

# OpenPathSampling Mini-Tutorial

SimStore and the OPS CLI

*Part 1: Setting up with SimStore*

[http://github.com/openpathsampling/mini-tutorials/  
simstore\\_and\\_cli](http://github.com/openpathsampling/mini-tutorials/simstore_and_cli)

# OPS Workflows



**Setup**

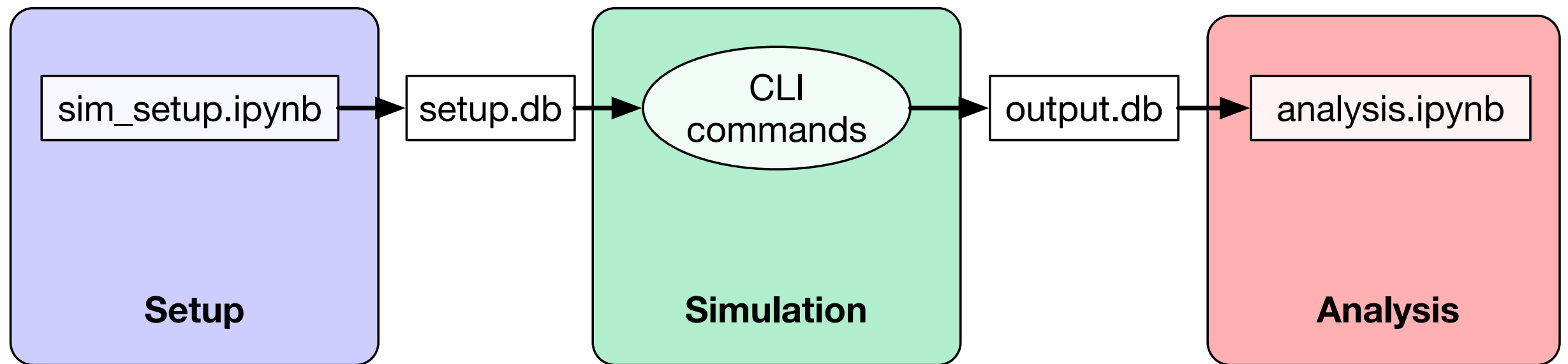


**Simulation**

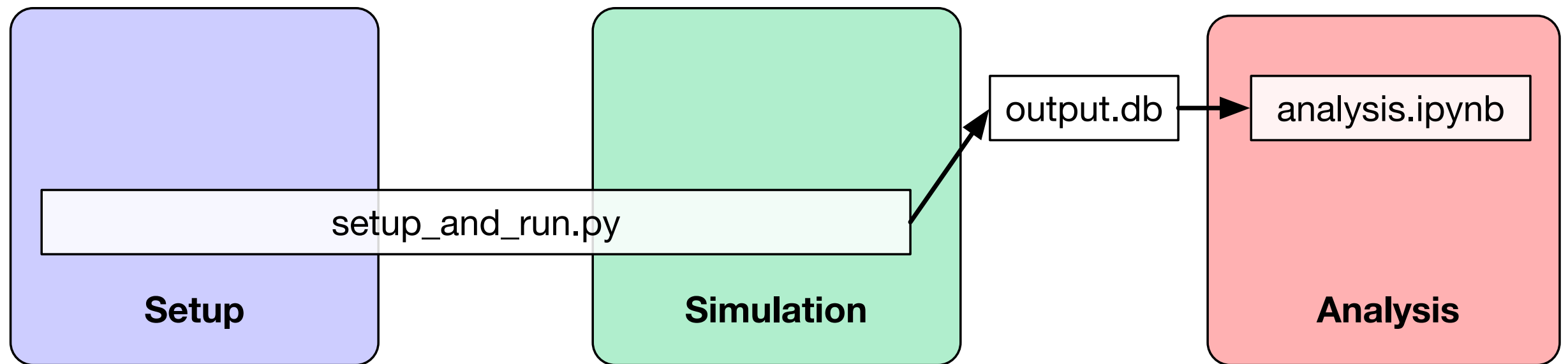


**Analysis**

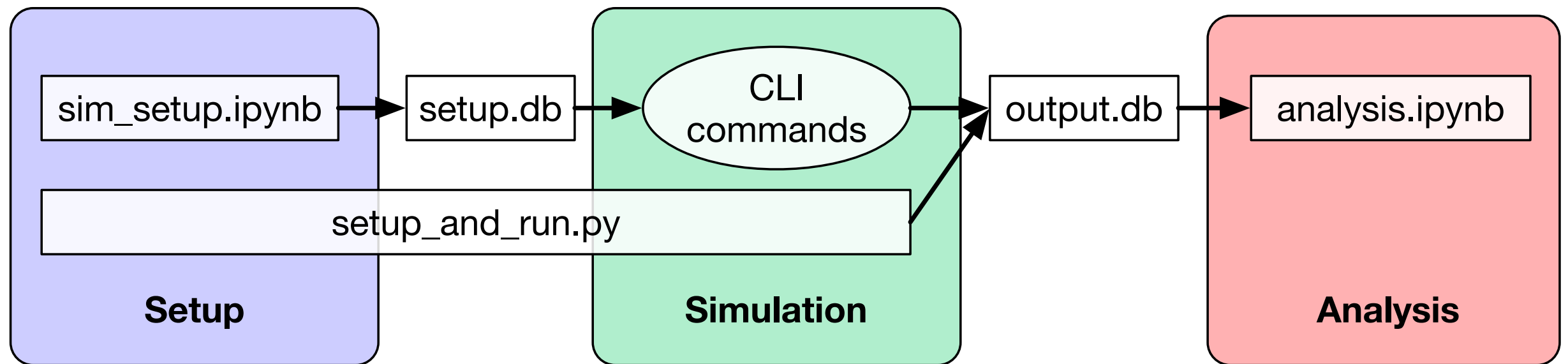
# OPS Workflows



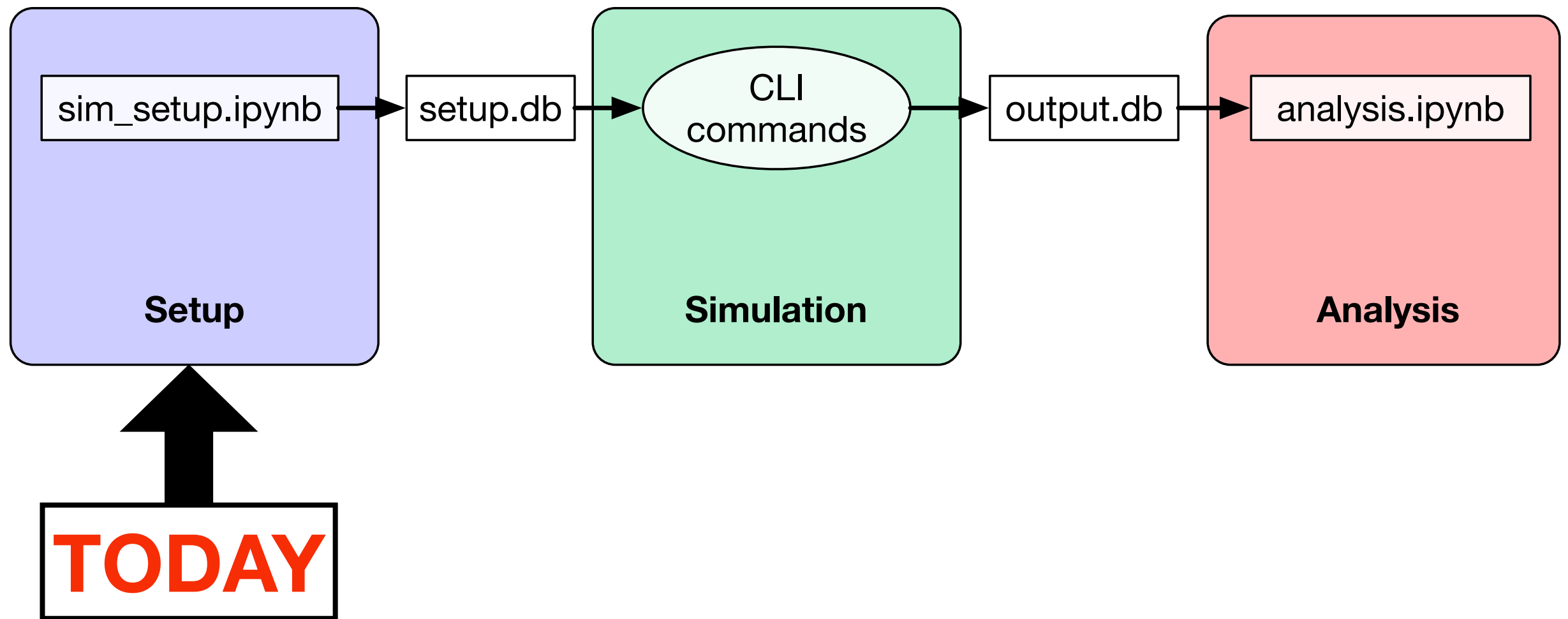
# OPS Workflows



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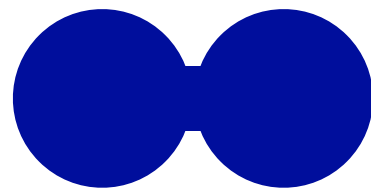
