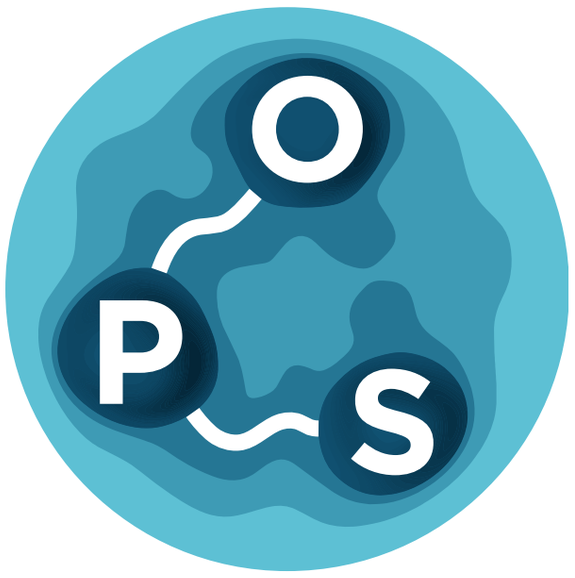


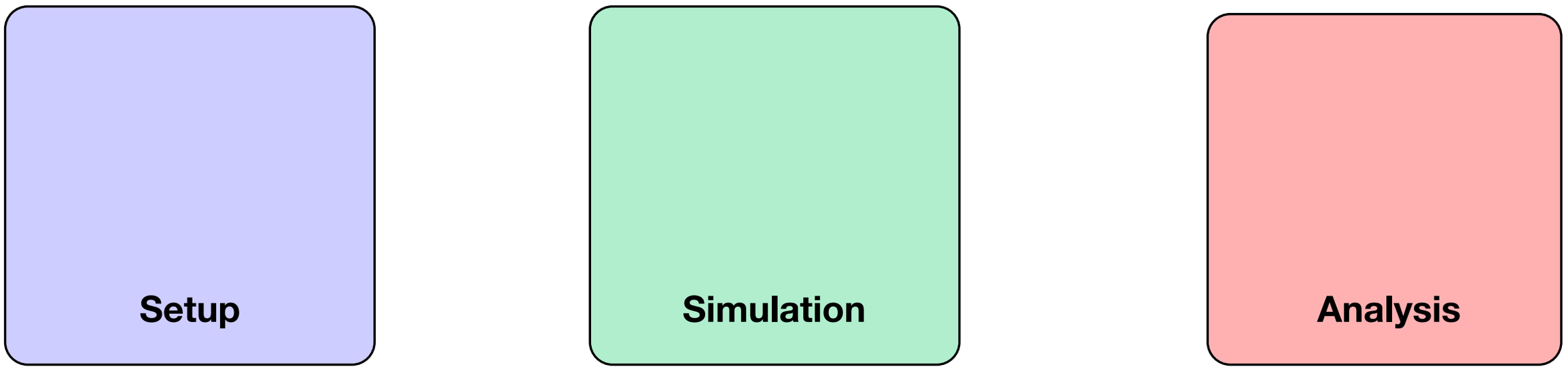

# OpenPathSampling Mini-Tutorial

## SimStore and the OPS CLI

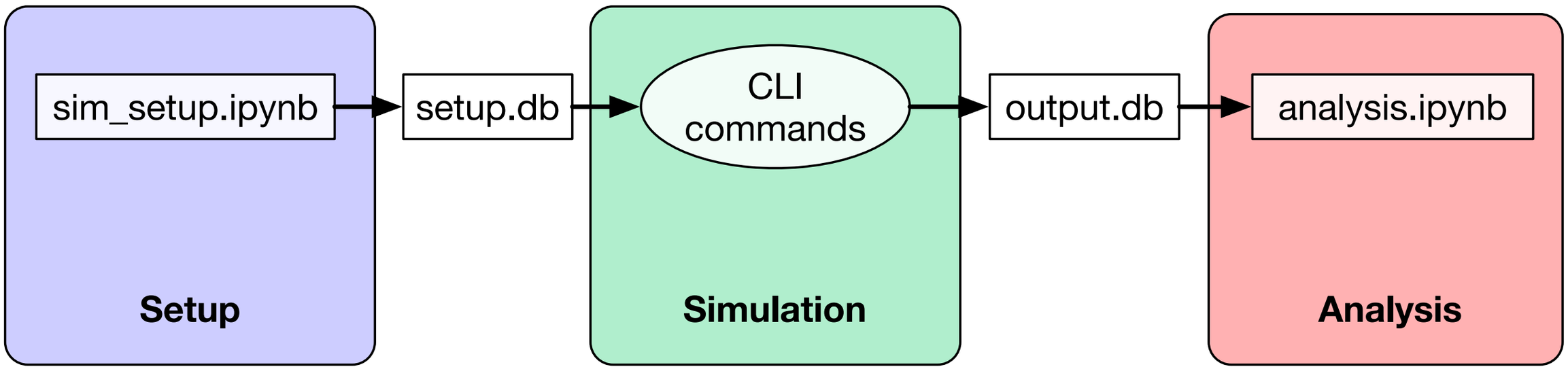
*Part 1: Setting up with SimStore*

https://github.com/openpathsampling/mini-tutorials/
**simstore_and_cli**

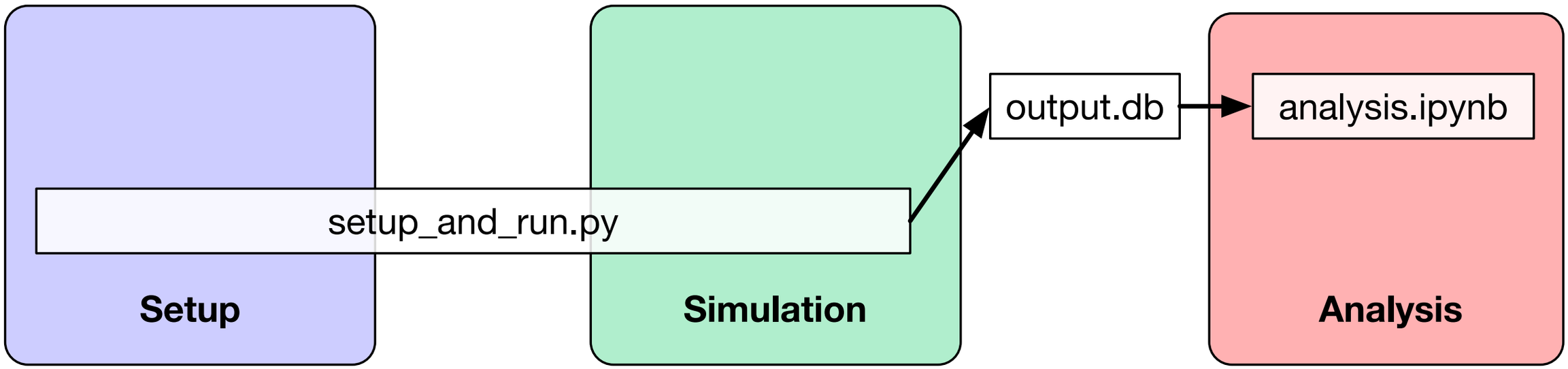
# OPS Workflows



# OPS Workflows



# OPS Workflows



