MetroTRPL GUI Tutorial – v.1.5.2

cfai2304 – HagesLab

February 6, 2024

About

MetroTRPL is a Python tool that aims to recover as many material parameters as possible by using Bayesian inference to compare characterization data measured from a physical system to simulations of the transient physics of that system. In our case, this would be photoluminescence or terahertz spectroscopy of semiconductors, but any other system could theoretically be analyzed with the appropriate physics simulation.

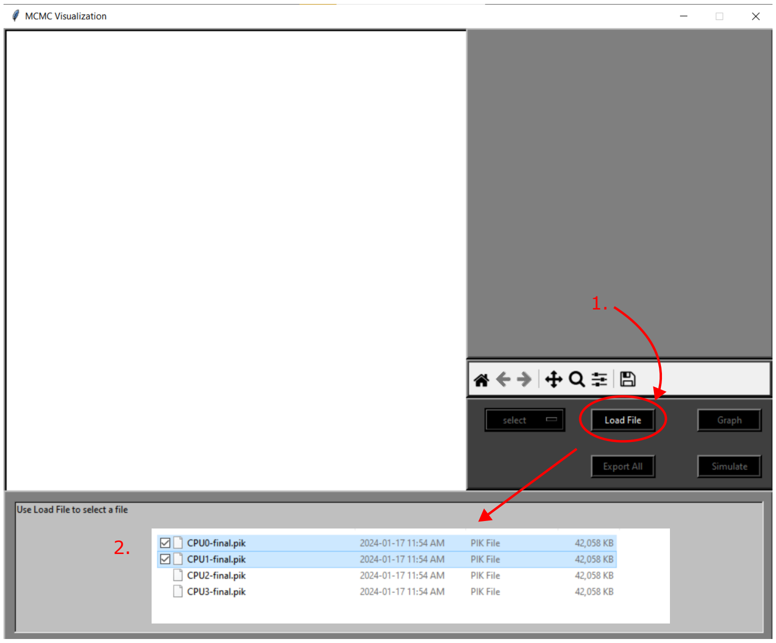
Regardless of your choice of physics simulation, MetroTRPL outputs results as a `.pik` file containing a sequence of all of the states that each chain in the ensemble has visited, the log-likelihoods of those states, records of which moves are accepted, and records of what settings were used during the run. This GUI allows you to visualize these states, do basic statistics on these states, and, if you already have a preferred data analysis tool, export these states as text files.

Contents

1. Quick Start

See the Github for required Python version and libraries.

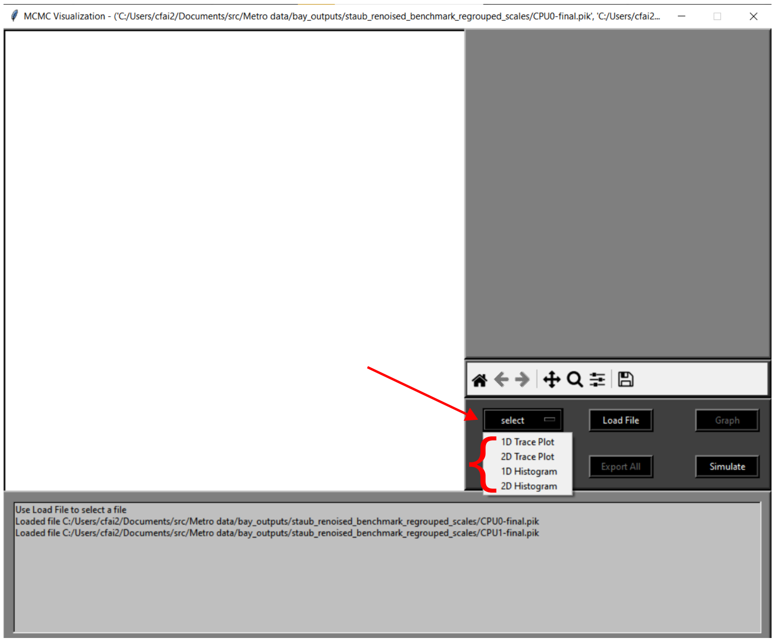
1. Navigate to the GUI directory and run `main.py`.
2. Click **Load File** and select `.pik` files.



Use Load File to select a file

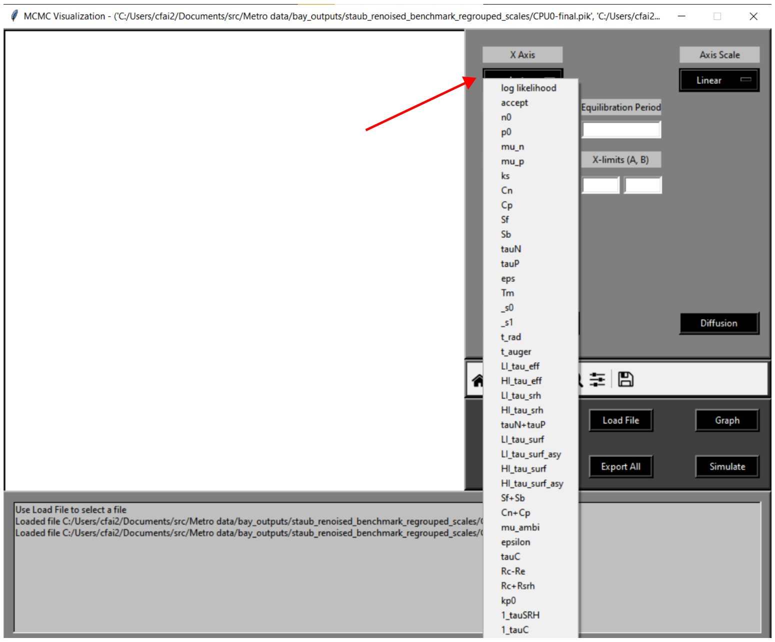
☑ CPU0-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
☑ CPU1-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
CPU2-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
CPU3-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB

3. Click **Select** and choose a visualization type.


MCMC Visualization - ('C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik', 'C:/Users/cfai2...
select
Load File
Graph
1D Trace Plot
2D Trace Plot
1D Histogram
2D Histogram
Export All
Simulate

```
Use Load File to select a file
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU1-final.pik
```

4. Choose a *state variable* from the **X Axis** dropdown menu.



MCMC Visualization - ('C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik', 'C:/Users/cfai2...