# OPS Workflows



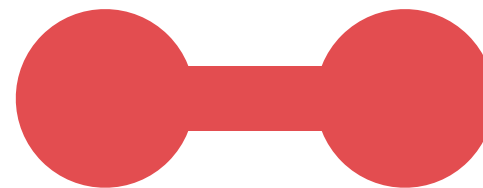
Setting up the simulation:

First phase of CLI workflow (but no CLI) and saving to SimStore

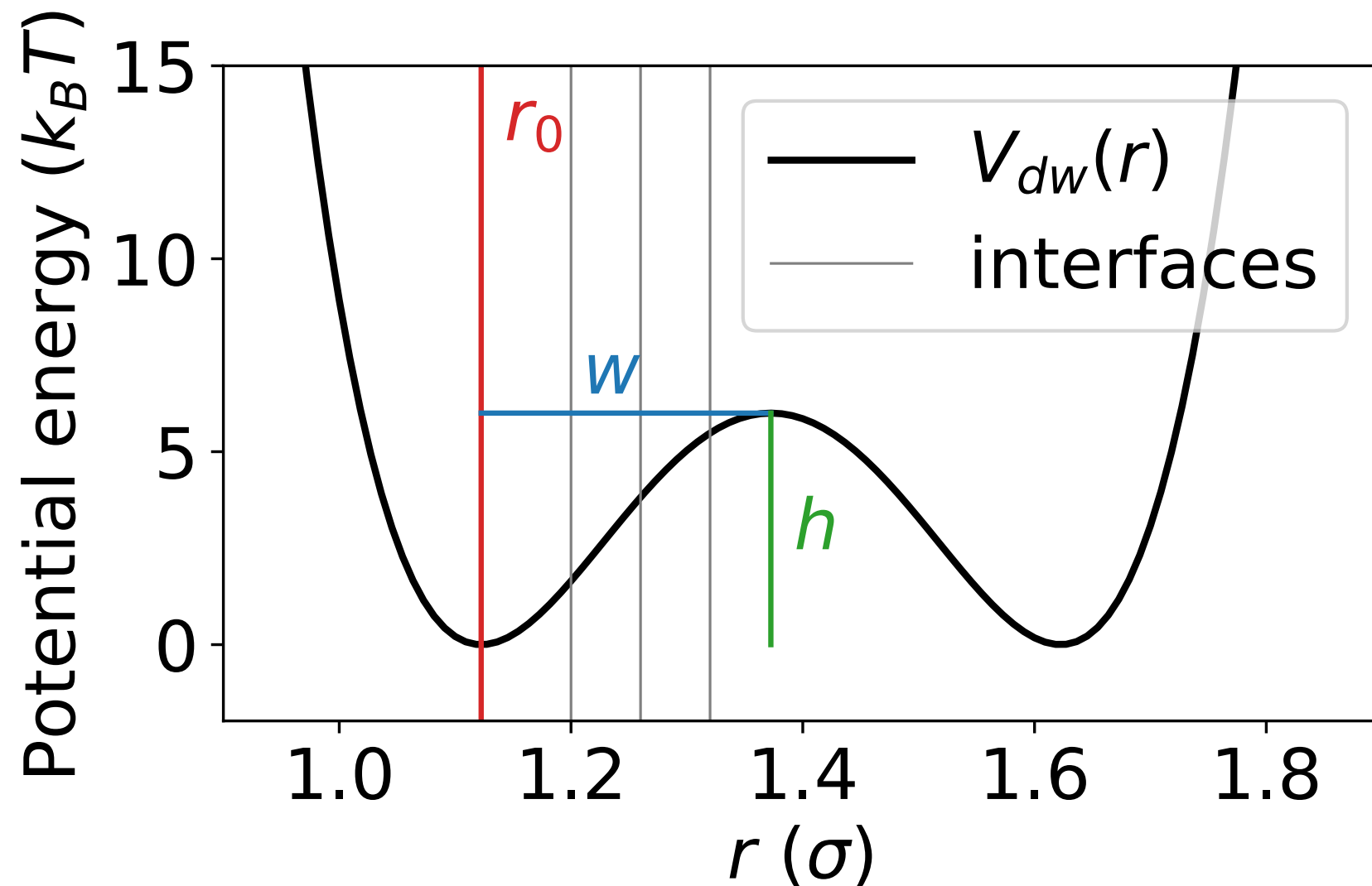
# Simple Bistable Model



condensed



extended



# SimStore

Files ending in .db instead of .nc

## Advantages

- Faster
- Smaller (especially small files)
- Ready for parallel

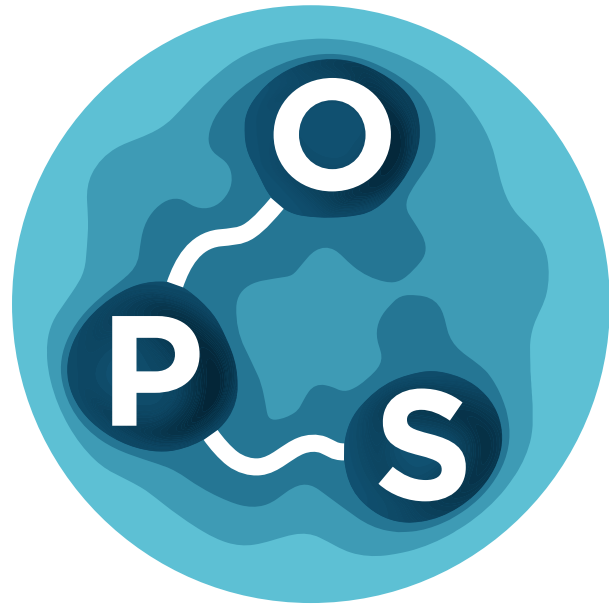
## Disadvantages

- Requires (small) changes to scripts
- May have problems in edge cases

Try it out and let us know what you find!







