60 Years

IAEA Atoms for Peace and Development

Progress on the development of gmapy

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Outline

- GMA(P) and its long history
- Reasons for the creation of gmapy
- Two operating modes: scipy.sparse or TensorFlow
- Implementation progress of agreed actions:
  - Renormalization of PFNS spectra and covariance matrices
  - Use of several spectra (e.g., ^{252}Cf(s.f) and ^{235}U(n_{th},f))
  - Modern readable format for GMA database
  - USU estimation
- Concluding remarks

The birth of GMA

A "Generalized Least Squares Method" developed by W. P. Poenitz

BNL-NCS-51363 VOL. I OF II
DOE/NDC 23
NEANDC(US)-209
INDC(USA)-85
UC-80 -
(General Reactor Technology - TIC-4500)

PROCEEDINGS OF THE CONFERENCE ON NUCLEAR DATA EVALUATION METHODS AND PROCEDURES

HELD AT
BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973
September 22-25, 1980

Conference Chairman:
R.J. Howerton
Lawrence Livermore National Laboratory

Proceedings Editors:
B.A. Magurno and S. Pearlstein
Brookhaven National Laboratory

March 1981

DATA INTERPRETATION, OBJECTIVE EVALUATION PROCEDURES AND MATHEMATICAL TECHNIQUES FOR THE EVALUATION OF ENERGY-DEPENDENT RATIO, SHAPE AND CROSS SECTION DATA*

W. P. Poenitz

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9700 South Cass Avenue
Argonne, Illinois 60439 USA.

ABSTRACT

The evaluation of several energy-dependent cross sections which are of importance for practical applications is considered. The evaluation process is defined as the procedure which is used to derive the best knowledge of these cross sections based on the available direct experimental data information, and, using theoretical models, on the auxiliary data base. The experimental data base represents a multiple overdetermination of the unknown cross sections with various correlations between the measured values. Obtaining the least-squares estimator is considered as the standard mathematical procedure to derive a consistent set of evaluated cross section values. Various approximations made in order to avoid the monstrous system of normal equations are considered and the feasibility of the exact solution is demonstrated. The variance - covariance of the result, its reliability and the improvements obtained in iterative steps are discussed. Finally, the inclusion of auxiliary, supplementary information is considered.

https://nds.iaea.org/standards/Reports/extract-from-indc-usa-85.pdf

GMA + PPP correction → GMAP

NUCLEAR DATA AND MEASUREMENTS SERIES

ANL/NDM-121

A Suggested Procedure for Resolving an Anomaly in Least-Squares Data Analysis Known as "Peelle's Pertinent Puzzle" and the General Implications for Nuclear Data Evaluation

by

Satoshi Chiba and Donald L. Smith

September 1991

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS 60439, U.S.A.

https://nds.iaea.org/standards/Reports/ANL-NDM-121.pdf

Update of GMA Code to Solve the PPP Problem (Technically)

D.L. Smith* and **V.G. Pronyaev**

Nuclear Data Section, IAEA, Vienna

*IAEA consultant

25 November 2003

The GMA code has been updated to introduce the Chiba-Smith option (see report ANL/NDM-121, 1991) to address the problem of PPP. To avoid confusion, we will refer to this code, and results obtained using it, as GMAP. This code revision was accomplished with a minimum of intervention to the original version of GMA in order to avoid introducing coding errors. The Chiba-Smith approach was implemented by means of simple renormalization of the experimental absolute errors (square roots of the variances) after

