

Convoys in Atomic and Molecular Trajectories

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Introduction

Problem

Drug manufacturers run molecular simulations to detect events of interest; we are looking for the formation of a hydrogen bond that persists over a certain period of time. Doing this manually takes extensive time and effort.

Solution

An application that will take the simulation data as an input and output the convoys and hydrogen bonds in a visually comprehensive way.

Intended Users & Usage

Chemical Engineers
Easily filter data & visualize results

Pharmaceutical Investors
Understand drug interactions without complex understanding of details

Educators
Use a safe environment to demonstrate chemical reactions.

Design Requirements

Functional

Take user input
Output results
Scales well with users & datasets
Server-side computation

Economic

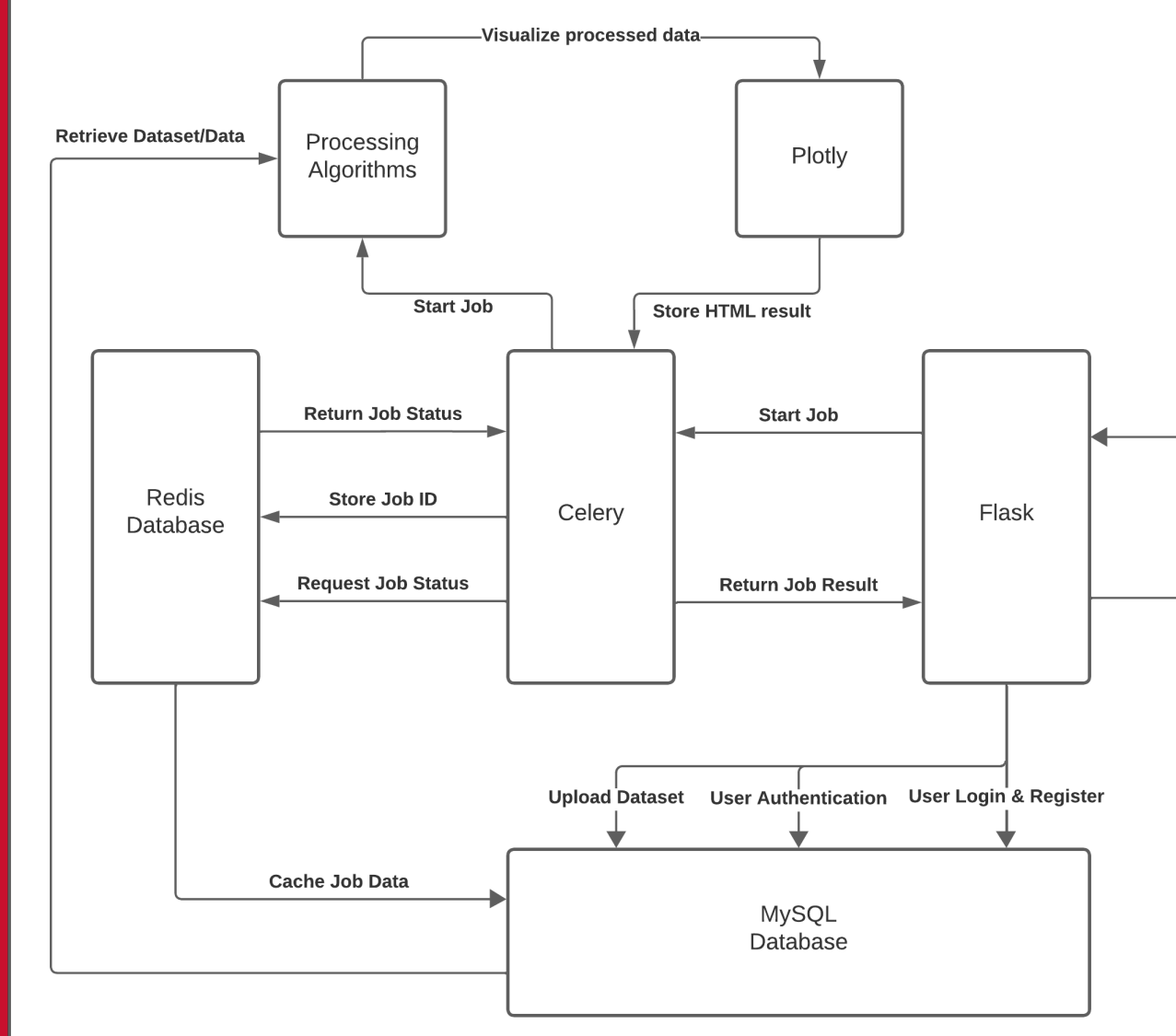
No unnecessary computations
Guarantee quality output

