

Readme File (ver14.1)

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1 Overview

This document provides instructions for using the attached files (Notebooks and data) for performing numerical analysis and visualization of the **Hill-Wheeler equation** in **Mathematica ver14.1**. Our previous investigations utilized **ver11.2** for optimization and parameter searches, but in this latest version, changes in the `FindMinimum` command have made it difficult to reproduce exactly the same results.

To address this, the folder includes Notebooks that incorporate **pre-computed results obtained with ver11.2**, providing an environment in which **analysis and visualization can be reused even under ver14.1**.

2 File List

- `HillWheeler_Main.nb`

A Notebook containing the main computational workflow of this study, compatible with ver14.1.

- `_Calculation_Results.nb` for each nuclide

For example: `U235_Calculation_Results.nb`, `U233_Calculation_Results.nb`,
...

Notebooks that load the results (data) already computed with ver11.2, enabling additional analyses and visualizations.

- A set of files named `_Data_JENDL5&Calculation_Data.m` for each nuclide
For example: `U235_Data_JENDL5&Calculation_Data.m`, ...
These files contain the nuclear data (JENDL-5) and the optimization results (parameters, etc.) calculated under ver11.2.
- `ReadmeFile_ver14_1.pdf` (this document)
A guide to all materials provided in this folder.

3 System Requirements

- **Software:** Wolfram Mathematica ver14.1
- **Operating System:** Windows 10 / Windows 11 / macOS, etc. (wherever ver14.1 operates)
- **Memory:** At least 8GB recommended (depending on the type of analysis)

4 Notes on Usage

4.1 Reproducibility

- In this research, the optimization and parameter searches were originally performed with `FindMinimum` under ver11.2. Due to internal algorithmic changes in ver14.1, it may be **impossible to reproduce the same results**, even if initial conditions and parameters are identical.
- **In this set of files, we have embedded the final results computed under ver11.2 as data files**, allowing you to visualize and carry out further analyses under ver14.1 by using those solutions.

4.2 Execution Steps

1. Place `HillWheeler_Main.nb` and each `_Calculation_Results.nb` file for each nuclide in the **same folder**.

2. Start Mathematica ver14.1 and open the aforementioned Notebooks.
3. Execute the cells at the top of each Notebook in sequence to load necessary parameters and functions. (The files `_Data_JENDL5&Calculation_Data.m` will be automatically loaded.)
4. By running all cells in the Notebook, you can view graphs, numerical comparisons, and other outputs that **take advantage of the ver11.2 results** in ver14.1.

5 Example of Execution

- **U235_Calculation_Results.nb:**

Open this Notebook and run all cells in sequence to visualize the eigenenergies, wavefunction distributions, mass parameters, and more for ^{235}U .

- **U238_Calculation_Results.nb:**

Follow the same procedure to view the analysis results for ^{238}U .

- The same steps can be applied to other nuclides as well.

6 Data License and Citations

- This research refers to **JENDL-5** nuclear data, which should be used in accordance with its license and terms of use.
- When utilizing the code or computational results in your own research, please **cite the authors' publications** (the source) accordingly.

7 Contact

For questions, bug reports, or requests for additional analyses, please contact us at:

(Example) E-mail: `etctransformation@jcom.zaq.ne`

This concludes the overview and usage instructions for the **ver14.1** files.

We hope it will be helpful for further comparison with ver11.2 results and for additional analyses.