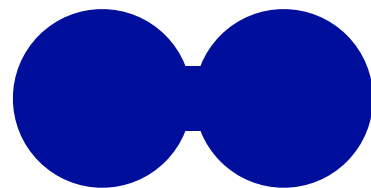
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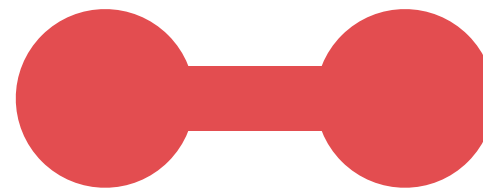
*Part 2: Running simulations with the CLI*

[http://github.com/openpathsampling/mini-tutorials/  
simstore\\_and\\_cli](http://github.com/openpathsampling/mini-tutorials/simstore_and_cli)

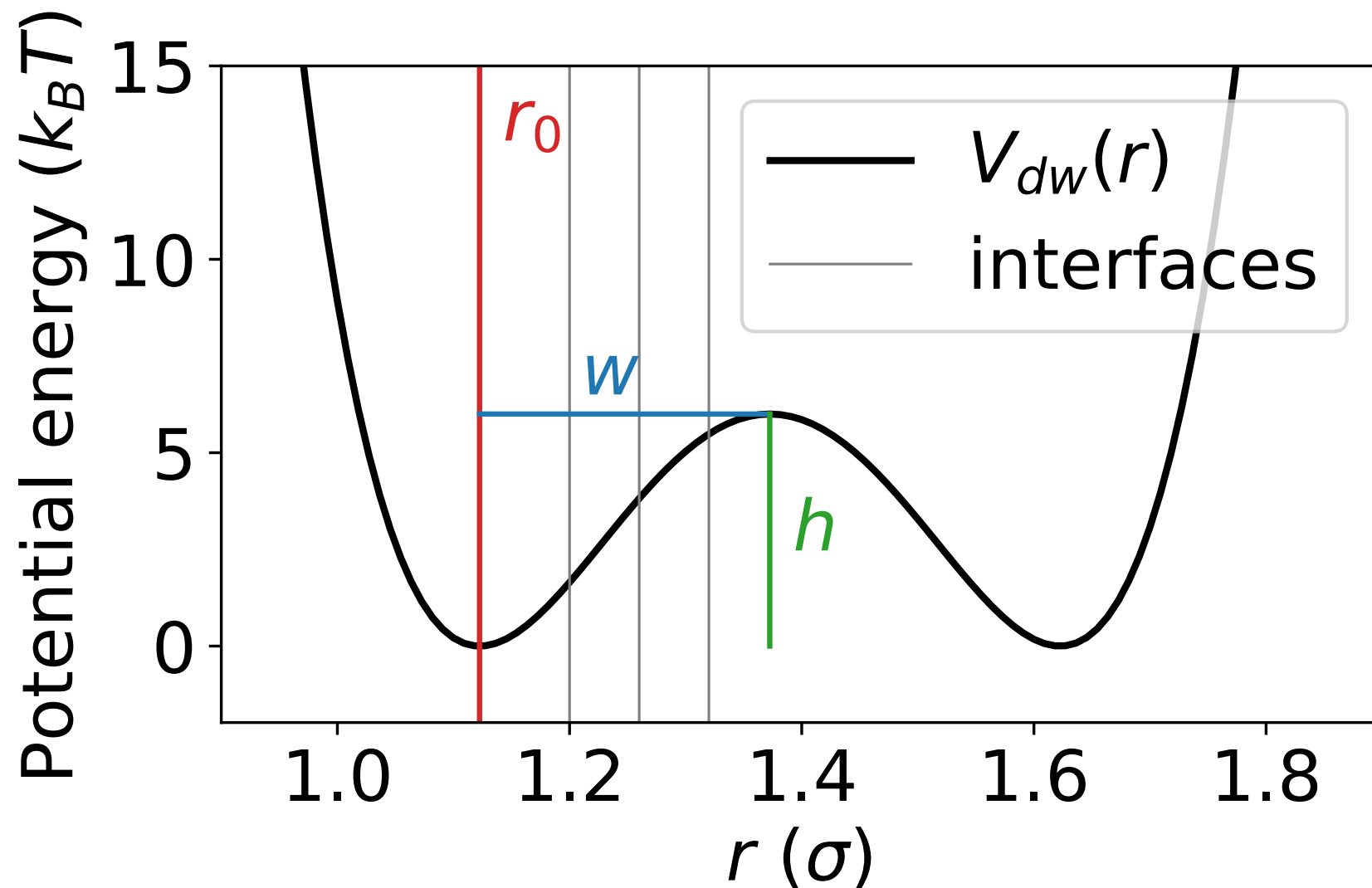
# Simple Bistable Model



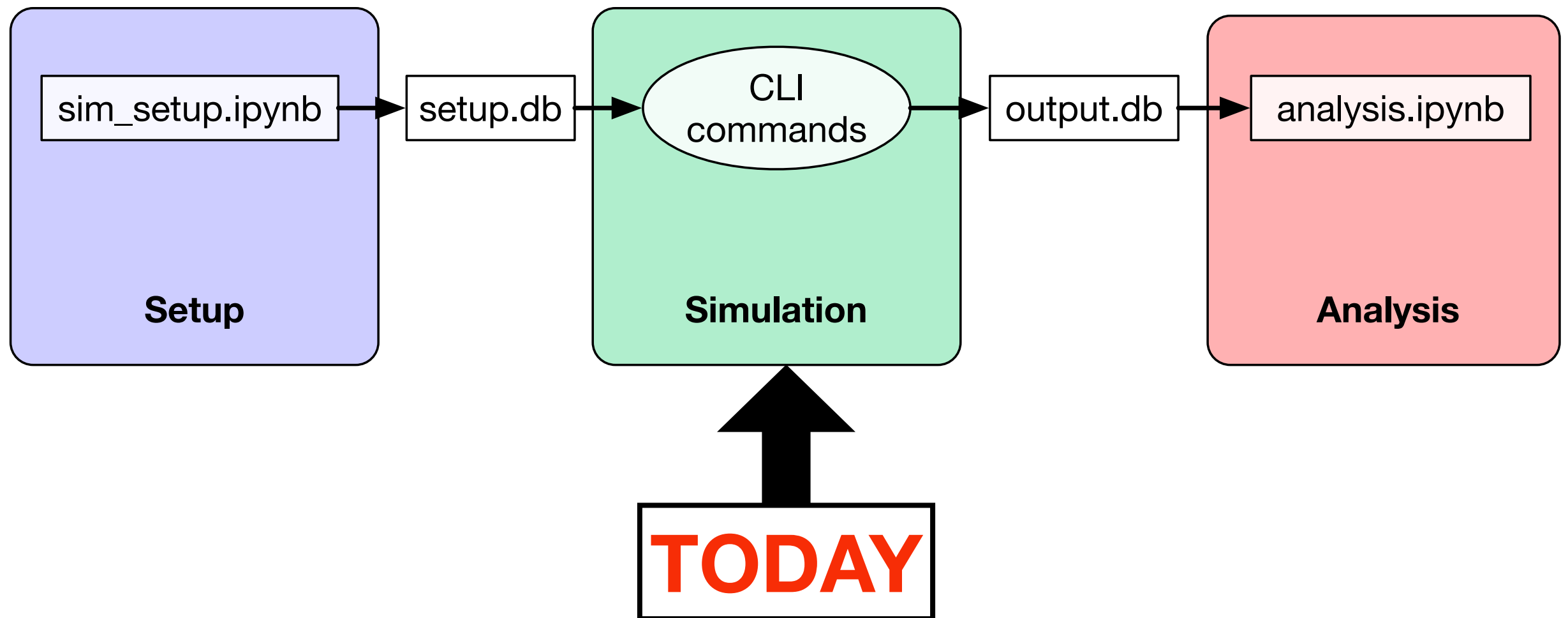
condensed



extended

