

WebDNA Project Proposal

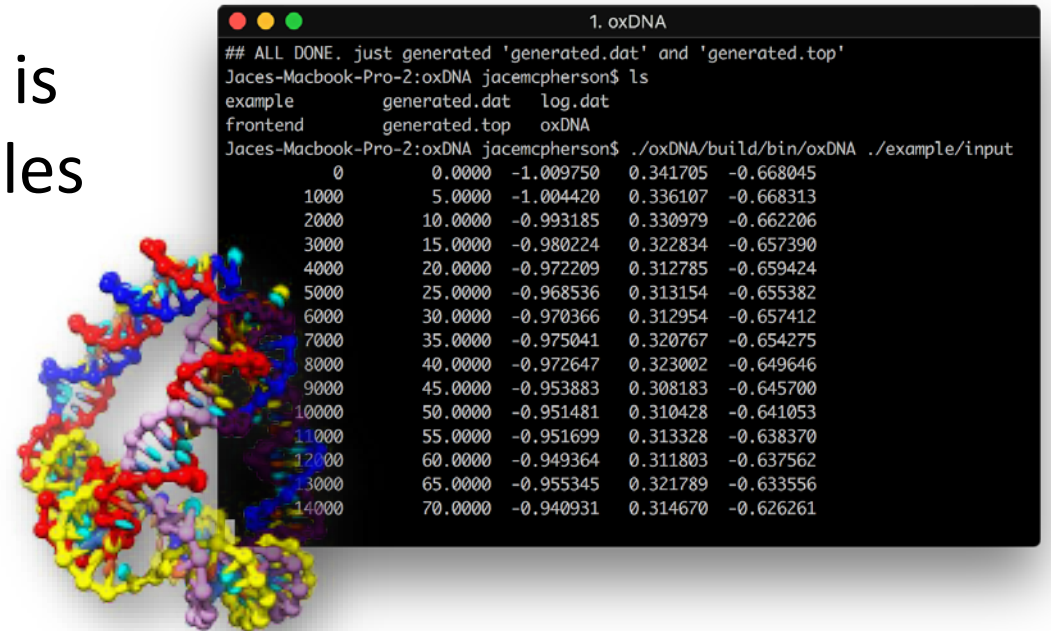
*Jace McPherson, Salvador Sanchez, Zack Fravel,
David Darling, Jonathon Raney*

November 6, 2017



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

An abstract background with a dark blue gradient. A bright blue arc curves across the upper portion of the image. A red dot is positioned on this arc, with a faint red glow around it. Below the arc, there are some faint, blurry light patterns.

Design Goals

Technologies

Server



Django Python Server

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



PostgreSQL DBMS

- Widely used SQL extension

Client

Angular2 Renderer



- Framework based on Javascript for rapid development of UIs.
- Adapts and extends HTML to present fully dynamic content.

Three.JS

- 3D Renderer for browsers (using WebGL)



Project Schedule

Tasks have been divided into two main sections to be worked on concurrently

Server

- Setup of hosting method January 26
- Initialization of database schema on hosted PSQL platform January 26
- Server Endpoints February 14
 - POST user authentication
 - GET projects
 - GET project configuration data
 - PUT project configuration data
 - POST specify simulation generation scripts
 - POST specify analysis pipeline
- Implementation of file generation February 16
- Script uploading and checking February 28
- Execute simulation from project data March 16

Client

- Login/Registration page January 22
- Project management page January 30
- Configuration page February 7
- Output file visualizer March 9
- Output pipeline editor March 23
- Custom script manager March 30
- Dashboard (integration of pages) April 6

Client: 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 titled 'Home > Test Project 1 > Configuration > Visualizer & Analysis'. It features a 'Required Configuration Settings' section with fields for 'Sequence File' (containing a DNA sequence), 'Strand Generator' (set to 'Script: DNA | Box Size: 13.0 | Notes: We Will...'), and 'Generic Parameters' (set to 'Interaction: DNA | Sim Type: MD | Precision: ...'). Below this is a 'Simulation Parameters' summary bar showing 'Steps: 1e6 | Newtonian Steps: 103 | T: 334K | ...'. The 'Optional Pre-processing Scripts (0)' section offers two options: 'Select an Existing Script' (with a .PY icon) and 'Upload Custom Script' (with an upload icon). A large green 'RUN SIMULATION' button is at the bottom. On the right, a blue sidebar titled 'Simulation Parameters' contains a list of 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).