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Use Load File to select a file
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/(
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/(
```

5. Edit the plot.

6. Rerun simulations from states.

7. Export state data.

2. Overview

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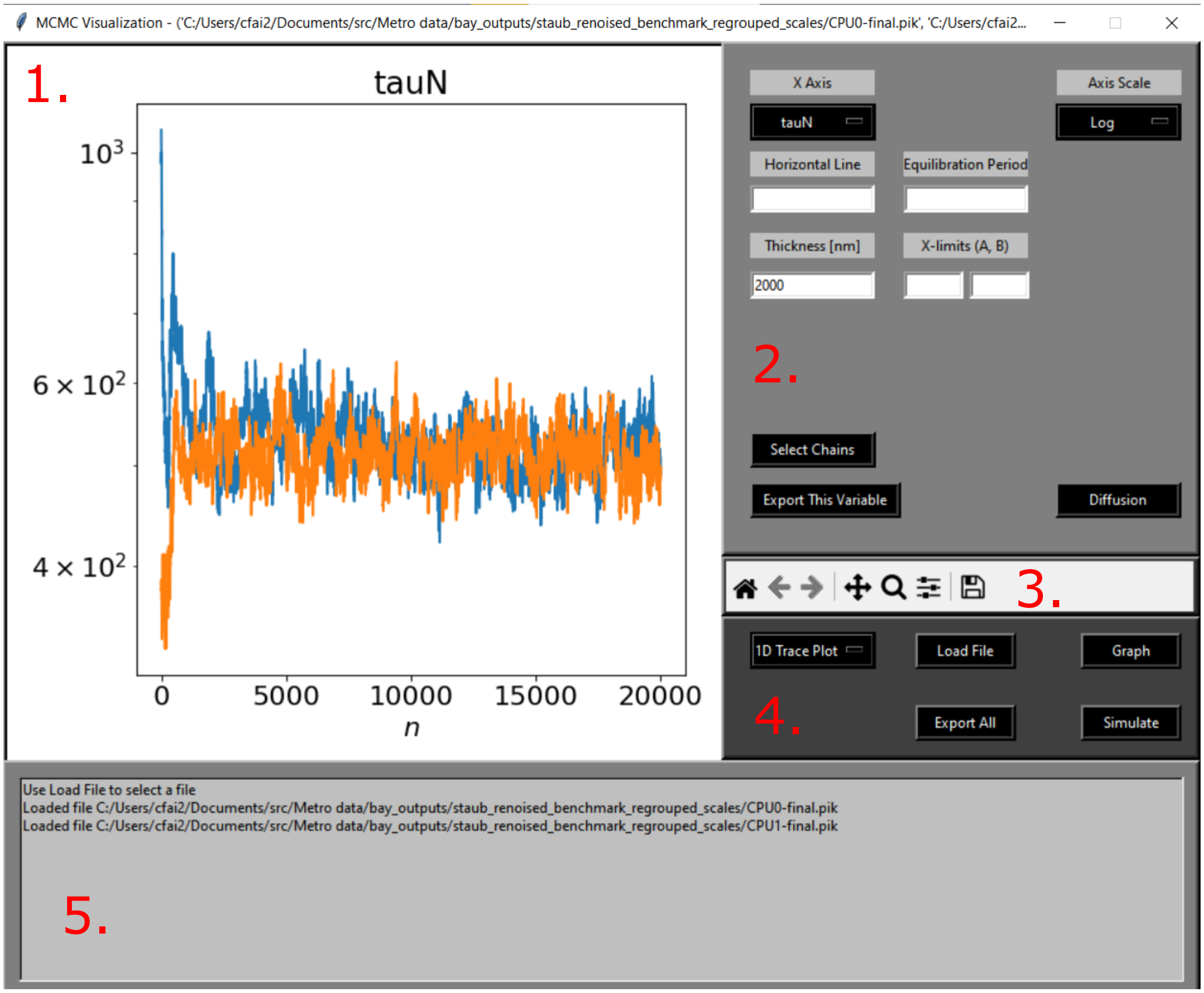


MCMC Visualization - ('C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik', 'C:/Users/cfai2...

X Axis: tauN

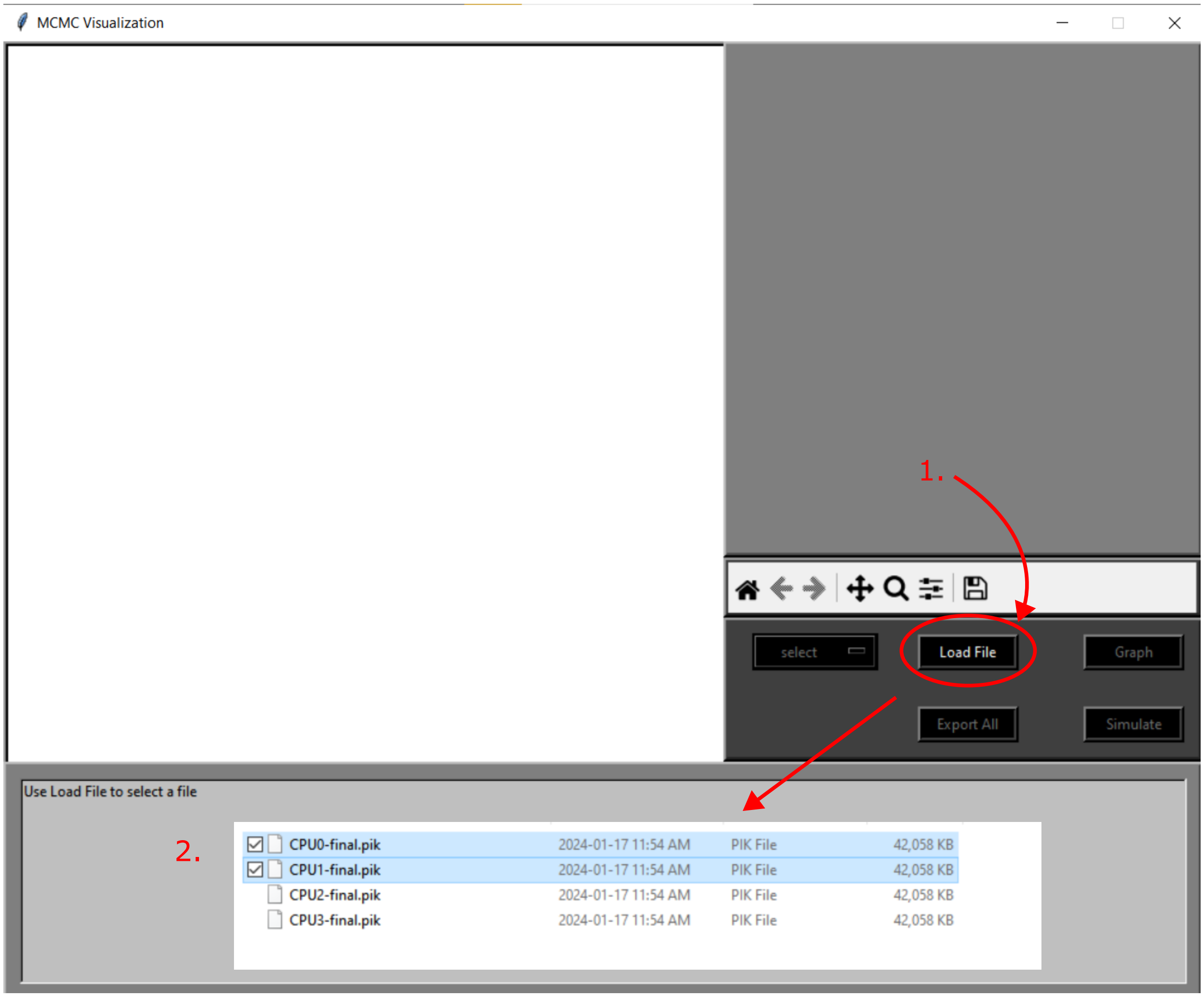
Axis Scale: Log

Thickness [nm]: 2000

