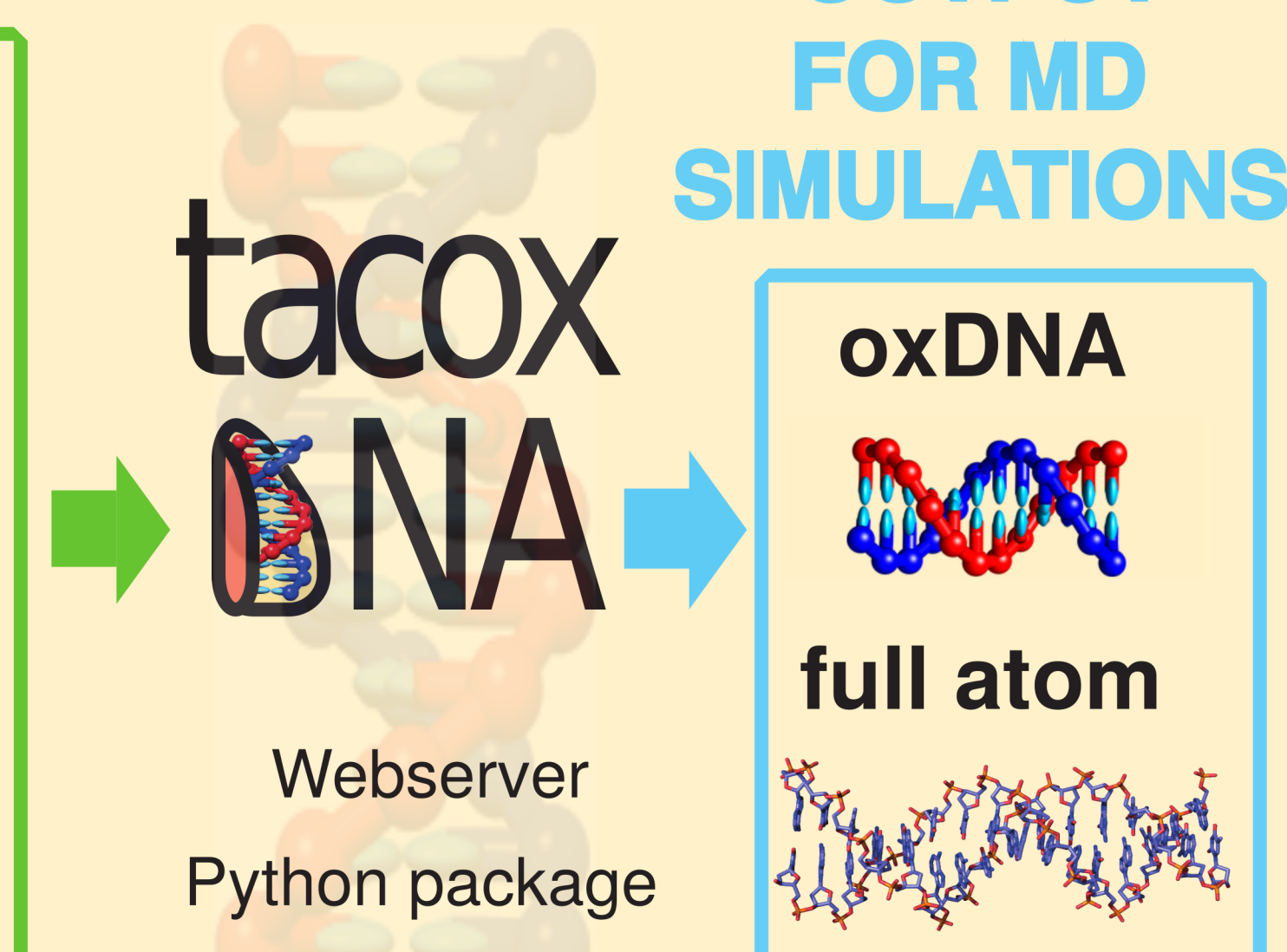
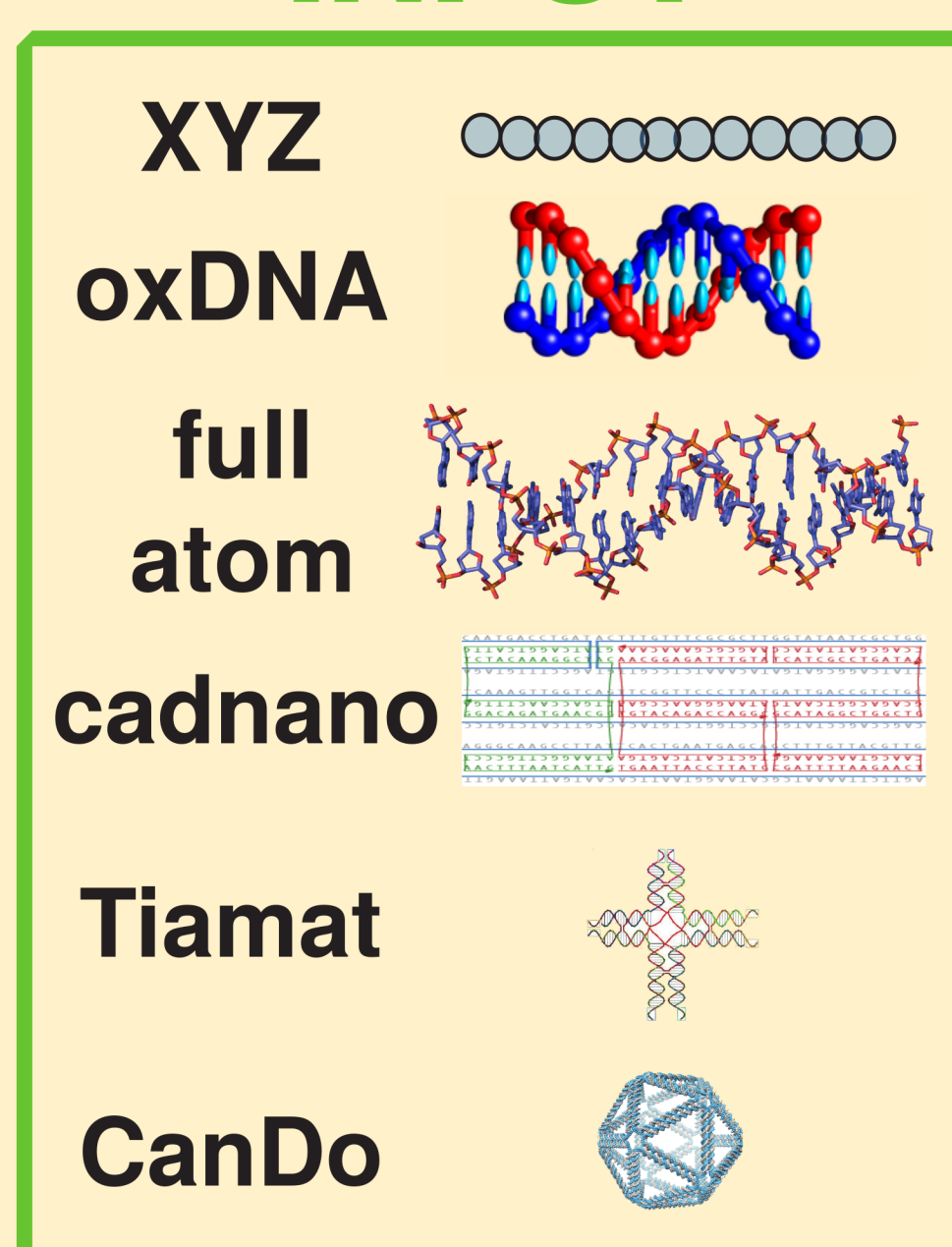


