Development of software to automate the computational analyses of fusion relevant benchmarks

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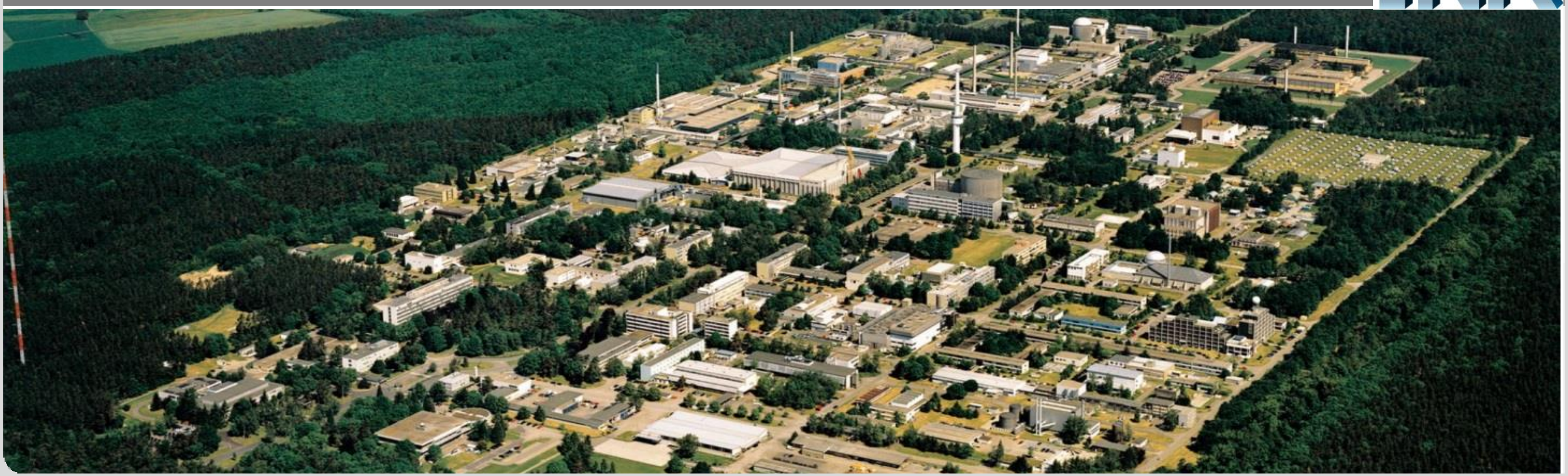


Motivation/Purpose

What do exist now for (quasi) automatic Validation of Evaluated data:

- "DICE/NEA" vs. ≈ hundreds criticality ICSBEP experiments/cases
= *pre-calculated (off-line) single parameter Keff , its sensitivities and comparison with measured ones, …*

- "van der Marck" vs. ≈ dozens Livermore 14 MeV pulsed spheres
= *MCNP on-the-spot calculation of neutron TOF arrays and graphical comparison with measured ones*

- "private scripts/suites" surely do exist …

What we try to implement: procedure which allows to run automatically on-the-spot spectral response (energy array) benchmark calculation sequence:

(i) modification (library selection) of MCNP input deck of experiment,

(ii) MCNP simulation,

(iii) processing of the MCNP output file,

(iv) read-in experimental data and comparison to MCNP calculations,

(v) assessment of evaluated transport data quality employing C/E array and single parameter = chi-squared criterion.

Here it will be demonstrated for the case:
ICSBEP neutron leakage spectra from Fe shell driven by ^{252}Cf(s.f.) source

