

WebDNA Project Proposal

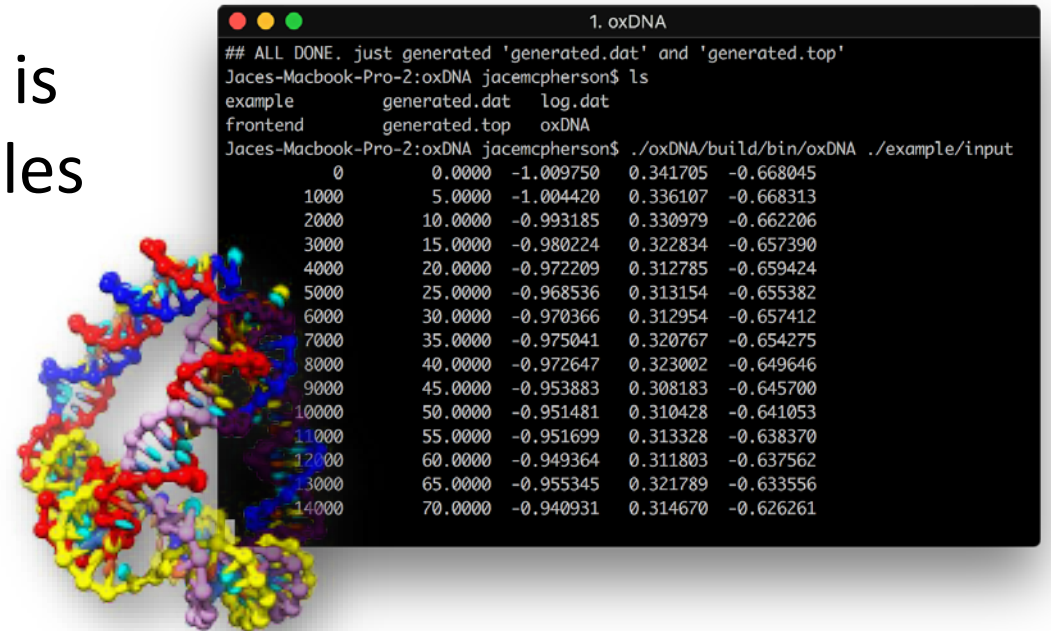
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Premise: Here's the Problem...

- oxDNA is a widely used DNA simulation software.
- It's clunky, and very inaccessible to most DNA researchers.
- Analysis of the oxDNA output is the main time-consumer for DNA related research.
- Because it lacks a UI, file management is also an issue. oxDNA produces many files and it's up to the user to figure out how to organize them.
- Difficult visualization of simulation results



Objective: How can we fix this?

- We plan to wrap oxDNA functionality with a website
- All input data, simulation visualization, and data analysis should take place in our controlled environment
- Guide the configuration experience with a clean, sensible UI
- Allow advanced users to download their results and perform offline analysis, if necessary.

UX + UI

The background is a deep blue gradient. A bright blue arc curves across the upper portion of the frame. A red dot is positioned on this arc, slightly to the left of the center. Below the arc, there are faint, blurry horizontal lines of light blue and white, suggesting a distant horizon or a reflection on water.

Design Goals

1. Provide simple user interface for generating input data to the oxDNA simulation environment.
2. Allow users to modify the execution parameters of the simulation
3. Provide a visualizer to show the DNA system state at different points in time.
4. Provide a visual *analysis platform* so that the user can easily perform analysis with no code experience necessary.

I promise, these will be clearer in a second...

Simulation Configuration

Required Settings

- Normally set up with Python scripts in a clunky workflow
- Now, reduced to simple series of steps with *same functionality*

Optional Settings

- Allows users to run built-in and/or custom scripts on their input

The screenshot displays the 'WebDNA - Configuration' web interface. The browser address bar shows 'https://webdna.uark.edu/configuration'. The main content area is divided into two columns. The left column contains a breadcrumb trail 'Home > Test Project 1 > Configuration > Visualizer & Analysis'. Below this is a section titled 'Required Configuration Settings' with three rows: 'Sequence File' (GCACGAGTCCTAAGC GCACGAGTCCTAAGC GCACGAGTCCTAA...), 'Strand Generator' (Script: DNA | Box Size: 13.0 | Notes: We Will...), and 'Generic Parameters' (Interaction: DNA | Sim Type: MD | Precision: ...). Below this is a blue bar for 'Simulation Parameters' showing 'Steps: 1e6 | Newtonian Steps: 103 | T: 334K | ...'. The next section is 'Optional Pre-processing Scripts (0)' with two buttons: 'Select an Existing Script' (with a PY icon) and 'Upload Custom Script' (with an upload icon). At the bottom of the left column is a large green button labeled 'RUN SIMULATION'. The right column is a blue sidebar titled 'Simulation Parameters' with a close button. It contains several settings: 'Steps' (1e6), 'Newtonian Steps' (103), 'Diffusion Coeff' (2.50), 'Thermostat' (john), 'Temperature' (334 K), 'dt' (0.005), 'Verlet Skin' (0.05), 'Fix Diffusion' (checked), 'Back in Box' (unchecked), and 'pt' (empty field).

