Kinetic TBN Simulator User Guide

1 Introduction

The Kinetic TBN Simulator is a web-based tool for exploring the behavior of thermodynamic binding networks under different kinetic approaches. Users can enter a monomer set, choose a start configuration, select an approach, and step through possible configurations.

This guide explains how to use the Kinetic TBNs web interface. It does not require installing Haskell, Cabal, or running commands in a terminal.

The next section gives a suggested workflow for a typical run. The remaining sections explain each feature in more detail.

2 Suggested Workflow

For a typical exploration:

1. Select an example system.
2. Click **Use Example** for the monomer set and start configuration.
3. Update the approach if needed.
4. Click **Start Simulation**.
5. Inspect the applicable and non-applicable next configurations.
6. Click **Next** to advance.
7. Label interesting configurations.
8. Use **List Saved** and **Load History** to review the run.
9. Export configurations or the full system when needed.

3 Interface Overview

The web interface is divided into three main areas:

- **Input panel:** used to select or enter a monomer set, start configuration, and approach.
- **Configuration display:** shows the current configuration and selected configurations.
- **Control panel:** contains buttons for starting, pausing, stepping through, saving, loading, and exporting simulations.

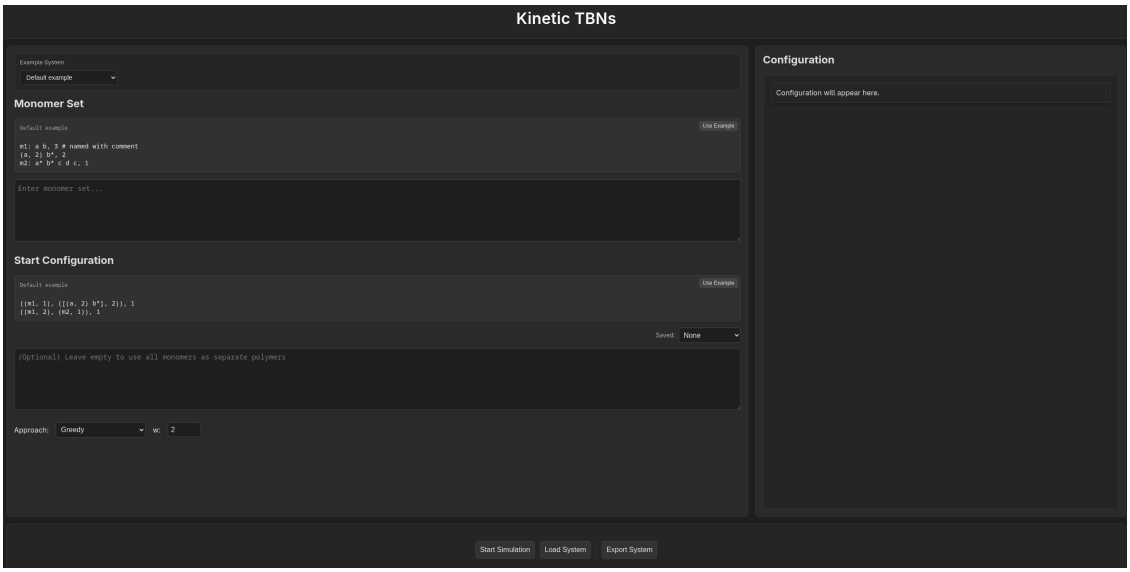

Figure 1: Main parts of the Kinetic TBN Simulator interface.

4 Setting Up a System

Before running a simulation, the user must provide a monomer set and optionally a start configuration.

4.1 Loading an Existing Example

The easiest way to begin is to load one of the built-in examples.

1. Open the **Example System** dropdown.
2. Select an example system.
3. The example preview boxes for the monomer set and start configuration will update.
4. Click **Use Example** under **Monomer Set**.
5. Optionally, click **Use Example** under **Start Configuration**.
6. Check the selected approach and the value of w, or k if a threshold approach is selected.
7. Click **Start Simulation**.

