Testing and Quality Assurance needs

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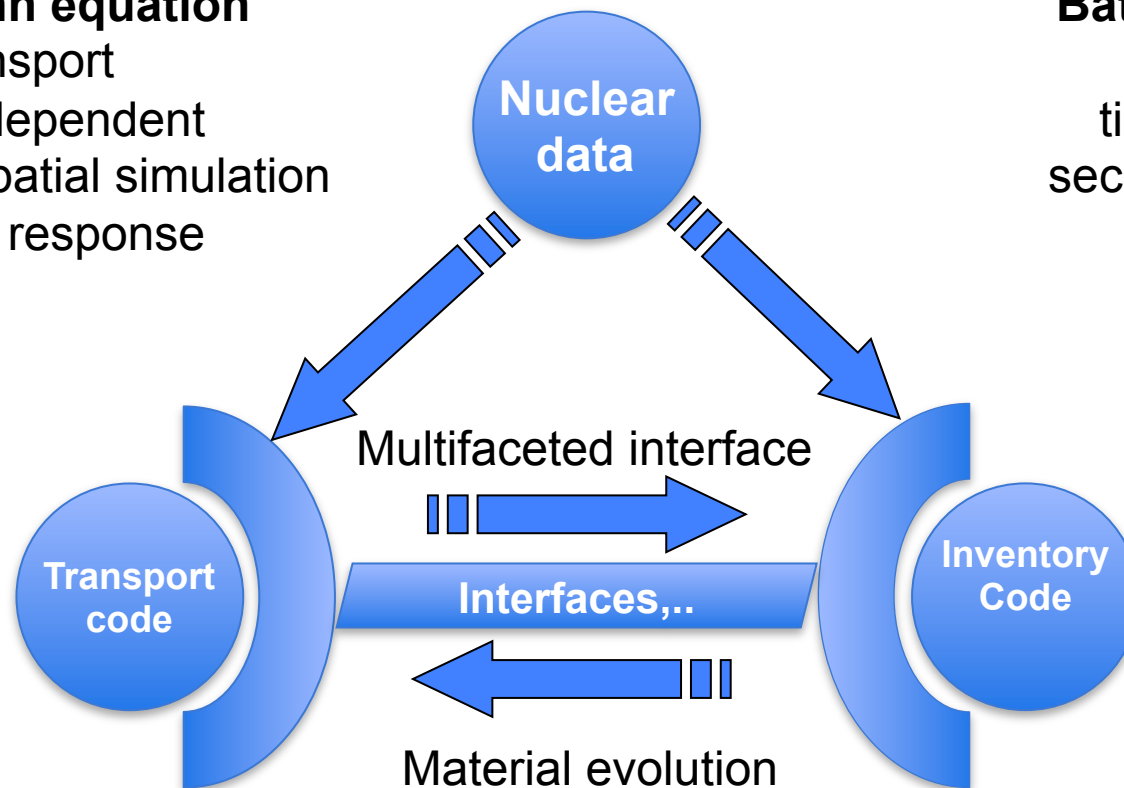
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CCFE is the fusion research arm of the United Kingdom Atomic Energy Authority

Boltzmann equation
transport
time independent
energy and spatial simulation
primary response

Bateman equation
inventory
time dependent
secondary response

Nuclear data

Transport code

Inventory Code

Multifaceted interface

Interfaces,..

Material evolution

Scripted interfaces to connect Boltzmann and Bateman solvers for non-linear t- and T-dependent transport

- to convert evaluations in the Evaluated Nuclear Data Files (ENDF) in ENDF-6 or GND format into form<u>s</u> useful for practical applications

- to pre-process ENDF, GND formatted data, for later, further processing for use in applications

- It is important at that stage to clearly differentiates between raw, evaluated data, data format and nuclear formalisms. The amalgam is been made, sustained, maintained during the ENDF, ENDF/B, ENDF-6 eras

➢ This has to evolve, progress during the GND format frame era

- ENDF-6 format manual: 397 pages !! How many for GND format manual??

- The BNL checker codes have done what they could, but still are failing to pickup trivial errors !! GND will have to be self checking, more robust than ENDF-6

- Many are satisfy when they see and evaluator's plots, e.g. cross section profile at 293K with EXFOR data and a good visual fit on a log-log graph !!

