IDataLib: INFN Data Library

Maria Grazia Pia, Paolo Saracco

Preventivi INFN 2019
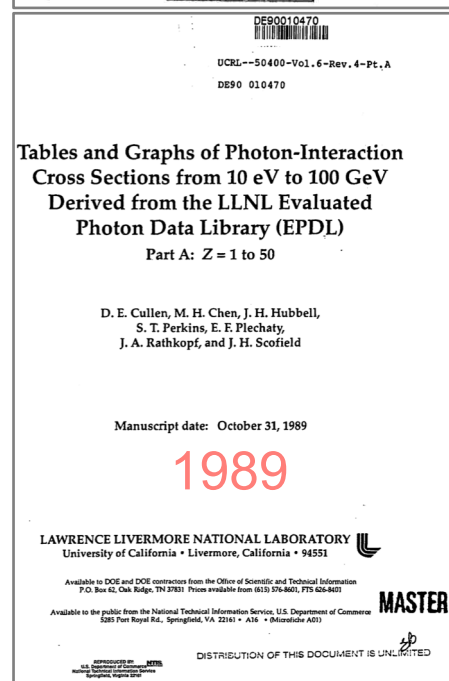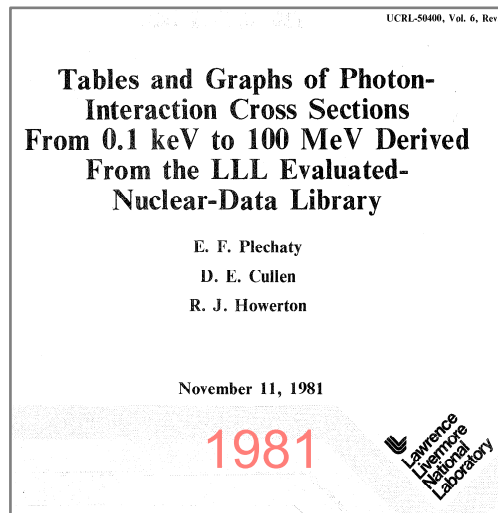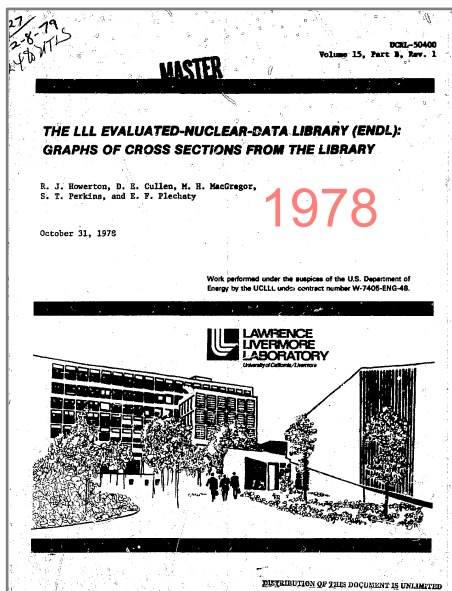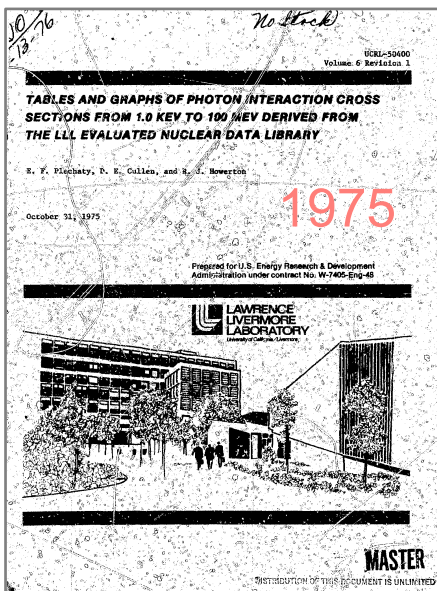
Genova, 1 luglio 2019

Evaluated data libraries

- Tabulations of physics quantities: cross sections, nuclear and atomic parameters, secondary particle spectra…

- Derive from the evaluation of the body of knowledge of **theoretical** computations, **experimental** measurements *or both*

- **Essential tool** for Monte Carlo particle transport, experimental physics and engineering applications

- Created and maintained as **national strategic projects**:
    - BROND *(Russian Evaluated Neutron Data Library):* Russia
    - CENDL *(Chinese Evaluated Nuclear Data Library):* China
    - ENDF/B *(Evaluated Nuclear Data File):* USA
    - JEFF *(Joint Evaluated Fission and Fusion File):* France
    - JENDL *(Japanese Evaluated Nuclear Data Library):* Japan

