Detecting molecular and atomic convoys

Group 33:
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Project Vision

- High cost to testing drug interactions with substrates over time
- Simulations lower these costs of this testing
- Interesting events in simulation data (e.g., Hydrogen bond)

- Main objective - Develop a system to visualize the convoys

Project Overview

Molecular Convoys

Groups of atoms and molecules

Figure 2: Convoys Versus Moving Clusters
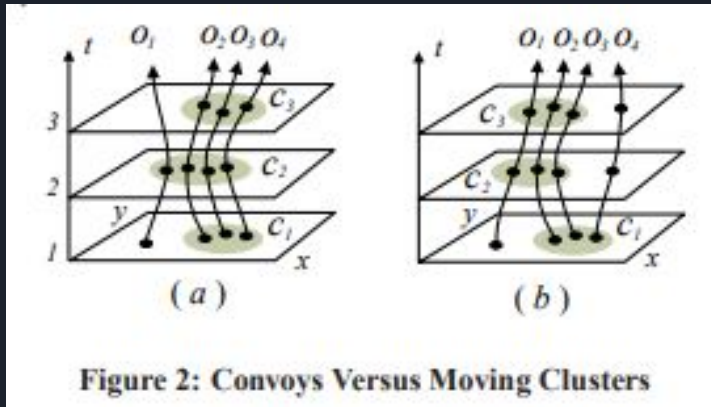
- Optimizing chemical research
- Simulating the molecular level
- Detecting convoys
- Finding trajectories
- Data analytics queries
- Algorithmic searching
- "Interesting Events"
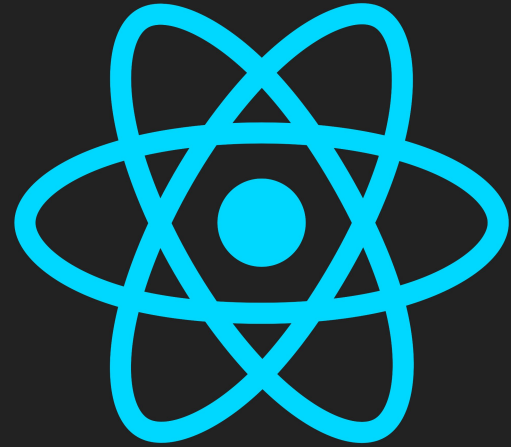- Graphical interface
- Frontend and backend design

