BUMS-Bonner sphere Unfolding Made Simple Modernized

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ABSTRACT

Neutron spectrum unfolding using Bonner sphere spectrometers has historically relied on specialized software environments with limited portability, platform dependence, and aging software architectures. This work presents a modernized implementation of the Bonner sphere Unfolding Made Simple (BUMS) framework through development of a unified Python-based architecture for neutron spectrum unfolding and dosimetry analysis. The framework preserves the original unfolding methodologies, detector response matrices, starting spectrum libraries, and dose conversion capabilities while extending maintainability, extensibility, deployment portability, and integration with contemporary scientific computing workflows. The updated implementation supports command-line, graphical user interface, and Docker-based deployment configurations for accessible and reproducible execution across computing environments. Validation was performed using legacy Oak Ridge National Laboratory test cases and additional generated unfolding configurations spanning multiple unfolding methods, response matrices, and starting spectra. Results from the modernized implementation were found to be numerically consistent with those produced by the original BUMS framework. The resulting open-source architecture provides a platform for continued development and deployment of neutron spectrometry and unfolding workflows within modern computational environments.

INTRODUCTION

Neutron spectrum unfolding using multisphere spectrometer measurements has traditionally relied on a collection of specialized unfolding methods that can be difficult to deploy and standardize. The Bonner sphere Unfolding Made Simple (BUMS) package was introduced to address these challenges by providing a web-based interface to established unfolding algorithms using the BUNKI framework. By centralizing execution and enforcing consistent input-output formatting through a HTML front end, BUMS reduced the need for local installation and simplified routine analysis. With modern software ecosystems evolving, the underlying foundation of Perl and Fortran subroutines poses a challenge for the maintainability, extensibility, and compatibility of the original BUMS package.

The following work focused on a modernized BUMS with the underlying Perl and Fortran subroutines being translated into a single Python package. The transition to Python enhances the modularity of the code base, simplifies integration with contemporary data analysis and visualization tools, and provides a framework that is easier for new users and developers to understand, modify, and enhance. Generative AI-assisted coding tools were utilized under author supervision during portions of the translation of legacy Perl and Fortran routines into Python. All translated implementations underwent debugging, regression testing, and validation against legacy BUMS outputs.

The goal of modernizing BUMS is to create an open-source, community-friendly version of BUMS that facilitates wider and ongoing development. The updated architecture supports easier customization of unfolding workflows, smoother deployment across platforms, and integration into broader neutron dosimetry or spectrometry tool chains. With this modernization, we aim to preserve the accessibility and algorithmic richness of the original BUMS package while ensuring its relevance and utility in present and future research environments.

BACKGROUND

Neutron unfolding is the process of estimating the neutron energy spectrum based on measured fluence data. This task constitutes an underdetermined inverse problem, as the number of detectors available is typically fewer than the number of energy groups used to discretize the neutron spectrum. The response of a detector to a given neutron field can be described in the following equation:

$$R_i = \int_{E_{min}}^{E_{max}} \sigma_i(E)\varphi(E)dE, \;\; i = 1, 2, ..., M \tag{1}$$

where R_i is the ith detector response, $\sigma_i(E)$ is the sensitivity of the ith detector to neutrons of energy E, $\varphi(E)$ is the incident neutron fluence of the surface of the detector, and M is the total number of detectors. This continuous equation can be transformed

into a discrete form in the following manner:

$$R_i = \sum_{j=1}^{M} j = \sum_{i=1,j=1}^{M} N\sigma_{i,j}\varphi_j,\ i = 1, 2, ..., M \tag{2}$$

where $\sigma_{i,j}$ is the ith detector sensitivity to the jth energy group, and N is the number of energy groups.

Unfolding methods differ in how they incorporate prior information. Two common modeling strategies include:

1. Representing the neutron spectrum as a vector of N discrete energy groups, initialized with a guess spectrum
2. Representing the neutron spectrum as a function of physically meaningful parameters, using estimated initial values.

The BUMS system adopts the first approach to perform neutron spectrum unfolding. It integrates access to four different algorithms: SPUNIT, BON, MAXED, and SAND-II. BUMS builds on the BUNKI framework, which originally included SPUNIT and BON methods, both of which use recursive minimization techniques. SPUNIT was first developed by Doroshenko et al.[1], while BON was created by Robert Sanna at the Environmental Measurements Laboratory[2].