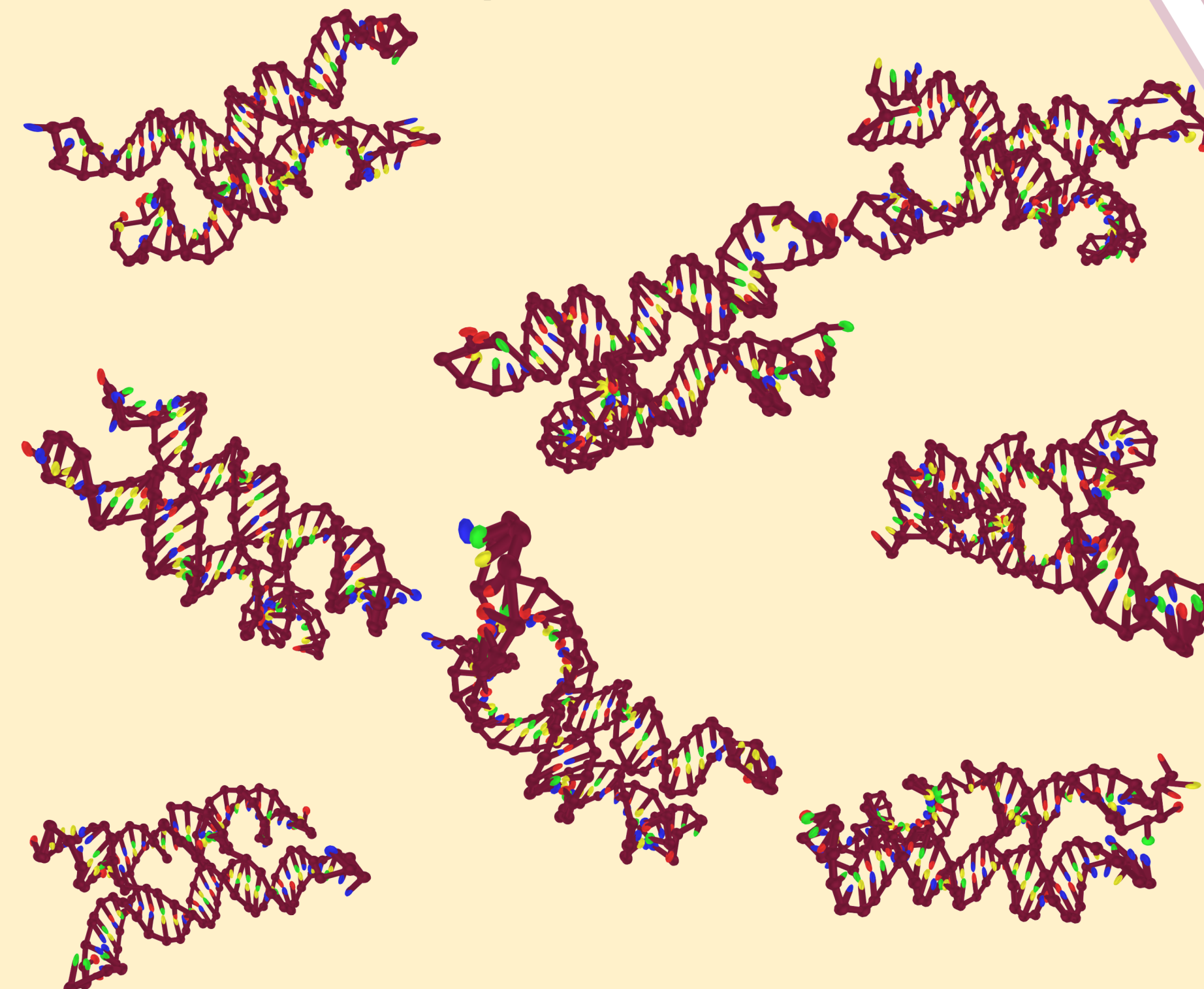
## Design and conversion to simulation format