```
Use Load File to select a file
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU1-final.pik
```

There are five main areas of the GUI. Clockwise from the top left, they are:

1. The **Plot window**. This is where the visualization appears once you choose a visualization type and enter all necessary settings for that visualization.
2. The **Visualization settings**. This is where you input settings for the visualization.
3. **Additional plot controls**. Pan, zoom, and export plots as images.
4. **Main menu**.
5. **Status box**. Status messages are written here.



Use Load File to select a file

☑ CPU0-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
☑ CPU1-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
CPU2-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB
CPU3-final.pik	2024-01-17 11:54 AM	PIK File	42,058 KB

The first thing you will want to do is load `.pik` files, and nearly everything in the **Main menu** will be disabled until you do. Start by clicking **Load File**–this will allow you to browse your computer for `.pik` files. You can click-and-drag or select the checkboxes to load in multiple `.pik` files at once.

This will enable the rest of the main menu. You can load new `.pik` files at any time by clicking **Load File** again. Note that doing so will *clear any plots or simulations you have previously made*, so be sure you have exported everything you need first.

3. Plotting

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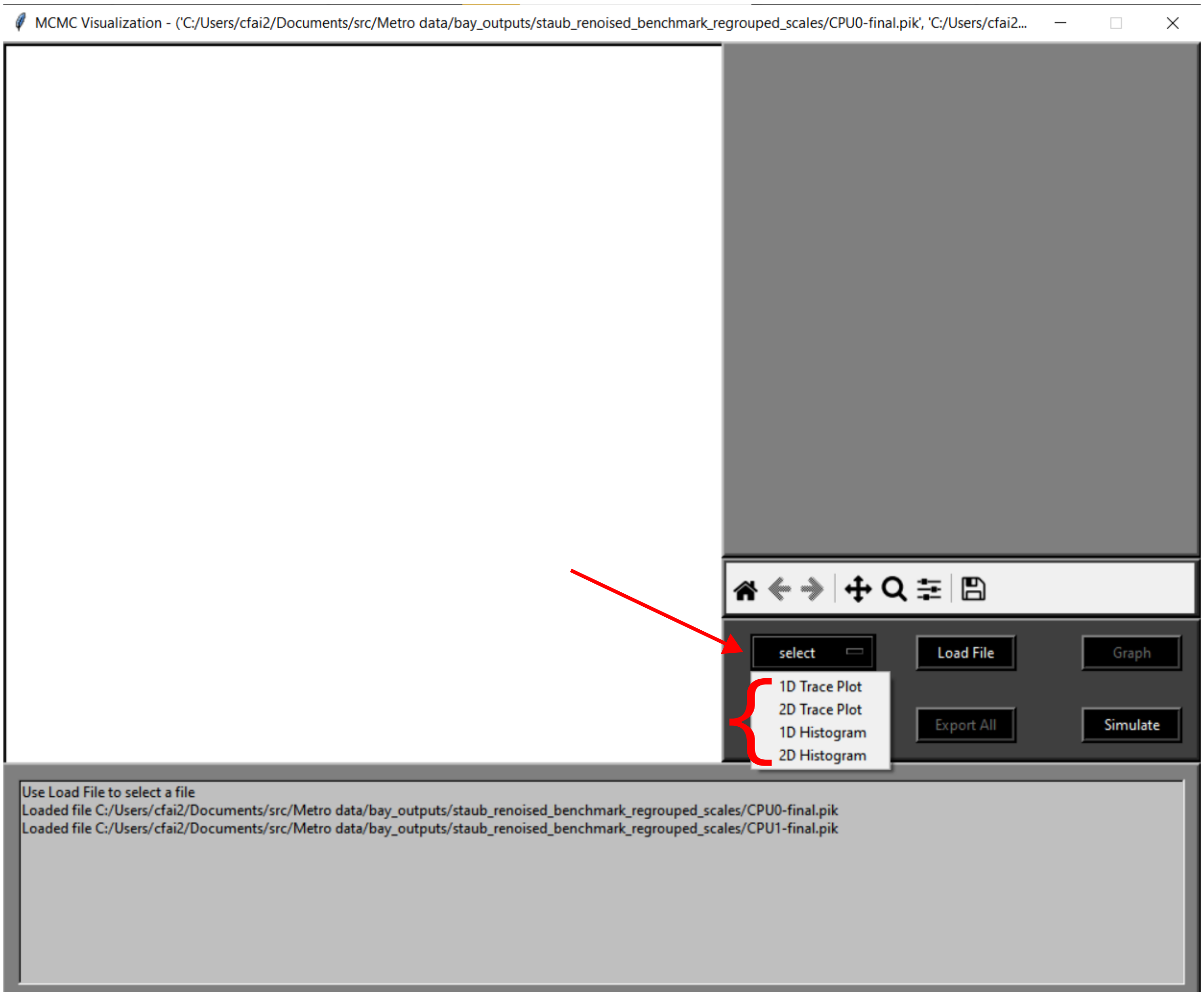
MCMC Visualization - ('C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik', 'C:/Users/cfai2...
select
Load File
Graph
1D Trace Plot
2D Trace Plot
1D Histogram
2D Histogram
Export All
Simulate

