

Project Documentation

Version: 1.1.0

Project Repo: https://github.com/bhavinjawade/ChemML_Web_UI

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 - left-menu-component
 - loading-component
 - nav-button
 - new-project-box
 - open-project
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 - results-page-component
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Architecture

Database structure:

MongoDB Collections > chemml_projects > projects

```

_id: ObjectId("5f5ef60606a5231ae56f8123")
project_name: "MaterialsLab Project"
project_desc: "Radial Distribution Function (RDF) defines the number of atoms present..."
created_date: 2020-09-14T00:48:06.708+00:00
✓ config: Object
  file: "/users/chemml/file.txt"
✓ project_properties: Object
  tag_list: Array
    0: "rdf"
    1: "materials"
    2: "solarcells"
    3: "some"
    4: "RDF"
  users: "bhavinjawade"
✓ files: Object
  > grad_ben_handbook-2020.pdf: Object
  > assignment2data.csv: Object
  > Boston.csv: Object
  > FL_insurance_sample.csv: Object
  > tempCSV.csv: Object
  ✓ testingCSV.csv: Object
    file_name: "testingCSV.csv"
    file_path: "./project_files/MaterialsLab Project/testingCSV.csv"
✓ results: Object
  > 1: Object
  ✓ 2: Object
    result: "Pipeline is still running. Results will be available after execution."
    run_status: "pending"
    scheduled_time: 2020-09-17T03:01:41.172+00:00
    time_exection: "not available"
    > pipeline_json: Object
  > 3: Object
  > 4: Object
✓ graph: Object
  ✓ 1: Object
    scheduled_time: 2020-09-17T03:01:40.283+00:00
  ✓ saved_graph: Object
    ✓ blocks: Object
      > tool_csv_0: Object
      > tool_dim-reduction_1: Object
      > tool_preprocessing-node_2: Object
      > tool_helper-functions_3: Object
    ✓ Arrows: Array
      0: "<div data-parent='tool_csv_0' data-child='tool_dim-reduction_1' class=..."
      1: "<div data-parent='tool_dim-reduction_1' data-child='tool_preprocessing..."
      2: "<div data-parent='tool_preprocessing-node_2' data-child='tool_helper-f..."
    ✓ blockarr: Array
      > 0: Object
      > 1: Object
      > 2: Object

```

Code Structure

To add a new API

1. Create a app.route and associated function in **server/api/api.py**.
2. Add API path in **app/helpers/api_url.ts**.
3. Add an Observable function in **data-service.service.ts**.
4. Subscribe to the observable in the component's constructor.

```

runPipeline(project_name: string, body: any): Observable<any> {
  var packet:any = {

```

```
        data : body
    }
    return this.http.post(API_URLS.runPipeline + project_name,
        JSON.stringify(packet)).pipe(
        catchError(this.handleError<any>('runPipeline', []))
    );
}
```

Angular Components:

1. **global-footer:** add it to every full page component.
2. **helpers:** contains chemml-sklearn-jsons, and api_url.ts
3. **home-page:** the main-landing page. contains redirection to tutorials and portal.
4. **input-output-component:** Opens when the user clicks on the arrows between tab. Handles output from previous node and input to next node.
5. **landing-page:** This is main page of the portal. Shows the listing of all projects.
6. **left-files-bar-components:** Show and upload files to the project.
7. **left-menu-components:** Not of any use. To be deleted.
8. **loading-component:** Import this component to create a loader in between component.
9. **nav-button:** Edit the navbar buttons in this component.
10. **new-project-box:** Opens the new project box.
11. **open-project:** Loads all the previous project.
12. **project-info-component:** Edit the project information name, description, and tags.
13. **results-page-component:** This component displays all the results of previous runs.
14. **tool-config:** Side config bar, to select configuration options for selected tool. Contains the json interpolator.
15. **toolbox:** left side toolbox that lists all tools
16. **toolbox-component:** Component that creates individuals tools. This works with flowy.js drag and drop.
17. **visualize-main:** The visualization component. Add more graphs in this component.
18. **app.component.ts:** The main component where portal canvas and drag drop functionalities work.

Celery pipeline uses mongoDB backend. **Mongodb > jobs collection.**

Description for individual functions will be added as comments in code files.

Project Deployment

Backend:

1. Clone repository:

```
https://github.com/bhavinjawade/ChemML_Web_UI
```

2. Activating environment and setting up flask API. The api code package requirements are written in requirements.txt

```
conda activate ./my_chemml_env
cd server
cd api
pip3 install requirements.txt
```

3. Install chemml

```
cd ..
cd chemml
pip3 install -e .
```

4. Start API Server

```
python api.py &
```

4. Setup Celery and MongoDB.

MongoDB is both our application database and celery backend and broker.

Celeryconfig is already written in a file called celeryconfig.py. So the next steps are to install MongoDB and install celery and create celery worker process.

If MongoDB and celery are installed, then run:

```
celery -A celery_task worker --loglevel=info --pool=eventlet
```

To install celery:

```
pip3 install celery
```

To install MongoDB community via terminal:

```
wget -qO - https://www.mongodb.org/static/pgp/server-4.4.asc | sudo apt-key add -
```

```
echo "deb [ arch=amd64,arm64 ] https://repo.mongodb.org/apt/ubuntu focal/mongodb-org/4.4 multiverse" | sudo tee /etc/apt/sources.list.d/mongodb-org-4.4.list
```

```
sudo apt-get update
```

```
sudo apt-get install -y mongodb-org
```

Start mongoDB server:

```
sudo systemctl start mongod
```

Frontend

Create production build of angular project.

```
cd client
cd chemmlAngular
ng build --prod
```

This will create the production build in dist folder.

Make sure angular.json baseUrl is set to point right url for static files.