### INPUT



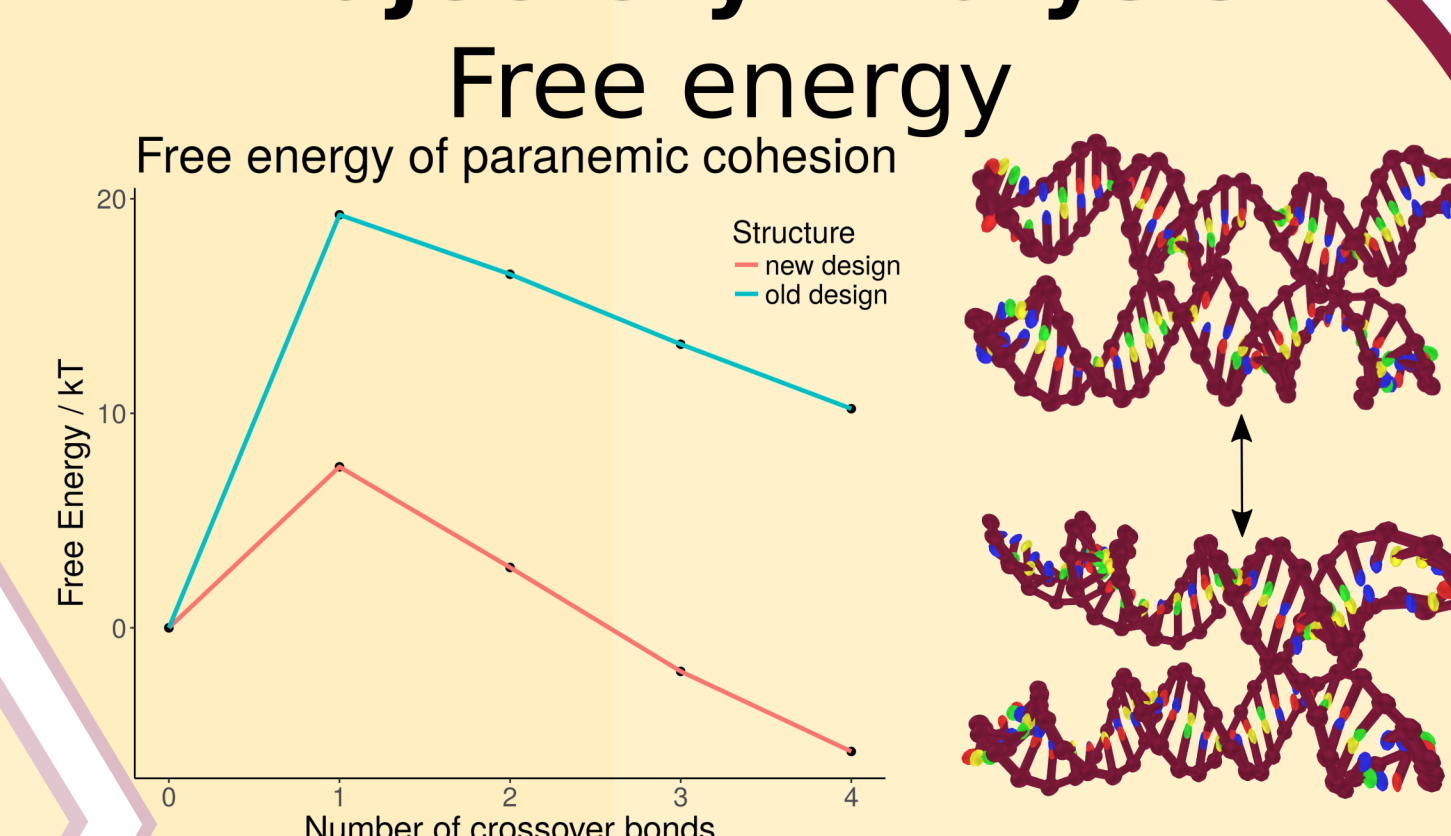
- The TacoxDNA webserver<sup>1</sup> provides tools to convert from nanotechnology design tools to the oxDNA format
- These files will not have physical geometry and must be relaxed prior to simulation
- Also supports conversion to and from PDB for use in other simulation software

## oxDNA/RNA simulation



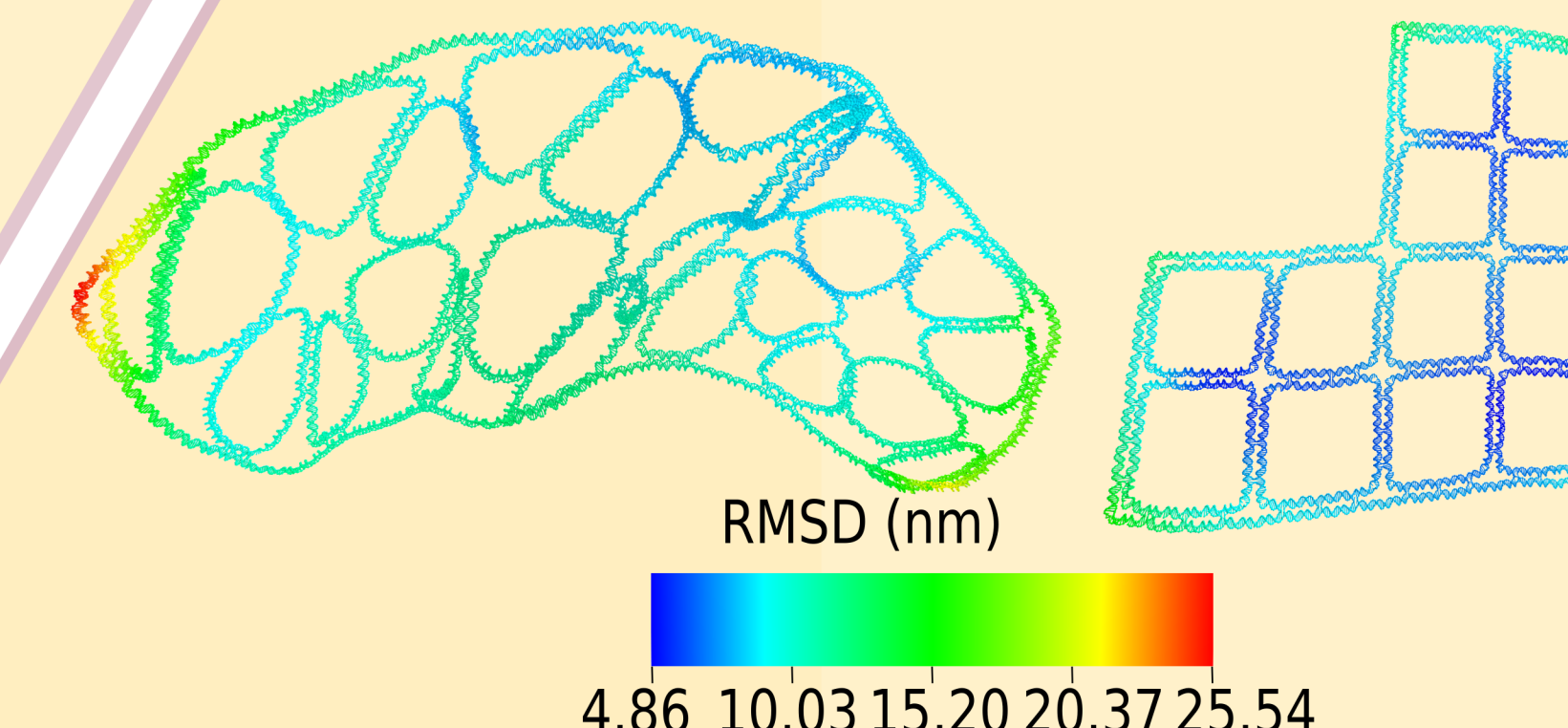
Studying unstable paranemic crossovers in RNA tiles  
Simulation identified the parts of the structure which were not forming as designed.

