Readme File (ver11.2)

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1 Overview

This document explains how to use the various codes and related files for execution and verification using **Mathematica ver11.2**. The following files are included in this folder.

2 File List

- `HillWheeler_Main.nb`
  Main code of the Hill-Wheeler equation used in this research.
- `U235_Calculation_Results.nb`
  Calculation results and visualization Notebook for ^{235}U.
- `U233_Calculation_Results.nb`, `U238_Calculation_Results.nb`
  Results and visualization Notebooks for other nuclides (^{233}U, ^{238}U, etc.).
- Set of `_Data_JENDL5.m` files for each nuclide
  Files for importing nuclear data from JENDL-5 into Mathematica, including cross-sections.
- `ReadmeFile_ver11_2.pdf` (this document)
  Documentation for this folder.

3 Execution Environment

- **Software**: Wolfram Mathematica ver11.2
- **OS**: Windows 10 / Windows 11 / macOS, etc. (environments where ver11.2 operates)
- **Memory**: Minimum 4GB or more recommended

4 Execution Procedure

Here, we demonstrate the execution method using `HillWheeler_Main.nb` as an example.

4.1 Opening the Notebook

1. Launch Mathematica ver11.2.
2. Open `HillWheeler_Main.nb`.

4.2 File Placement

- Place `_Data_JENDL5.m` for each nuclide in the same directory as `HillWheeler_Main.nb`.
- When executing other Notebooks (e.g., `U235_Calculation_Results.nb`), similarly place necessary data files in the same directory.

4.3 Code Execution

1. Execute cells from the top of the Notebook in order to define parameters and functions.
2. Upon completion, analysis results based on the Hill-Wheeler equation will be output, including energy eigenvalues and wavefunction visualization.
3. Follow the same procedure for other Notebooks (e.g., `U235_Calculation_Results.nb`) to analyze each nuclide.

5 Important Notes

- **Critical Computational Environment Constraint**: The numerical calculations using the Hill-Wheeler equation in this research operate correctly **only in Mathematica versions 9 through 11.2**. Due to fundamental specification changes in the `FindMinimum` command from version 11.3 onwards, it is **absolutely impossible** to correctly reproduce the same calculations.

  This constraint is not a limitation of our methodology but a direct consequence of the command specification changes. Therefore, using **Mathematica versions 9 through 11.2 is essential** for reproducing this research's calculations. In particular, we **strongly recommend using version 11.2**, which has been extensively verified in this study.

- **Computation Time**: Depending on CPU performance, executing each Notebook sequentially may take from several minutes to tens of minutes.

- **Data License**: Please observe the license regulations for nuclear data (JENDL-5) usage.

- Memory usage may increase due to large-scale calculations. Please secure sufficient memory or adjust calculation parameters as needed.

6 Contact Information

For questions or bug reports, please contact:

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

This concludes the overview and usage instructions for **ver11.2** files.

For reproducibility purposes, we strongly recommend execution in the specified Mathematica version environment.