Changing the example dropdown only changes the preview. The monomer and start configuration input boxes are not filled until the user clicks **Use Example**.

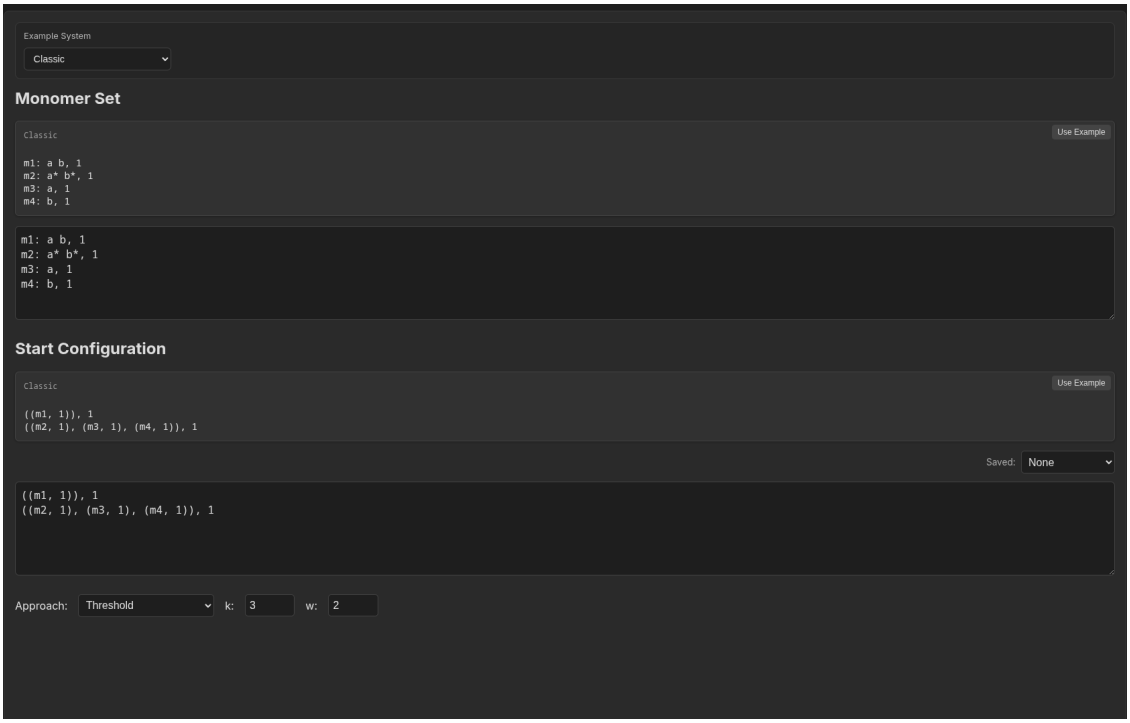

Figure 2: Selecting an example system from the dropdown.

4.2 Adding Your Own System

Users may also type their own monomer set and start configuration.

The **Monomer Set** box defines the available monomers and their counts. A named monomer has the form

```
name:  domains, count of monomer
```

For example:

```
m1:  a b, 3
```

An unnamed monomer may also be entered directly:

```
a* b* c, 1
```

Users can also define a monomer with multiple counts of a domain. Each of the following monomers have 2 $a*$.

```
a* a* b* c, 1
```

```
a* b* a* c, 1
```

```
(a*, 2) b* c, 1
```

The **Start Configuration** box is optional. If it is left empty, the simulator creates a default start configuration in which all monomers begin as separate polymers.

A start configuration consists of polymers and their counts. For example:

```
((m1, 1), (m2, 1)), 1
```

represents one polymer containing one copy of `m1` and one copy of `m2`.

4.3 Loading a System from File

A previously exported system can be loaded from a JSON file.