## Trajectory Analysis



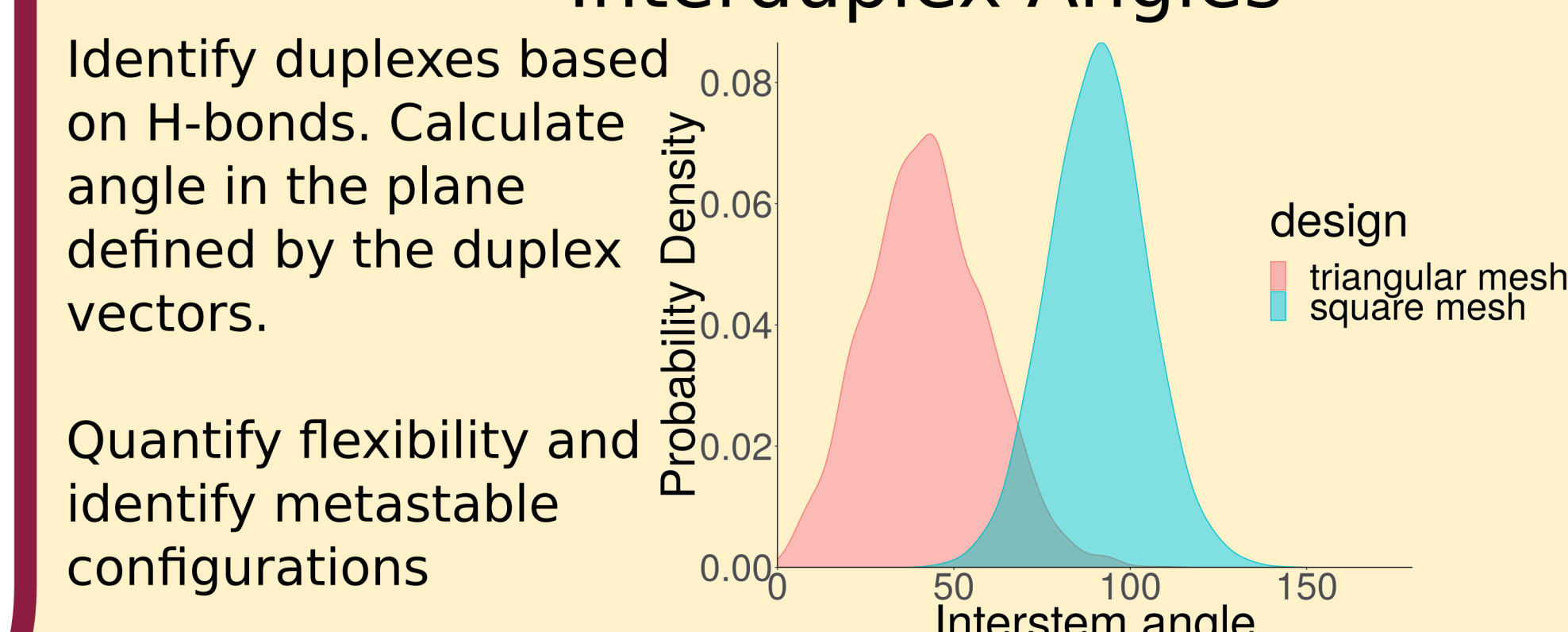
Understanding energy barriers between states can inform design choices