```
Use Load File to select a file
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU0-final.pik
Loaded file C:/Users/cfai2/Documents/src/Metro data/bay_outputs/staub_renoised_benchmark_regrouped_scales/CPU1-final.pik
```

Four types of visualizations are available by clicking the **select** dropdown menu in the **Main menu**:

1. 1D trace plots, which track the value of one state value over the run.
2. 2D trace plots, which track the values of two state variables in a 2D representation over the run.
3. 1D histograms, which display how frequently one state variable's values were visited over the run.
4. 2D histograms, which display how frequently two state variables' values were visited over the run, as a 2D heatmap.

The visualization may not appear automatically when you select it. Some visualizations require you to enter additional settings. Once all of the required settings are entered, the visualization will appear automatically. The visualization will also update automatically when any of these settings are changed.

*If the visualization fails to update, click the **Graph** button in the **Main menu**.*

3.1. 1D Trace Plots

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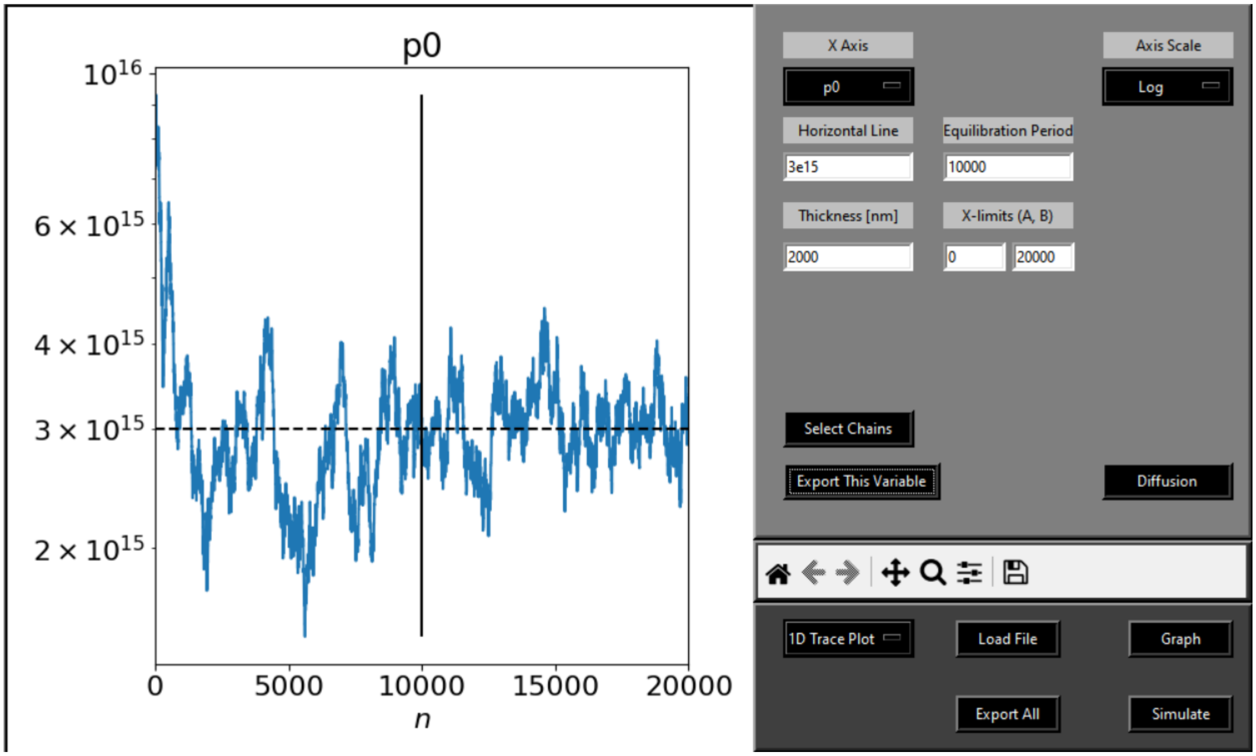

X Axis: p0

Axis Scale: Log

Horizontal Line: 3e15

Equilibration Period: 10000

Thickness [nm]: 2000

X-limits (A, B): 0 20000

- **X Axis** – Selects the state variable to be plotted in the visualization. The log-likelihood and acceptance rate can also be selected here.
- **Axis Scale** – Toggle logarithmic or linear scale for the y axis. Symlog works better for log-likelihood plots.
- **Horizontal Line** – Adds a dashed line marker at a specified state variable value.
- **Equilibration Period** – Adds a vertical solid marker at a specified iteration number. Use this to mark when the run has equilibrated.
- **Thickness [nm]** – Thickness of the material. This only affects some calculated state variables that depend on the thickness, such as surface lifetimes.
- **X-limits (A, B)** – Left and right limits for the x axis.
- **Select Chains** – Toggle the visibility of specific chains in the collection of loaded `.pik` files. Inactive chains will not be plotted or used in calculations/simulations.
- **Diffusion** – Computes the state space diffusion constant of each active chain. Counts only samples after the equilibration period. See our paper on Metropolis sampling for details.

