Installation:

This code was developed in 3.9. It utilizes the following external packages:

* numpy 1.21.6
* numba 0.55.1
* scipy 1.8.0
* matplotlib 3.5.1
* tqdm 4.64.0
* PyQt5 5.15.6

Usage:

After installing all the prerequisite packages to your environment of choice, you can use any of the python scripts to run a simulation. Most are different methods of distributing the calculation load to different computing resources. Alternatively, the GUI (PPPP\_calculation\_numba\_gui.py) can be opened, which utilizes the numba parallel CPU compute suite.

Upon opening the GUI, the user is greeted with the following screen:

Graphical user interface, application, Word

Description automatically generated

To add a calculation, simply edit the simulation parameters of choice and click “Add Calculation”. This will add the parameters to the calculation queue table, as shown below:

Graphical user interface, application

Description automatically generated

When ready, click “Run Calculation”, which initializes the calculation and begins printing progress in the consol:

A picture containing text

Description automatically generated

Data is saved in a .json format, with metadata on the first list and the results of the calculation in the second list. The dictionary terms are ‘Run\_Properties’ and ‘Results’. The order of the run properties are as they appear in the calculation table.

The analysis tab allows the editing and saving of figures.

Graphical user interface, chart

Description automatically generated with medium confidence

When a calculation is complete, the analysis side will update with the most recently finished calculation.

A picture containing graphical user interface

Description automatically generated

Old data can be loaded in .json format, as demonstrated:

Graphical user interface, text, application

Description automatically generated