## Mean Structure and Flexibility

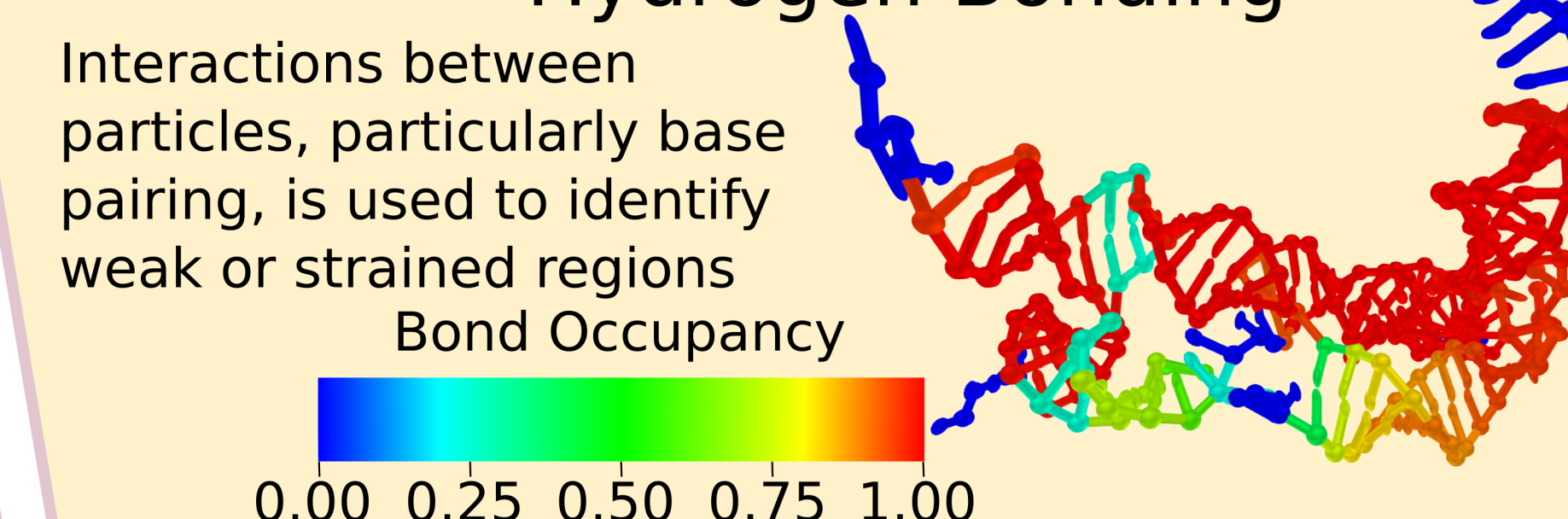


Singular value decomposition for rigid structures.  
Multidimensional scaling for small, flexible structures.