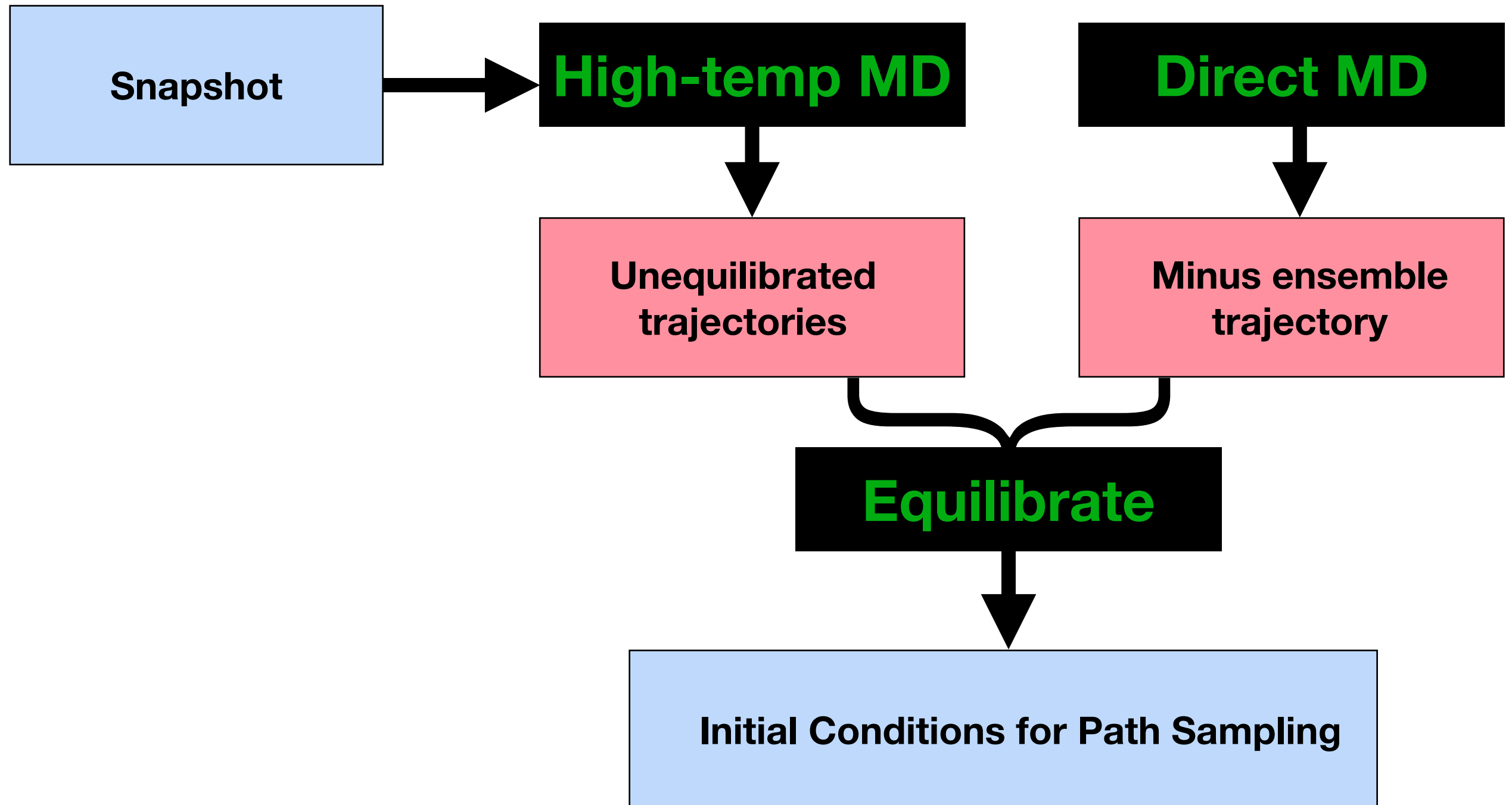


# OPS Workflows

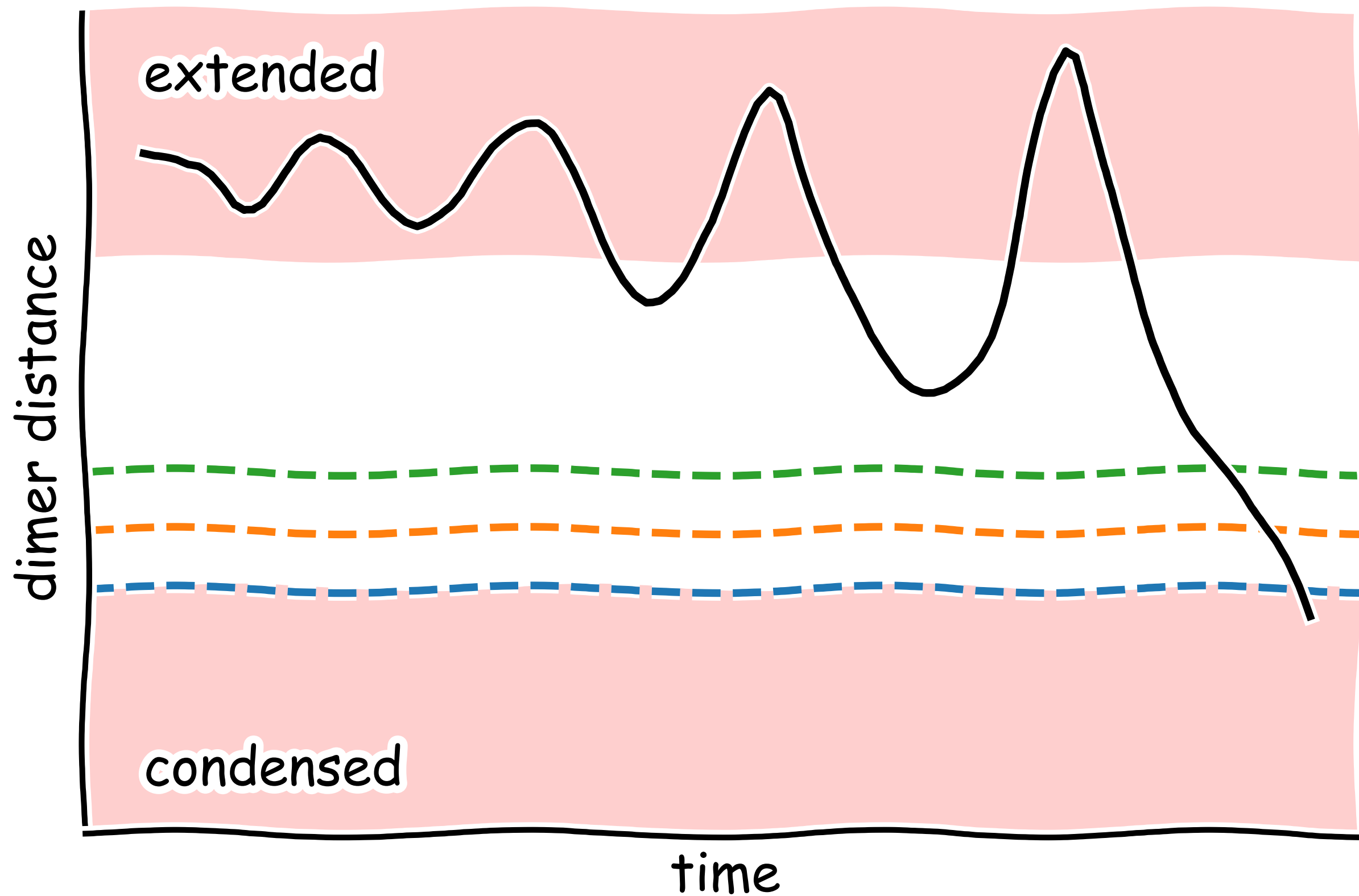


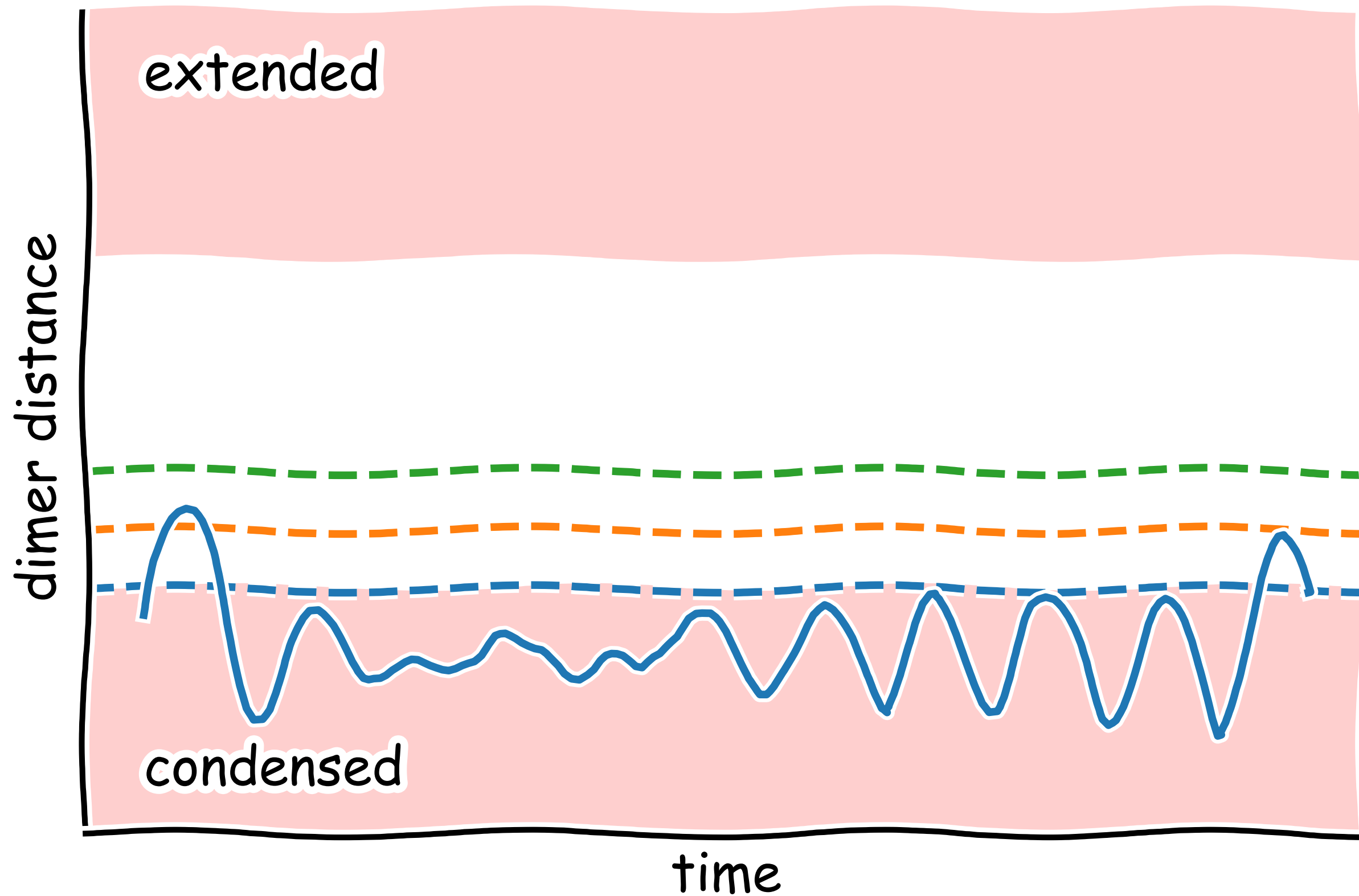
Running the simulation with the CLI:  
From a snapshot to path sampling (no Python!)