- Proprietary and personal compilations *(usually of specialized scope)*

EGS, FLUKA, Geant4, MCNP, Penelope, PHITS…

Evaluated Atomic Libraries

- **EADL** (atomic)   **1991**
- **EEDL** (electron)   **1991**
- **EPDL** (photon)   **1997**

1966

TID-4500, UC-34,
Physics

CFSTI PRICES

H.C. $3.00; MN .65

Lawrence Radiation Laboratory
UNIVERSITY OF CALIFORNIA
LIVERMORE

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

UCRL-50178

PHOTON CROSS SECTIONS 1.0 keV TO 15.0 MeV

Ernest F. Plechaty
John R. Terrall

September 20, 1966

Lawrence Radiation Laboratory
UNIVERSITY OF CALIFORNIA
LIVERMORE

UCRL-50400 Vol. VI

PHOTON CROSS SECTIONS
1 keV TO 100 MeV

Ernest F. Plechaty
John R. Terrall

October 22, 1968

1968

MP 310:7-184

Siemens AG
ZFE GR FID B
Fachbibliothek
Postfach 3240
Erlangen

8. 10. 89
Von der
UB/TIB Hannover
übernommen

UB/TI
118 93

1975

UCRL-50400
Volume 6 Revision 1

TABLES AND GRAPHS OF PHOTON INTERACTION CROSS SECTIONS FROM 1.0 KEV TO 100 MEV DERIVED FROM THE LLL EVALUATED NUCLEAR DATA LIBRARY

E. F. Plechaty, D. E. Cullen, and R. J. Howerton

October 31, 1975

Prepared for U.S. Energy Research & Development Administration under contract No. W-7405-Eng-48.

LAWRENCE LIVERMORE LABORATORY
University of California/Livermore

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

1978

UCRL-50400
Volume 15, Part B, Rev. 1

MASTER

THE LLL EVALUATED-NUCLEAR-DATA LIBRARY (ENDL):
GRAPHS OF CROSS SECTIONS FROM THE LIBRARY

R. J. Howerton, D. E. Cullen, M. H. MacGregor,
S. T. Perkins, and E. F. Plechaty

October 31, 1978

Work performed under the auspices of the U.S. Department of Energy by the UCLLL under contract number W-7405-ENG-48.

LAWRENCE LIVERMORE LABORATORY
University of California/Livermore

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

UCRL-50400, Vol. 6, Rev. 3

Tables and Graphs of Photon-Interaction Cross Sections From 0.1 keV to 100 MeV Derived From the LLL Evaluated-Nuclear-Data Library

E. F. Plechaty
D. E. Cullen
R. J. Howerton

November 11, 1981

1981

Lawrence National Laboratory

DE90010470

UCRL--50400-Vol.6-Rev.4-Pt.A

DE90 010470

Tables and Graphs of Photon-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Photon Data Library (EPDL)
Part A: Z = 1 to 50

D. E. Cullen, M. H. Chen, J. H. Hubbell,
S. T. Perkins, E. F. Plechaty,
J. A. Rathkopf, and J. H. Scofield

Manuscript date: October 31, 1989

1989

LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California • Livermore, California • 94551

Available to DOE and DOE contractors from the Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831 Prices available from (615) 576-8401, FTS 626-8401

Available to the public from the National Technical Information Service, U.S. Department of Commerce
5285 Port Royal Rd., Springfield, VA 22161 • A16 • (Microfiche A01)

MASTER

REPRODUCED BY
U.S. Department of Commerce
National Technical Information Service
Springfield, Virginia 22161

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

- **Originally released by LLL/LLNL**
- Released in **ENDF/B** since version **VI.8**
- *Currently in the hands of a LLNL retiree*

Formats:
ENDL
ENDF

The world changes… 1991/1997 ⟶ 2018

- Kissel's S-matrix calculations of photon elastic scattering
- Electron ionisation cross sections (Deutsch-Märk, Kim-Rudd, Bote-Salvat…)
- Scofield's Hartree-Fock calculations of atomic parameters
- Effects of theoretical/experimental atomic binding energies
- Salvat's electron elastic scattering calculations
- Photoelectric cross sections, relativistic scattering functions etc.