- The file format may be OK, but one still find inconsistent values, ENDF file steadiness never has been on the agenda

- Nobody ever unit test, sample an entire file and look at the results. However, TENDL's fabric show the way

- Unit (drawer) test for
    - resonance parameter (e.g. CALENDF's messages,…)
    - physical constants (<u>one</u> consistent numerical value,..)
    - cross sections (against energy, total, partial, macro,…)
    - multiplicity (against incident particle energy range, not only at the thermal fission energy,…
    - emitted spectra (against incident particle energy range,..)
    - angular distribution (complete cover, no more high order numerically instable Legendre polynomials,…)
    - direct derived forms
        » energy grid, temperatures
        » thresholds, normalisation "window"
        » dilutions, self-shielding factors
        » decay data, energy levels and their consistency

- Global (file) test for
  - group matrices
  - variance and covariance existence, coverage, handling, extraction, visualisation
  - energy balance, KERMA, PKA,…
  - ….

- Numerical Monte Carlo and deterministic test
  - single isotope sphere, fluxes and leakage spectra
    - look at the spectra (un-physical features,..)

- It is the responsibility of the evaluator(s) to experience and test the processing steps, look at the results

- the processing code developer have for too long cover for the sloppiness and arrogance of the evaluator
  - Correct the file at the origin, not during the processing steps, i.e. not like JEF-2.3 Pu239 (partial fiss. ≠ total fiss.)

- Output a full set of plots and unit test results from repeatable, open benchmarking steps

- Comment clearly any evolution

- A GND file would only be accepted once vetted by an expert in multi-processing, or a group of "expert, knowledgeable users"

- Not one……not two ….but three processing codes should be used in sequence and in parallel to produce, shape, check and compare the nuclear data
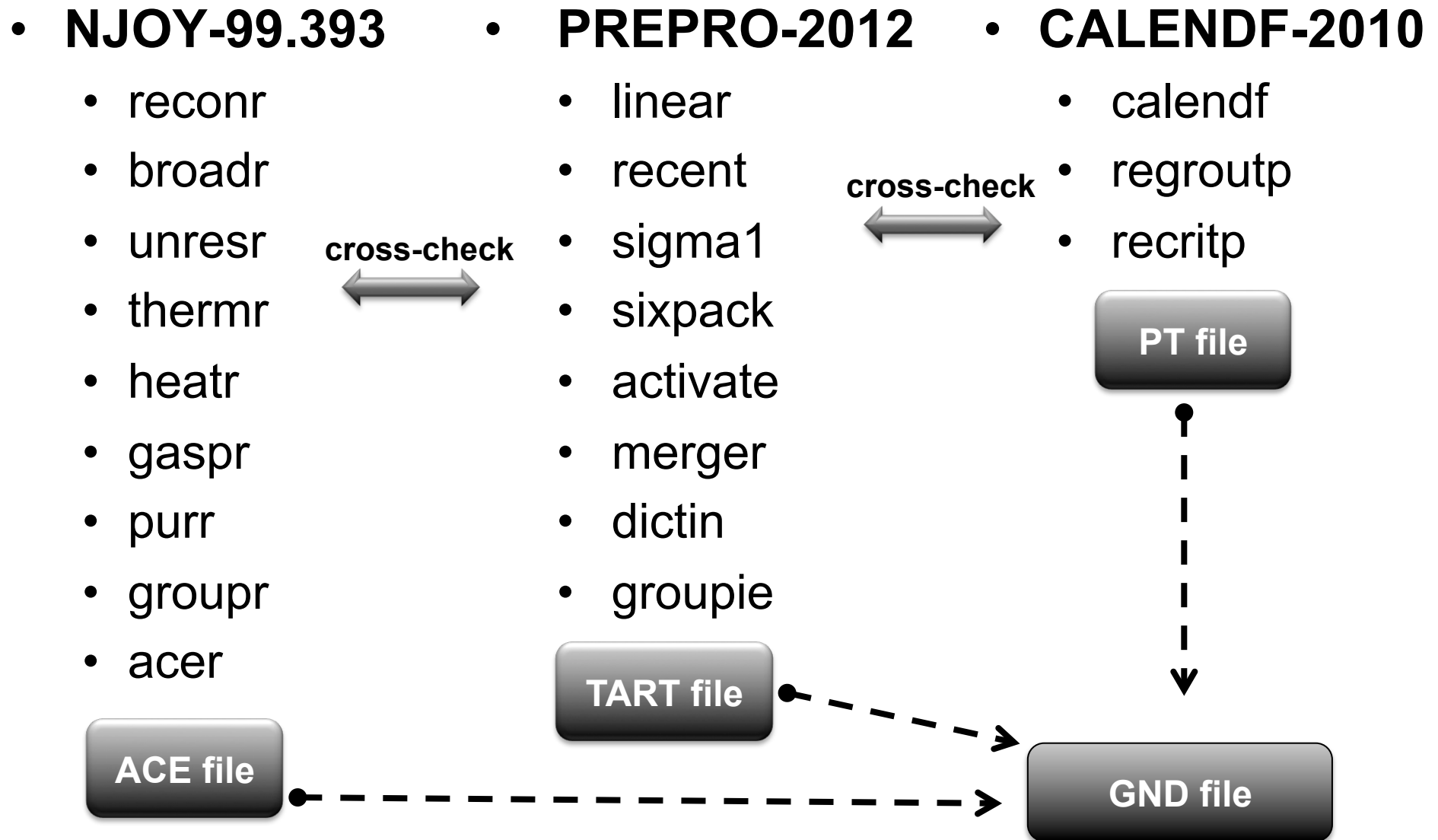
NJOY, PREPRO and CALENDF