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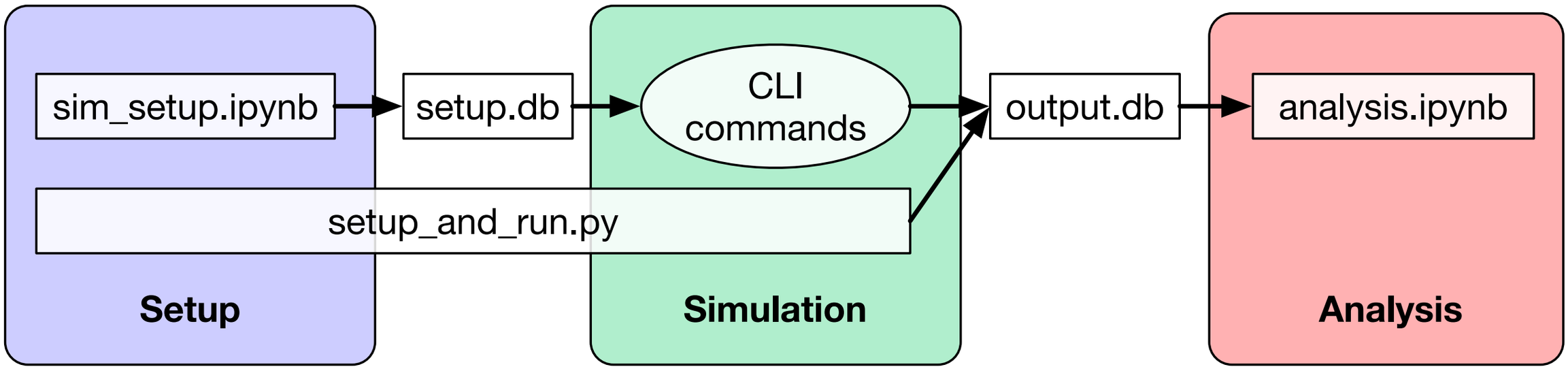
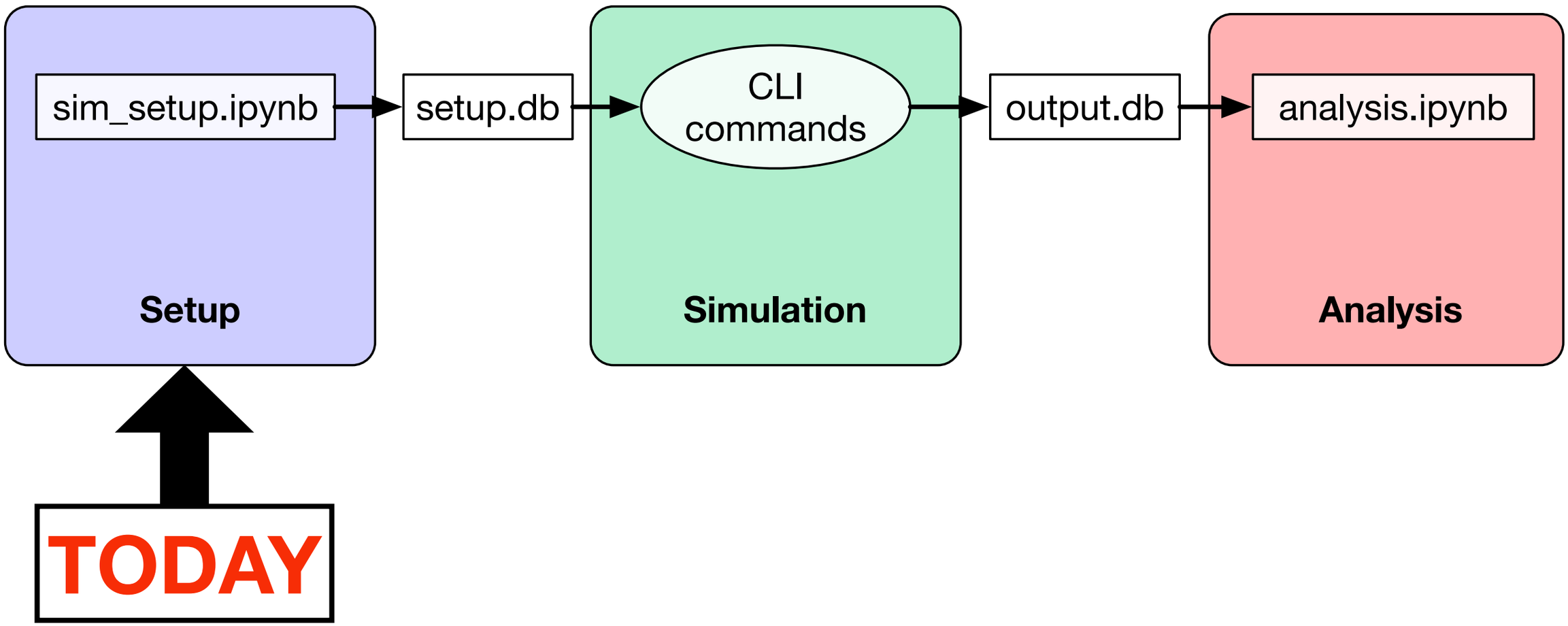
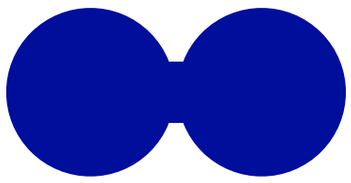


# OPS Workflows




Setting up the simulation:
First phase of CLI workflow (but no CLI) and saving to SimStore

# Simple Bistable Model



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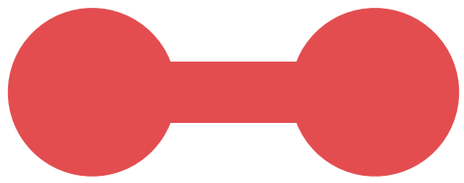