1. Click **Load System**.
2. Select the exported JSON file.
3. The simulator restores the saved system state.

Loaded systems may include the current configuration, saved configurations, history, the active approach, and other simulator state.

5 Choosing an Approach

The approach determines which next configurations are considered applicable and how the simulator chooses a next step.

Common approaches include:

- **Greedy:** allows transitions that do not increase energy and chooses among the lowest-energy applicable configurations.
- **Threshold:** allows transitions within a specified energy barrier k.
- **Stochastic:** chooses among applicable configurations with probabilities based on counts.
- **Weighted:** chooses among all next configurations using probabilities proportional to an exponential weighting based on energy and configuration counts.
- **Favorable:** chooses among configurations that do not increase energy using probabilities proportional to an exponential weighting based on energy and configuration counts.
- **Guided:** lets the user manually select the next configuration.
- **Thermal (τ) approaches:** use a sequence of w-values and attempt the base approach at different values of w.

The w-input controls the energy parameter used by most approaches. For thermal approaches, the input changes to a sequence of values, such as:

```
<2, 3, 0.5, 1>
```

6 Running a Simulation

After setting up the system, click **Start Simulation**. The simulator displays the current configuration and computes possible next configurations.

6.1 The Current Configuration

The current configuration appears in the main configuration display. It includes a diagram of the polymers and the energy value.

For thermal examples or cases where different w-values are relevant, the display may also show the w-value used to compute the configuration.

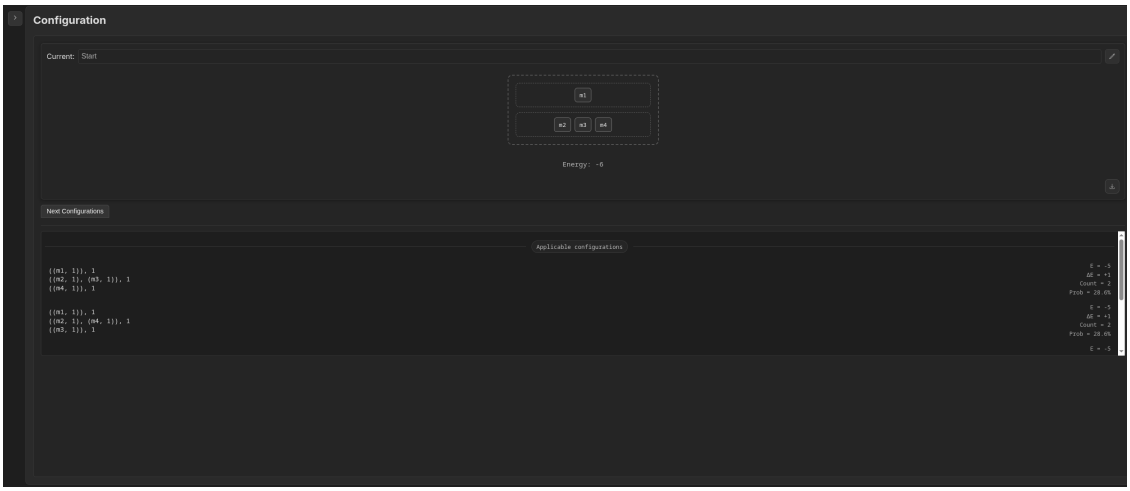

Figure 3: The current configuration and possible next configurations.

6.2 Next Configurations

The **Next Configurations** panel lists possible configurations that can be reached from the current configuration in one step.

The panel may be divided into:

- **Applicable configurations:** configurations allowed by the selected approach.
- **Non-applicable configurations:** configurations that are possible one-step changes, but are not allowed by the current approach.

Each next configuration may display:

- its energy E,
- the energy change ΔE,
- its count, except for transitional or guided approaches,
- its probability, for all approaches, except for the guided approach.

The non-applicable configurations can be shown or hidden using the divider button.