Robustness, redundancy, portability, availability, accessibility, repeatability, legacy and maturity
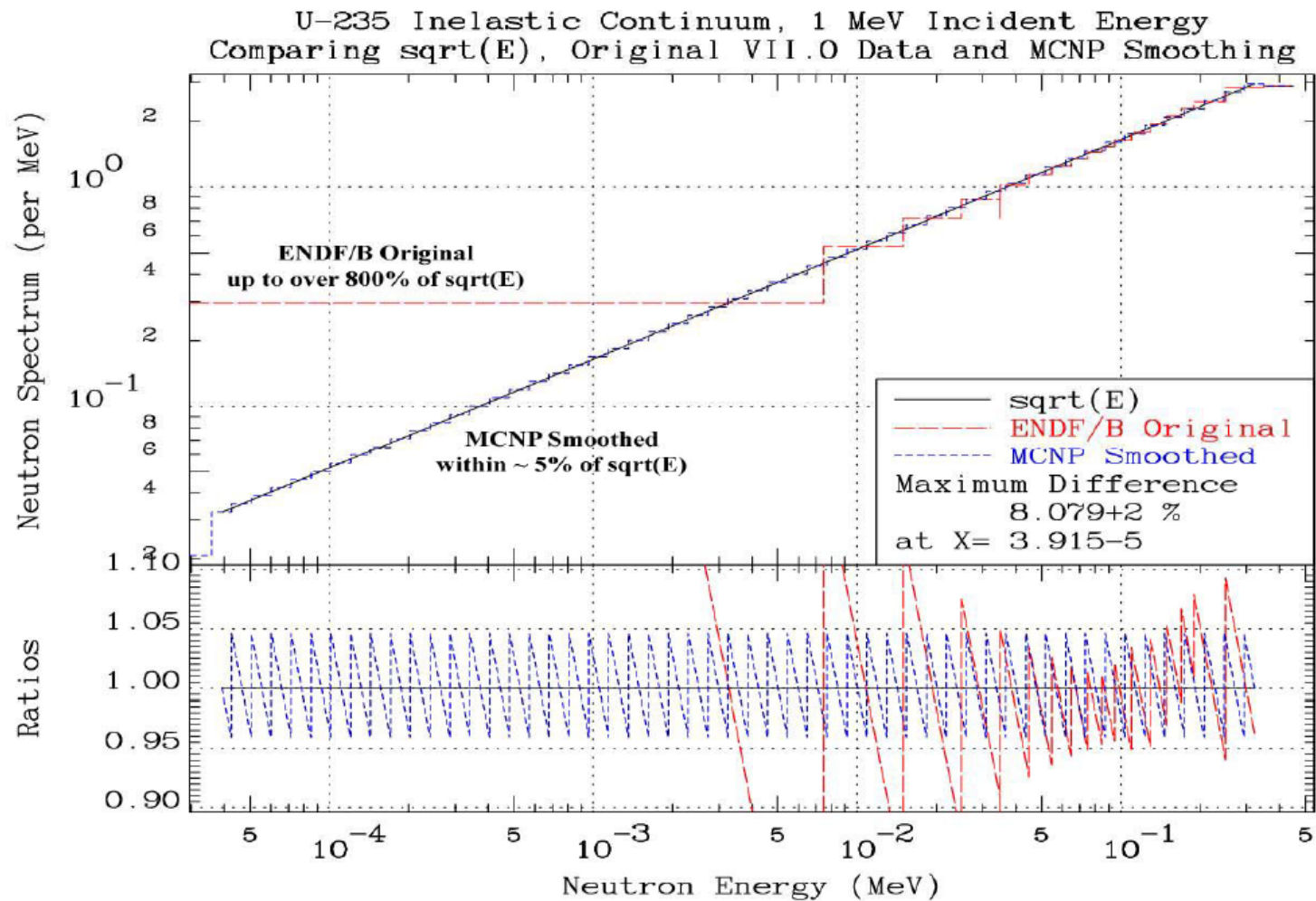
All processing steps cannot be handle by only one or