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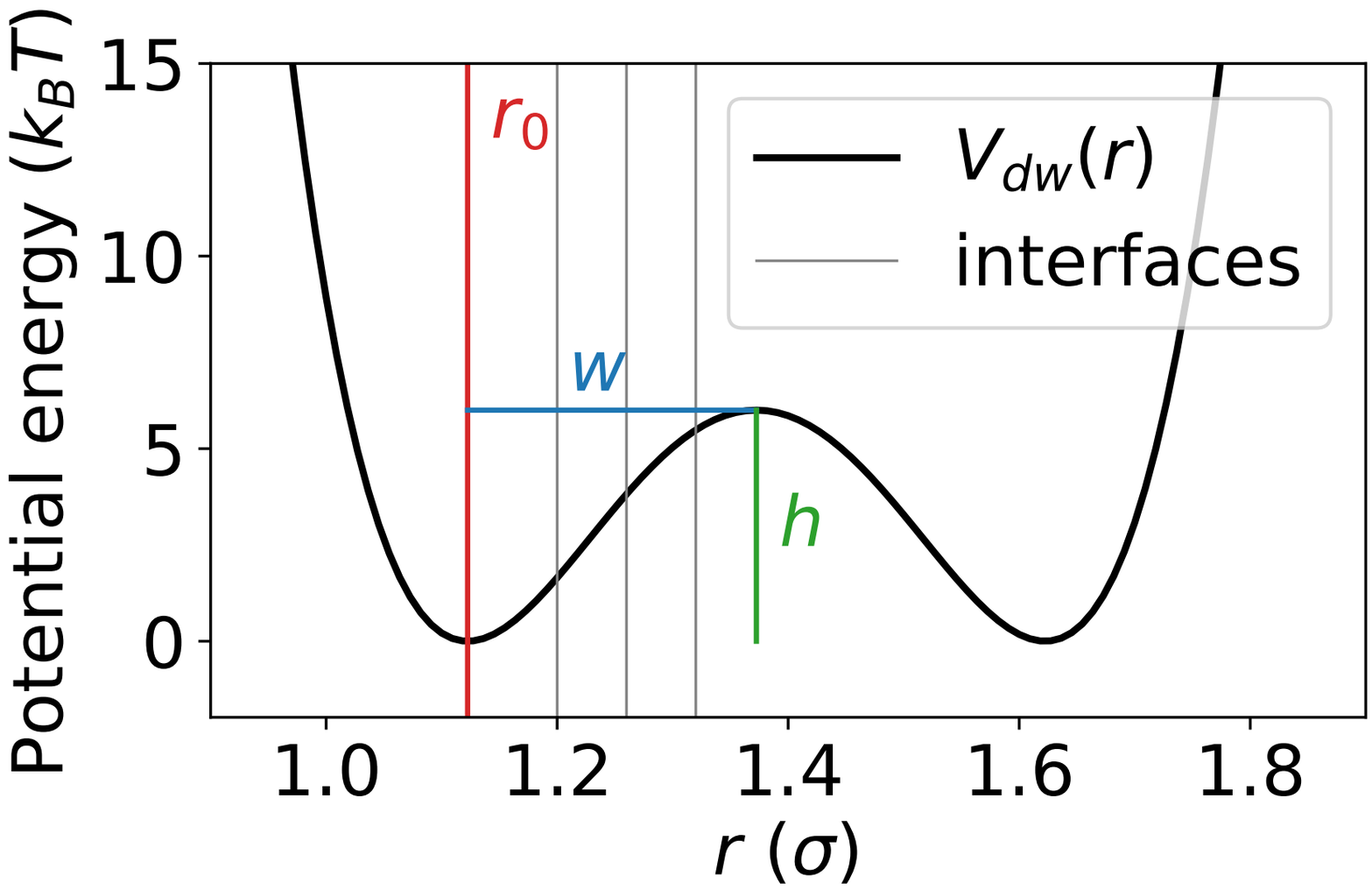


# SimStore

Files ending in .db instead of .nc

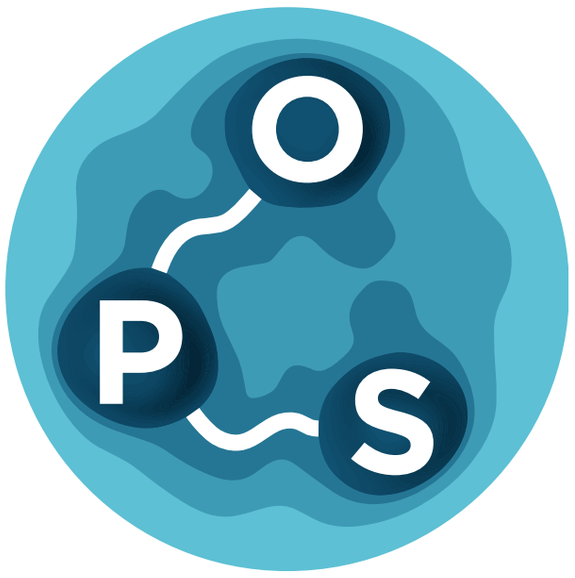
**Advantages**

- 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!



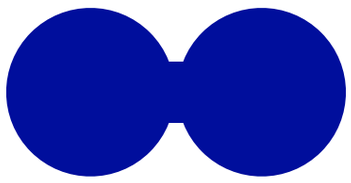

# OpenPathSampling Mini-Tutorial

## SimStore and the OPS CLI

*Part 2: Running simulations with the CLI*

https://github.com/openpathsampling/mini-tutorials/
**simstore_and_cli**

# Simple Bistable Model



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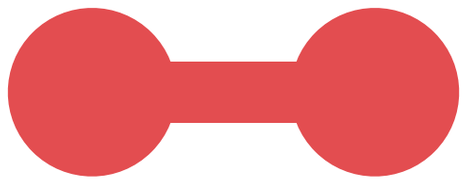