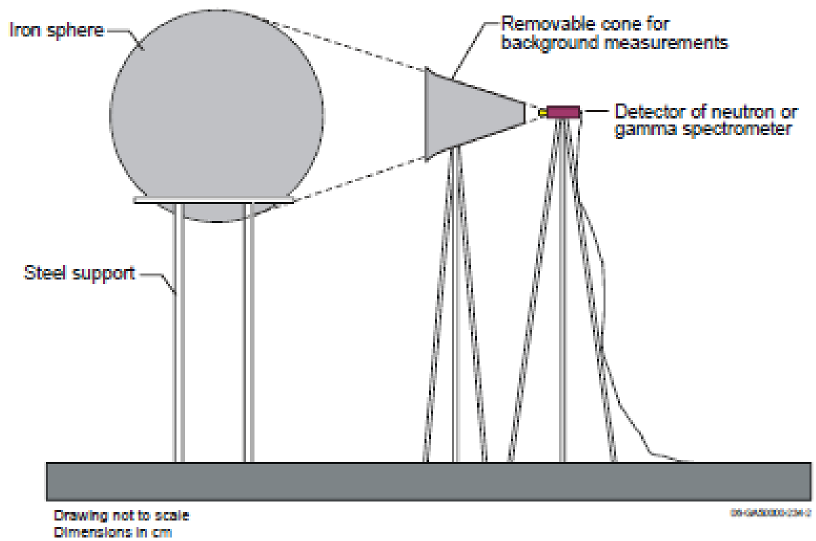
The case: IPPE neutron and γ-ray leakage spectra from six Fe spheres of Ø10, 20, 40, 50, 60, 70 cm with ^{252}Cf(s.f.) in centre

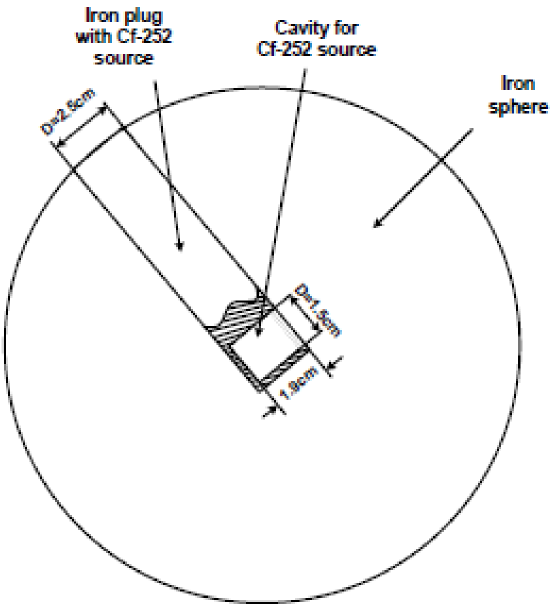
Primary publication: *L.A. Trykov et al., "Experimental Researches of Outflow Spectra of Neutron and Gamma Radiations for Spheres from Iron", Preprint FEI-943, Obninsk, 1979*

ICSBEP Handbook: *G. Manturov et al. (Evaluators), "Neutron and photon leakage spectra from Cf-252 source at centers of six iron spheres of different diameters", ALARM-CF-FE-SHIELD-001, 2006*

<u>IPPE Iron shells experimental lay-out</u>

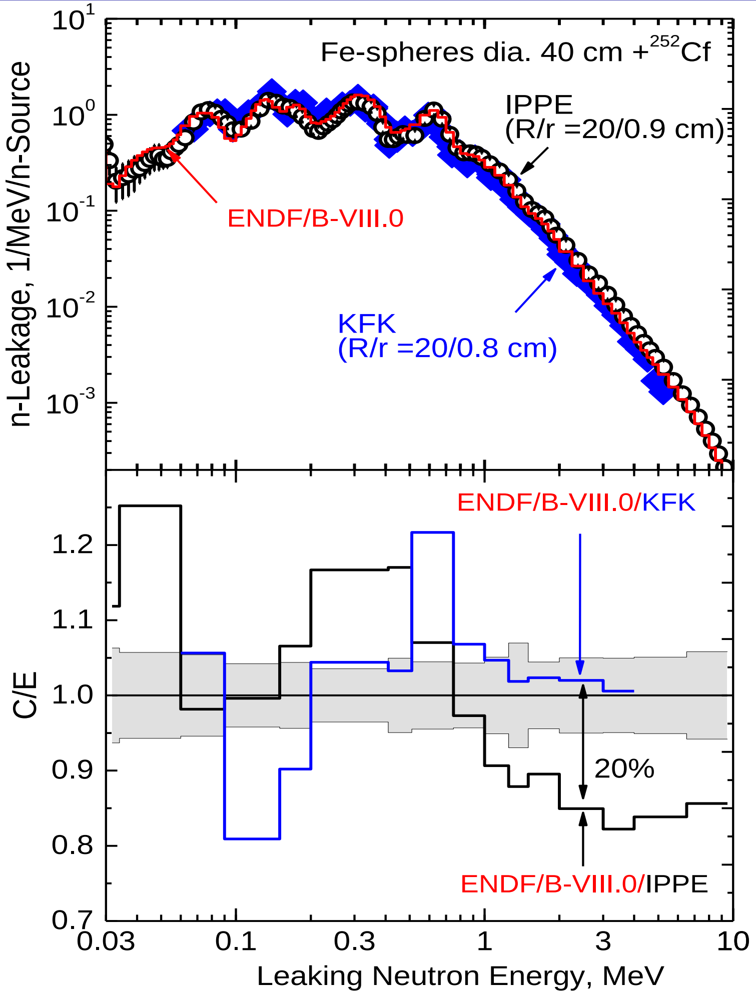
(Shell Diameter and Detector-to-Source distance vary)