The MAXED algorithm, introduced by Marcel Reginatto and Paul Goldhagen at the same laboratory[3], employs the maximum entropy method to stabilize and solve the unfolding problem. Lastly, the SAND-II algorithm, originally developed by McElroy et al.[4] [5], incorporates components of the MAXED Fortran routines and is included as part of the modified MAXED implementation in BUMS.

METHODOLOGY

Starting with BUMS

The modernized version of BUMS is available on GitHub, with the main branch containing the newly translated Python code intended for general use. In addition to the main branch, the repository includes a development branch, where ongoing edits and new features are tested before integration. As well as a legacy branch, which preserves the original Perl and Fortran implementation for archival and comparative purposes.

The new version of BUMS was developed using Python 3.9.6, and depends on two core libraries: NumPy and Matplotlib. These dependencies are managed through a requirements.txt file included in the repository, allowing for a straightforward installation via standard Python tools.

Both the original and modernized versions of BUMS can be executed from the command line or through graphical user interface (GUI). While the original BUMS was designed to run entirely through a browser without requiring local installation, that architecture could not be preserved in the modern implementation. To enhance portability and reproducibility, Docker containers have been created for both versions of BUMS. Docker enables platform-independent deployment by providing a consistent, isolated runtime environment across operating systems. It also simplifies setup and installation, ensuring all users interact with the software in a uniform way.

Unfolding Process

To initiate the unfolding process, BUMS provides users with a broad selection of predefined starting spectra. This includes a library of 58 spectra, primarily sourced from the *Compendium of Neutron Spectra and Detector Responses for Radiation Protection Purposes*[6]. The library encompasses a diverse range of spectra, including those from calibration sources and benchmark fields, operational field measurements, neutron scattering from facility walls, neutron scattering in air, and natural background. Users may also extend this library with additional spectra to suit specific applications.

In addition to the predefined library, BUMS offers three alternative methods for specifying the starting spectrum: MAXIET, automatic search, and user input. MAXIET is an algorithm originally developed for use with the BON and SPUNIT methods. It generates an initial spectrum by assuming a general spectral shape and adjusting key physical parameters based on user-provided inputs. The resulting spectrum consists of a high-energy Maxwellian peak, and intermediate component with a $(1/E)^X$ dependence, and a thermal peak[7]. MAXIET simultaneously estimates the Maxwellian temperature, the exponent of the intermediate region, and the intensity of the thermal component.

The automatic search method selects a starting spectrum by evaluating each option in the available library. It calculates the detector response for each candidate spectrum and selects the one that minimizes the chi-squared deviation from the measured responses. Finally, the user input option allows users to define a custom initial spectrum directly through the GUI or as a separate file input for the command line, offering the greatest flexibility for advanced or specialized cases.

The modernization of BUMS retains the original set of 14 detector response matrices provided in the initial release[8]. These include widely used matrices such as UTA4 and UTA13 (both consist of the 31- and 171-group representation), SAN4, ARK1, and HEVE4 and VHS, which were developed using detailed three-dimensional models and MCNP simulations[8]. No modifications have been made to these response datasets in the current work, but they remain integral to the unfolding process and are available for selection during spectrum reconstruction.

RESULTS

Regardless of whether BUMS is executed via the GUI or command line, the unfolding process produces a structured output page containing all relevant results. If the user selects either automatic search or MAXIET as the initial spectrum method, the corresponding starting spectrum parameters will be included at the beginning of the output.

The unfolding results include the scale factor determined during spectrum fitting, the number of iterations performed by the unfolding algorithm, and the percent error associated with the final solution. In addition, the output provides the expected detector counts for each Bonner sphere, along with the associated uncertainty estimates.

The neutron fluence and dose equivalent values are computed for the full spectrum, and further broken down by energy group, enabling energy-resolved dosimetry analysis. The output also includes results from standard dose conversion functions, presenting equivalent dose quantities based on commonly used radiation protection models. Additionally, the output presents the detector responses of commonly used detectors in accordance with the given problem. Both methods of BUMS will generate plots showing the initial guess spectrum selected during the initialization of the run, and the unfolded spectrum generated during the unfolding process.