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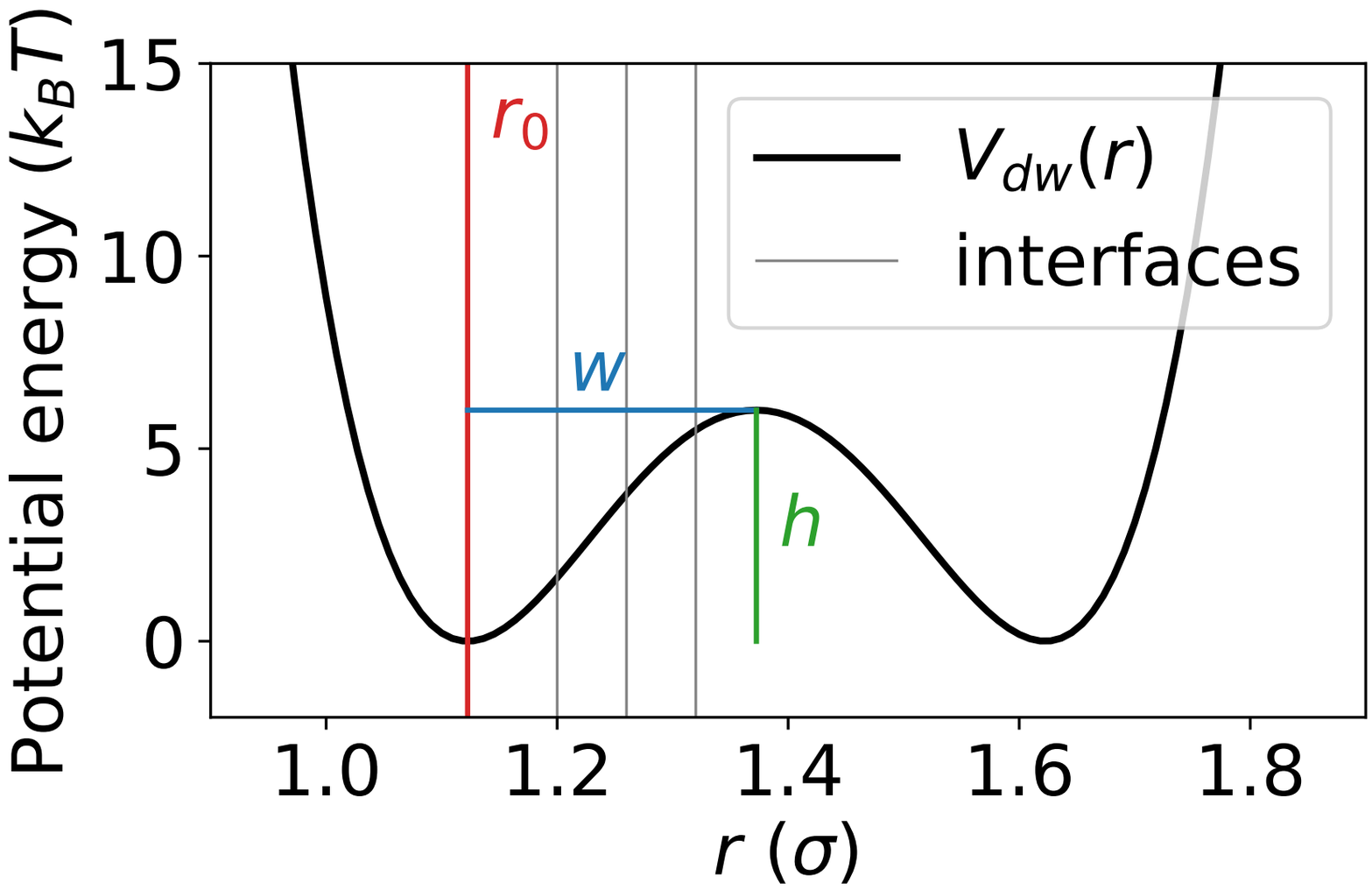
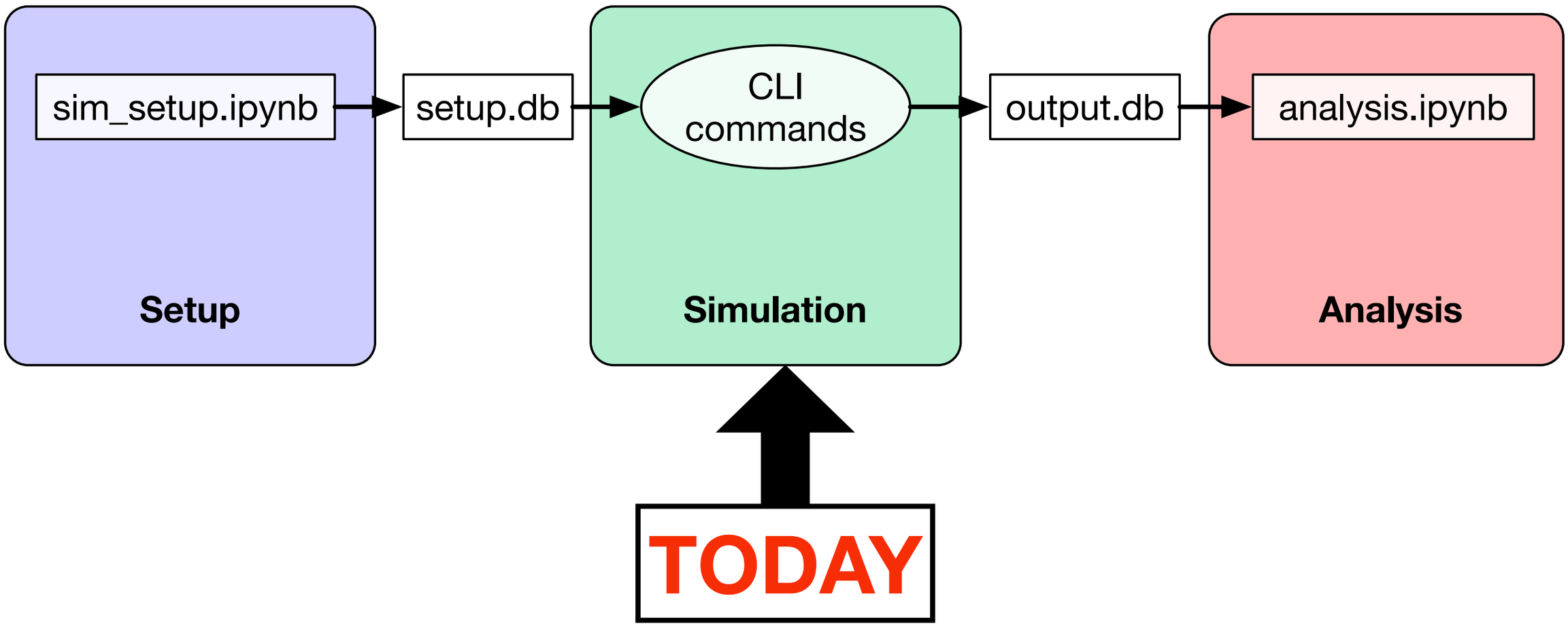
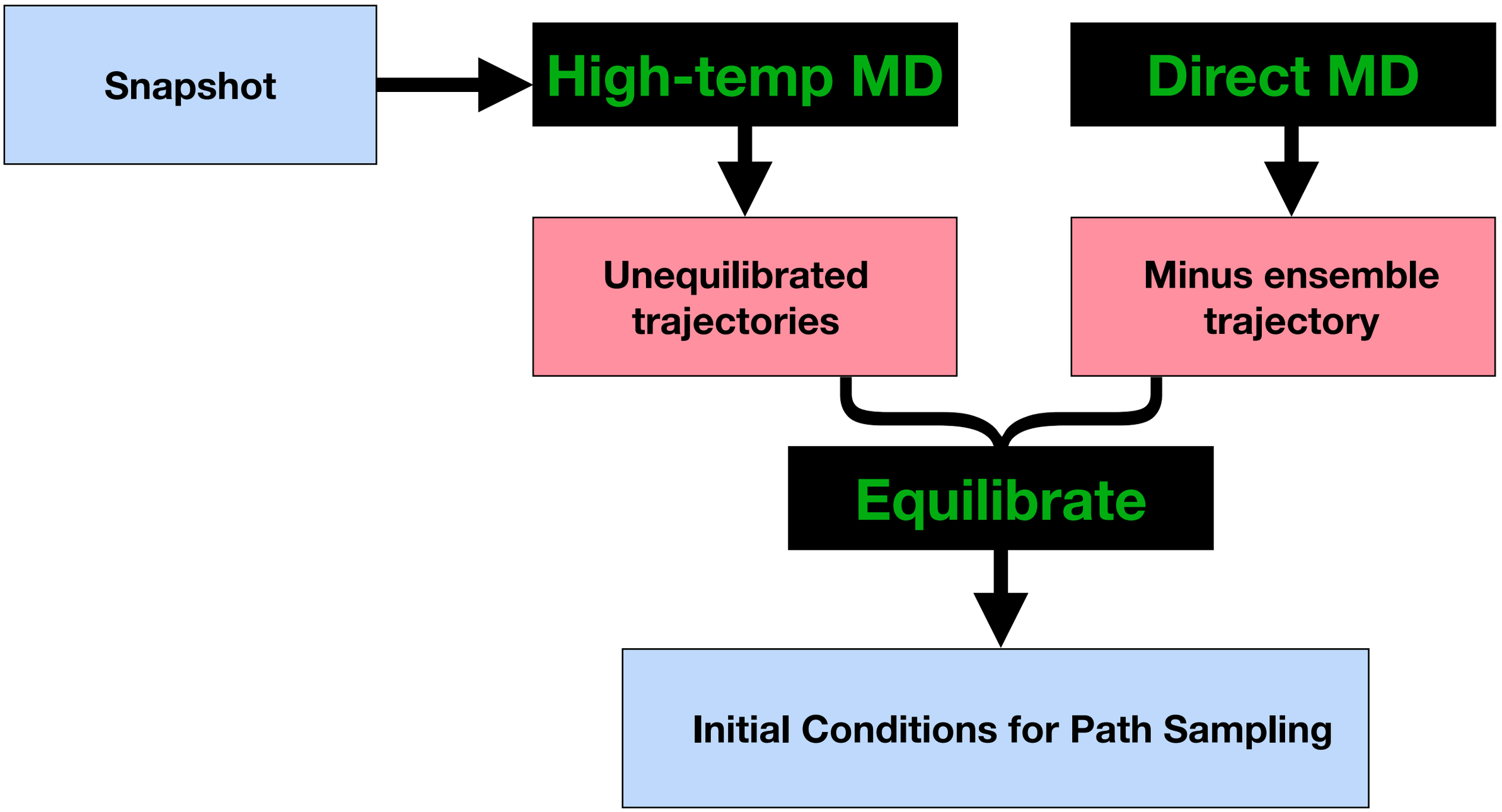