EPICS2017
Released in January 2018 by IAEA
Released in February 2018 in ENDF/B-VIII.0

2268   IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 65, NO. 8, AUGUST 2018

First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries

Min Cheol Han, Maria Grazia Pia, Paolo Saracco, and Tullio Basaglia

Physics   Software engineering

e.g. does not conserve energy!   e.g. changes w/o version control

References

- M. C. Han et al., First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries, *IEEE Trans. Nucl. Sci.,* vol. 63, no. 8, pp. 2268-2278, 2018.
- T. Basaglia et al., Validation of Shell Ionization Cross Sections for Monte Carlo Electron Transport, *IEEE Trans. Nucl. Sci.,* vol. 63, no. 8, pp. 2279-2302, 2018.
- M. C. Han et al., "Validation of Cross Sections for Monte Carlo Simulation of the Photoelectric Effect", *IEEE Trans. Nucl. Sci.*, vol. 63, no. 2, pp. 1117–1146, 2016.
- M. Batič, et al., "Photon elastic scattering simulation: validation and improvements to Geant4", *IEEE Trans. Nucl. Sci.*, vol. 59, no. 4, pp. 1636–1664, 2012.
- H. Seo et al., "Ionization cross sections for low energy electron transport", *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3219–3245, 2011.
- M. G. Pia et al., "Evaluation of atomic electron binding energies for Monte Carlo particle transport", *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3246–3268, 2011.
- M. G. Pia et al., "Validation of K and L shell radiative transition probability calculations", *IEEE Trans. Nucl. Sci.,* vol. 56, no. 6, pp. 3650–3661, 2009.
- S. Guatelli et al., "Validation of Geant4 Atomic Relaxation against the NIST Physical Reference Data", *IEEE Trans. Nucl. Sci.,* vol. 54, no. 3, pp. 594-603, 2007.
- G. Weidenspointner et al., "Validation of Compton Scattering Monte Carlo Simulation Models", *Proc. IEEE Nucl. Sci. Symp.,* 2013.
- M. Begalli et al., "Validation of Geant4 Electron Pair Production by Photons", *Proc. IEEE Nucl. Sci. Symp.,* 2013.

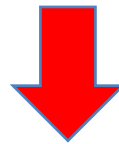etc.

What's next?

WANDA

Workshop for Applied Nuclear Data Activities
DOE strategic workshop
Washington DC, January 22-24, 2019
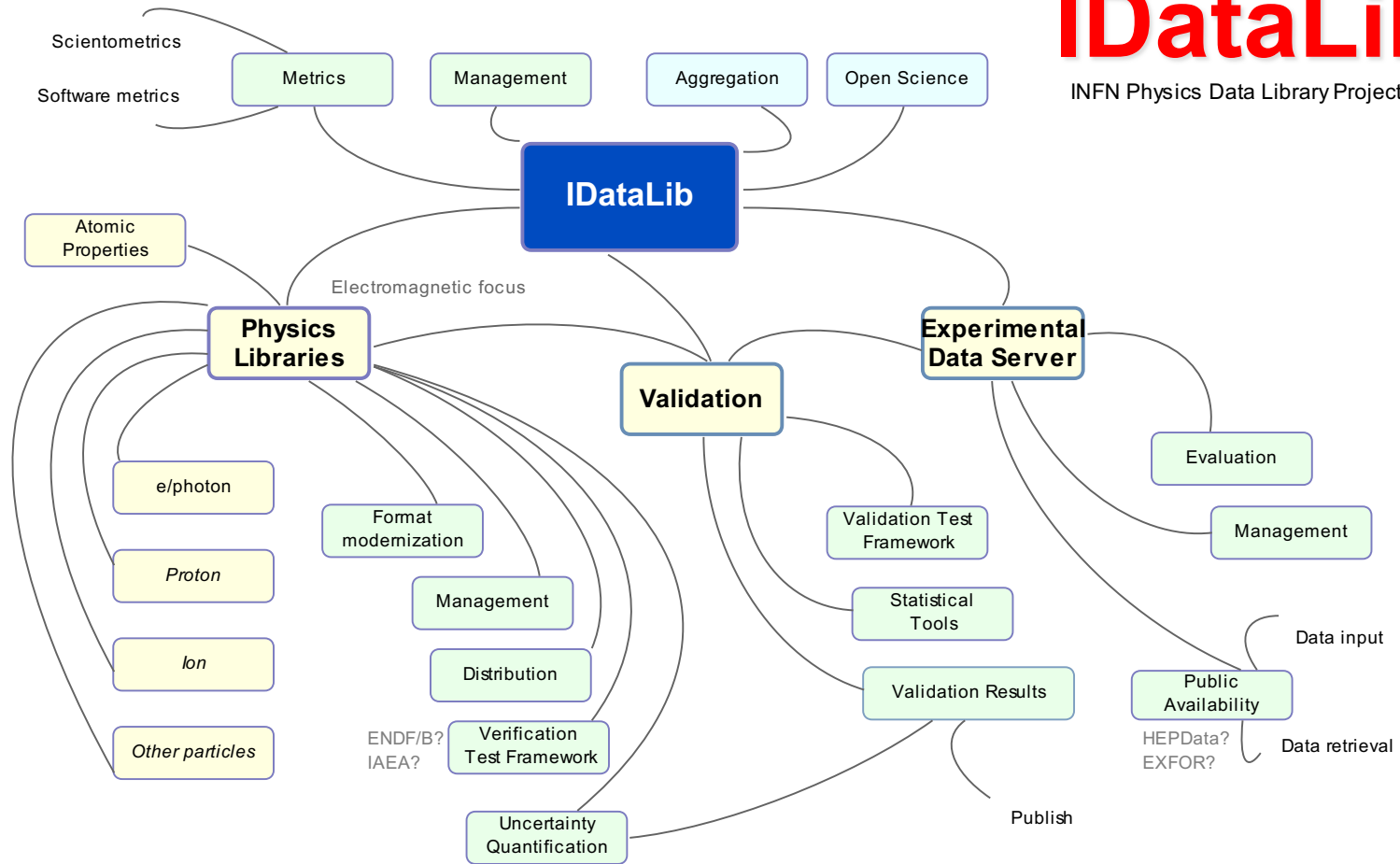