even two of those quite unique processing codes !!!
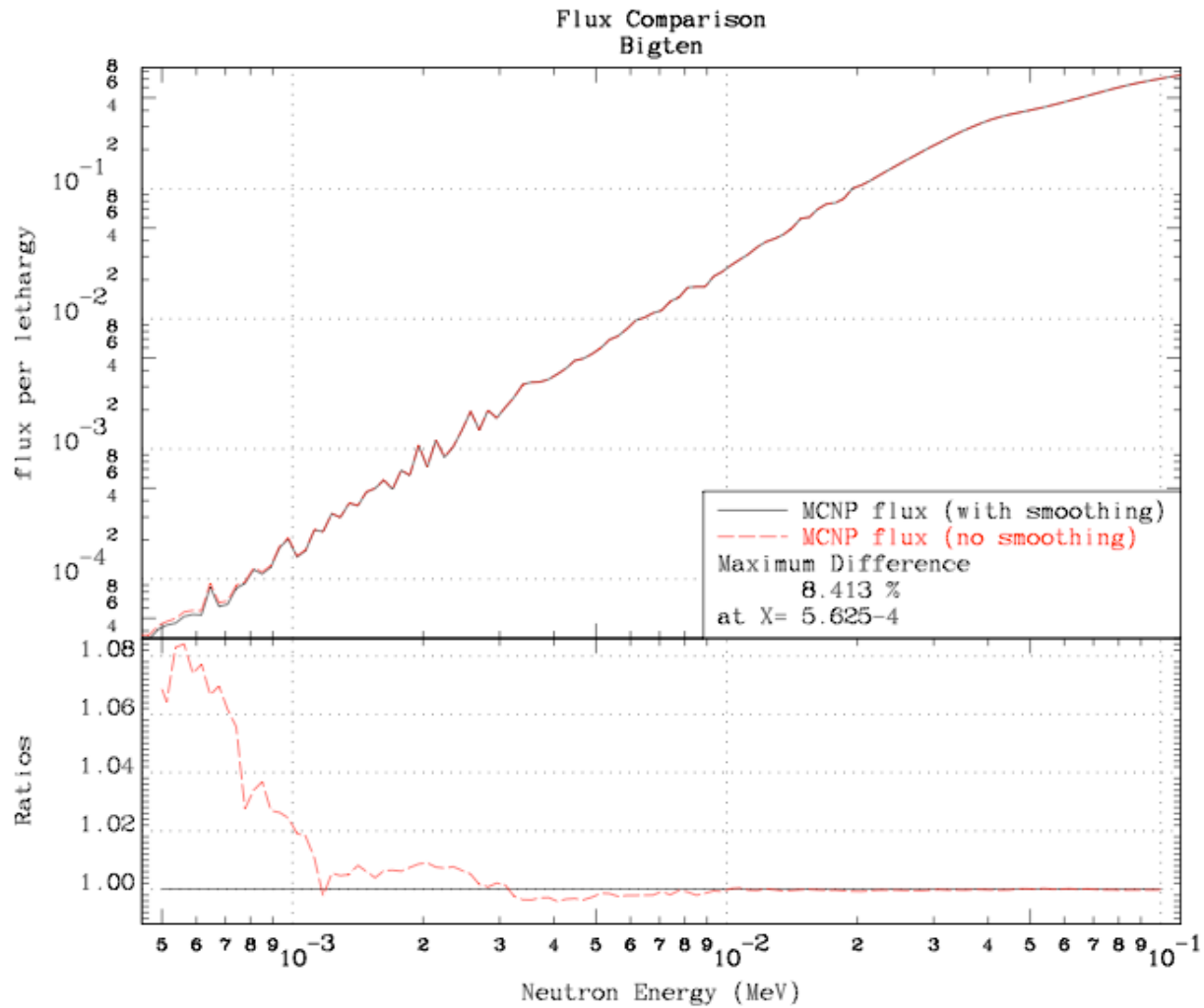
- Monte Carlo pointwise multi-particle, multi-temperature libraries with probability tables in the URR