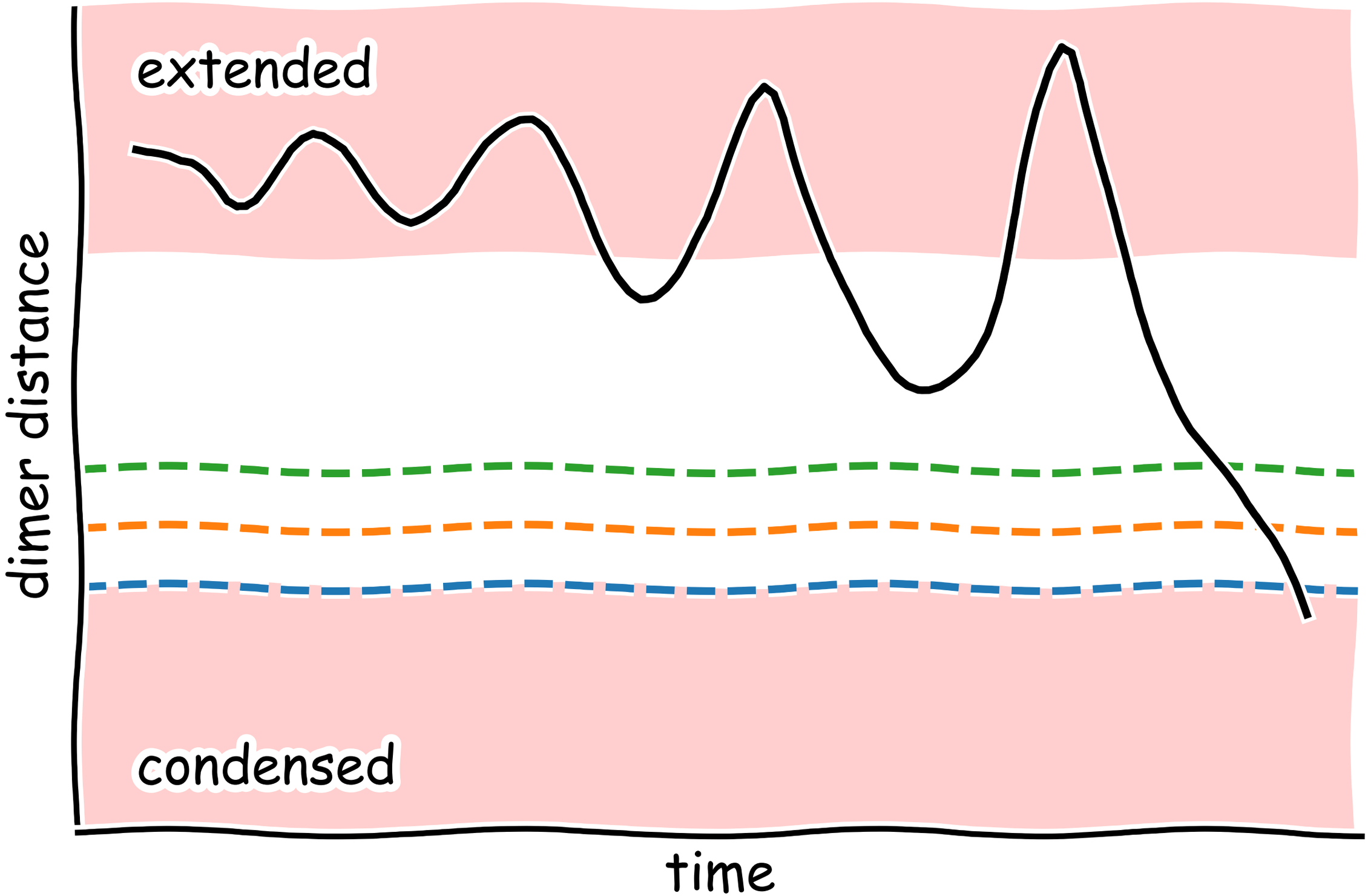
# OPS Workflows

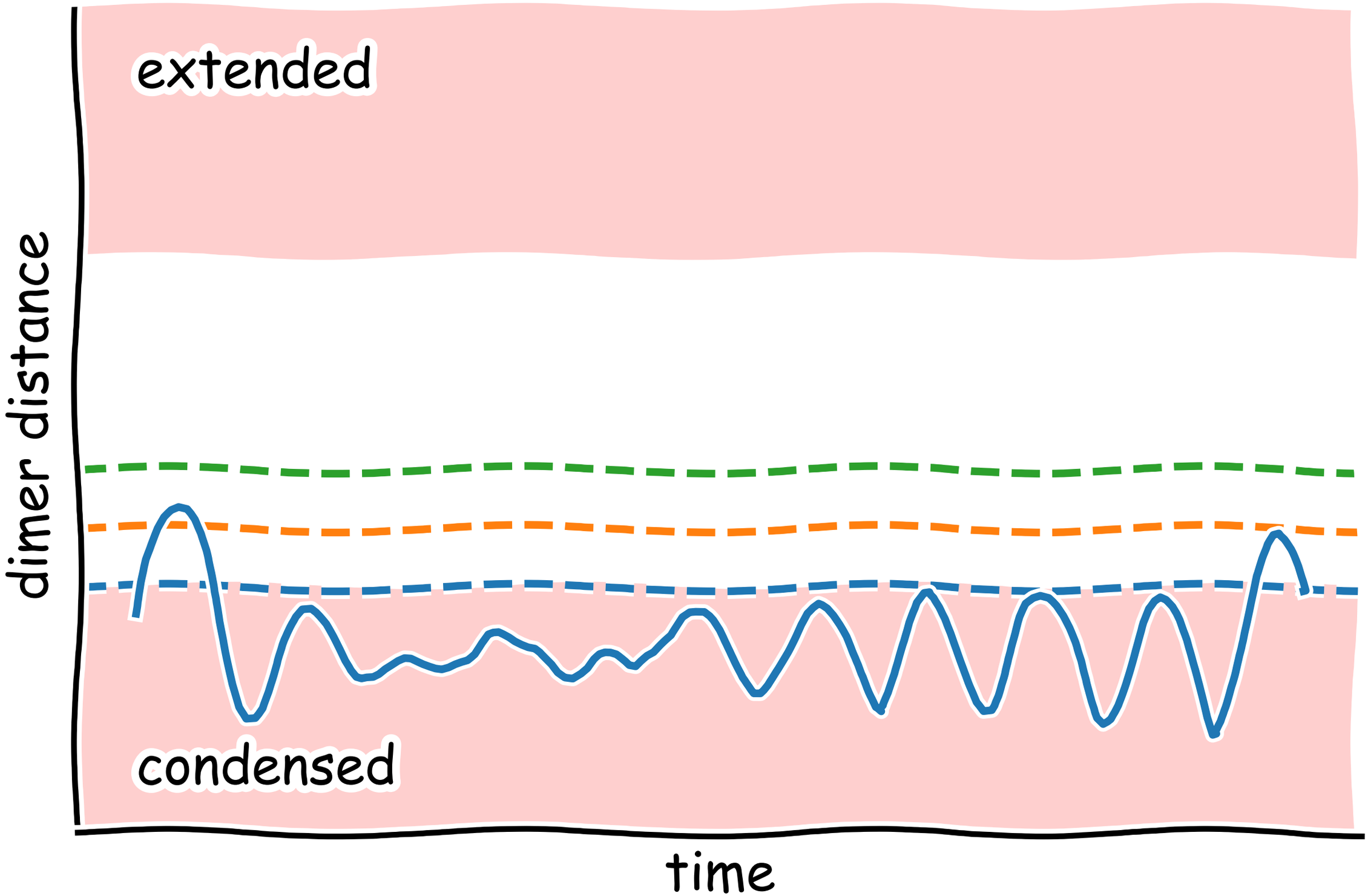



Running the simulation with the CLI:
From a snapshot to path sampling (no Python!)

# Snapshot to Path Sampling




extended
dimer distance
condensed
time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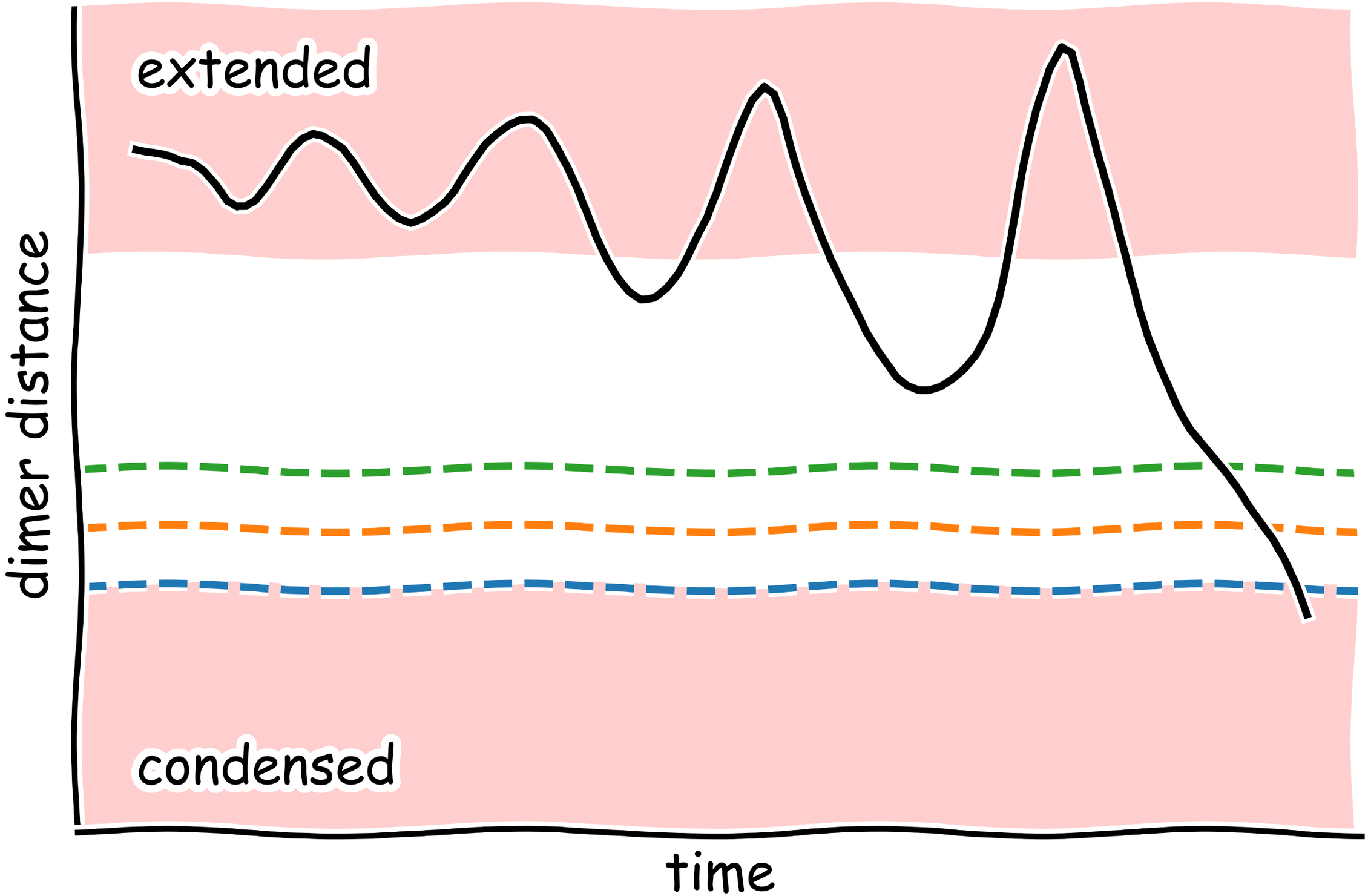
