WebDNA Documentation

1. User Profiles

Registration

The landing page of the site allows new users to register for an account as well as links existing users to the login page.

Users enter their First and Last name, Username, Email, and Password.

Password must have at least 1 [A-Z], [0-9], and one special character.

Logging In

Use this page if you're an existing user and wish to log in with your username and password.

Log out on the dashboard using the button in the top right.

2. Projects

Creating (and Deleting) Projects

Creating new projects is simple. From the dashboard, just click "Add New Project" at the top of the project list and you'll be asked to name and create your new project.

Projects can be deleted clicking the "Delete Project" icon at the far right of the project's entry on the dashboard list.

Editing Projects

Simulation Settings

Whenever a user clicks "Edit Project," they're brought first to the "Simulation Settings" page. Here, users can specify their inputs to all the various oxDNA simulation parameters. See the oxDNA documentation for more information about each of these settings.

Generation Options

Users are asked to provide a "sequence.txt" file that oxDNA is expected to read. This contains the strands being simulated in the system.

Users specify the system box size here. Smaller box sizes will take longer to initialize, since the chance of strands colliding is much higher with a smaller box.

Generic Options

We've provided the ability to specify interaction type, simulation type, floating point precision, backend type (CPU/GPU), as well as enabling or disabling debugging.

Simulation Options

These options are frequently used for most simulations.

Molecular Dynamics Simulation Options

These settings are specifically for modifying the behavior of "MD" simulations. This is the only type of simulation the WebDNA currently supports.

Output Analysis

Users can navigate to the output analysis portion of editing their project by clicking "Configure Analysis" at the top right of the page at any time.

Built In Analysis

We've provided a number of default oxDNA analysis scripts that can be added one at a time to the pipeline by clicking "Insert Row" under the Project Pipeline section.

When ready, users can click "Execute Analysis" to initialize the output pipeline.

Once an analysis is running, the pipeline output can be observed in the dialogue box in the center of the page.

User-Defined Analysis Scripts

Users have also been given the ability to upload their own Python scripts to be added to the pipeline by clicking “Upload New Script” in the section at the top left of the page. We’ve kept the handholding to a minimum with the script uploading, so be safe and double check for errors!

Downloading Project Files

Users have the ability to download everything associated with their project to a .zip file by clicking “Download Project” on the Dashboard under the desired project entry.

3. Running Simulations

Running a Job

Simulations can be run by clicking the “Run Simulation” button in the “Simulation Settings” page.

Clicking this button also begins generating the system state, which can take a while depending on your specific box size. Be patient while the server initializes the simulation.

Jobs are handled per processor core on the server, so the maximum number of jobs is determined by the number of processor cores available.

Viewing Job Output

Your current running job’s oxDNA console output log can be viewed by clicking “View Output” on the project’s list entry on the Dashboard.

This output can be viewed in real time and is also saved to a file that is accessible to the user later through a download.

4. Visualization

How to Visualize a Simulation

Your current project can be visualized using HTMoL by clicking the "Visualizer" button on the left hand side of the Dashboard.

Users can specify which project they want to visualize using the provided dropdown menu.

Note on Browsers and Compatibility

Currently our visualizer only works on **Mozilla Firefox,** other browsers have a tendency to crash the website. Our recommendation for now is to stick with Firefox until a solution is found.

5. Reference Information

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Created as part of the University of Arkansas Computer Science / Computer Engineering Department Capstone Course.