User Interface

Ease of navigation
Intuitive to understand
Provide input validation

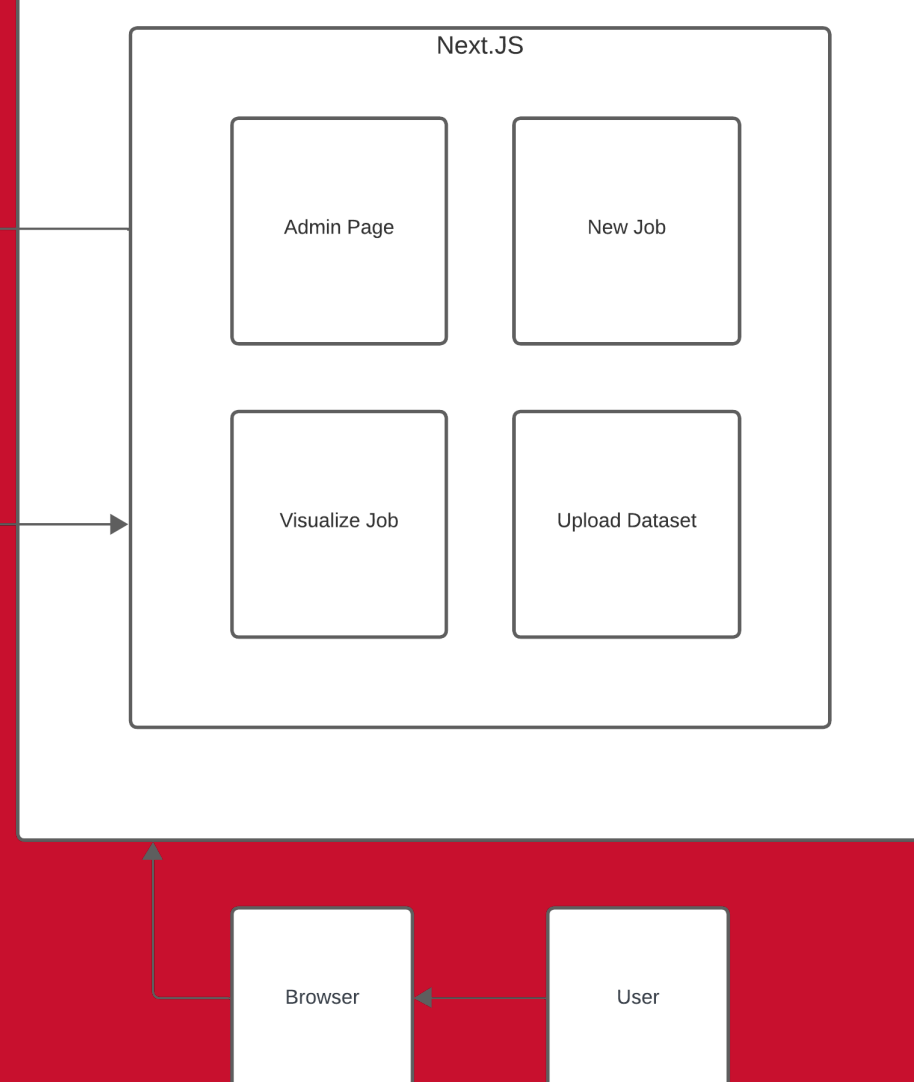
Design Overview

Backend Design



block diagram

Frontend Design



Technical Details

Technologies Used

Next.JS
Frontend framework

Flask