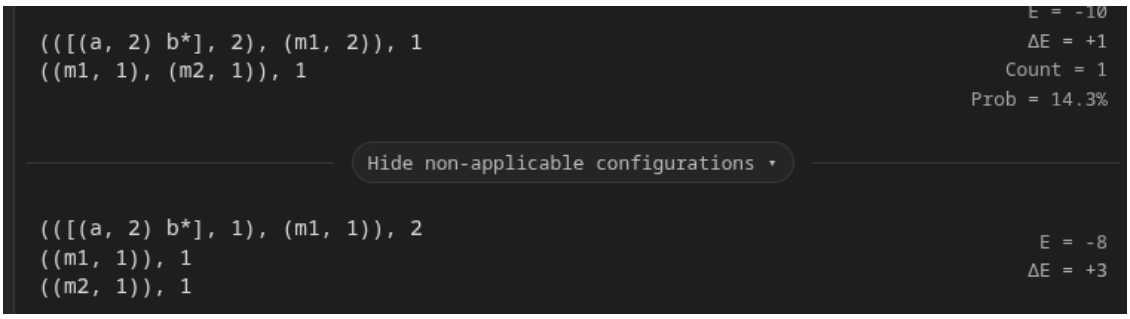

Figure 4: Non-applicable configurations.

6.3 Taking a Step

Click **Next** to advance the simulation.

The simulator chooses one applicable next configuration according to the selected approach. The chosen configuration becomes the new current configuration, and it is added to the simulation history.

If the **Next** button is disabled, then there are no applicable configurations under the current approach.

6.4 Guided Steps

When using the **Guided** approach, radio buttons appear next to applicable configurations.

1. Select the configuration you want to take.
2. Click **Next**.

The selected configuration becomes the new current configuration.

6.5 Changing Approach During a Run

The **Change Approach** button allows the user to switch approaches without restarting the simulation.

This keeps:

- the current configuration,
- the history,
- saved configurations.

Only the approach is changed, and the next configurations are recomputed using the new approach.

This is useful when a user wants to explore with one approach and then switch to another approach to test stability or continue the run.

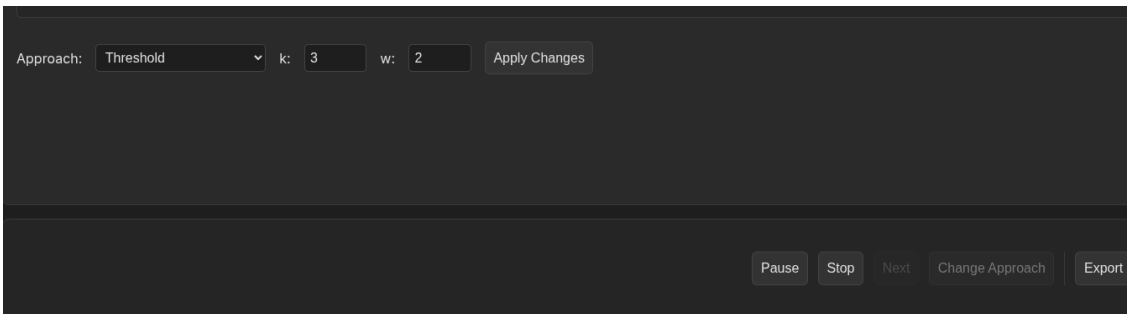

Figure 5: Changing the approach without restarting the simulation.

7 Saving and Labeling Configurations

Configurations can be saved by assigning them labels.

7.1 Labeling the Current Configuration

To save the current configuration:

1. Click the pencil icon next to the current configuration label.
2. Type a label.
3. Click the checkmark to save the label.

Once labeled, the configuration is added to the saved configurations.

If there is an error, such as using a reserved or conflicting label, the error appears near the label input.