3.2. 2D Trace Plots

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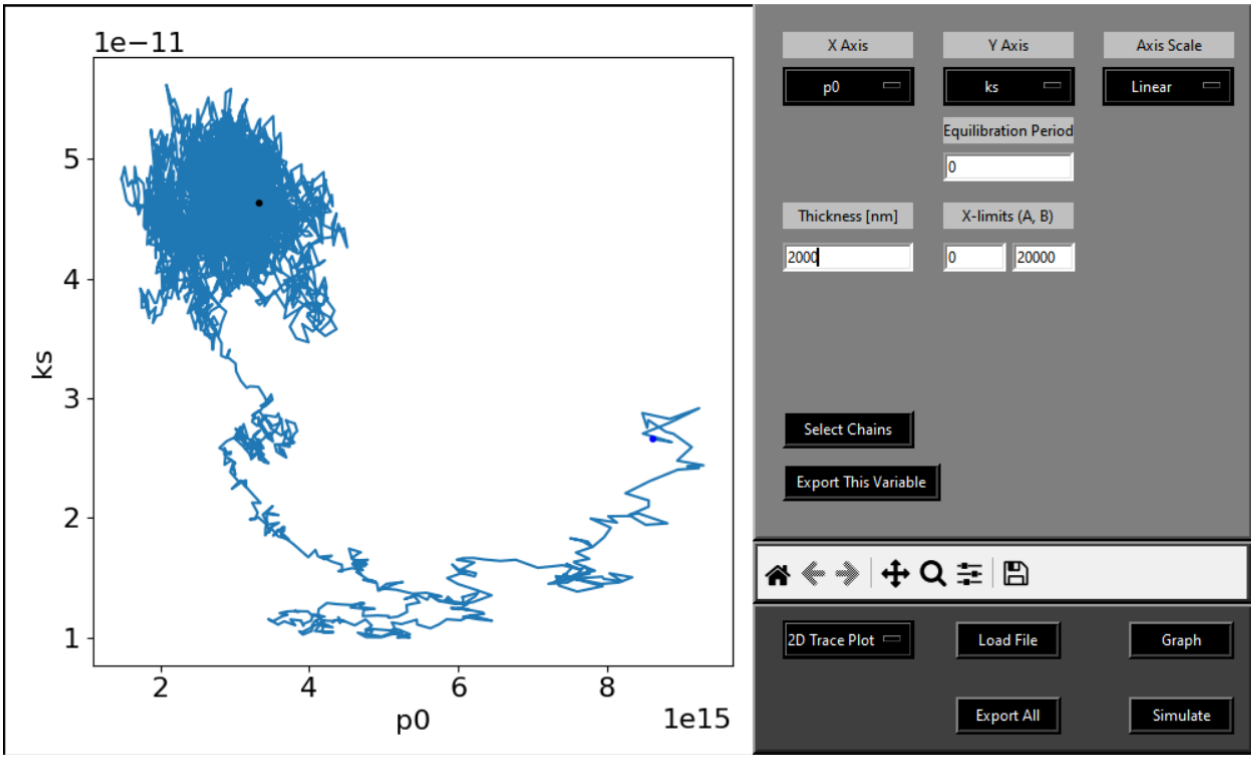

X Axis: p0

Y Axis: ks

Axis Scale: Linear

Equilibration Period: 0

Thickness [nm]: 2000

X-limits (A, B): 0 20000

- **X Axis** – Selects the state variable to be plotted along the x axis of the visualization.
- **Y Axis** – Selects the state variable to be plotted along the y axis of the visualization. Both **X Axis** and **Y Axis** must have state variables selected for the visualization to display.
- **Axis Scale** – Toggle logarithmic or linear scale for both axes.
- **Equilibration Period** – Truncates the iterations. Only samples at iteration greater than this value will be displayed.
- **Thickness [nm]** – Thickness of the material. This only affects some calculated state variables that depend on the thickness, such as surface lifetimes.
- **X-limits (A, B)** – Left and right limits for the x axis.
- **Select Chains** – Toggle the visibility of specific chains in the collection of loaded `.pik` files. Inactive chains will not be plotted or used in calculations/simulations.

3.3. 1D Histograms

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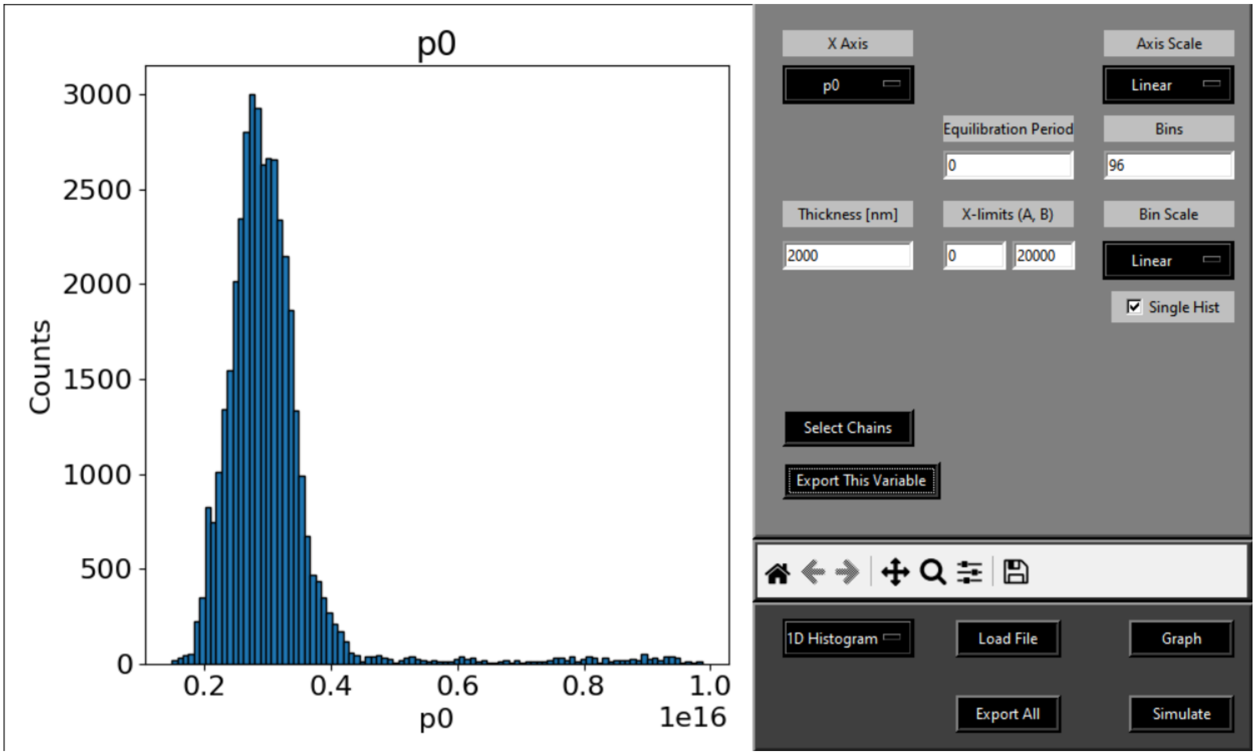

X Axis: p0

Axis Scale: Linear

Equilibration Period: 0

Bins: 96

Thickness [nm]: 2000

X-limits (A, B): 0 20000

Bin Scale: Linear

☑ Single Hist

- **X Axis** – Selects the state variable to be plotted in the visualization.
- **Axis Scale** – Toggle logarithmic or linear scale for the y axis.
- **Equilibration Period** – Truncates the iterations. Only samples at iteration greater than this value will be counted in the histogram. Use the 1D trace plot to determine where the equilibration period should be set.
- **Bins** – Number of bins to draw in the histogram.
- **Bin Scale** – Whether the bins will be partitioned equally in linear or log space.
- **Single Hist** – If selected, samples from all chains will be counted under a single histogram. Also computes the mean and standard deviation of the state variable in the status window. Otherwise, different histograms will be shown for each chain.
- **Thickness [nm]** – Thickness of the material. This only affects some calculated state variables that depend on the thickness, such as surface lifetimes.