WebDNA - Configuration

https://webdna.uark.edu/configuration

Home > Test Project 1 > Configuration > Visualizer & Analysis

Required Configuration Settings

Sequence File GCACGAGTCCTAAGC GCACGAGTCCTAAGC GCACGAGTCCTAA...

Strand Generator Script: DNA | Box Size: 13.0 | Notes: We Will...

Generic Parameters Interaction: DNA | Sim Type: MD | Precision: ...

Simulation Parameters Steps: 1e6 | Newtonian Steps: 103 | T: 334K | ...

Optional Pre-processing Scripts (0)

Select an Existing Script Upload Custom Script

RUN SIMULATION

Simulation Parameters

Steps 1e6

Newtonian Steps 103

Diffusion Coeff 2.50

Thermostat john

Temperature 334 K

dt 0.005

Verlet Skin 0.05

Fix Diffusion ☒

Back in Box ☐

pt

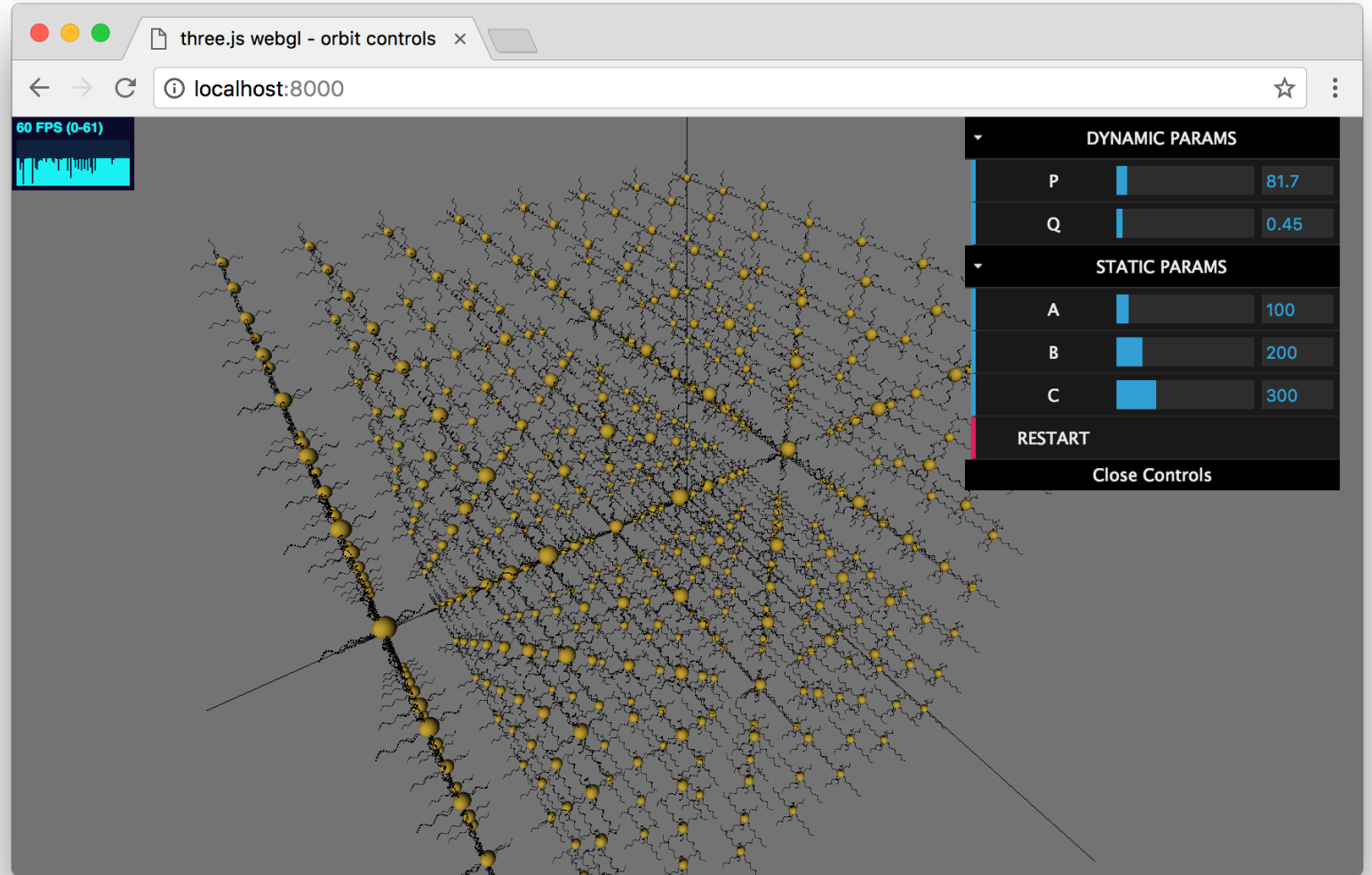
Simulation Visualization

Current Visualizer

- Simple nanoparticle visualizer already implemented
- We can use the current visualizer as a base for our more flexible oxDNA simulation visualizer.