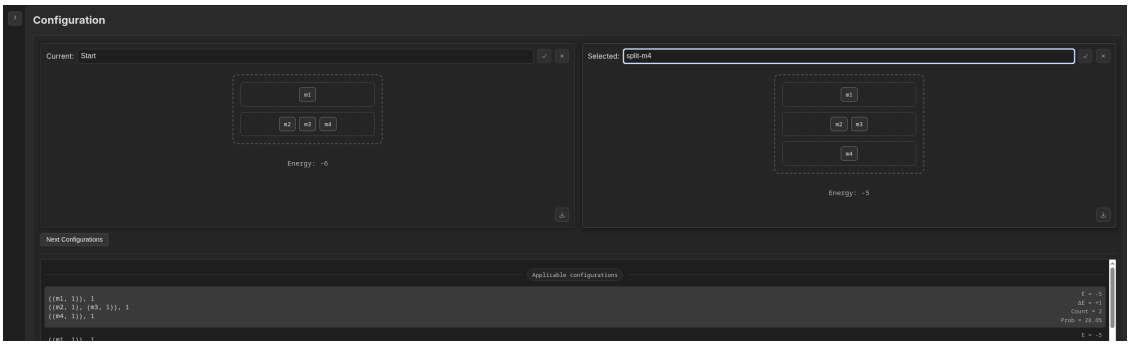

Figure 6: Saving configurations by labeling them.

7.2 Labeling a Selected Configuration

Users can also click a next, saved, or history configuration to view it beside the current configuration. The selected configuration can also be labeled.

This is useful for saving interesting configurations that are not necessarily current. If the current configuration is selected, the user can also update its label here.

8 Saved Configurations

8.1 Listing Saved Configurations

Click **List Saved** to open the saved configurations panel.

Saved configurations are configurations that have been assigned labels. Clicking a saved configuration displays it in the selected configuration view.

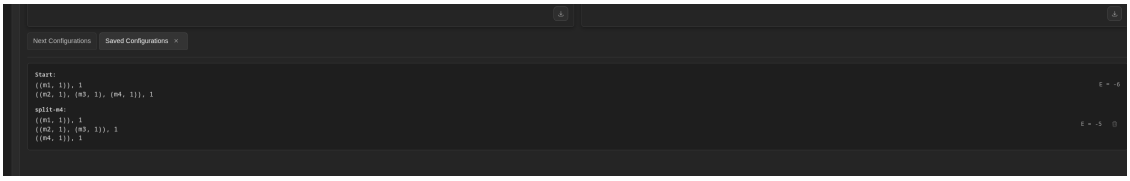

Figure 7: Viewing saved configurations.

8.2 Deleting Saved Configurations

Saved configurations can be deleted from the saved list. Deleting a saved label does not remove the configuration from the history. It only removes the saved label.

The start configuration cannot be deleted.

9 Using the History

The simulator stores the sequence of configurations visited during a run.

9.1 Loading History

Click **Load History** to display the history panel.

Each history item represents a configuration that appeared as the current configuration during the run.