  - For TRIPOLI-4.9, MCNP6, MCNP5 1.60, MCNPX 2.7.0, SERPENT, MONK, MC21, TART, MERCURY, etc..

- Deterministic groupwise neutron, multi-temperatures, multi-dilutions libraries

  - For CASMO, WIMS, APOLLO, etc..

- Multi-particles groupwise, multi-particles multi-temperature libraries with probability tables in the RR & URR

  - For FISPACT-II, ACAB, CINDER, ORIGEN, etc…

- Transport, activation, astrophysics, medical applications libraries will have to stem from a unique, truly general purpose this time, GND formatted file
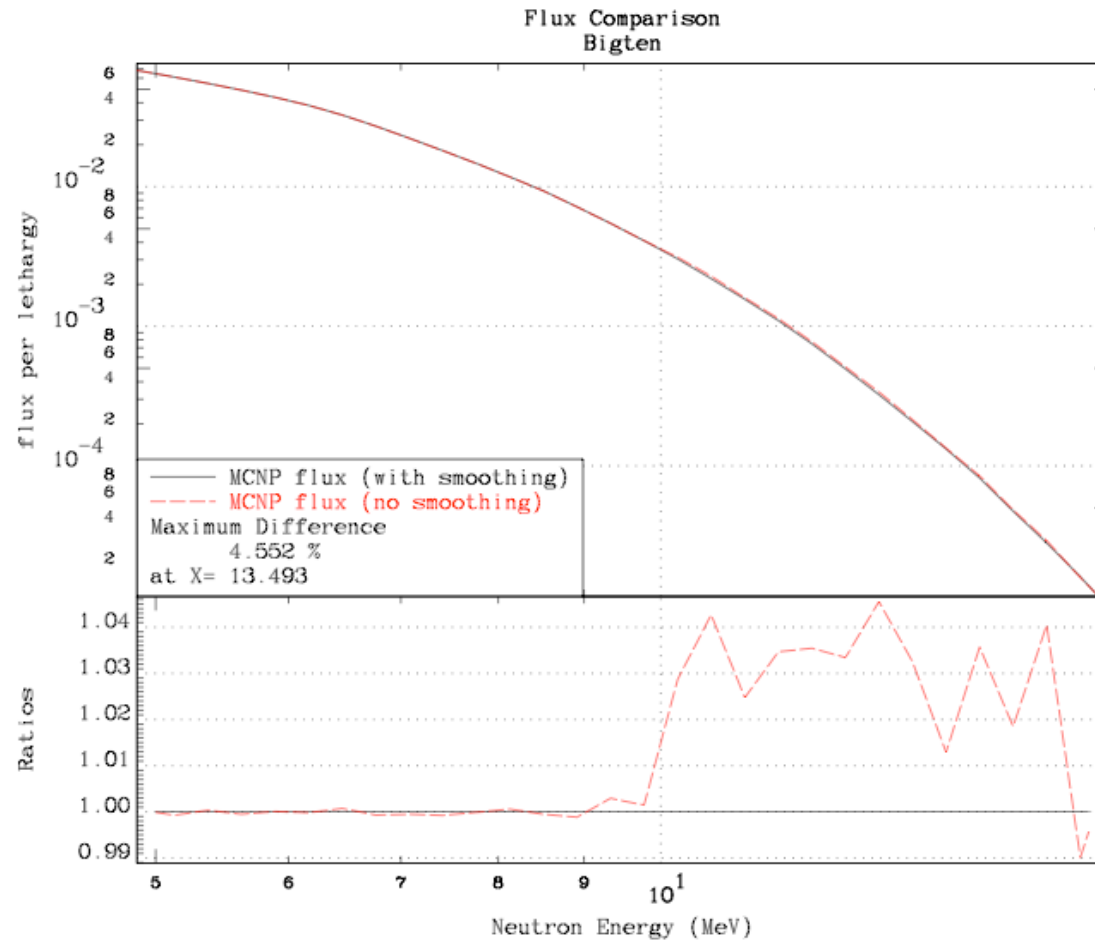
- **NJOY-99.393**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
  - purr
  - groupr
  - acer