Added Features

- Scrubbing through simulation over time



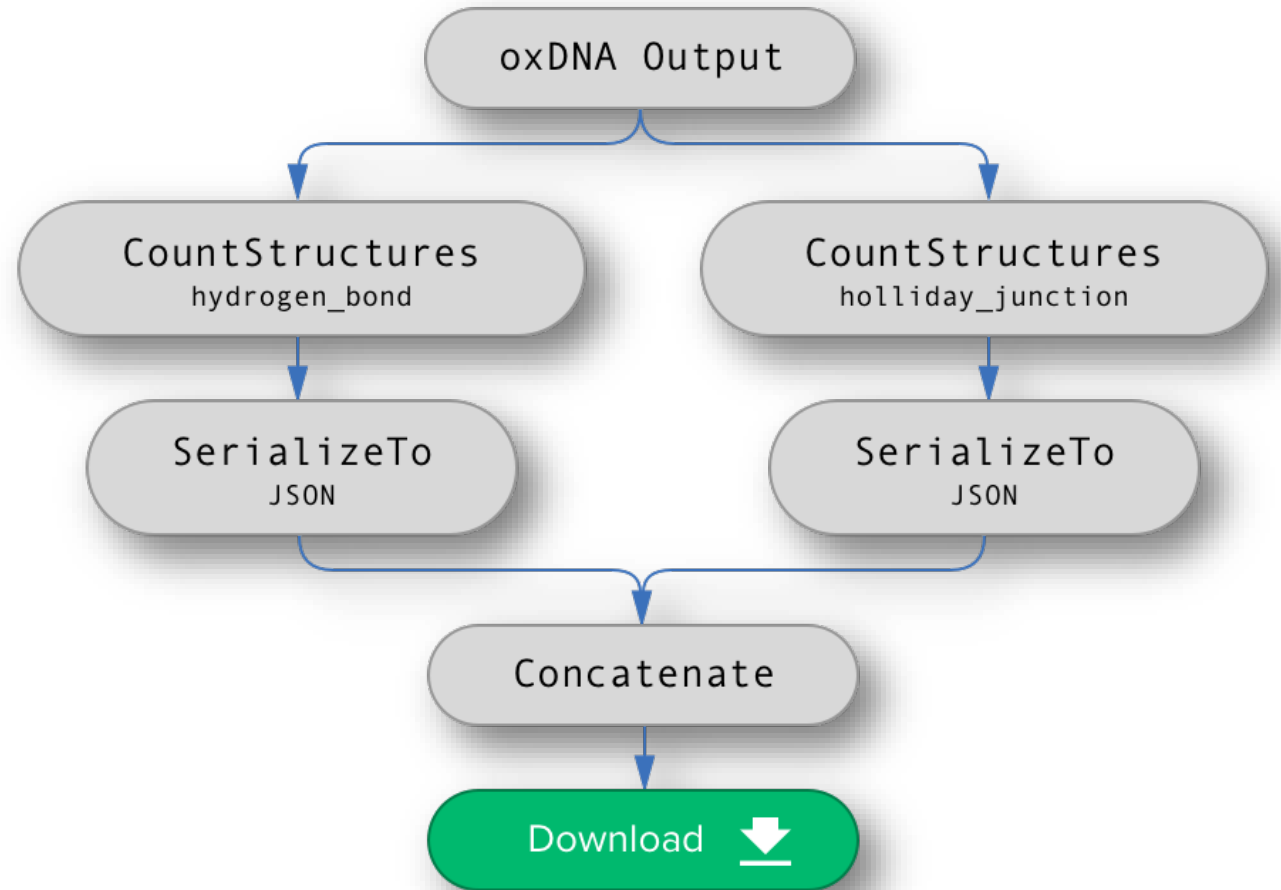
Analysis Editor

Current Analysis Pipeline

- NONE! Researchers have to write their own analysis code to extract meaningful data from simulations

Our Analysis Solution

- Create a drag-and-drop style interface for users to pipe their simulation data through a series of analysis steps
- Allow downloads of data at *each of the steps*, including the final output, for full customizability.



Technologies

Server



Django Python Server

- Listens for HTTPS requests
- Serves web pages using the Django HTML renderer



PostgreSQL

PostgreSQL DBMS

- Widely used SQL extension

Client

Django Python Renderer

- Renders HTML, CSS, and Javascript using logic written in Python

Three.JS

- 3D Renderer for browsers (using WebGL)