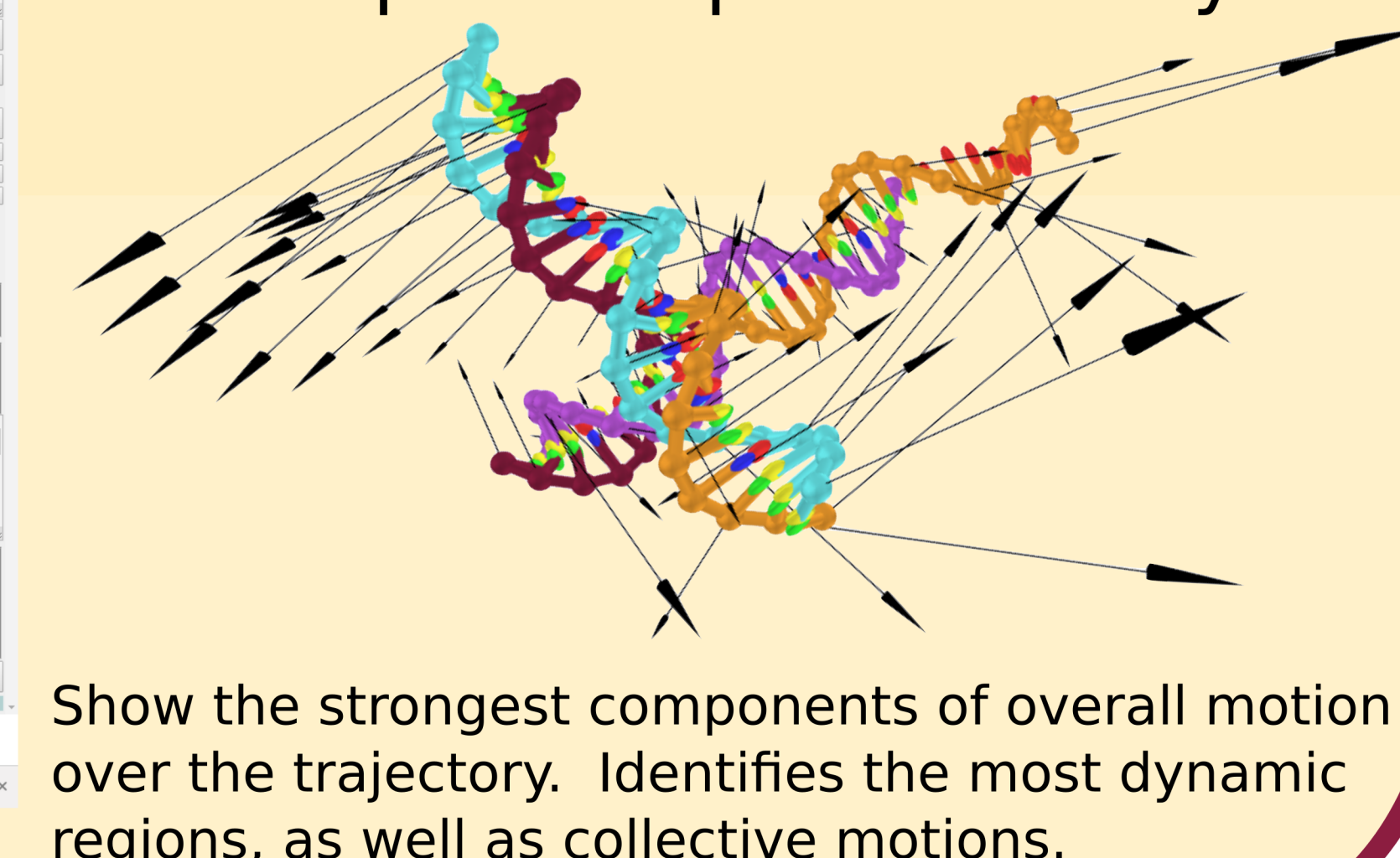
## Interduplex Angles



## Hydrogen Bonding



## Principal Component Analysis



# General-Purpose analysis package for coarse-grained simulations of DNA/RNA nanotechnology

**ASU** Biodesign Institute

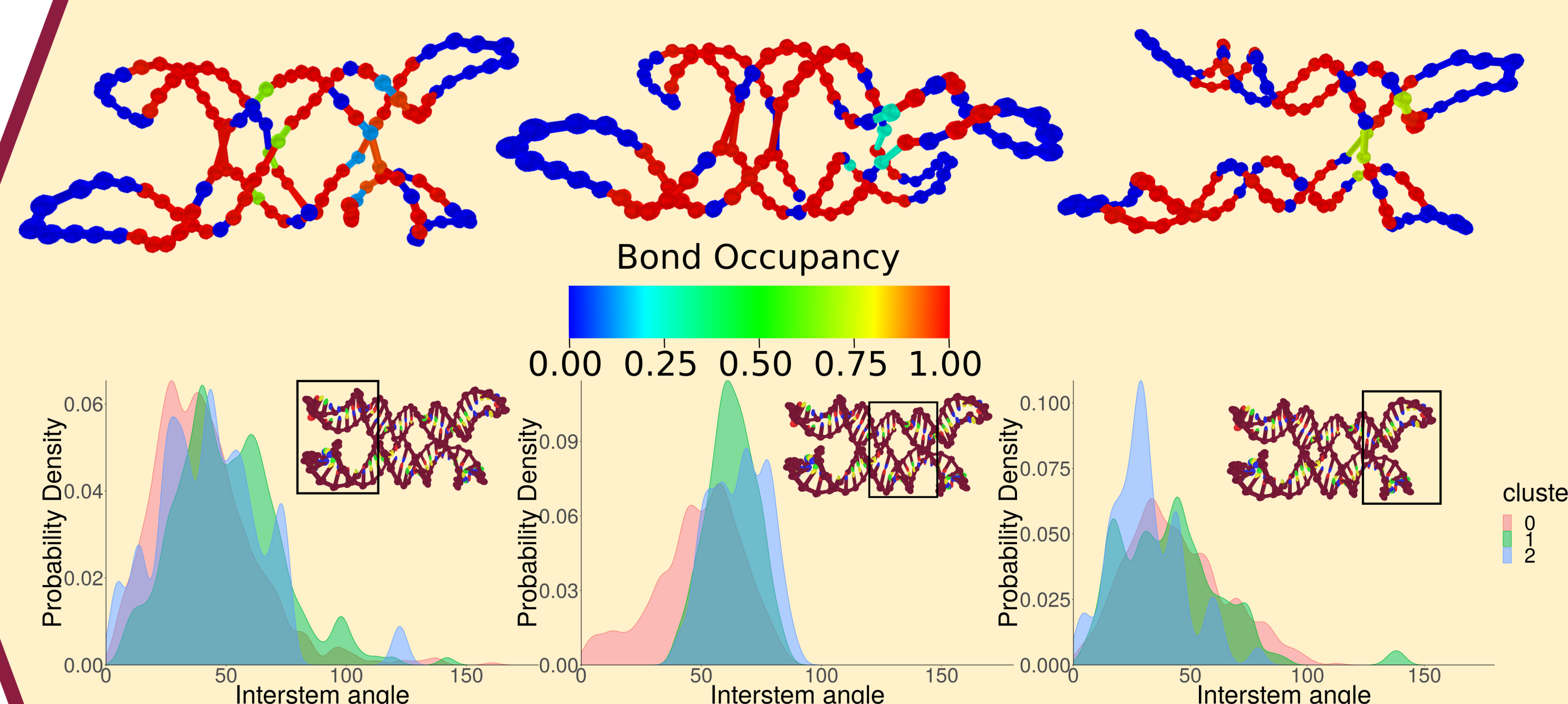
Arizona State University

Erik Poppleton<sup>a</sup>, Michael Matthies<sup>a</sup>, Shuchi Sharma<sup>a</sup>, Joakim Bohlin<sup>b</sup>, Petr Šulc<sup>a</sup>

<sup>a</sup> Center for Molecular Design and Biomimetics, The Biodesign Institute, Arizona State University, Tempe, AZ, USA