Python-based API framework

Celery
Asynchronous task queue library

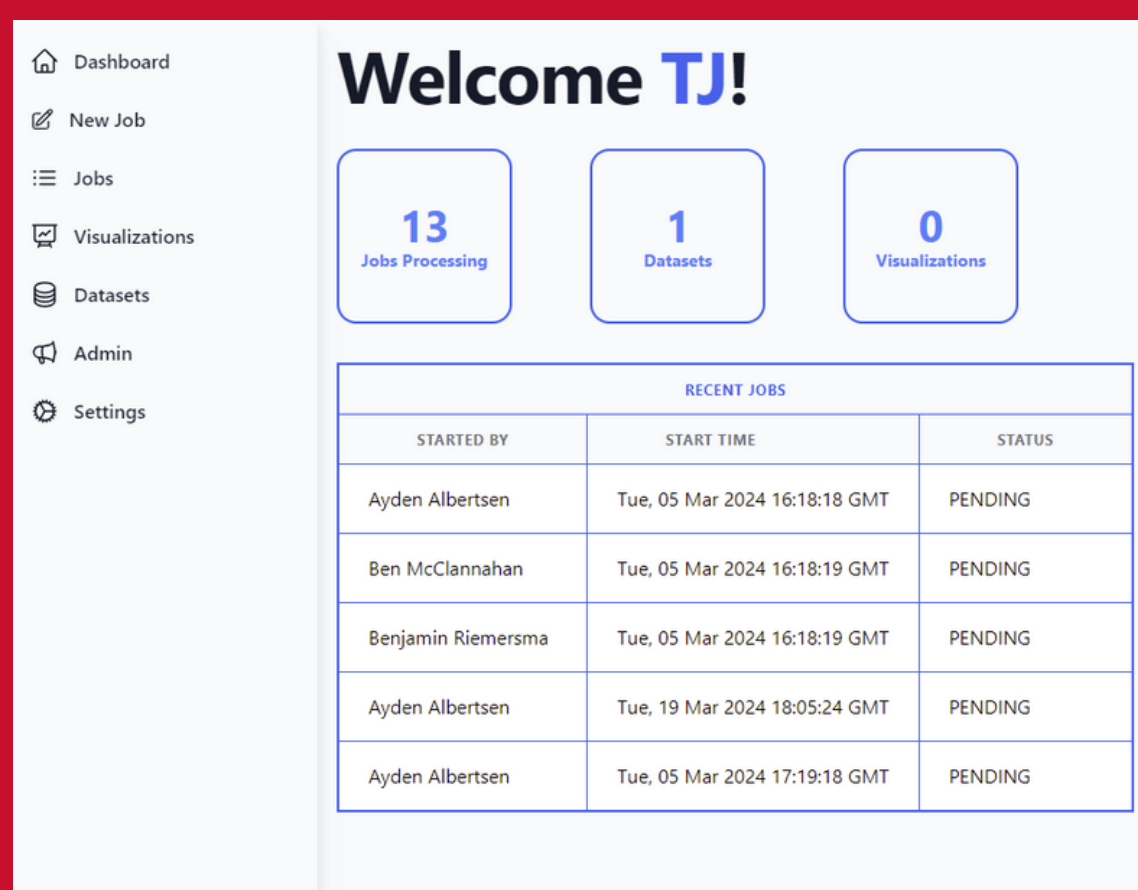
Redis
In-memory database for Celery

MySQL
Relational database for persistent data

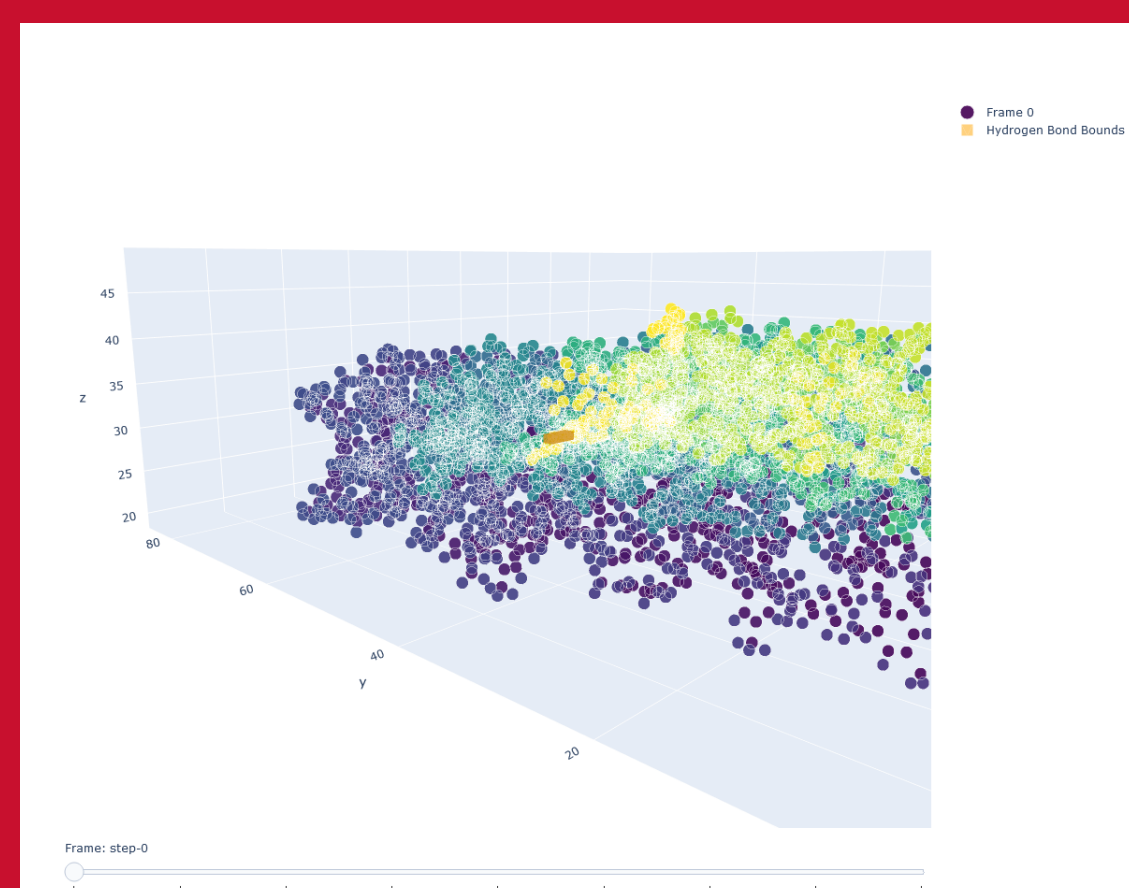
Plotly
Python-based data visualization library