https://nds.iaea.org/standards/Reports/Min-Max-PPP.pdf

GMAP Features

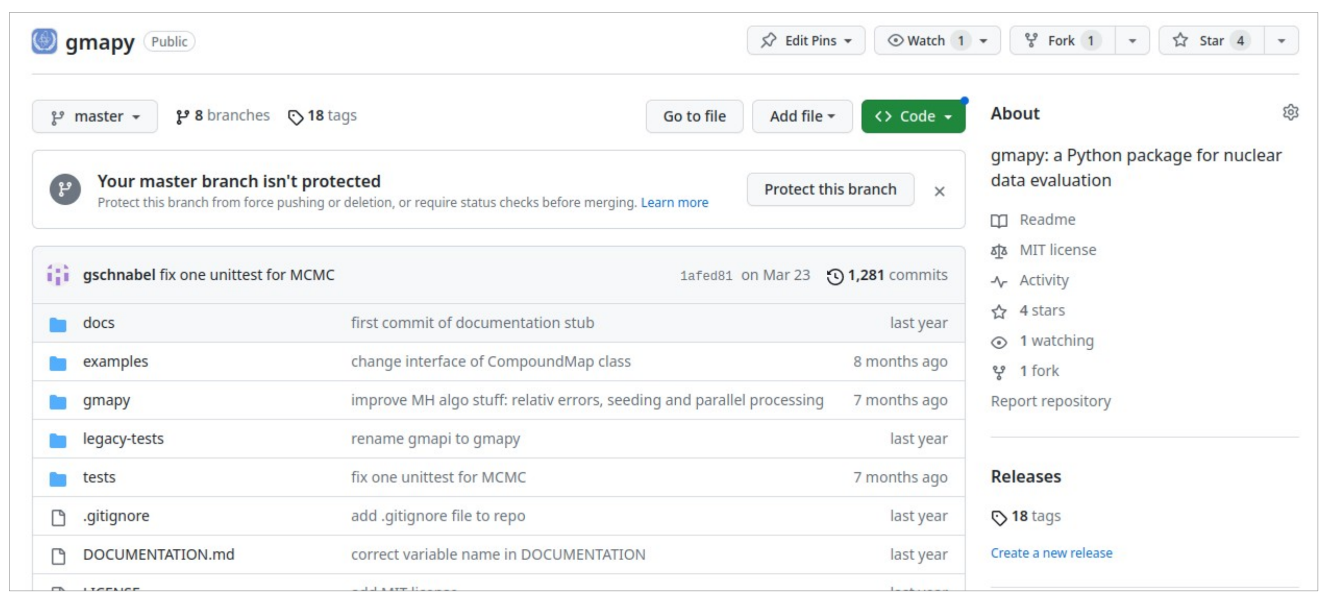
- Written in Fortran-77
- Two modes of inference:
  - Generalized Least Squares (GLS)
  - Iterative GLS scheme (to address PPP)
- Reads in comprehensive GMA database !

Why modernize?

- It's difficult to extend GMAP (with confidence)
- Fortran for high-performance computing and not data analysis
- Popular package ecosystems (e.g. of Python) not usable
- GMA database a treasure of information yet not easily accessible
- Only way to easily "analyze" data is GLS via GMA

gmapy

- Python package backwards-compatible with GMAP
- Many verification & validation tests to prove that
- Many limitations of GMAP removed
- Flexible and advanced inference algorithms beyond GLS
- Design and modularity facilitate extensions
- On GitHub at https://github.com/iaea-nds/gmapy



Two operating modes: scipy.sparse versus Tensorflow

SciPy

TensorFlow

Implementation of Action: Spectrum and Covariance Renormalization

$$\phi'(E) = N\phi(E)$$

Prior covariance matrix imposed on unnormalized and discretized Φ(E)

$$\vec{\phi} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$

Spectrum normalization performed during propagation, e.g.,

$$\mathrm{SACS} = \frac{1}{\sum_i \phi_i} \sum_i \omega_i \phi_i \sigma_i$$

Implementation of Action: Possibility of Several Spectra

- Motivation: Make also use of 235U(n_{th}, f) measurements in the fit
- Technically, not yet implemented
- Code extension straight-forward
- GMA Database needs to be extended as well

Implementation of Action: Modern readable GMA format


```
{
  "prior": [
    {
      "type": "legacy-prior-cross-section",
      "ID": 1,
      "CLAB": " 6Li(n,a)       ",
      "EN": [
        2.53e-08,  9.4e-06,  0.00015,  0.00025,  0.00035,  0.00045,  0.00055,  0.00065,  0.00075,  0.00085,
         0.00095,   0.0015,   0.0025,   0.0035,   0.0045,   0.0055,   0.0065,   0.0075,   0.0085,   0.0095,
           0.015,     0.02,    0.024,     0.03,    0.045,    0.055,    0.065,    0.075,    0.085,    0.095,
             0.1,     0.12,     0.15,     0.17,     0.18,     0.19,      0.2,     0.21,     0.22,     0.23,
           0.235,     0.24,    0.245,     0.25,     0.26,     0.27,     0.28,      0.3,    0.325,     0.35,
           0.375,      0.4,    0.425,     0.45,    0.475,      0.5,     0.52,     0.54,     0.57,      0.6,
            0.65,      0.7,     0.75,      0.8,     0.85,      0.9,     0.94,     0.96,     0.98,      1.0,
             1.1,     1.25,      1.4,      1.6,      1.8,      2.0,      2.2,      2.4,      2.6,      2.8
      ],
      "CS": [
         938.1,  48.64,  12.16,  9.413,  7.954,  7.012,  6.341,  5.832,  5.428,  5.098,
         4.822,  3.835,   2.97,   2.51,  2.215,  2.005,  1.845,  1.719,  1.617,  1.531,
         1.227,  1.072, 0.9852, 0.8921, 0.7565, 0.7066,  0.674, 0.6547, 0.6476, 0.6499,
        0.6542, 0.7019, 0.8901,  1.156,   1.36,  1.629,  1.973,  2.381,  2.803,  3.132,
         3.222,  3.246,  3.203,  3.102,  2.781,  2.399,  2.036,  1.479,  1.055, 0.8104,
         0.662,  0.564, 0.4972, 0.4484, 0.4123, 0.3826, 0.3653, 0.3499, 0.3308, 0.3153,
        0.2953, 0.2805, 0.2691, 0.2598, 0.2522, 0.2466, 0.2421, 0.2401, 0.2384, 0.2368,
        0.2303,  0.224, 0.2208, 0.2194, 0.2207, 0.2193, 0.2145, 0.2069, 0.1861, 0.1685
      ]
    },
```