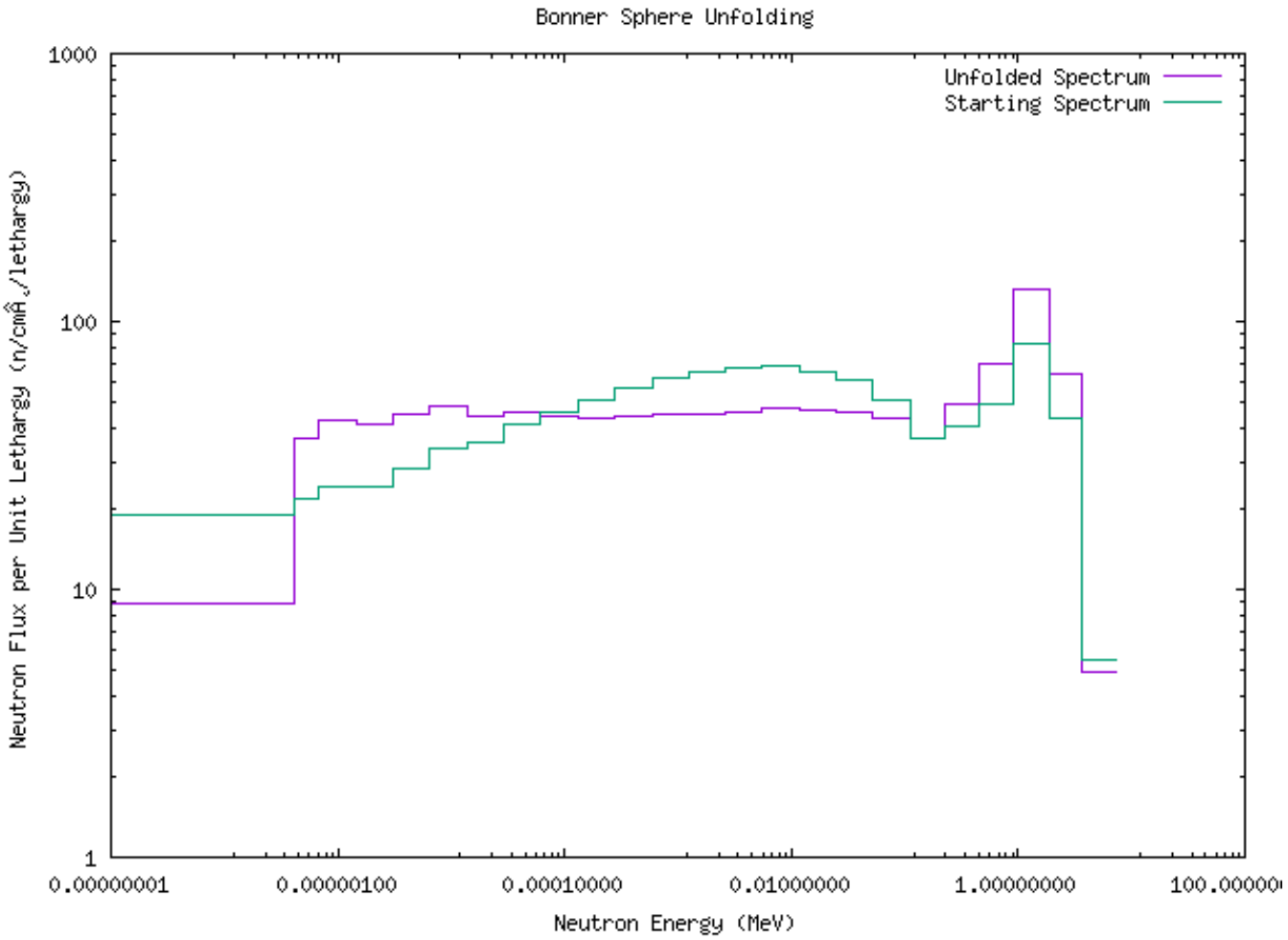

Fig. 1: Perl BUMS command line plot output

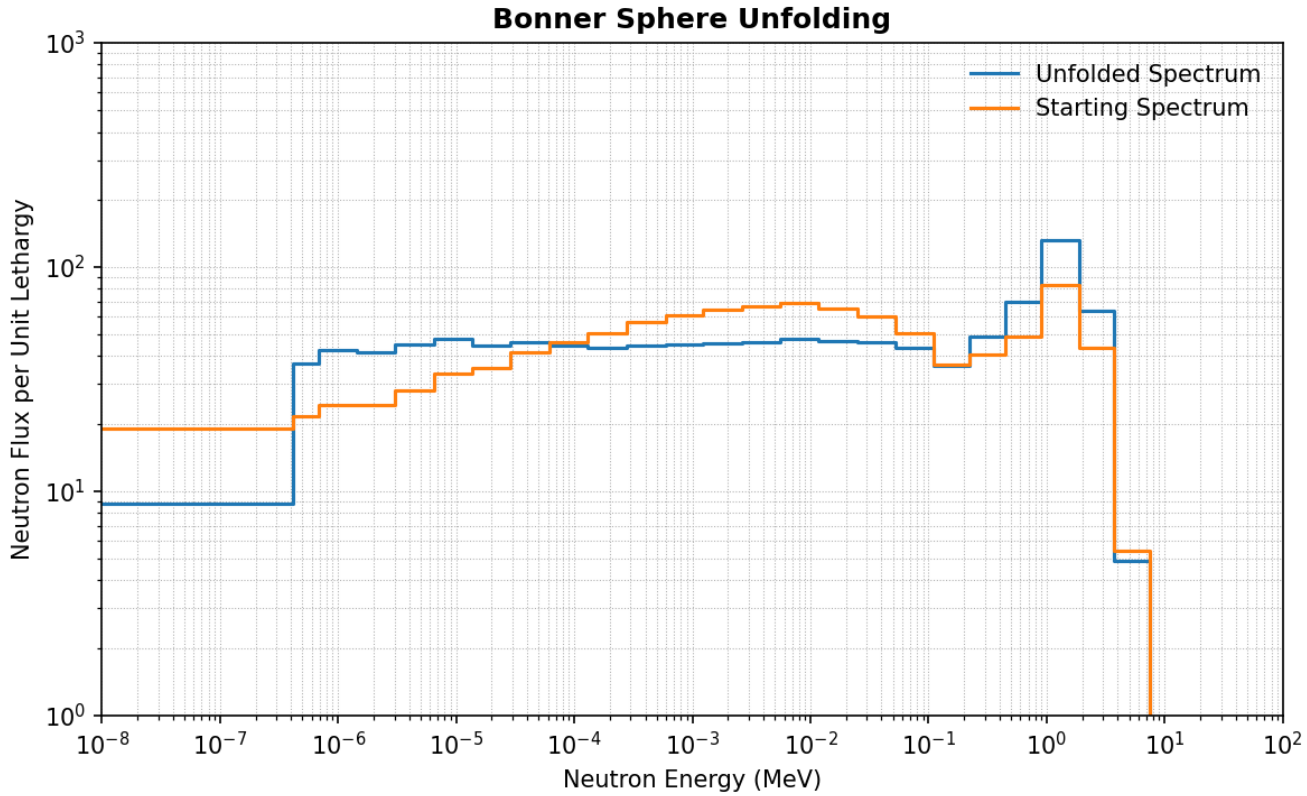

Fig. 2: Python BUMS command line plot output

CONCLUSIONS AND FUTURE WORK

The latest version of BUMS was validated using a series of test cases from an Oak Ridge National Laboratory internal test report[9] that were generated with the original BUMS program, and with a series of generated test cases that iteratively selects different starting spectra, responses matrices, and unfolding methods. The outputs from each version were compared and found to be numerically identical, with minor differences in the format of the final output. Likewise, the outputs between the command line interface and graphical user interface were compared for content and accuracy. The assumed accuracy of the modern BUMS system is reliant on the accuracy of the original BUMS.

Minor stylistic changes exist between the original and modernized version of BUMS. The modern BUMS GUI was created to emulate the appearance of the original, with some added features. The BUMS GUI provides an option to the user to download an input template that will autofill the page when uploaded and selected, with the same layout as the file needed for using the command line. The input page also provides the option to autofill the uncertainty column with the most frequently used forms of uncertainty as seen in the test cases from ORNL[9]. The input page has been further enhanced to include hoverable tool tips and an improved user spectrum upload feature that expands the input page when the option is selected. The output page has been updated to include all calculated parameters on a single page for a more concise display of information for users.

The remaining inputs to fine-tune the unfolding such as max number of iterations, iterations before test error, final error percentage, Maxwellian temperature, smoothing factor, shape, perturbation, calibration factor, and maximum energy were left untouched between the original and modern version of BUMS. Similarly, the neutron unfolding methods, detector matrices, and dose correlations were retained in the modern version to ensure numerical consistency with the legacy BUMS. Users are encouraged to incorporate their own updates and methodologies within this framework, fostering an open-source community for continued development. The public repository can be found at https://github.com/larnold34/BUMS2.

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