<sup>b</sup> Physics Department, University of Oxford, Oxford, UK

## Unsupervised clustering

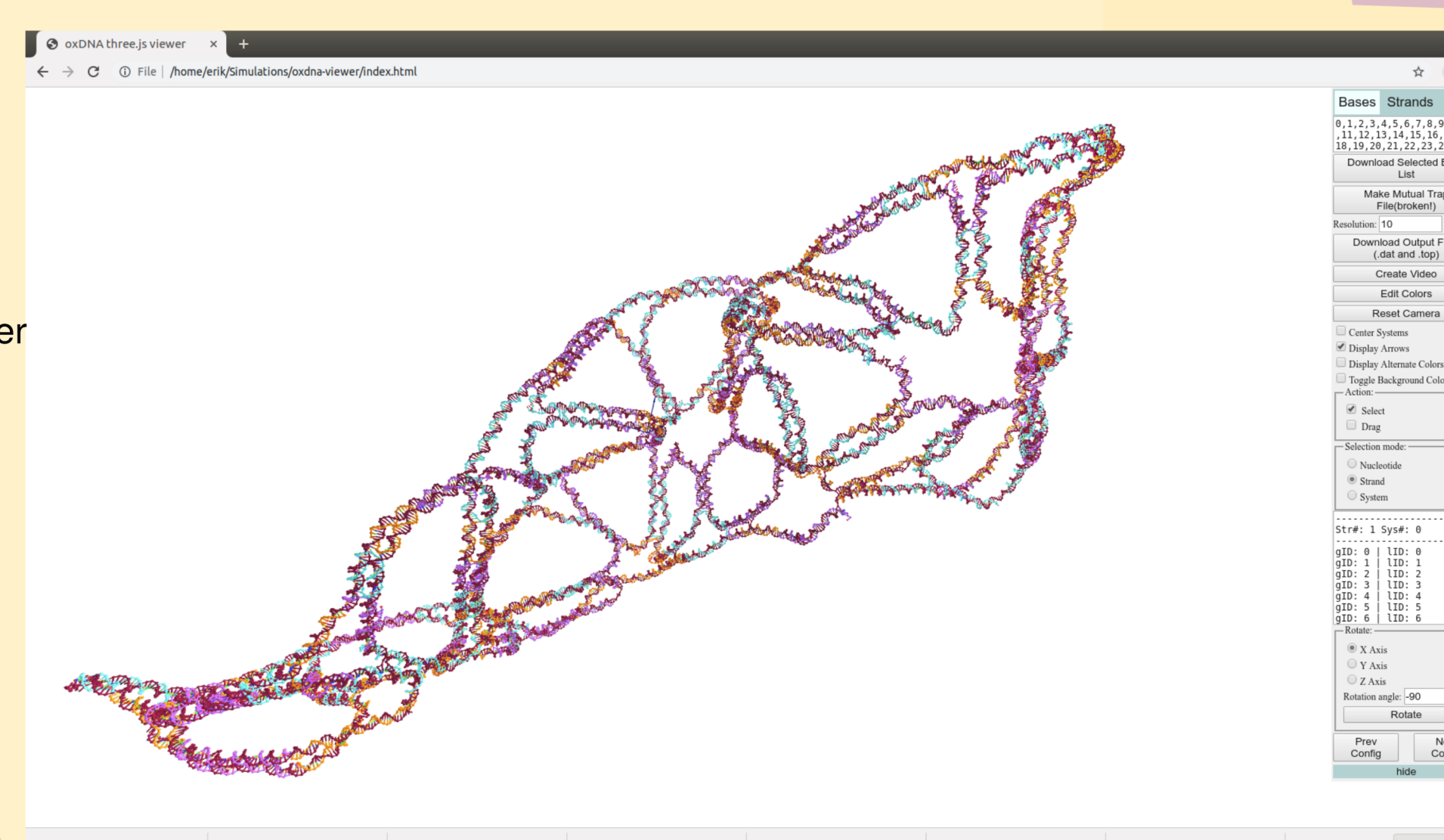


Using DBSCAN<sup>2</sup>, an unsupervised machine learning algorithm, to identify structurally distinct subpopulations in a trajectory and exploring differences in bonding and angles

## Visualization

OxDNA Viewer is a Three.js browser app that reads, edits, and writes oxDNA simulation files. Modify single configurations, create videos from trajectories, and overlay data from other analyses

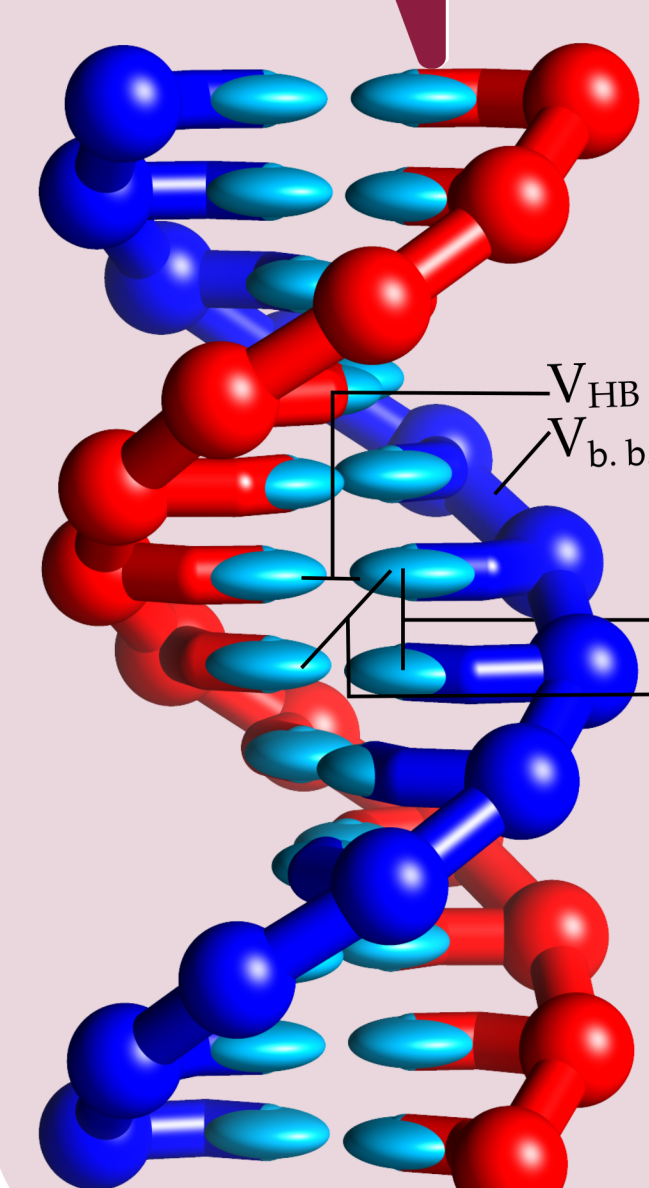
Download at:  
<https://github.com/sulcgroup/oxdna-viewer>