# Snapshot to Path Sampling

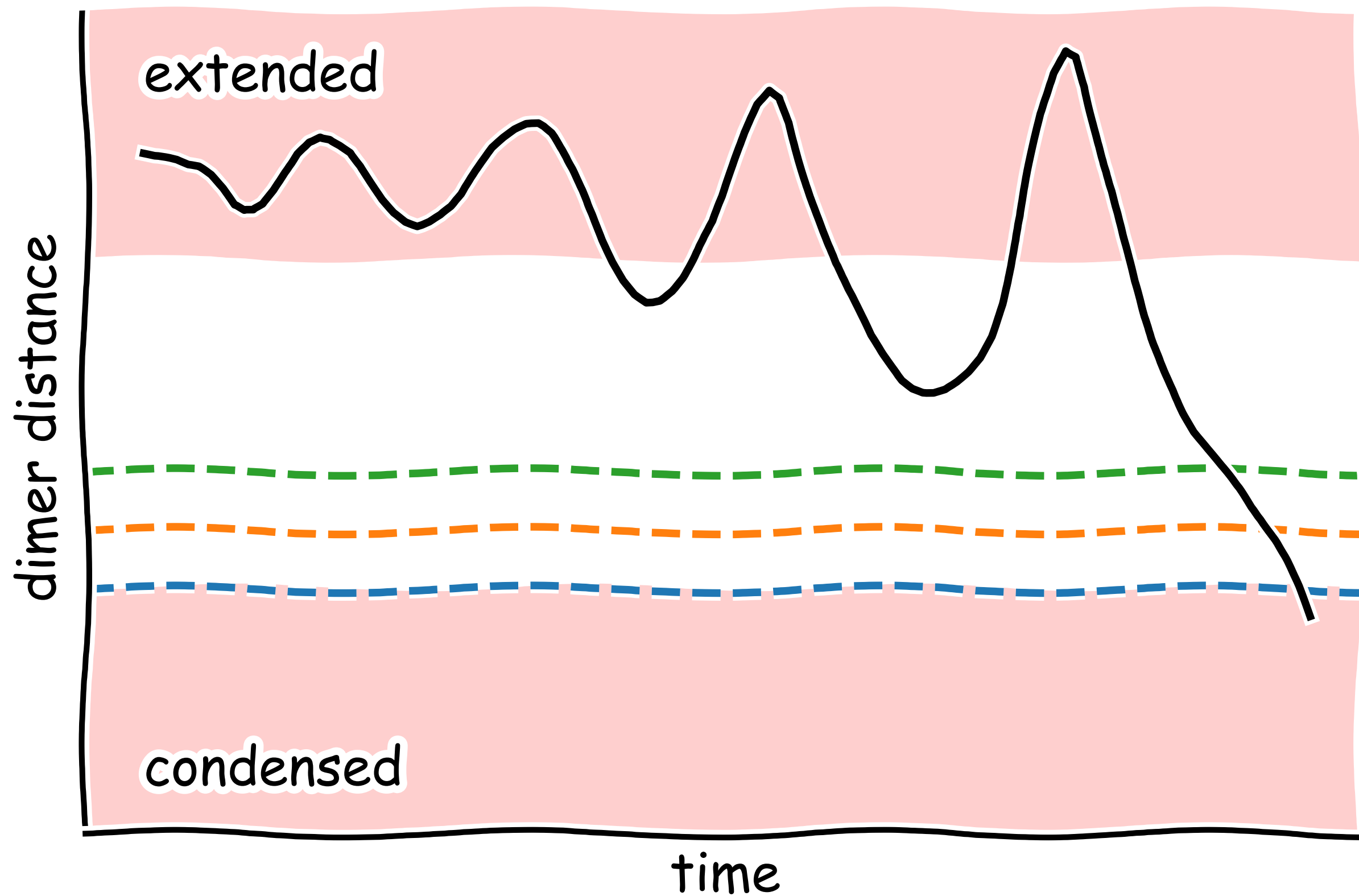


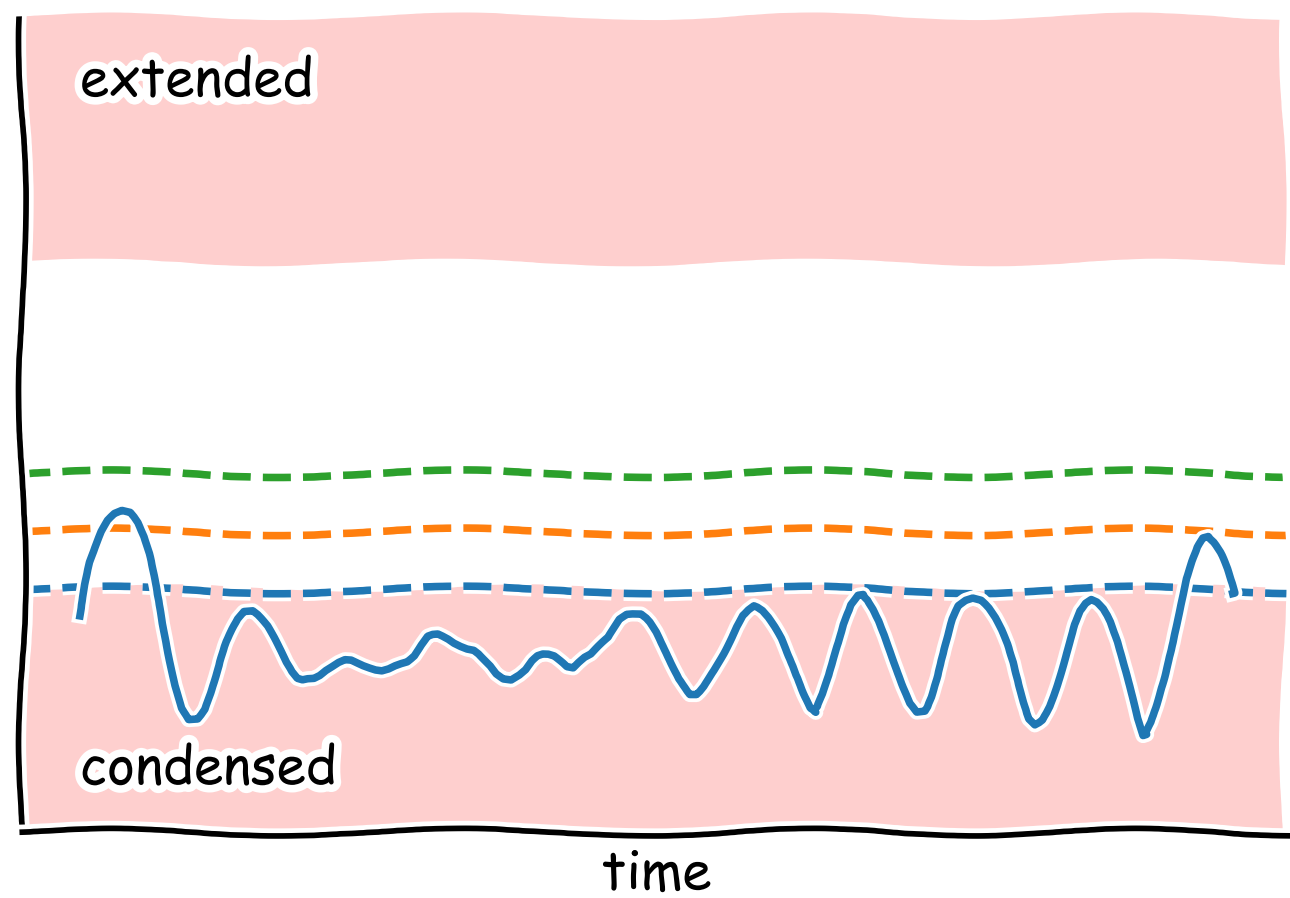
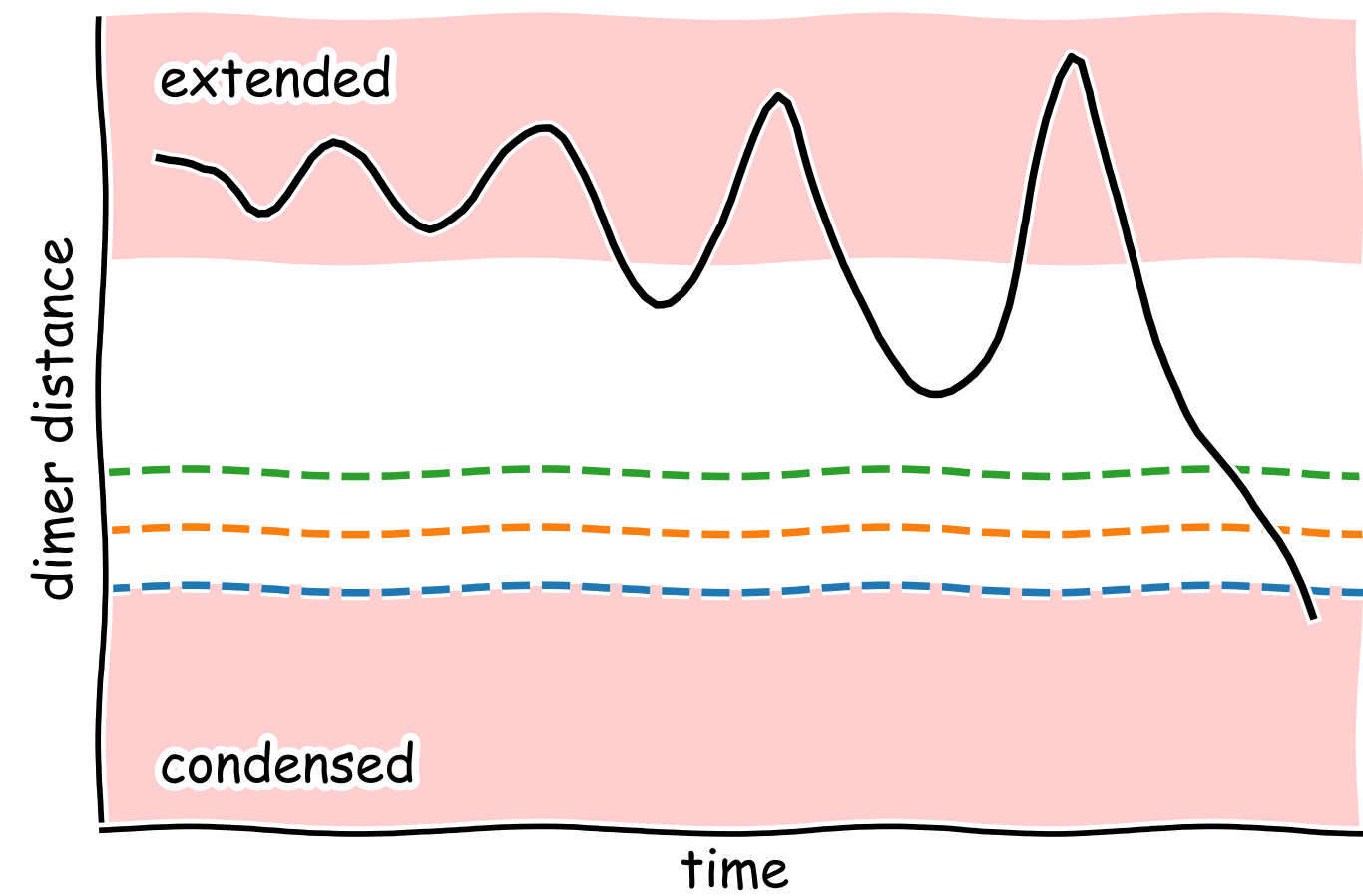