- **PREPRO-2012**
  - linear
  - recent
  - sigma1
  - sixpack
  - activate
  - merger
  - dictin
  - groupie

- **CALENDF-2010**
  - calendf
  - regroutp
  - recritp

cross-check (between NJOY-99.393 and PREPRO-2012)

cross-check (between PREPRO-2012 and CALENDF-2010)

PT file

TART file

ACE file

GND file

- The actual processing codes are modular, each having unique capability, provide for specific form<u>s</u>

  - NJOY: heatr, acer

  - PREPRO: sixpack, merger, fixup

  - CALENDF: regroutp, mixisotp, seffnra

- Do not try re-inventing those 'Swiss clock' style wheels, start by making use of the most robust, core modules, but also providing in parallel for an even better future processing steps
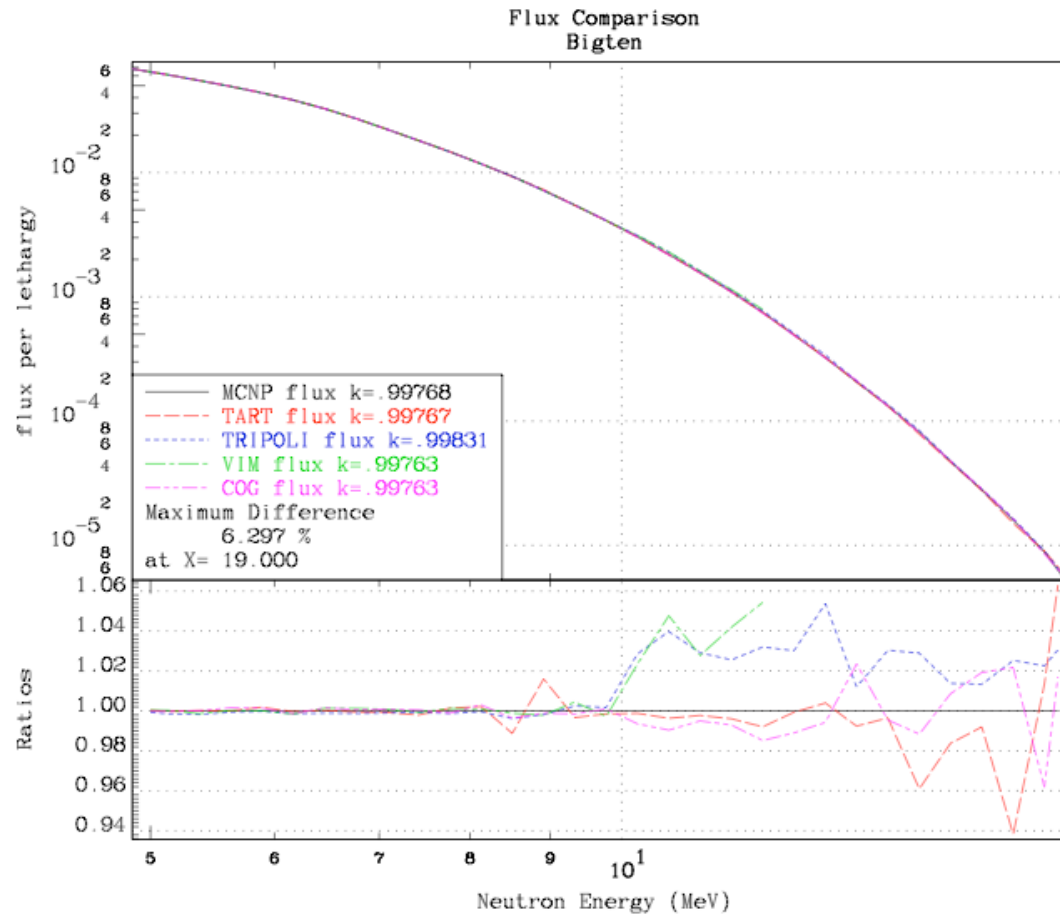
U-235 Inelastic Continuum, 1 MeV Incident Energy
Comparing sqrt(E), Original VII.0 Data and MCNP Smoothing