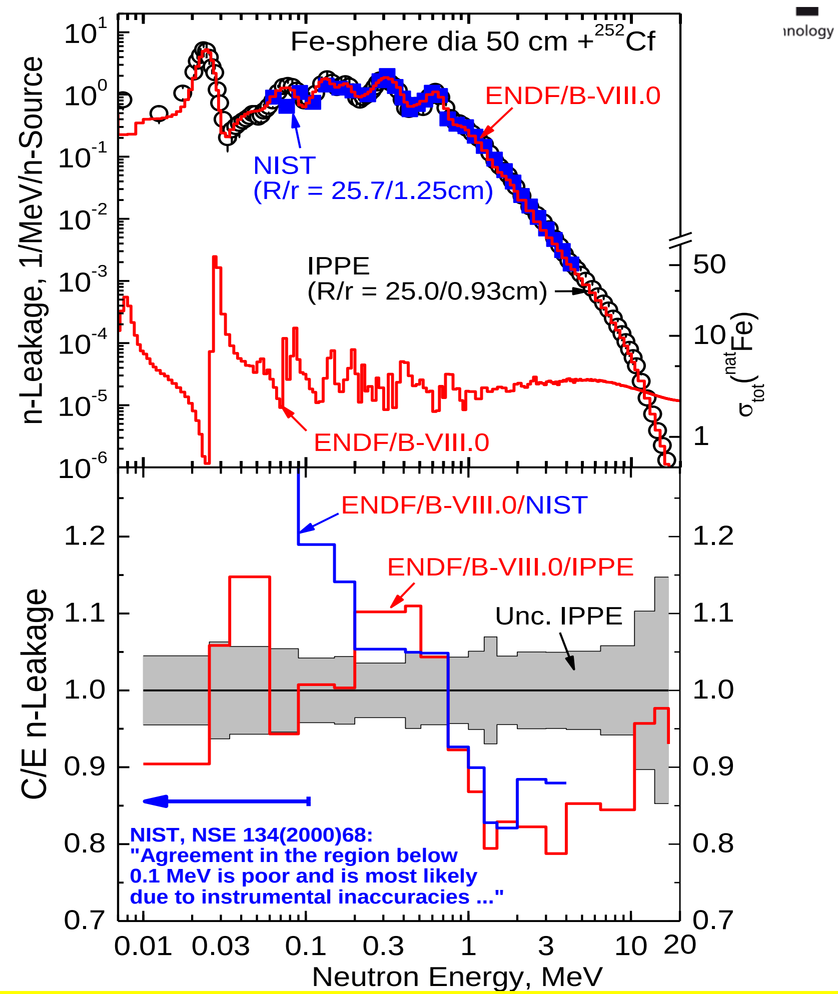


IPPE Fe n-leakage spectra: cp. to KFK, NIST & impact on Validation

Fe shell Ø40cm: IPPE'1985 cp. KFK'1977



Fe shell Ø50cm: IPPE'1985 cp. NIST'2000



Observations/Findings:

- **IPPE experiment covers the largest secondary neutron energy range where it either agrees or not (sometimes the reasons could be found) with other independent experiments**
- **objective 20% underestimation in 1 - 3 MeV since it was also observed by NIST**
  (this was reported in EFFDOC-1342 (2017), IAEA TM Dec 2017 and used to validate ENDF /B-VIII.0 in M.Herman et al. NDS 148(2018)214)

