Getting Started with 4D Genome Browser Workbench (workflow version 0.3)

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Instructions v3

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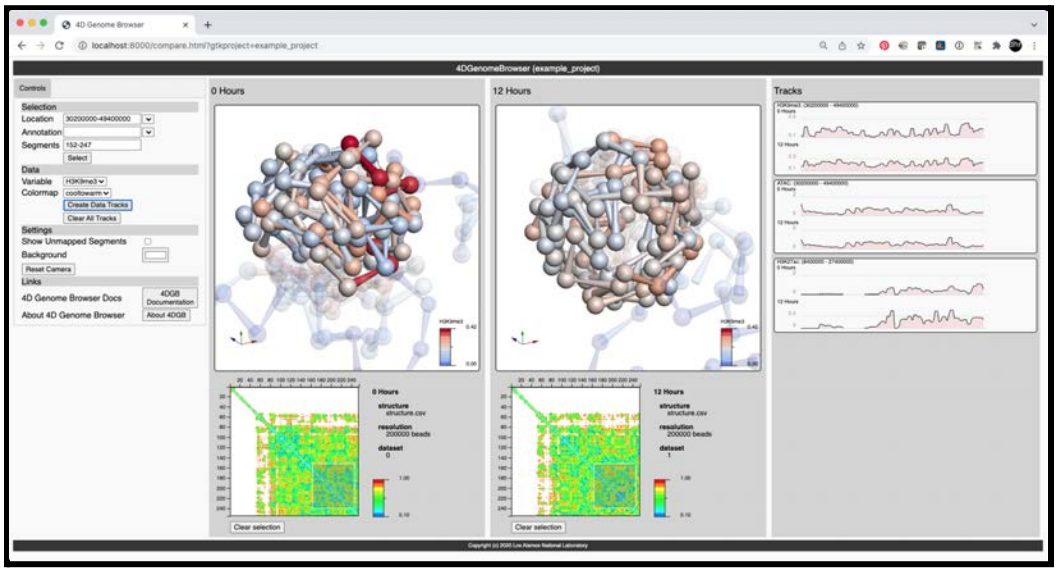

Figure 1: Screen capture of the result of running the 4DGenomeBrowser Workflow on the example project. The user can compare two collections of data side-by-side, manipulating the view, contact map and tracks of data displayed. This screenshot shows several detailed tracks, and a new colormap applied to the data.

Overview

The 4D Genome Browser Workflow is an application that takes `.hic` data and tracks as input, runs a molecular dynamics simulation to determine a 3D structure for that data, and constructs an instance of a browser to view the resulting information.

The first task we'd like people to do is to try to download and install the workflow, run it on an example dataset. The development team is seeking feedback on how that process works, as well as bugs and features in the browser.

Getting started

The workflow requires the application Docker to be installed on your machine. This is the engine that runs the workflow. To get started with Docker:

1. Create an account on docker hub and send the login name to dhr@lanl.gov
2. Install docker on your machine. Instructions are here.
3. Download the example project from github.

Running the workflow

- **Run docker on your machine.** How you do this depends on the operating system you're running on:
    - Mac: Click on Docker Desktop and wait until it reports that it is running
    - Linux: Most likely, it will be running automatically, if not, you can run:

      ```
      systemctl start docker
      ```

    - Windows: Click on Docker Desktop and wait until it reports that it is running

- **Login to DockerHub.** In a shell or terminal window, login to DockerHub (you'll be asked to enter your username and password):

  ```
  docker login
  ```

- **Update to the most recent workflow** Each time you run the workflow, make sure you've got the latest version. To do this, open a shell and **`cd`** to the directory with the **`example_project`** data in it, then run the following command. The workflow will update, and you'll be ready to test again.

  ```
  docker pull 4dgb/workbench:latest
  ```

- **Extract the `4DGBWorkflowExamples-0.3.tar.gz`** file you downloaded into the current directory, which will result in a directory with a script (`4dgb-workflow`) and a project directory (`example_project`) inside it. This is the command to extract the files:

  ```
  tar -xzvf 4DGBWorkflowExamples-0.3.tar.gz
  ```

- **Run the example project.** The first time you run this, it will download the Docker image and run the LAMMPS simulation. It will take a few minutes, but it will go quickly on subsequent runs because it will not need to re-run the simulation.

  ```
  cd 4DGBWorkflowExamples-0.3
  ./4dgb-workflow example_project
  ```

- After the workflow is complete, a URL will be printed to the shell (see Figure 2). Copy and paste that URL into a browser (Chrome, Safari and Firefox), and you should see the browser running on the data (see Figure 1).

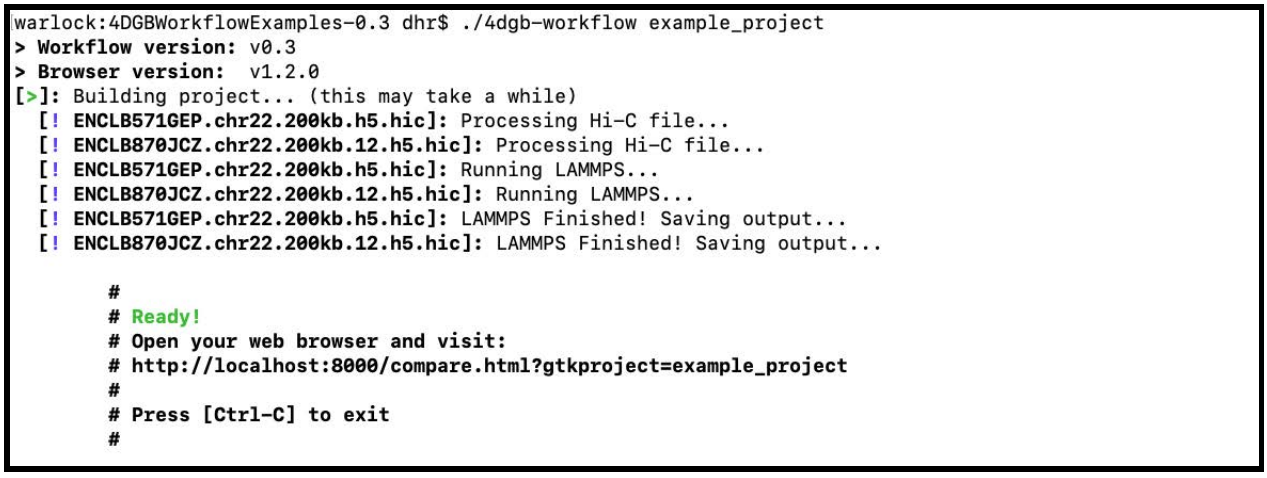

Figure 2: Screenshot of the output from running the workflow on the example project.

Sending feedback and suggestions

If you run into any problems, or have suggestions about browser features that would be helpful, contact the group:

- 4dgbworkflow@lanl.gov — general discussion with the group
- dhr@lanl.gov — David Rogers
- ctauxe@neptuneinc.org — Cameron Tauxe
- croth@lanl.gov — Cullen Roth