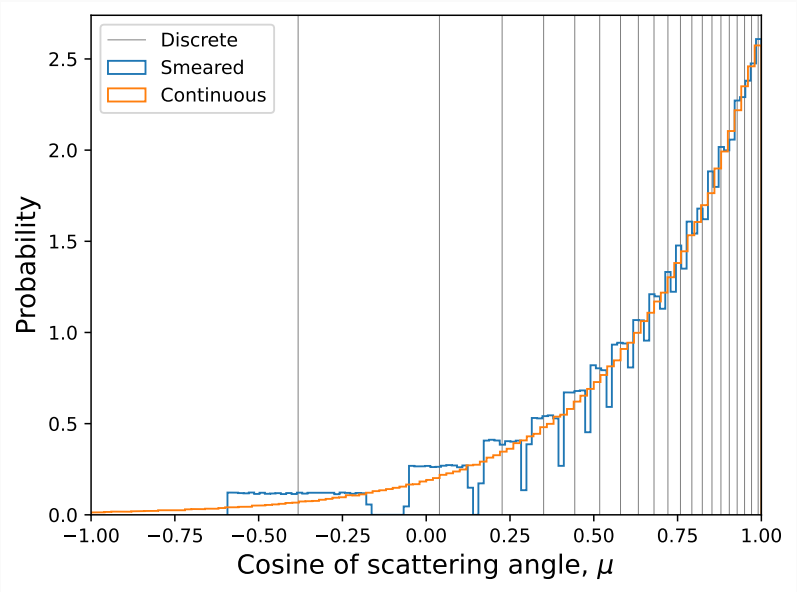


Figure 2: Samples at E=1.56 $\times$ 10^{-1} eV

Other notable features

- OpenMC allows $S(\alpha, \beta, T)$ tables to apply to some fraction of nuclides
- For multitemperature problems, stochastic interpolation is performed between temperatures
- Support for mixed coherent/incoherent elastic has recently been added to OpenMC

Conclusions

- OpenMC provides automated generation of HDF5-based thermal scattering libraries through the `openmc.data` module
- Implementation of thermal scattering in OpenMC is simplified by adopting same class hierarchy used for other nuclear data
- A novel treatment of incoherent elastic angle distribution faithfully represents original data, avoiding artifacts from NJOY-produced discrete distributions

Acknowledgments

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[1] This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.

Thank you!