IPPE n-leakage spectra: necessary Modifications of ICSBEP MCNP input prior to use in automatization

The original MCNP input file, given for IPPE experiment in ICSBEP, was modified to allow automation of Validation procedure as following:

(1) Default Material card for All Nuclides (C, Mn, Fe, Cu) was added:

m0 nlib= plib=04c $ setting default n and g libraries for all materials

(2) Elemental Carbon was replaced by ^{12}C and ^{13}C, since main major evaluation libraries have no data for natural carbon:

m1 6012.80c 0.000388870 $ "6000 0.000393076 " was replaced by 0.000393076*0.9893 = 0.000388870

6013.80c 0.000004206 $ isotope 6013 was added 0.000393076*0.0107 = 0.000004206

PS. Obsolete Fröhner' ^{252}Cf(s.f.)PFNS spectrum was replaced by Mannhart' Standard for PFNS plus ENDF/B-VII.1 for delayed (DFNS)

IPPE n-leakage spectra: Linux batch script for automatic substitution of evaluated ACE data, running MCNP & post processing

(1) At first step, User has to select desirable evaluation by ordering the proper ACE files extension: in this example JEFF-3.3 ACE files will be used by MCNP for All nuclides in Iron sphere (C, Mn, Fe, Cu) :

```
echo " 1: ===  selection of ace data from needed library  === "
  ext="03"   #  "80" for ENDF/B-VIII.0    or   "03"  for  JEFF-3.3
```

Linux stream editor *sed* will replace string *"nlib="* by ordered library *"nlib=03c"* and will produce input file *"mcnp.inp"* for MCNP:

```
sed  "s/nlib=/nlib=${ext}c/g"  Trykov_Cf_n  >  mcnp.inp
```

(2) At second step, Linux batch file launches the MCNP code *"mcnp.mpi":*

```
echo " 2: ===  run mcnp  === "
  mpirun  mcnp.mpi   i=mcnp.inp  o=output   m=mctal    x=xsdir
```

Applicable for the further processing is a file *"mctal"*

IPPE neutron leakage spectra: Linux batch script for substitution of Evaluations, running MCNP and post processing (cont.)

(3) At third step, the Fortran code "*read_mctal.f95*" is invoked together with its input file "*read_mctal.inp*" to process MCNP *mctal*:

echo " 3: === run read_mctal read_mctal.inp to process mctal === "

./read_mctal read_mctal.inp

Input file "*read_mctal.inp*":

```
mctal              Name of File mctal produced by MCNP
1.                 Scaling Factor for Tally, Fn  (default = 1.)
0                  Convert in Energy spectrum or keep Grouped, KeyConv (1/0)
0                  Reverse the order of argument array or not, KeyRev  (1/0)
2                  Tally Number, NumTally
Trykov_d50n.dat    Name of File with Experimental Data
2                  No. of Energy columns in Exp. Data file ? (2/1)
2                  Errors type for Exp. Data, Abs/Rel/No  ? (2/1/0)
```

that will produce output file "*read_mctal.res*" with results of "*mctal*" processing, calculation of C/E array = comparison with experim. "*Trykov_d50n.dat*" and χ^2.

(4) At last fourth step the Linux script copies "*mctal*" and "*read_mctal.res*" into files labelled with "*ext*" for checking and savings, e.g.: "*mctal_03*" and "*read_mctal_03.res*"

IPPE neutron leakage spectra: Validation Outcome - criterion χ^2

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To qualify the level of agreement we employed the standard metric for testing nuclear data libraries - the "reduced" chi-squared:

$$\chi^2 = \frac{1}{n}\sum_{i=1}^{n}\frac{\left({C_i}/{E_i} - 1\right)^2}{\sigma_i^2}$$

