

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.

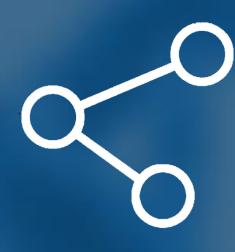
FEATURES



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

Jace McPherson | Computer Science
David Darling | Computer Science
Zack Fravel | Computer Engineering
Salvador Sanchez | CS, Mathematics
Jonathan Raney | Computer Science

MENTOR

Matthew Patitz, PhD Computer Science



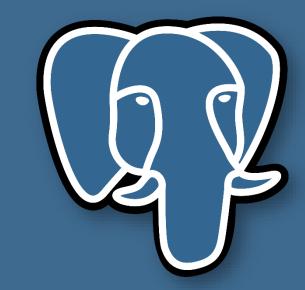
ENABLING TECHNOLOGIES

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



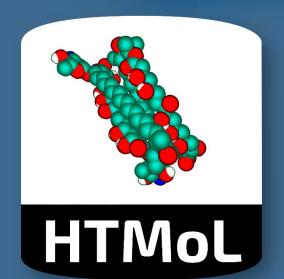
PostgreSQL

Database Management System



Angular

Front-end Web Application Platform



HTMoL

HTML Embeddable Simulation Frame



We DNA