time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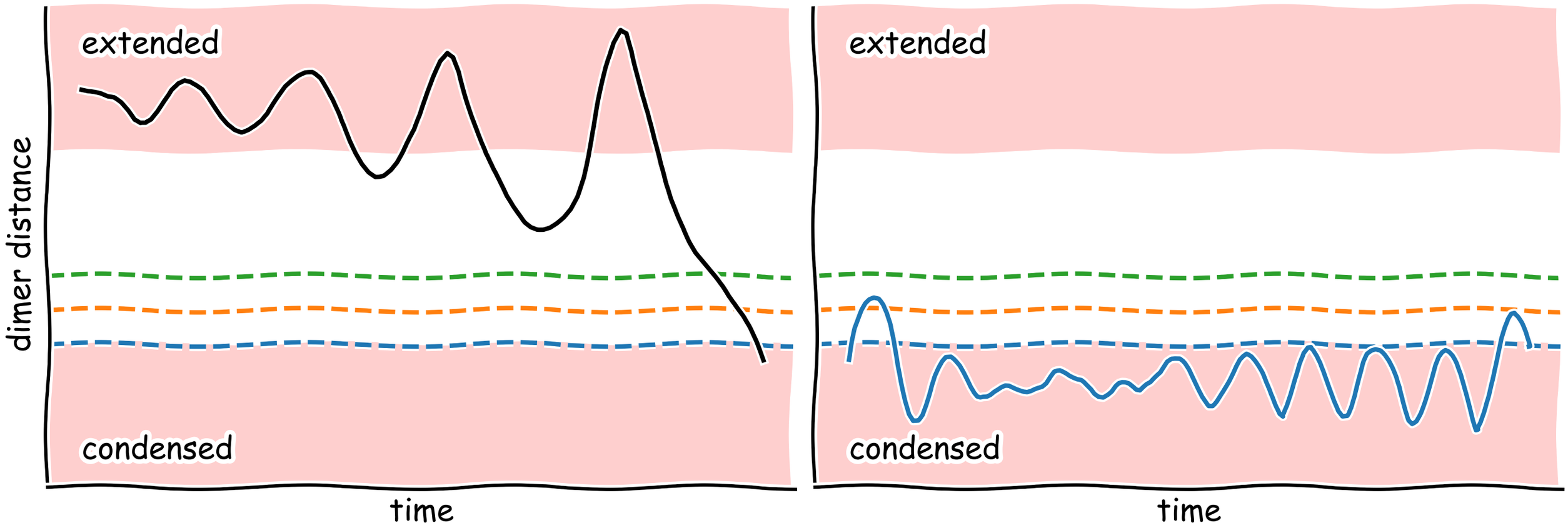
dimer distance
condensed
time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condensed
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time
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condensed
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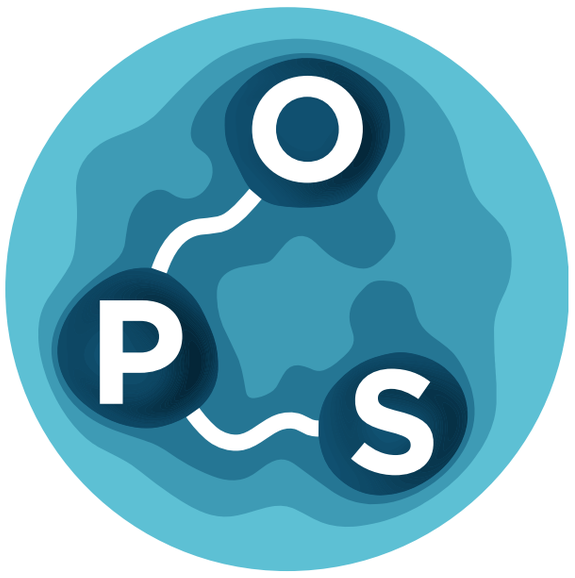



