Computer Science & Computer Engineering

WebDNA

an oxDNA simulation interface

THIS PROJECT

oxDNA is a widely-used molecular dynamics simulation software. While powerful, it's prohibitively difficult for non-programmers to use. We have built a web-based user interface, called *WebDNA,* that exposes the immediately useful information, such as simulation ***configuration***, ***visualization***, and ***analysis*** to the average researcher. With this project, we hope to have made a useful and user-friendly tool for efficiently and effectively running and analyzing DNA simulations.

FEATURES

Take advantage of the rich feature-set of oxDNA with **no programming requirements**! We've provided researchers with the ability to set simulation configuration options using a web-based GUI. These options are then sent off to the server to perform the requested oxDNA simulation.

Once results are ready, play back the simulation using the integrated **HTMoL** molecular visualization software. This visualization is generated directly from **`.pdb`** files provided by oxDNA at different steps in the simulation.

The final feature we've provided is the ability to run various **analysis scripts** on your results. Our site hosts a variety of default analysis scripts provided by oxDNA, as well as the ability for users to **upload their own scripts** to be executed on the server securely.

TEAM

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MENTOR

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ENABLING TECHNOLOGIES

These technologies are the building blocks that make WebDNA work as well as it does.

Django & Python
Server-side REST API and oxDNA Execution Server

PostgreSQL
Database Management System

Angular
Front-end Web Application Platform

HTMoL
HTML Embeddable Simulation Frame