## The oxDNA/RNA<sup>3,4,5</sup> model

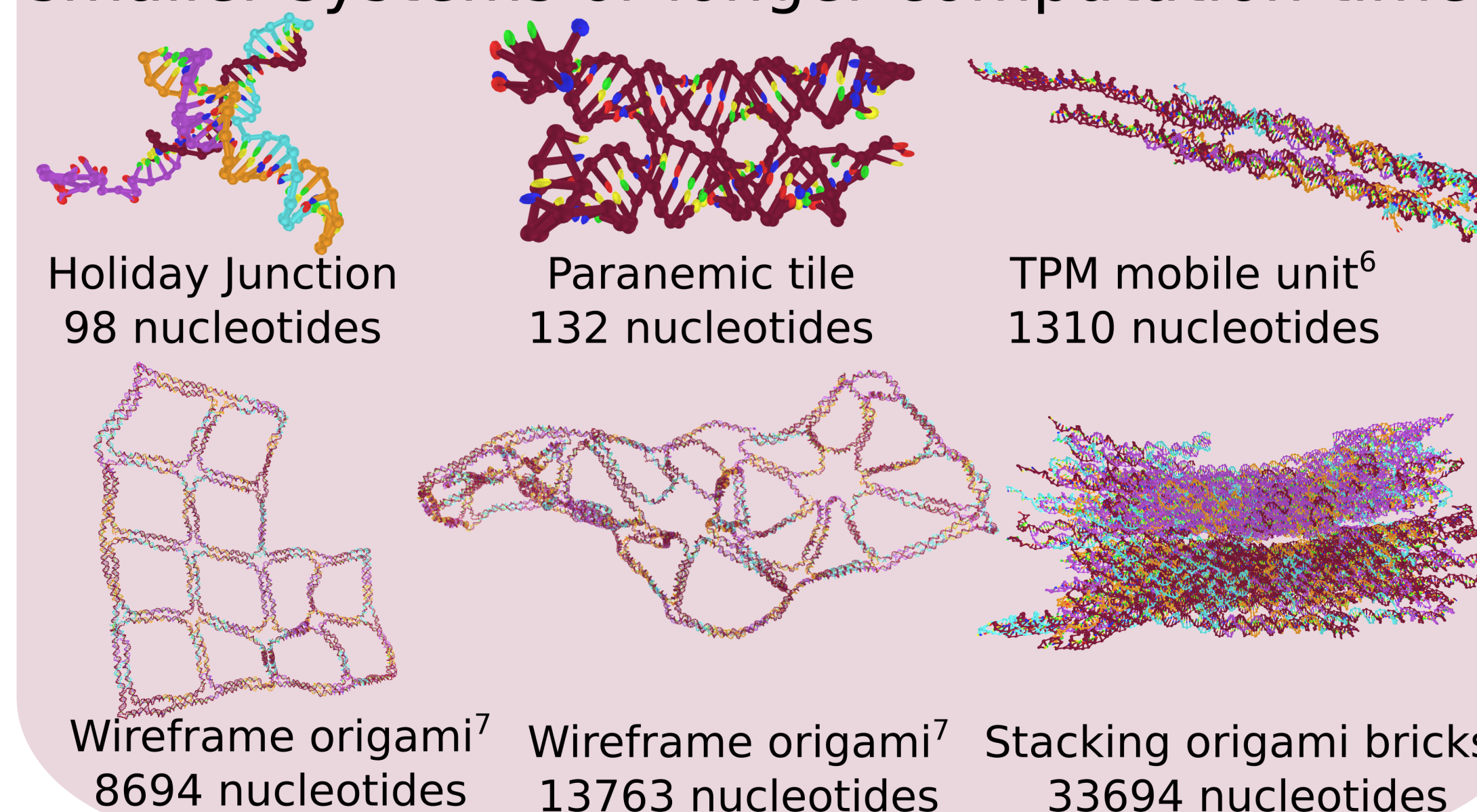
- Coarse-grained models built for nanotechnology
- Accurately reproduces structure, thermodynamics, and mechanics of single- and double-stranded DNA/RNA
- Monte-Carlo and Molecular Dynamics methods
- Efficiently sample systems up to 2 million nucleotides

Download: **[dna.physics.ox.ac.uk](http://dna.physics.ox.ac.uk)**



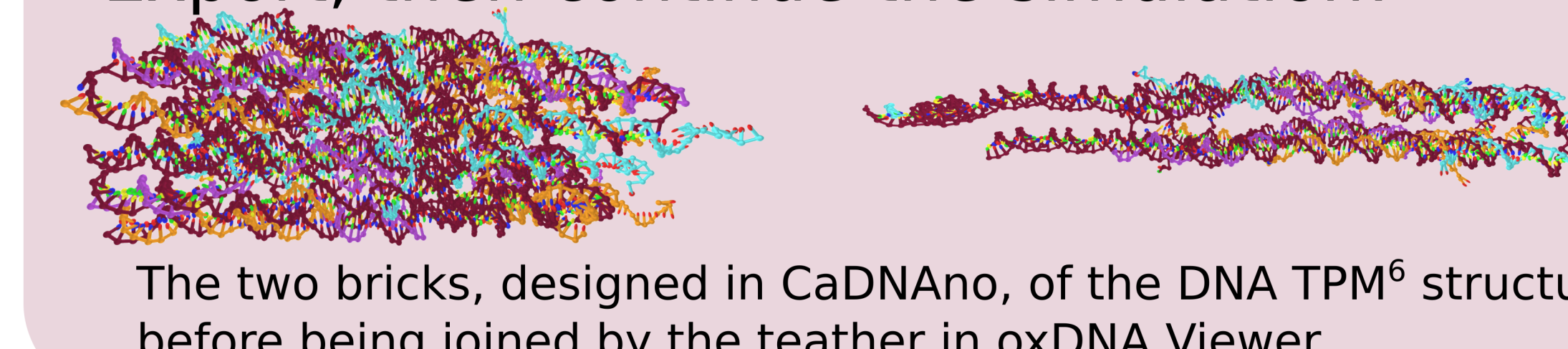
## Scale and sampling

- More complete sampling is possible with smaller systems or longer computation time



## Editing in the visualizer

- One strength of DNA/RNA nanotechnology is the modularity of components.
- oxDNA viewer has basic editing functions
  - Translation, rotation, nicking, ligation, deletion
- Export, then continue the simulation!



## Input vectors for DBSCAN

- Clustering can be performed on any vector space that has density differences.
- This example uses each snapshot's representation in principal component space

## Code structure

- These are generic tools for most structures
- Functions like file reading and parallelization are modular for use in custom applications
- Written in Python 3 and TypeScript

## References

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