i-ViDa: An interactive visualization tool for DNA reaction trajectories

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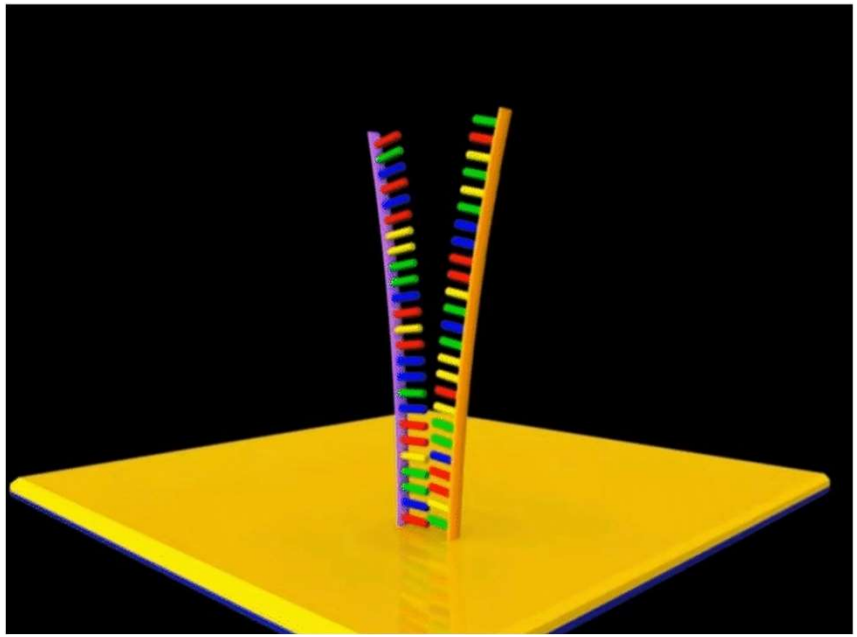
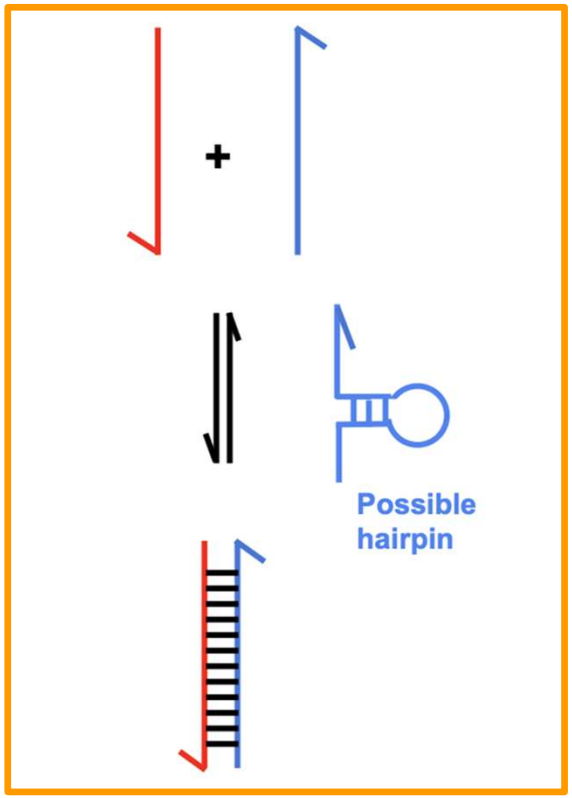
What is DNA hybridization?





The fundamental ingredient in the self-assembly of DNA nanostructures and in the operation of DNA nanomachines is the hybridization of single-stranded DNA to form duplexes

Gif cites from https://www.youtube.com/watch?v=0qoqzErrae4

Why DNA trajectories?

Help to understand mechanisms of DNA reaction kinetics.

Further make contributions to DNA nanotechnologies, such as DNA computing, DNA robots, and etc.

The goal

Visualize different reaction pathways laying out on the top of the energy landscape.

Each simulation generates a different pathway.