# OpenPathSampling Mini-Tutorial

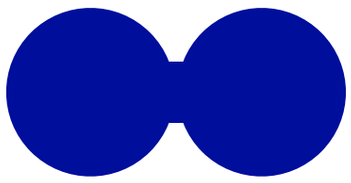
## SimStore and the OPS CLI

*Part 3: Analyzing results*

https://github.com/openpathsampling/mini-tutorials/

**simstore_and_cli**

# Simple Bistable Model



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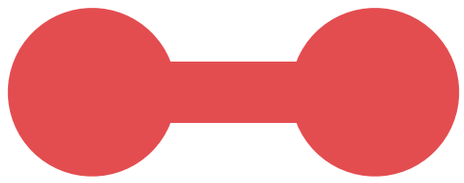

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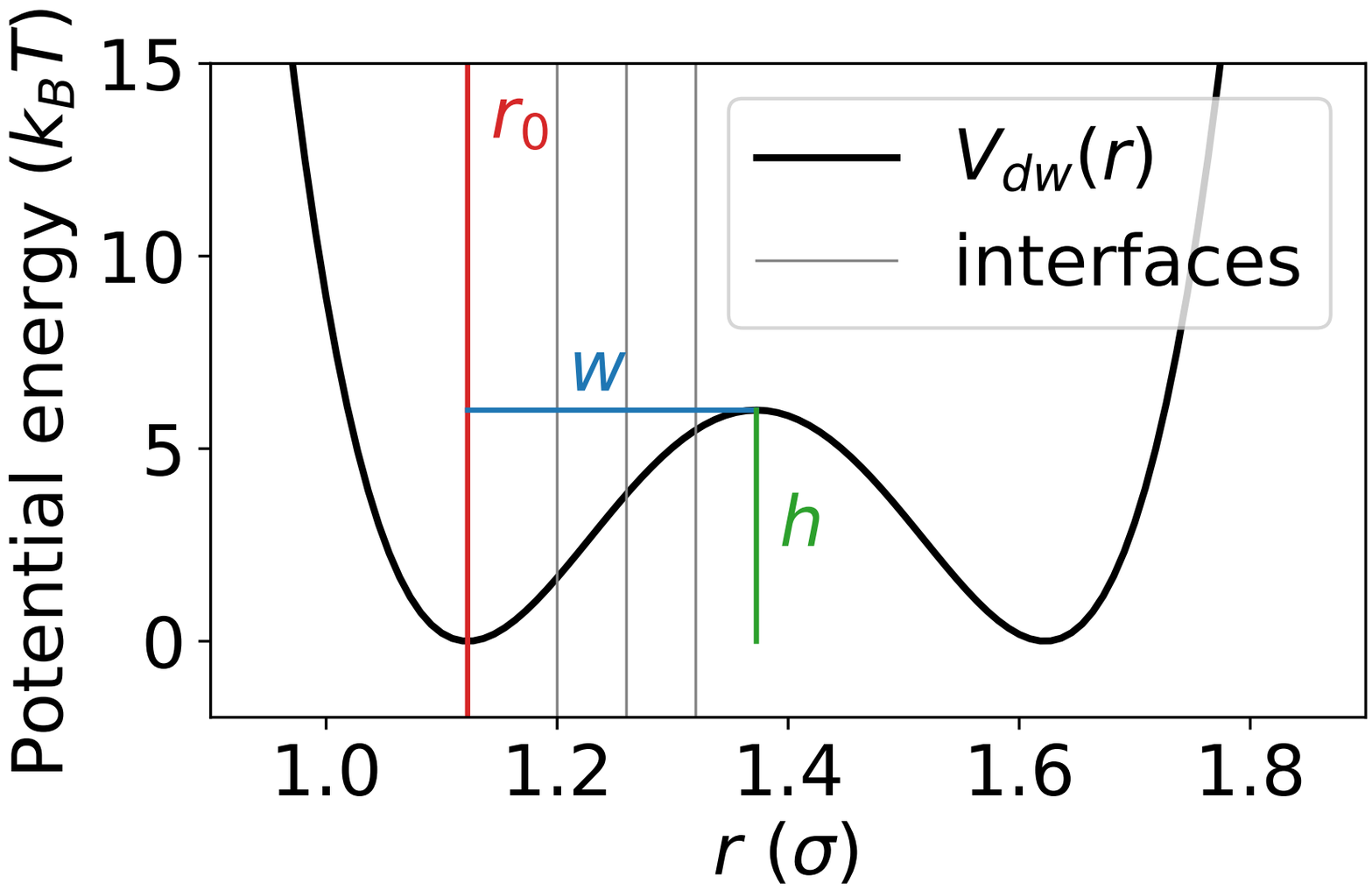
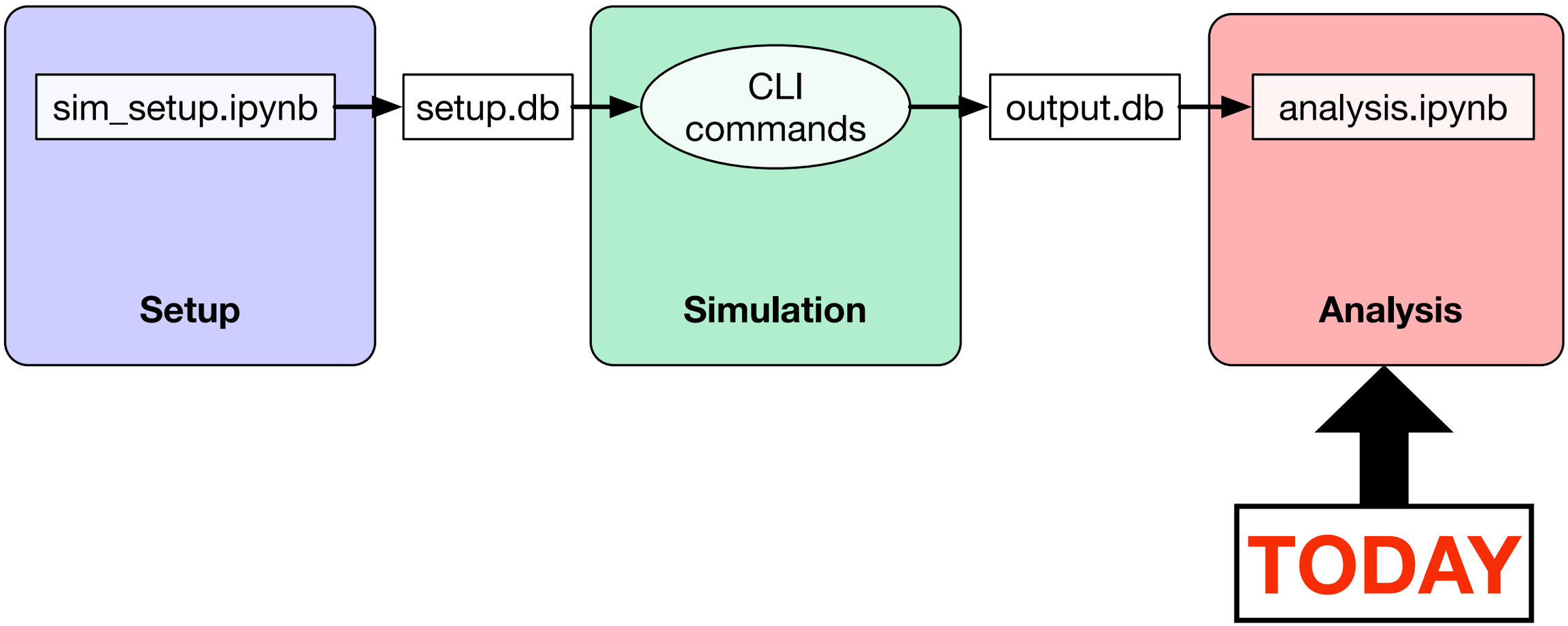
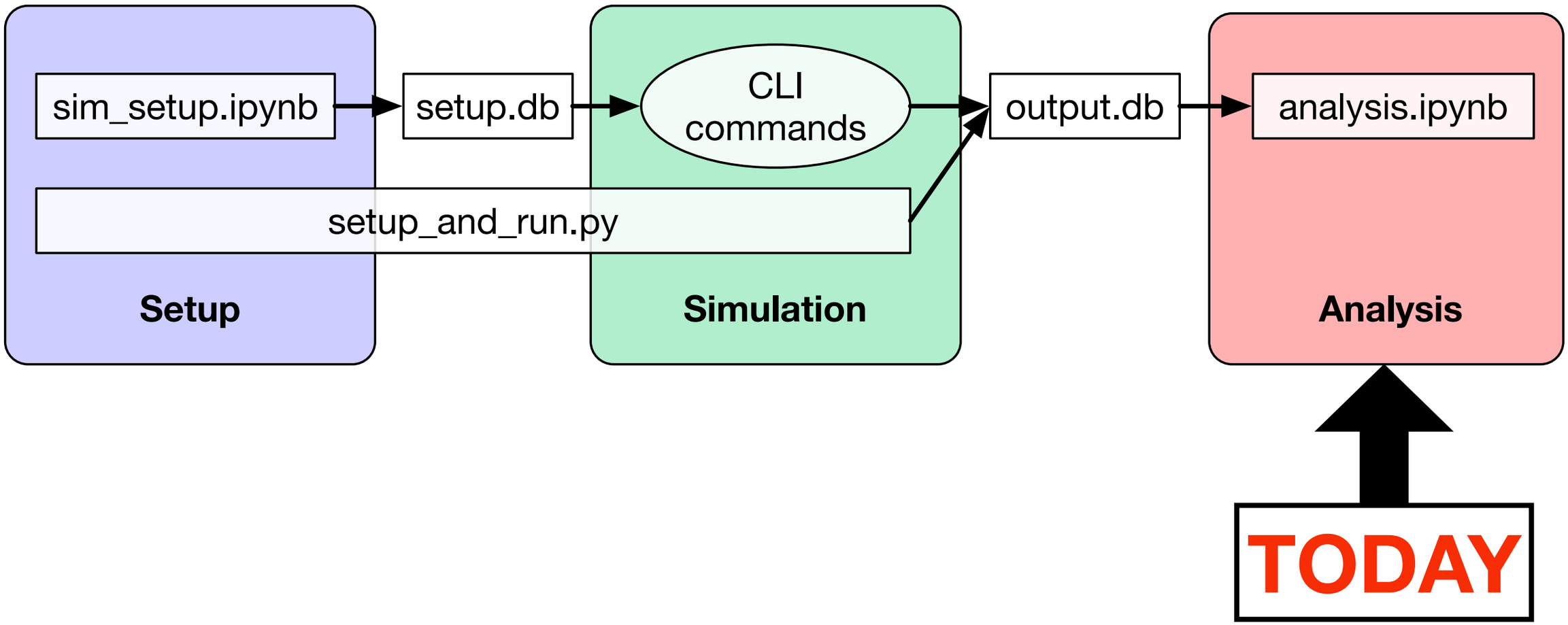


# OPS Workflows




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

# OPS Workflows




Analysis: Slight changes with SimStore;
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