More important for fusion studies
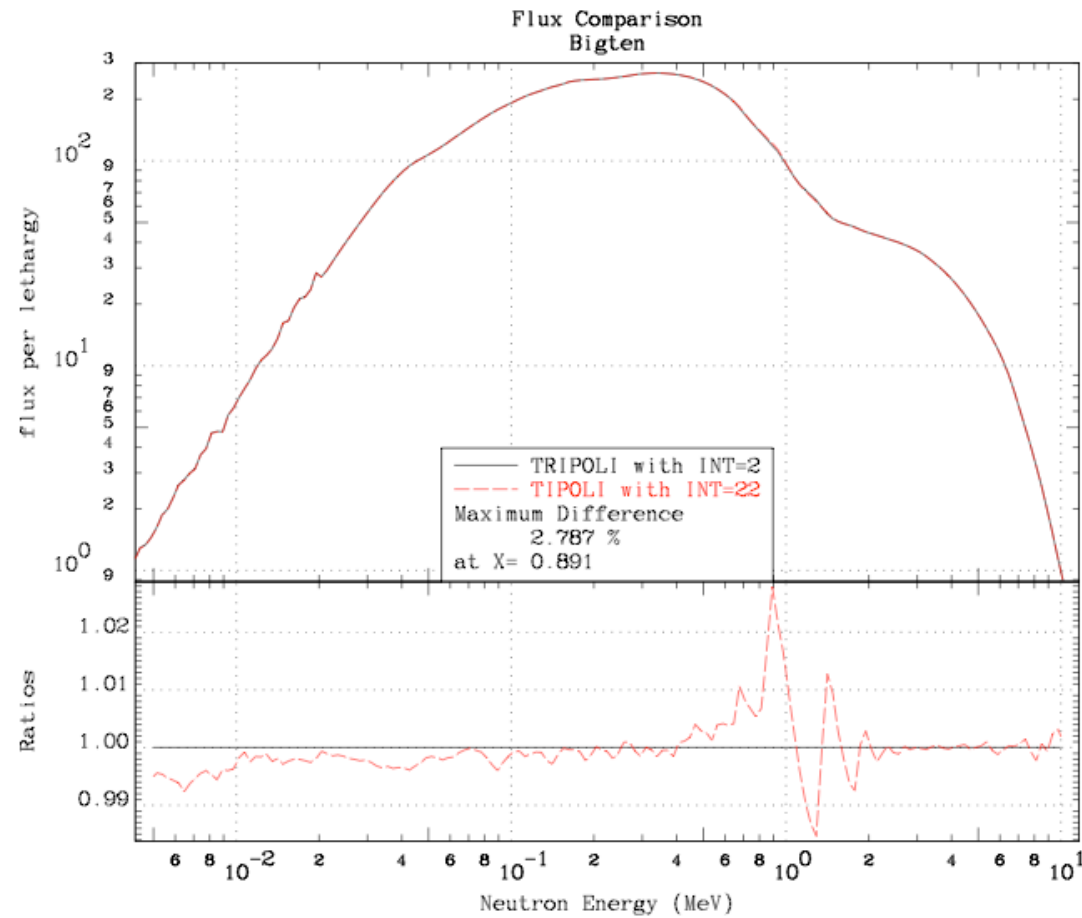
The fusion energy range, 200 KeV grid

Note that MCNP, TART, and COG all use smoothing for the fission spectra above 10 MeV, but TRIPOLI and VIM do not.

Incorrect "INT=2" in U-238 was changed to "INT=22,"

- If you do not Verify and Validate your computer tools, code system, nuclear data, your results are worthless

- If you do not document your V&V work, your results are worthless

- If you do not document your work, you are worthless

- V&V work is absolutely necessary, but not glamorous or fun

- Well-known data, codes, processes must <u>still</u> be validated for your work, nuclear system

Journal publications are not V&V Documents

- are all Doppler broaden files identical ??

- are all dilution levels calculated in the same way ??

- ENDF's interpretation are not unique !!

- emitted particle spectra edge's !!

- above 30 Legendre coefficients !!

➢ We have reached with ENDF-6 the stage where some nuclear data uncertainties may be of the same magnitude of the error one can make in processing or when using reactor physics codes knobs

➢ GND should need to take care of those deviations

- embrace technologies

  - well defined processes, automatic repeatability

  - sturdy programming, reporting, logging

  - open access, redundancy

  - repeatability in testing

  - team work, worldwide !!