- **X-limits (A, B)** – Left and right limits for the x axis.
- **Select Chains** – Toggle the visibility of specific chains in the collection of loaded `.pik` files. Inactive chains will not be plotted or used in calculations/simulations.

3.4. 2D Histograms

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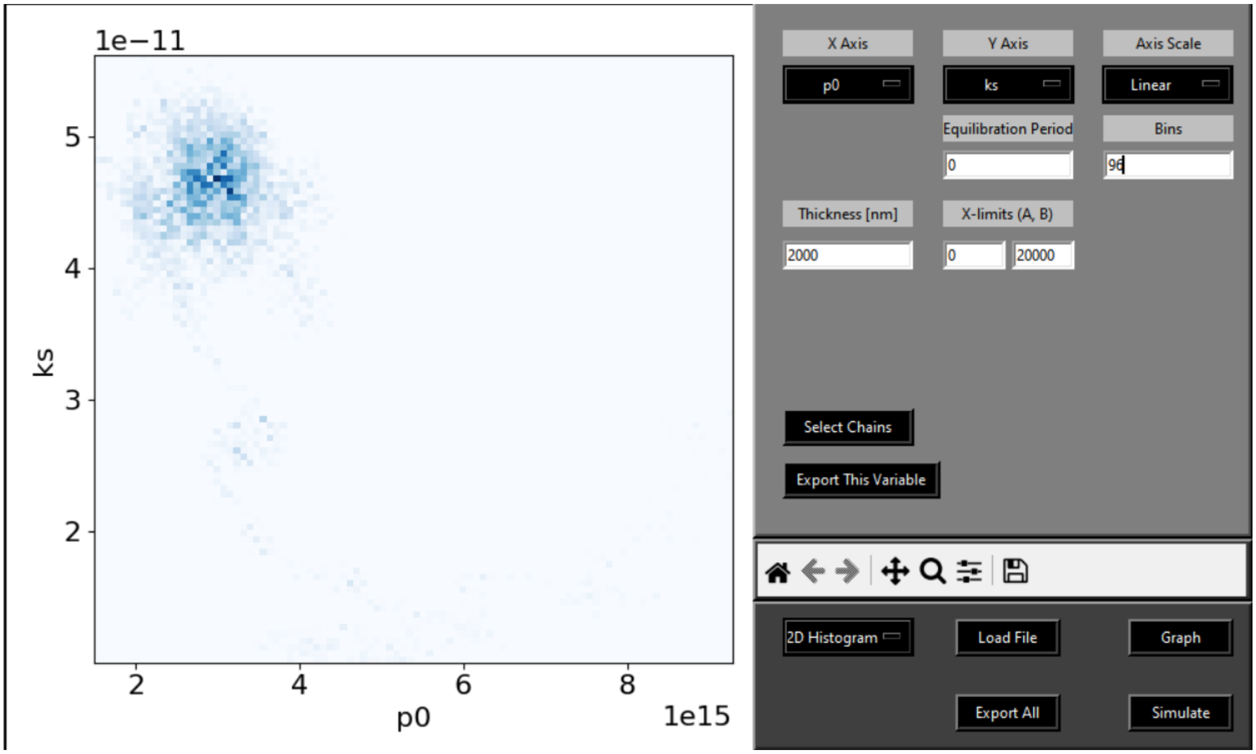

X Axis: p0

Y Axis: ks

Axis Scale: Linear

Equilibration Period: 0

Bins: 96

Thickness [nm]: 2000

X-limits (A, B): 0 20000

- **X Axis** – Selects the state variable to be plotted along the x axis.
- **X Axis** – Selects the state variable to be plotted along the y axis.
- **Axis Scale** – Toggle logarithmic or linear scale for both axes.
- **Equilibration Period** – Truncates the iterations. Only samples at iteration greater than this value will be counted in the histogram. Use the 1D trace plot to determine where the equilibration period should be set.
- **Bins** – Number of bins to draw in the histogram.
- **Thickness [nm]** – Thickness of the material. This only affects some calculated state variables that depend on the thickness, such as surface lifetimes.
- **X-limits (A, B)** – Left and right limits for the x axis.
- **Select Chains** – Toggle the visibility of specific chains in the collection of loaded `.pik` files. Inactive chains will not be plotted or used in calculations/simulations.

4. Running Simulations

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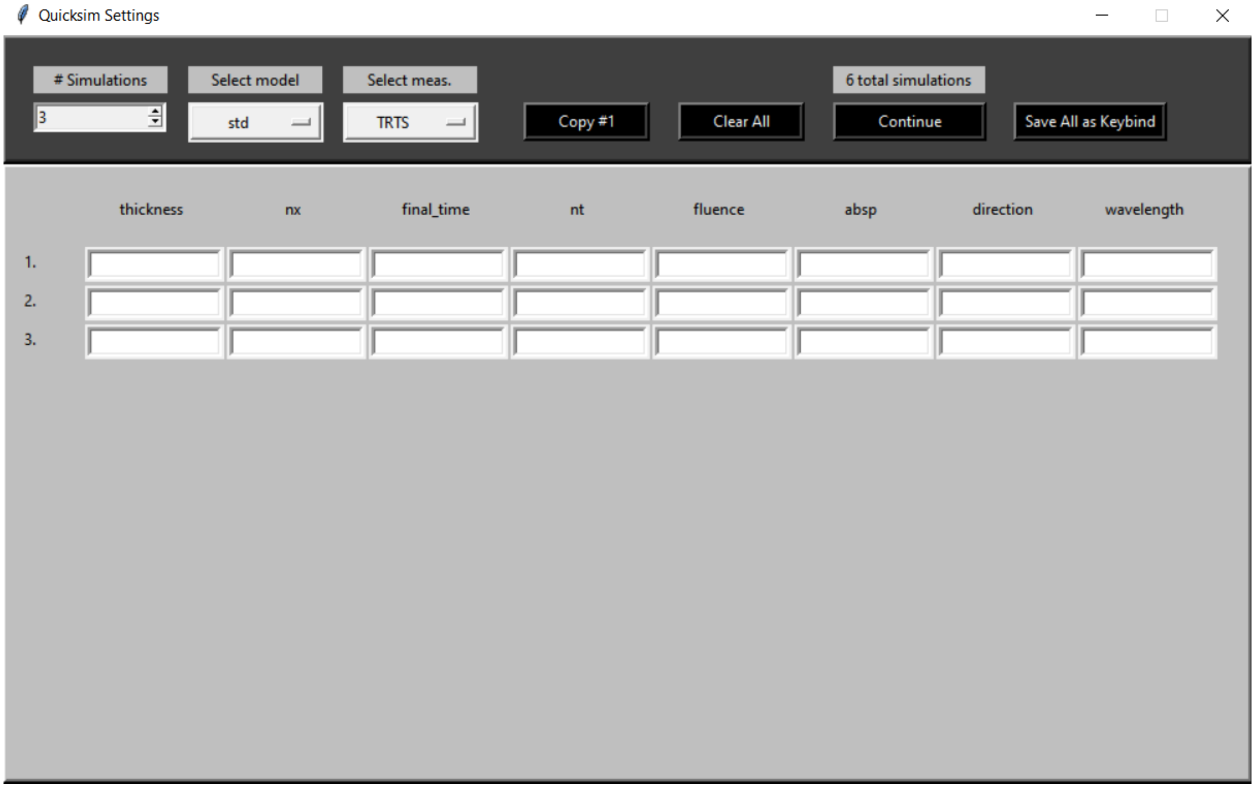


Simulations: 3

Select model: std

Select meas.: TRTS

This feature, accessed by clicking the **Simulate** button on the **Main menu**, allows you to repeat the simulations of any state variable and verify whether they fit the measurement data well.

Note: simulations take state variable values from the *final iteration*.

A popup window opens with two regions - an upper region listing the type and number of simulations to run, and a lower region where the parameters for each simulation is entered.

Each simulation requires the following parameters:

- **thickness** – Thickness or length value, in nm.
- **nx** – Number of space discretization nodes.
- **final_time** – Final time to be reached by the simulation, in ns.
- **nt** – Number of time discretization nodes.
- **fluence** – Fluence for initial carrier profile, in cm^{-2}.