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	<input checked="" type="checkbox"/>
Back in Box	<input type="checkbox"/>
pt	

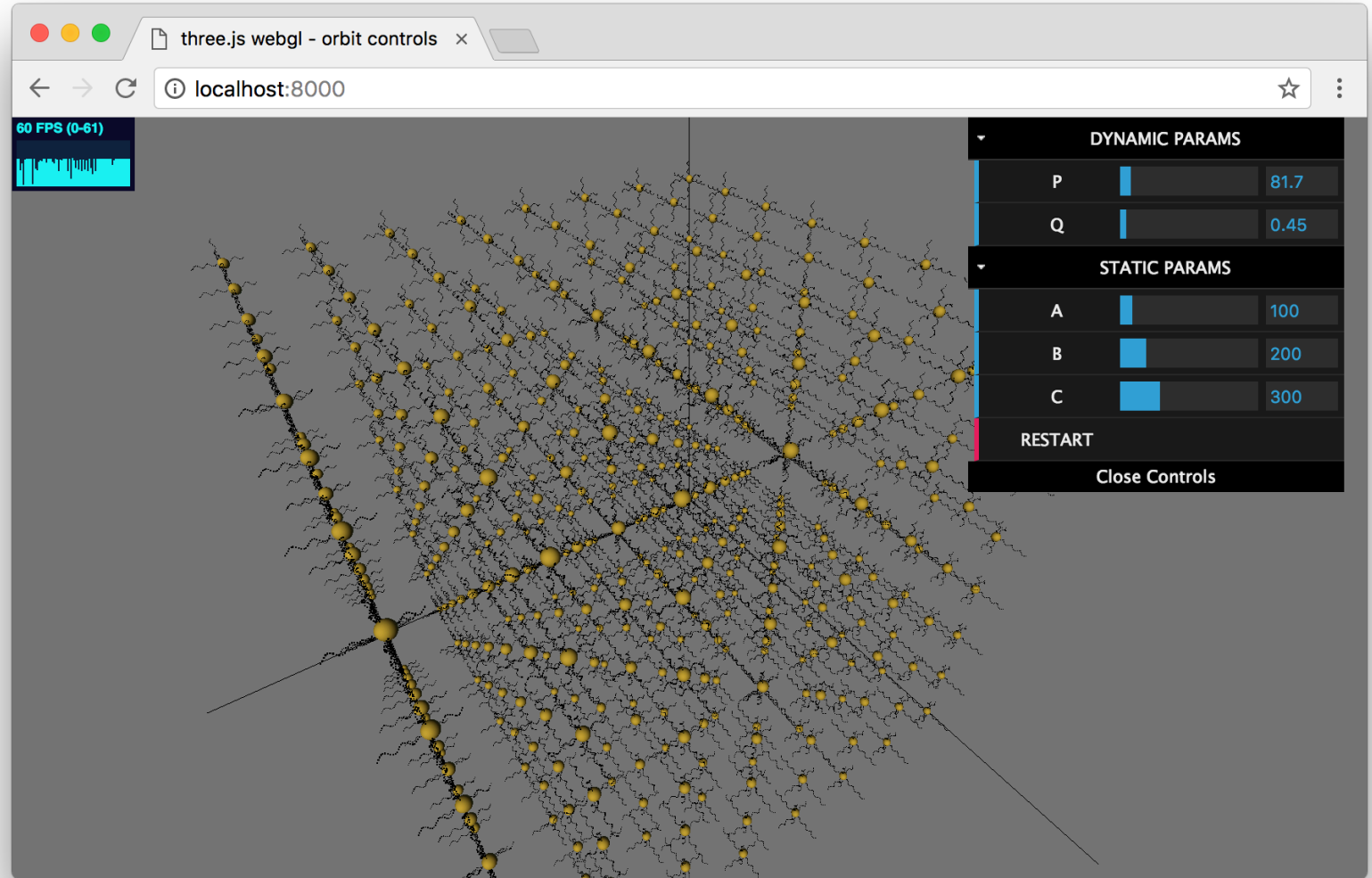
Client: Simulation Visualization

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



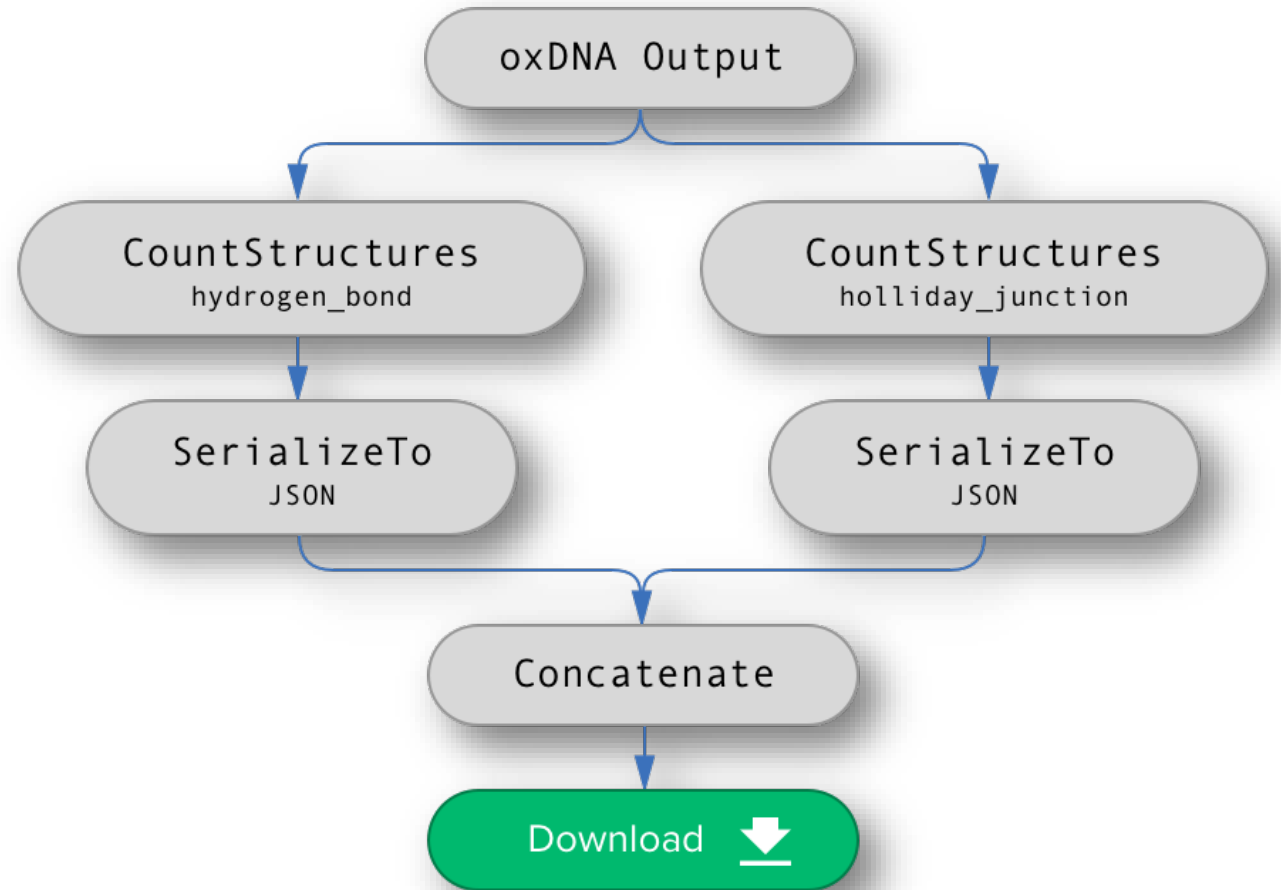
Client: Output Pipeline Editor

Current Analysis Pipeline

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

Our Analysis Solution

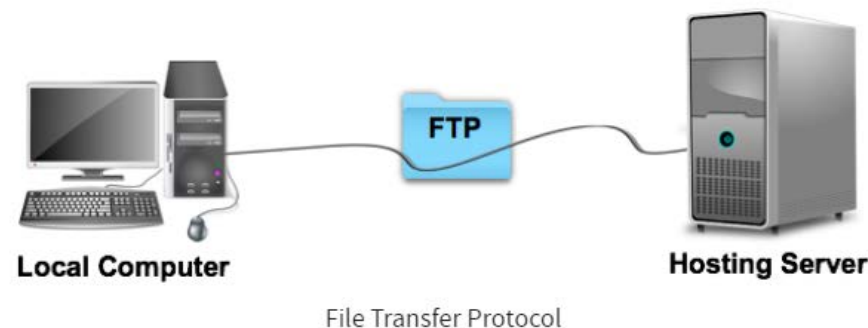
- Create a drag-and-drop style interface for users to pipe their simulation data through a series of analysis steps
- Allow downloads of data at *each of the steps*, including the final output, for full customizability.