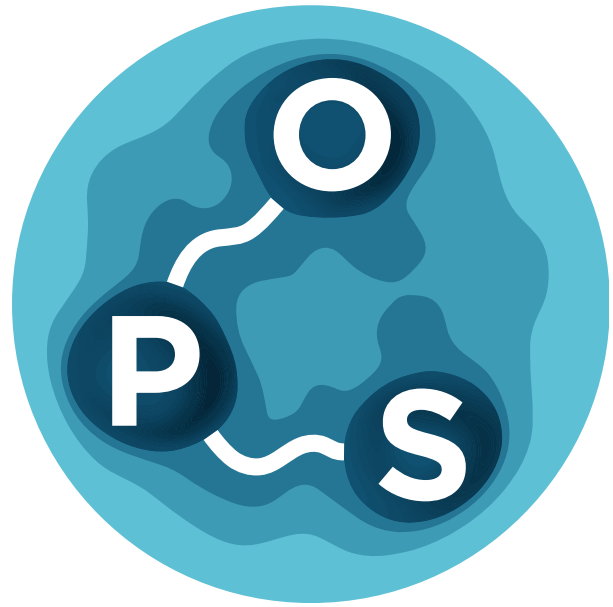












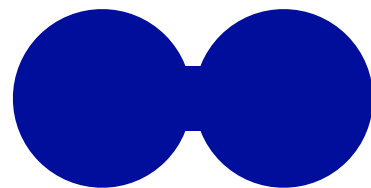
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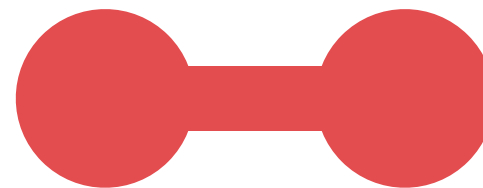
*Part 3: Analyzing results*