- **absp** – Absorption coefficient for initial carrier profile, in cm^{-1}.
- **direction** – Orientation of carrier profile. Input 1 to make the carrier profile descend from z=0 to z=thickness, and -1 to make the carrier profile descend from z=thickness to z=0.

- **wavelength** – Wavelength used to generate initial carrier profile. *This is not used to calculate the carrier profile – only to determine what instrument response function to convolve simulations with.*

The upper region lists the following options:

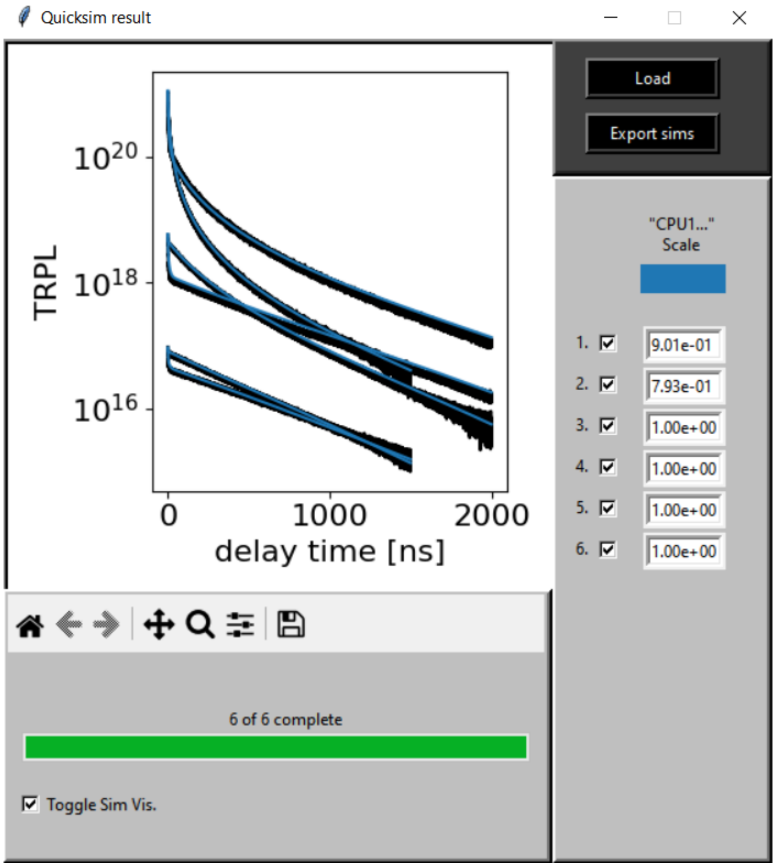
- **# Simulations** – Number of simulations to run per chain. The requested simulations will be run once per active chain, with the state variable values from each chain.

  Note: The **Select Chains** button can still be accessed while this popup is open, if you need to modify which chains are active.

- **Select model** – Select physics model to be used for simulations.
- **Select meas.** – Select type of measurement.
- **Copy #1** – Duplicate the simulation parameters entered for simulation # 1 across all other simulations.

  Note: To duplicate parameters for other simulations, *right click* the region to the right of the wavelength box for that simulation to access a `copy` and `paste` menu.

- **Clear All** – Clear all simulation parameters for all simulations.
- **Continue** – Start the simulations. Also lists the total number of simulations that will be run – **# Simulations** × the number of active chains.
- **Save All as Keybind** – Saves the current simulation parameters as a keybind (shortcut) file. Keybind files are text files named with single keyboard character names. The next time simulations are run, that keyboard character can be pressed to automatically reload the simulation parameters.



"CPU1..."
Scale

1. ☑ 9.01e-01
2. ☑ 7.93e-01
3. ☑ 1.00e+00
4. ☑ 1.00e+00
5. ☑ 1.00e+00
6. ☑ 1.00e+00

Once the simulations are started, a new popup will appear to display the results of the simulation. Clockwise from the top left, this popup contains a plot window, an export menu, a simulation options area, a progress bar, and additional plot options.

The plot window starts blank but is populated with results when all simulations are complete.

The **Load** button allows you to select measurement data to plot alongside the simulations. Measurement data should come from the same `.csv` files that were originally inputted to the Monte Carlo run.