International cooperation
is necessary to address the wide and complex needs of atomic data for Monte Carlo simulation *(i.e. for nearly all basic and applied experimental nuclear/particle/astro/medical physics), for experimental and industrial applications*

Workshop on Open Physics Data Libraries, IEEE Nucl. Sci. Symp., Manchester, Oct. 2019
Chairs: D. Brown, MGP

2020: WANDA, IEEE NSS…

IDataLib

IDataLib

INFN Physics Data Library Project

Scientometrics

Software metrics

Metrics · **Management** · **Aggregation** · **Open Science**

IDataLib

Atomic Properties

Electromagnetic focus

Physics Libraries · **Validation** · **Experimental Data Server**

e/photon

Proton

Ion

Other particles

Format modernization

Management

Distribution

Verification Test Framework

ENDF/B? IAEA?

Uncertainty Quantification

Validation Test Framework

Statistical Tools

Validation Results

Publish

Evaluation

Management

Public Availability

Data input

Data retrieval

HEPData? EXFOR?

Innovation: validation process embedded in data library

| **UQ** Ongoing R&D | **Metrics** QA Scientometrics | **Aggregation** Experimental communities and theoretical expertise | **Open Science** *not yet involved in physics data libraries* |

Maria Grazia Pia, INFN Genova

7

2020 research program

## Define and document the process
- Disciplines, development cycles, phases, iterations
- Work products
- Tools

EADL/EEDL/EPDL: coordinate consistent release with ENDF/B

Verification test framework: *1st cycle*
- *Configuration and change management*
- *Requirements*
- *Analysis and design*
- *Implementation*
- *Test*
- *Deployment (prototype)*
- *Continuous integration*
- *Quality metrics and related analysis*
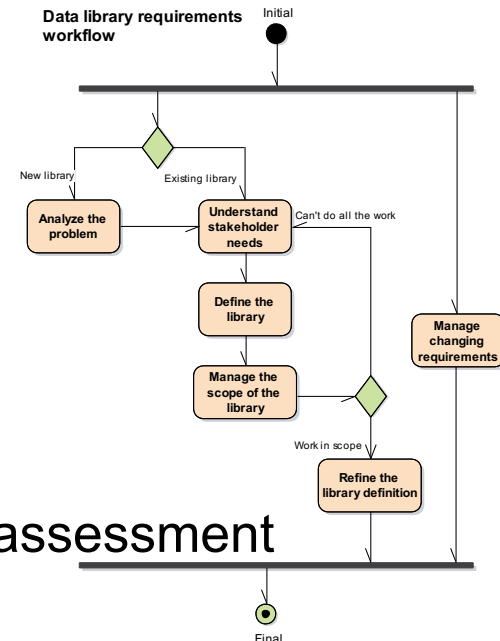
Physics requirements: elicitation, in EA model, assessment
Validation test
Compton scattering cross section OR e+e- production total cross section

Partecipazione, finanze e servizi

Partecipazione
ex CCR-UQ: M.G. Pia [1], P. Saracco [0.4] (Genova), E. Ronchieri (CNAF)
Contatti in corso: LNGS, Trieste
Nucleo inizialmente piccolo, prevista espansione quando l'attività sarà avviata
Multidisciplinare: teorici, sperimentali, informatici
Collaborazione con ENDF/B (DOE) *(+NEA, IAEA, EXFOR, HEPData…)*

Richieste finanziarie "ordinarie":
Workstations di sviluppo, Mac per analisi, storage di dati, missioni per contatti nazionali e internazionali, consumo informatico e metabolico
Nodi e storage di farm: sostituzione di materiale obsoleto
Richieste per Experimental Data Server: quando sarà progettato
Risorse umane: assegnisti/borsisti/studenti

Richieste per i **servizi di sezione**: nessuna
Ringraziamo il Servizio Calcolo per l'ordinario supporto degli utenti e delle attività della sezione