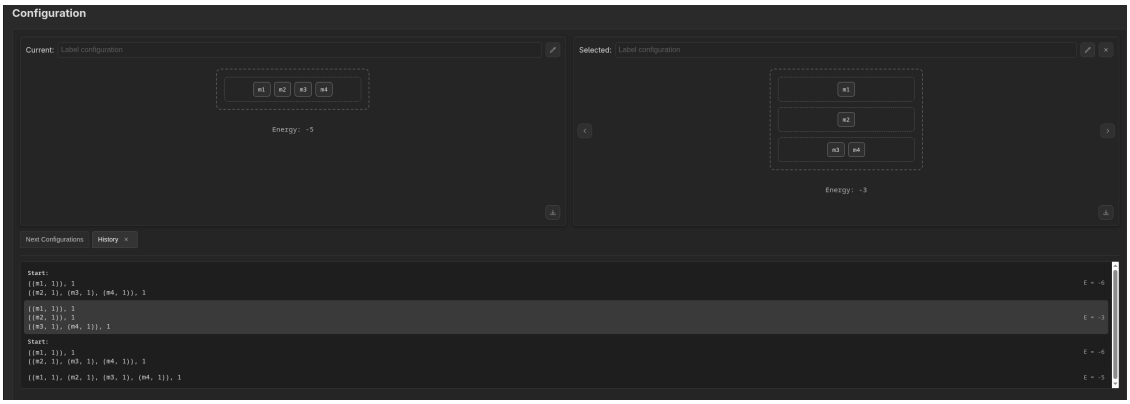

Figure 8: Viewing the simulation history.

9.2 Viewing Previous and Next History Items

Clicking a history item displays it beside the current configuration. When viewing a history item, the arrow buttons can move to the previous or next item in the history sequence.

This is useful for reviewing how the simulation reached its current state.

10 Exporting Results

10.1 Exporting a Configuration as SVG

Each rendered configuration has a download icon. Clicking this icon exports the visible configuration diagram as an SVG file.

This is useful for including configurations in reports, presentations, or notes.

10.2 Exporting the System

Click **Export System** to download the current simulation state as a JSON file.

The exported system may include:

- the monomer set,

- the start configuration,
- the current configuration,
- saved configurations,
- the history,
- the current approach.

The exported file can be loaded later using **Load System**.

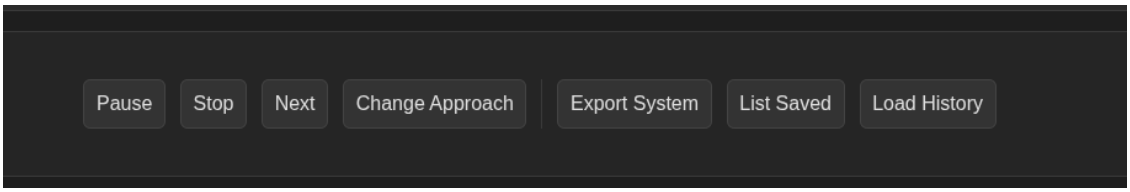

Figure 9: Running controls, including export, history, saved configurations, and pause buttons.

11 Pausing and Resuming

11.1 Pausing a Simulation

Click **Pause** to pause the simulation.

While paused, users may edit the start configuration and approach. This is different from **Change Approach**. Pausing is used when the user wants to restart the run from a new start configuration.

The dropdown next to the start configuration input panel can be used to choose one of the saved configurations as the new starting point.

11.2 Resuming with a New Start

After editing the start configuration or approach, click **Resume**.

When resuming:

- the simulation restarts from the edited start configuration,
- the edited start configuration becomes the new current configuration,
- the history is reset for the new run,
- saved configurations are preserved.

This allows users to keep important saved configurations while starting a new run from a different starting point.

12 Common Issues

12.1 The Next Button Is Disabled

If **Next** is disabled, then there are no applicable configurations under the current approach.

Try one of the following:

- switch to a different approach using **Change Approach**,
- use a threshold approach with a larger value of k,
- inspect the non-applicable configurations,
- restart from a different start configuration.

12.2 The Start Configuration Does Not Parse

Check for common syntax mistakes:

- missing parentheses,
- missing commas,
- unmatched brackets,
- misspelled monomer names,
- using a monomer type when the type is ambiguous.

12.3 Ambiguous Monomer Types

If two monomers have the same type, the simulator may not know which monomer is intended.

For example, if both `input` and `output` have the same domains, then writing the type directly may be ambiguous. In that case, use the monomer name:

```
(input, 1)
```

instead of writing the type directly.

12.4 Changing an Example Does Not Fill the Input Boxes

Selecting an example from the dropdown changes the preview only. To copy it into the input box, click **Use Example**.

12.5 Exported Systems Store the Current State

Exported systems store the current simulation state and the current approach used to continue the simulation. They do not store a full log of every approach previously used during the run.