The **Export sims** button allows you to export the simulation results as a `.csv` file.

If you are working with experimental data or have defined scaling factors in the Monte Carlo run, the simulations will probably not coincide well with the measurement data. The GUI will attempt to populate the simulation options area with scaling factors taken from the state variable lists–you should double check these by reviewing the 1D trace plots for each scaling factor. Simulations for each chain are color coded, and the checkboxes can be used to toggle visibility of specific simulations.

The **Toggle Sim Vis.** button under the progress bar also allows you to toggle the visibility of all simulations.

5. Exporting State Data

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The **Main menu** contains an **Export All** button, which exports all state variables for all active chains as `.csv` files. These files are all stored within a single timestamped directory.

Additionally, the **Visualization settings** contains an **Export This Variable** button, which exports data regarding the currently displayed state variable. The data depends on the visualization type:

- For **1D trace plots**, a list of values indexed by iteration to recreate the line shown in the trace plot.
- For **2D trace plots**, a list of (x, y) coordinates indexed by iteration to recreate the line plotted in 2D.
- For **1D histograms**, a list of bin centers and counts to recreate the histogram bars.
- For **2D histograms**, a frequency matrix to recreate the heatmap.

6. Advanced Users

6.1. Adding and enabling new state variables

To add new state variables that can be calculated from existing state variables, open the `secondary_params.py` file and add a method to the `SecondaryParameters` class detailing how the new variable should be calculated. This method should accept two arguments: 1) `self`, and `p`, a dictionary keyed by names of other state variables, and should return an array-like of the new variable's values.

Then, add an entry to the `func` attribute of the SecondaryParameters class. This entry should have the name of the new variable as a key and a 2-tuple as its value - first element the method, and second element a tuple of the state variables needed to calculate the new variable.