i-ViDa: Visualizing Energy Landscapes and Trajectories of DNA Reactions

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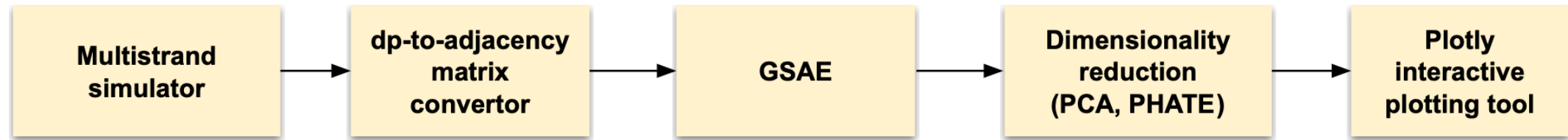
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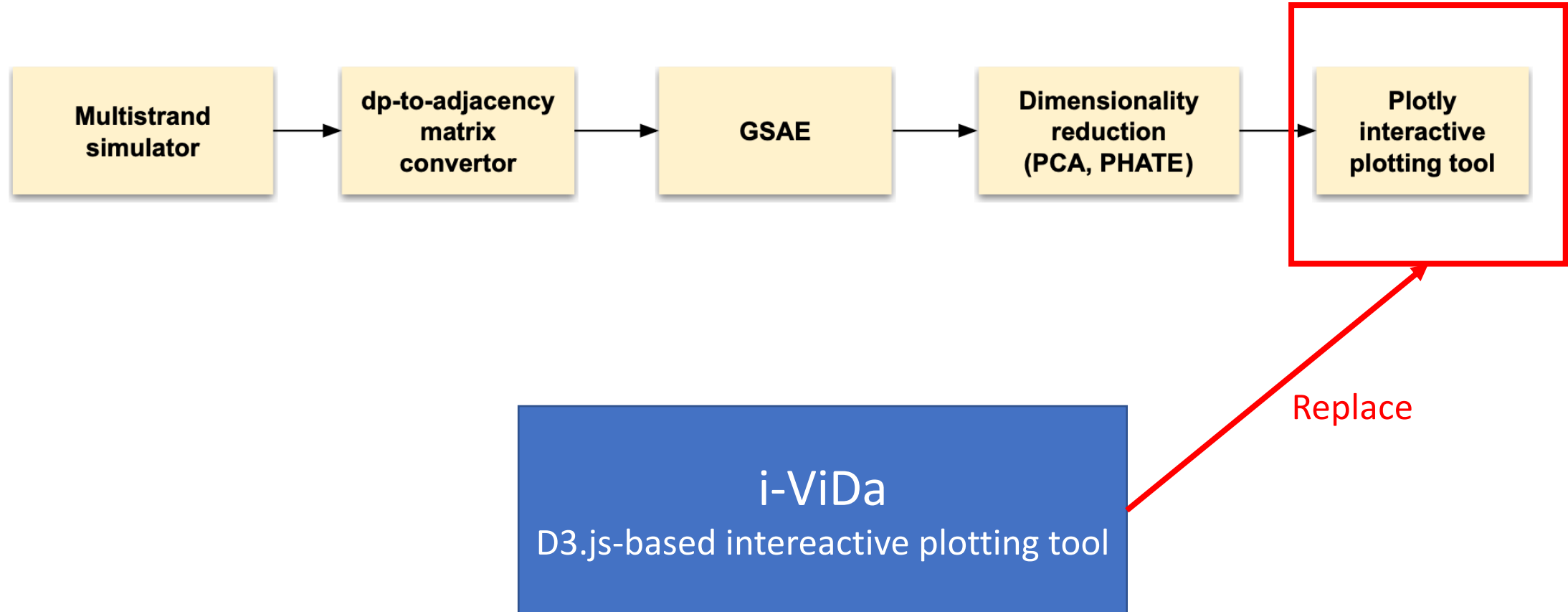**UBC** THE UNIVERSITY OF BRITISH COLUMBIA

Motivation

- Help domain experts to make the output from the reaction simulators more comprehensible.

- Help synthetic biologists and molecular programmers design novel DNA reactions with more potential applications.

Framework of ViDa

Framework of i-ViDa

Background

- **DNA reaction:**
  - Strand interactions: strands folding from initial to final secondary structures
- **Secondary structure:**
  - A set of strands with their base pairs formed via hydrogen bonding
  - Dot-parenthesis notation: ..((..)))…
- **Reaction trajectory:**
  - A sequence of secondary structures from the initial to the final of a DNA reaction
- **Energy landscape:**
  - Comprised of a set of secondary structures visited in the sampled trajectories.
- **State and trajectory space:**
  - Name energy landscape as the state space; laying out the trajectories on the state space, then we call it trajectory space
- **Kinetic traps:**
  - Stable hairpins which can slow down the reaction

Data Abstraction

Table 1. Data abstraction for secondary structure information.

Attribute	Type	Range
ID	categorical	[1, 46606]
DP notation	categorical	N/A
Coordinate X	quantitative	[-9.7, 13.3]
Coordinate Y	quantitative	[-6.7, 12.9]
Energy	quantitative	[-39.47, 10.87]
Average time	quantitative	[0, 3.60 e-8]
Occupancy density	ordinal	[1, 100]
Intra-strand bp (top)	quantitative	[0, 7]
Intra-strand bp (bot)	quantitative	[0, 7]
Corrected inter-strand bp	quantitative	[0, 25]
Total inter-strand bp	quantitative	[0, 25]
Binding	categorical	{0, 1}

Table 2. Data abstraction for trajectory information.

Trajectory	Type	Range
List of indices (List length of indices, m)	quantitative	[104, 54762]
List of times (List length of times, m)	quantitative	[104, 54762]

Occupancy density equation

$$d(S_j) = \sum_{i=0}^{100} b(S_j, i)$$

$$b(S_j, i) = \begin{cases} 1, & if\ ID(S_j) \in I_i \\ 0, & otherwise, \end{cases}$$

Task Abstraction

- **State space tasks:**
  - See latent space of secondary structures and retrieve the selected state with various features
  - See the reduced latent space by manipulating some controllable parameter
  - Aggregate similar states into one group to see coarse-grained latent space

- **Trajectory space tasks:**
  - See simulated trajectories in latent space and retrieve the related information such as the reaction time of specific trajectories
  - Compare the spatial shapes of trajectories with notably different reaction times
  - Compare different trajectories in terms of their corresponding energy flows
  - Identify the number of kinetic traps in trajectories and capture the traps' information
  - Identify the significant reaction pathways

Overview of i-ViDa

i-ViDa: Visualizing Energy Landscapes and Trajectories of DNA Reactions

YiBo is showing demo

Limitations

- Trajectories are too long and hard to track each transition

- Cannot find exact kinetic traps

- Constrained by specific DNA reactions

Future Work

- Find better way to showing trajectories on state space

- Implement more accurate analysis for finding kinetics traps

- Do K-means to partition the state space

Thank you for listening!

Q&A