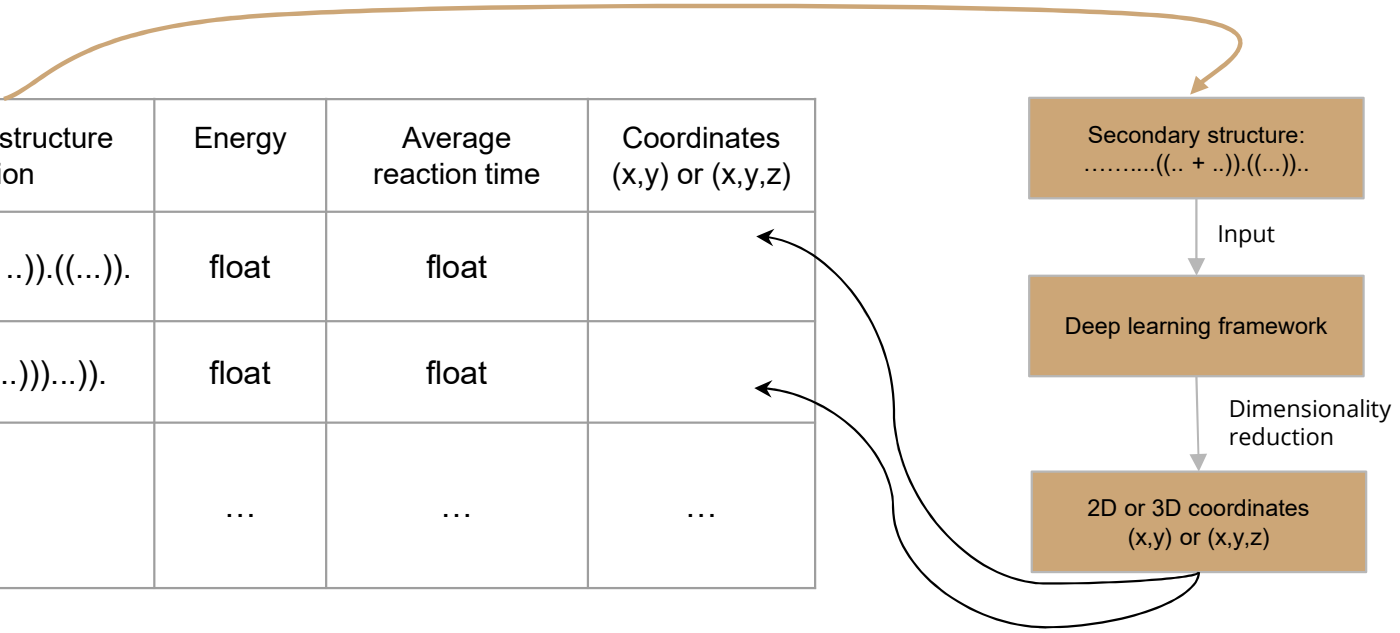
How to visualize them on a energy map to get a sense of which reaction is fast, where the reaction stucks, and why it fails ...

Gif cites from https://maps.tnc.org/migrations-in-motion/#4/19.00/-78.00

Datasets

Dataset

Item	Secondary structure notation	Energy	Average reaction time	Coordinates (x,y) or (x,y,z)
1	..(…)...((.. + ..)).((...)).	float	float	
2	..((..(((.. + ..)))...)).	float	float	
… (hundreds of thousands items)	…	…	…	…

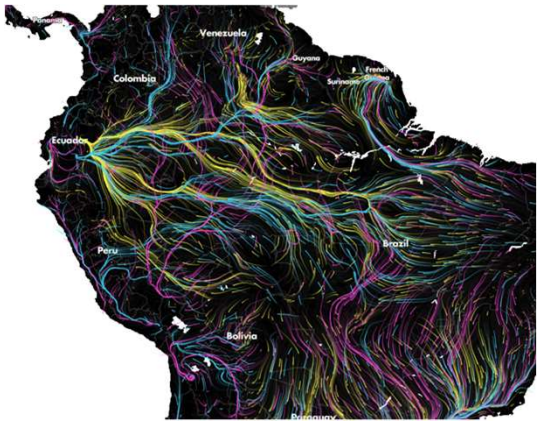


Trajectory	Indx	Time
1	list: [1,4,6,9,...]	list: [float, float, …]
2	list: [0,1,6,8,…]	list: [float, float, …]
… (hundred of trajectories)	…	…

Vis Tool Design

Scatter Plot + Graph for DNA States

1. Graph
    a. Node - DNA state (secondary structure)
    b. Edge - Elementary step
    c. Path - Reaction trajectory
2. Layout: scatter plot - reduced into 2D
    a. Add time slider
    b. Animation
3. Concerns:
    a. Efficiency - Scalability
    b. Technique - Visualizing flows(svg?canvas?)



Algorithm of Visualizing DNA Structure

Current methods of visualizing DNA structures:

- Focused on single-strand DNA
- No interaction, return a image display

Our goal:

- Develop a standard algorithm of visualizing multiple-strand DNA with interaction
- Input DP(text) -> Output vis