Client: Custom Script Manager



- The goal is to provide a simple way for users to upload and make use of their own locally-written python scripts for use within the pipeline editor.
- A remote file exchange protocol such as FTP will be used to allow users to directly upload files
- These files will be screened to ensure they meet server requirements and then made available to users



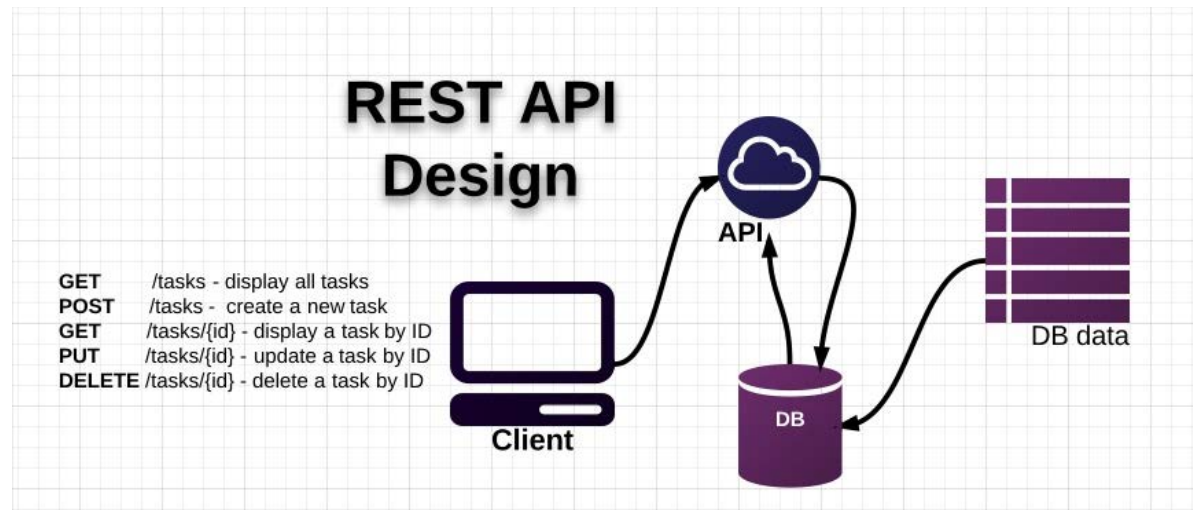
Server: Hosting and Database

- Server will be hosted on either UARK's Turing or a 3rd party platform such as AWS or Heroku
- The PSQL Database will be similarly hosted and will store data such as user information and script metadata



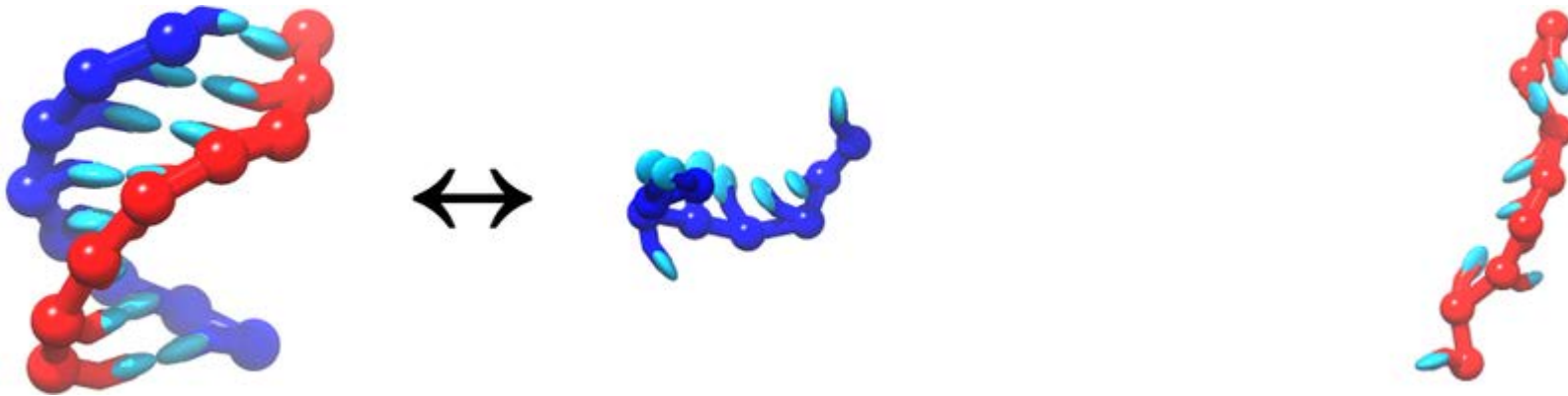
Server: URL Endpoints

- The server will rely on RESTful URL endpoints to provide functionality to clients.
- Endpoints will be defined to perform many different tasks such as authenticating users and specifying analysis pipeline information



Server: Executing Simulations

- The user will be able to submit a Job for queuing to the server
- The Job is initialized using only the desired project ID.
- An instance of oxDNA will be executed according to the parameters specified in the project corresponding to the supplied project ID.



Final Product

- By the end of the course, we hope to deliver a robust and extensible web server capable of launching highly customizable oxDNA simulations.
- 3D analysis tools and custom output scripts will offer useful and intuitive functionality for researchers.
- Using oxDNA will become much more streamlined and simplified