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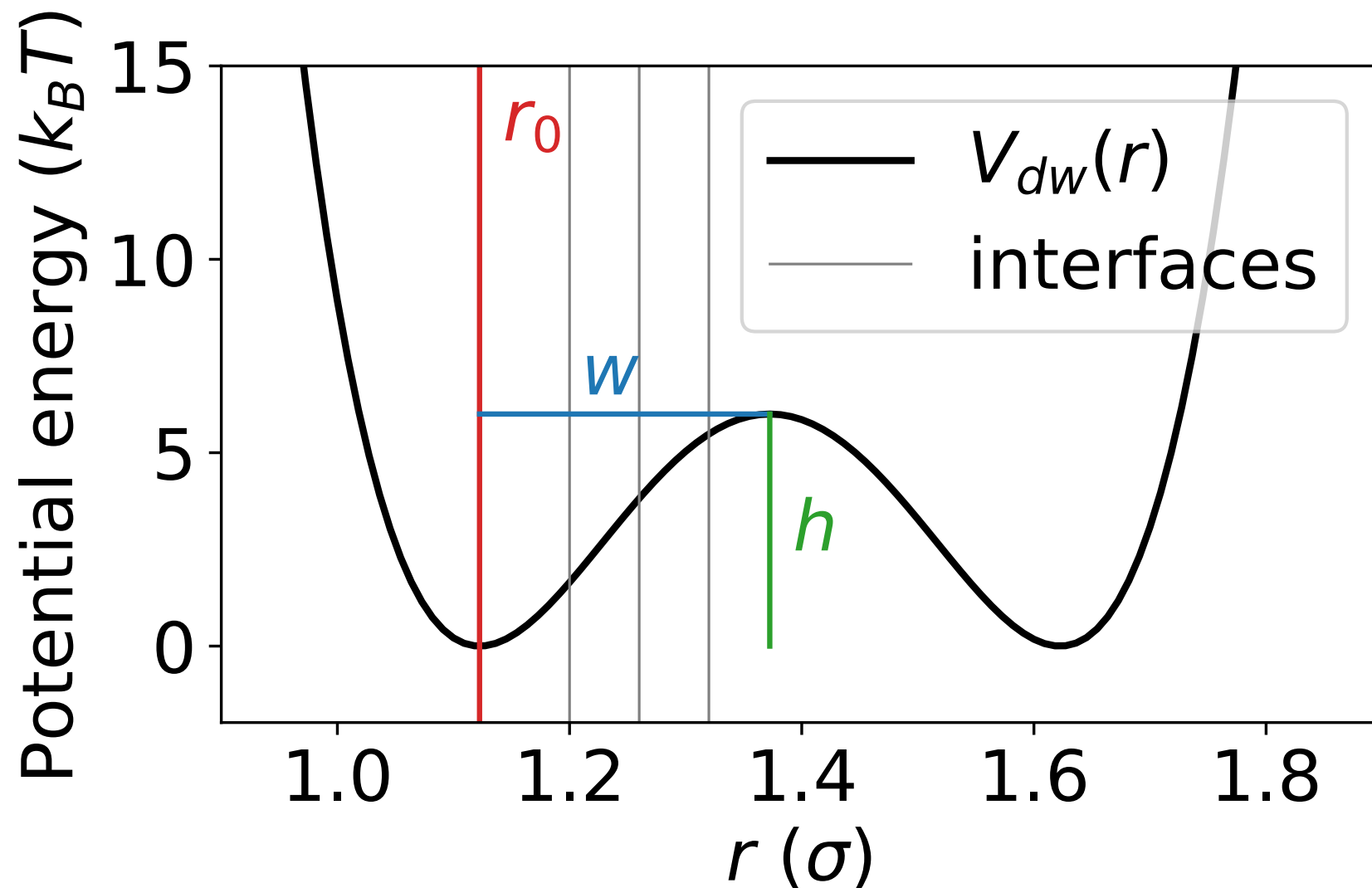
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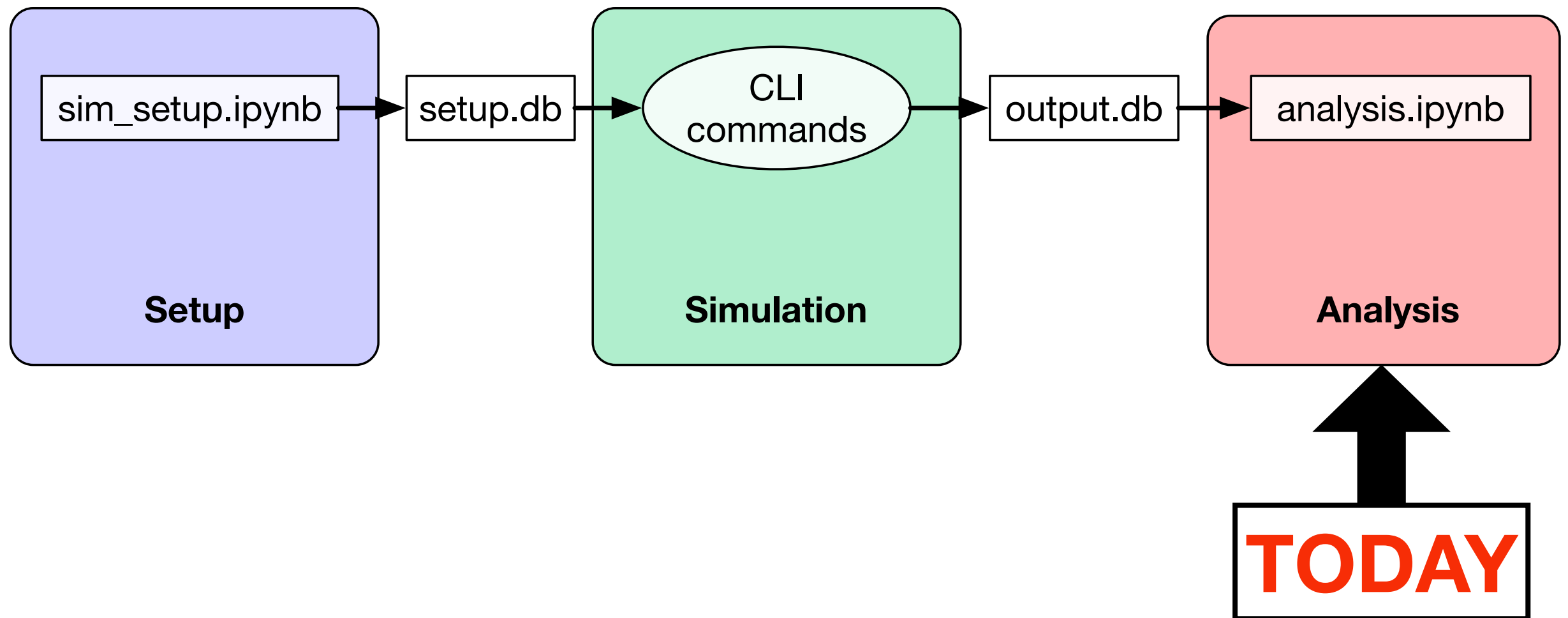
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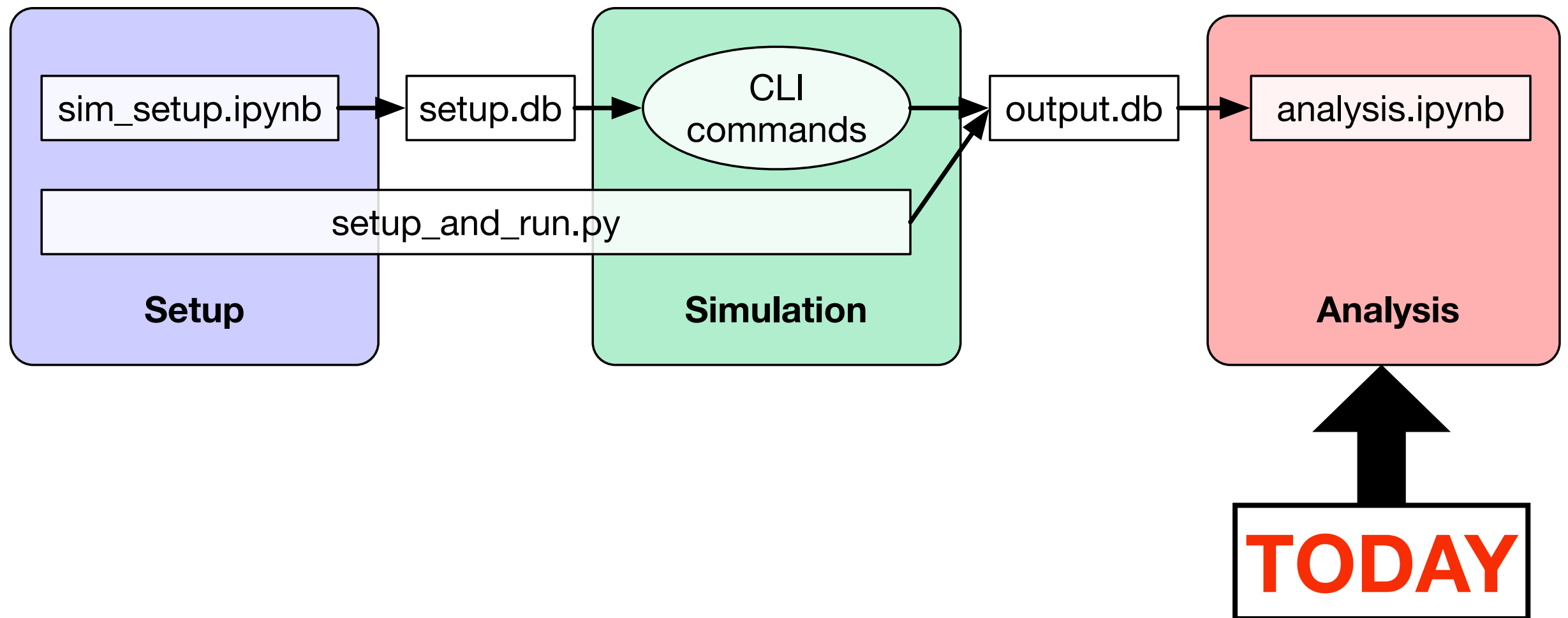


# OPS Workflows



Analysis: Slight changes with SimStore;  
No differences with CLI workflow

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