

LLNL Report for USNDP

Nuclear Data Week, December 2020

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LLNL-PRES-817213

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC



LLNL contributions to USNDP

- 0.25 FTE for \$138k
- Coordinate LLNL nuclear data efforts with CSEWG
- Make, Verify, Validate R-matrix evaluations
 - With IAEA, R-matrix workshops, and GNDS-interchange codes
 - Apply Machine-Learning methods to R-matrix modeling.
- Leverage LLNL programmatic funding to provide evaluations for inclusion in ENDF

FY20 Metrics Table

NSR Compilations	0
EXFOR Compilations	0
XUNDL Compilations	0
ENSDF Evaluations submitted	0
ENDF Evaluations	1 review
Disseminations (in thousands)	5 (approx)
Articles	2
Reports	0
Invited Talks	2

FY20 FTE Table

PhD Permanent	0.20
PhD Temporary	0
Tech. & Admin.	0.05
Grad. Student	0
Total	0.25

\$138k FY21 funding

\$24k FY19 carry over

\$133k FY20 total costs

\$29k rollover into FY21

Activity with Current Funding

- National Coordination
 - Coordinate Nuclear Data Efforts with USNDP/CSEWG
 - Attend USNDP/CSEWG meetings
 - Use R-matrix GNDS tools to translate, verify and improve proposed evaluations
 - R-matrix methods: validate use of Brune basis (now in SAMMY!)
 - CSEWG reviewer of LANL candidate evaluation $n+{}^6\text{Li}$ (not yet complete).
- International Coordination
 - One of organizers of “R-matrix Workshop on Methods and Applications”
 - Online in 2020
 - Planning for Ohio in June 2021.
 - On organizing committee for ND2022 in Sacramento, CA.
 - Continuing INDEN work of light-ion neutron models
 - Projects underway for new evaluations $n+{}^9\text{Be}$, $n+{}^{14}\text{N}$, $n+{}^{15}\text{N}$, $n+{}^{23}\text{Na}$.
- Provide LLNL evaluations for ENDF
 - USNDP funds the translation over to ENDF
 - Support LLNL reports on TPC and actinide evaluations for CSEWG (Rob Hoffman, Gregory Potel).

RFLOW

a code using GNDS parameters with EXFOR data

- Code **Rflow** to read R-matrix parameters from a GNDS file (i.e. from any modern R-matrix code, using Ferdinand.py). For neutrons as well as charged particles.
- Calculate χ^2 for all given data
- Tensorflow used on GPUs for fast ‘tensors’: multidim arrays.
- Tensorflow, can given a function yielding chisq, automatically calculate gradients by

```
return(chisq, tf.gradients(chisq, searchpars) )
```
- Then search for χ^2 for minimum using ML optimizers, and produce parameter covariance matrix with positive eigenvalues.
- A variant can be used for pointwise reconstruction of cross-sections on given energy & angle grids. Useful in making statistical instances for gathering URR statistics

R-matrix representation in GNDS

- Using and checking LLNL changes in GNDS formulations.
- Eg. use `.ComputerCodes` module to store data normalizations for fast replication of data fits.
- Encouraging facility for future developments:
 - Brune parameters for R-matrix fits.
 - Overlapping R-matrix and statistical sections (to use 'optical R-matrix' method I proposed at CNR18 meeting to go to higher energies.