Meaning based on keywords, not positions

Implementation of Action: Modern readable GMA format


```
{
  "type": "legacy-experiment-dataset",
  "NS": 1014,
  "MT": 3,
  "YEAR": 1998,
  "TAG": 1,
  "NT": [9, 8],
  "NNCOX": 0,
  "CLABL": "P. STAPLES, K. MOORLEY          ",
  "BREF": "    NSE,129,P.149(1998)         ",
  "EPAF": [
    [ 0.0,  0.0,  0.0,  0.5,  0.5,  0.5, 0.99,  0.5,  0.9,  0.5,  0.5],
    [ 0.0,  0.0,  0.0,  0.5,  0.5,  0.5, 0.01,  0.5,  0.1,  0.5,  0.5],
    [ 0.0,  0.0,  0.0,  0.5,  0.5,  0.5,  0.5,  0.5,  0.5,  0.5,  0.5]
  ],
  "NETG": [0, 0, 9, 1, 1, 1, 1, 1, 1, 0, 1],
  "ENFF": [1.2, 0.1, 0.1, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0],
  "NENF": [1, 1, 1, 0, 0, 0, 0, 0, 0, 0],
  "NCSST": [8002],
  "NEC": [
    [
      [15], [16], [17], [18], [19], [2], [31], [0], [0], [0]
    ],
    [
      [15], [20], [17], [21], [16], [18], [8], [0], [0], [0]
    ]
  ],
  "FCFC": [
    [0.5], [0.2], [1.0], [0.2], [0.2], [0.5], [0.5], [0.0], [0.0], [0.0]
  ],
```

Implementation of Action: Modern readable GMA format


```
  {
    "type": "modern-experiment-dataset",
    "api_version": "0.1",
    "identifier": 2515,
    "quantity": "legacy_sacs_ratio",
    "reaction_identifier_numerator": 9,
    "reaction_identifier_denominator": 8,
    "measured_value": 1.475,
    "authors": "Adamov",
    "publication": "NA",
    "year": 9999
  }
],
"percentual_uncertainties": [1.62,  1.2,  0.9,  1.6, 1.32,  1.2,  0.8, 1.45, 1.79, 2.26, 1.66,  1.5],
"lower_triagonal_correlation_matrix": [
  [100],
  [ 23, 100],
  [ -9,  36, 100],
  [  0,   0,   0, 100],
  [  0,   0,   0,  60, 100],
  [  0,   0,   0,   0,   0, 100],
  [  0,   0,   0,   0,   0,  39, 100],
  [  0,   0,   0,   0,   0,   0,   0, 100],
  [  0,   0,   0,   0,   0,   0,   0,   0, 100],
  [  0,   0,   0,   0,   0,   0,   0,   0,  59, 100],
  [  0,   0,   0,   0,   0,   0,   0,   0,   0,   0, 100],
  [  0,   0,   0,   0,   0,   0,   0,   0,   0,   0,  39, 100]
]
```


Straight-forward addition of new datablock and dataset types

Implementation of Action: USU estimation beyond GLS

- **Motivation**:
  - Data inconsistencies in GLS don't impact uncertainties
  - Low evaluated uncertainties in STD2017 led to addition energy-independent, fully correlated uncertainties (USU)
- **Goal**: Implementation of a statistically sound and data-driven way to assess USU in the Neutron Standards Project
- Extension of the GLS method to a Bayesian hierarchical model accounting for "uncertain uncertainties" **accomplished**

Concluding remarks

- Significant progress in the development of gmapy
- Modular Python code facilitating extensions
- Easier programmatic access to GMA database