Docker
Dynamic deployment of backend

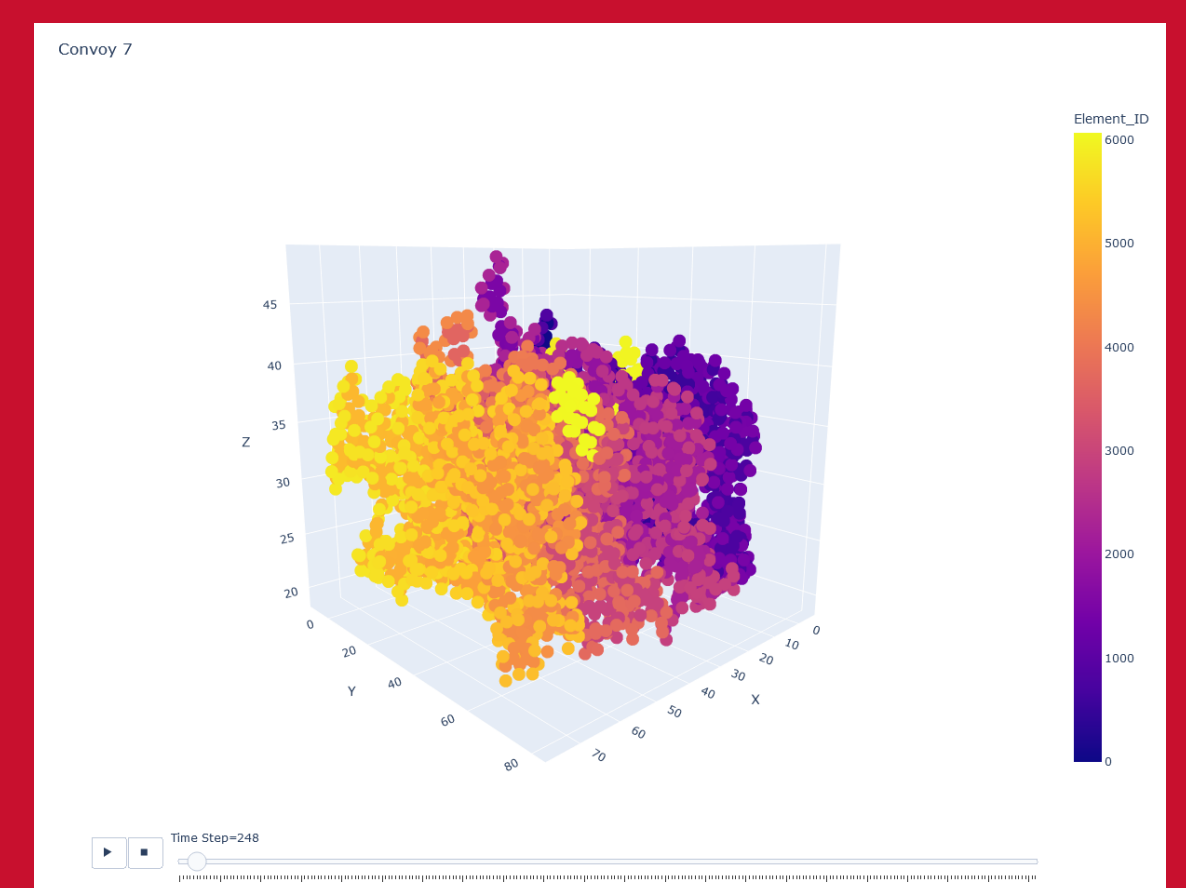
Visualizations



job dashboard



hydrogen bond visualization



convoy visualization

Testing

Unit Testing

PyTest
Backend Tests

Selenium
Frontend Test

Other Testing

Performed manual reviews for accuracy and completion with client and advisor

Standards IEEE/ISO/IEC 12207-2017