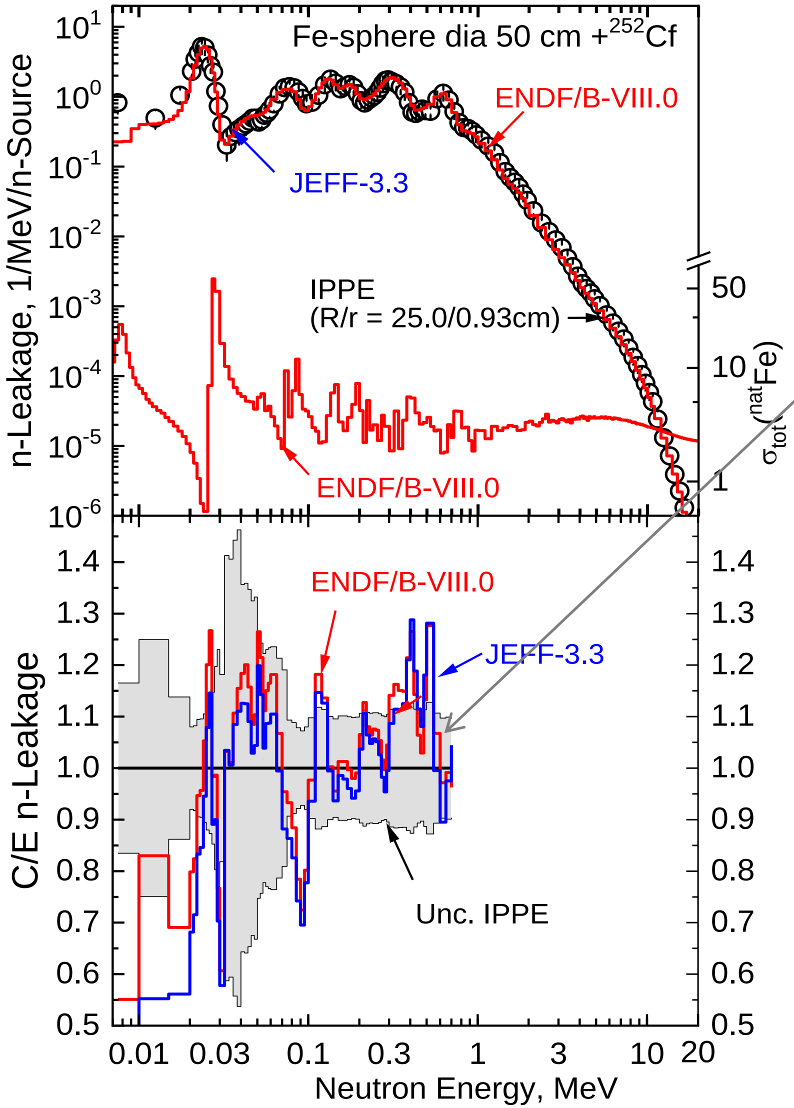
where calculated C_i and experimental E_i arrays are compared with 1, mediated by experimental uncertainty σ_i (MC statistics is small)
Degree of freedom, n, is considered to be equal to number of Energy bins in experimental and calculated neutron leakage spectra.

For present validation example (Fe sphere Ø50cm), χ^2 turns out to be 2 times lower for ENDF/B-VIII.0 than for JEFF.3.3, thus confirming better quality of ENDF/B-VIII.0 evaluation for Fe isotopes:

Library	En range, MeV	No. of Points	χ^2
ENDF/B-VIII.0	0.005 – 0.750	72	2.76
JEFF-3.3	0.005 – 0.750	72	4.18

IPPE neutron leakage spectra: Validation Outcome - C/E array

IPPE Fe shell Ø50cm: Spectra and C/E



Neutron Leakage were measured by:

- H proportional counter in 0.001 - 0.7 MeV

- stilbene scintillator in 0.2 - 17. MeV

and presented in ICSBEP as one n-spectrum

However ICSBEP MCNP model has 2 tallies with different energy range and resolution, which correspond to the two physical detectors

Therefore:

⇒ further modifications of ICSBEP MCNP will be applied to compute χ^2 in the whole energy range

⇒ computing of C/E and χ^2 for the energy intervals wider than experimental bins likely have more sense for validation

Summary/Overlook

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- Example of automatic procedure for shielding benchmark with response as energy array is given:
  User select ACE library, then procedure does routine job itself (modifies MCNP *input*, runs MCNP, reads *mctal*, compares with measured spectra) and reports to User the single parameter χ^2 = quality of Evaluation

- However some adjustment of the MCNP input file archived in ICSBEP is necessary in advance to implement such automation

- Further upgrade of this procedure (adjustment of input files, inclusion of all six IPPE spheres and γ-ray leakage spectra, …) is planed