Overview Diagram
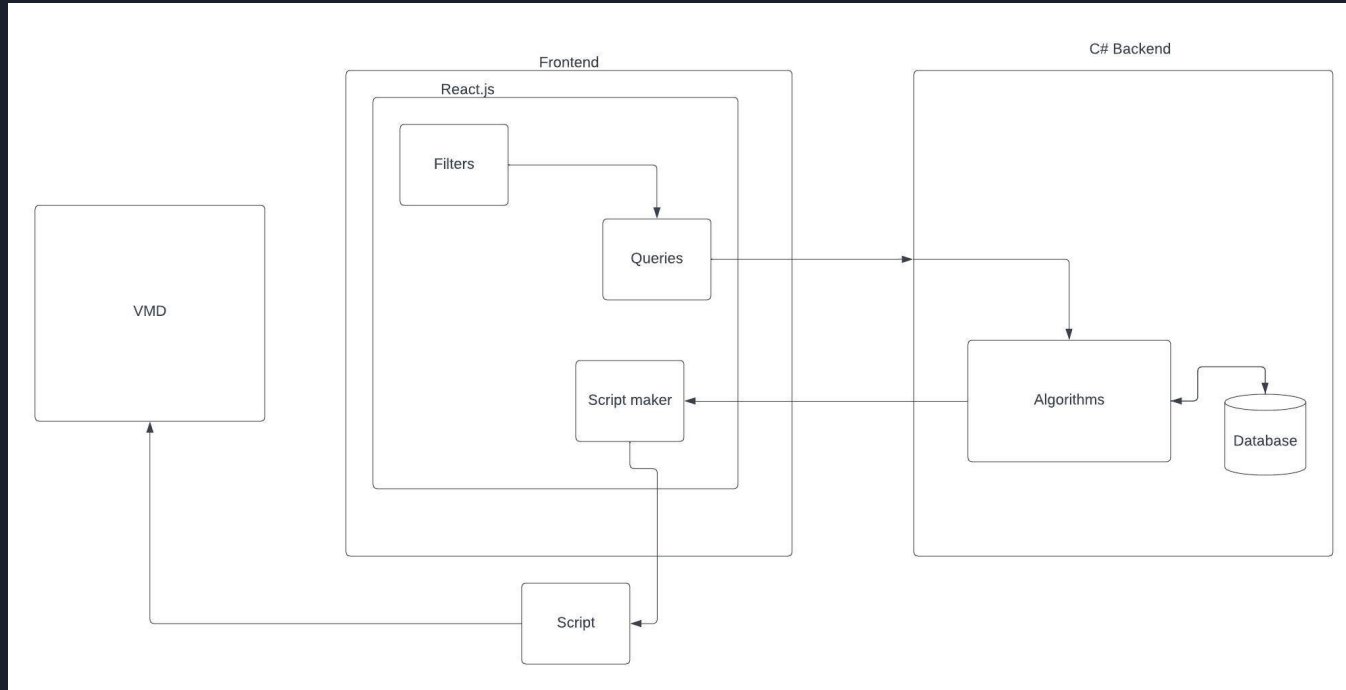
Frontend Implementation
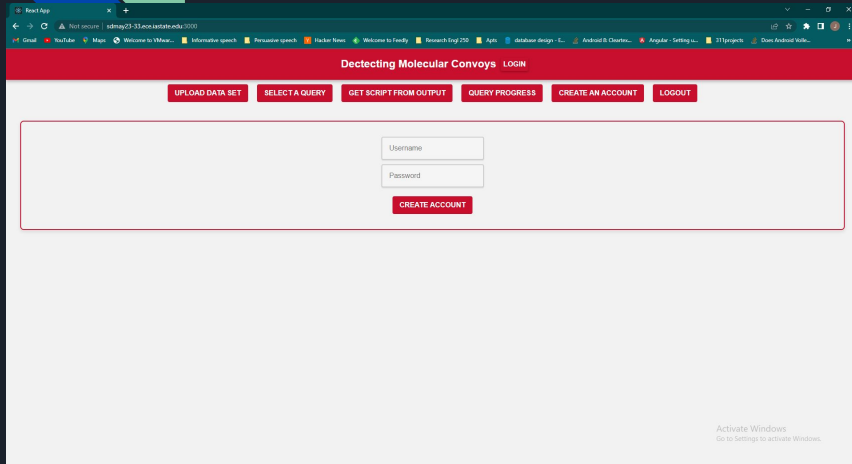
- React.js
- VMD
- .TCL

Backend Implementation

- Backend - C#/.NET
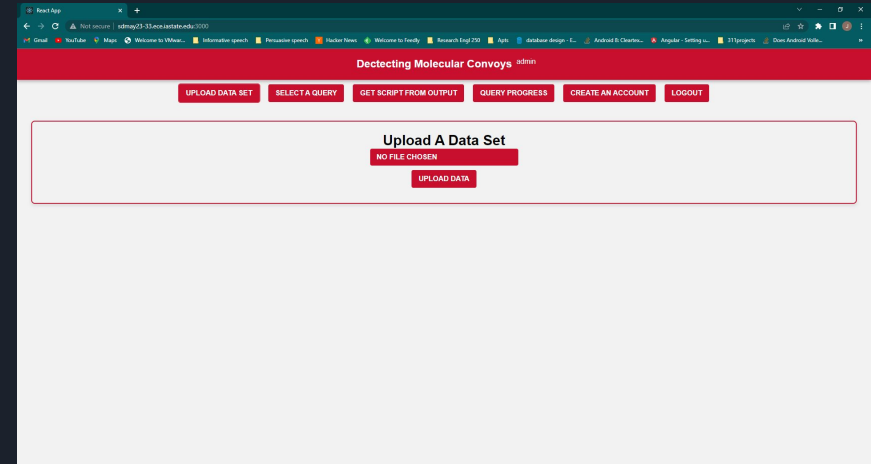- Database - Microsoft SQL Server

Key Points:

- Supporting frontend user actions
- Handling files
- Query setups
- Returning result files

Work Accomplished

- Login system

- Upload Data

Work Accomplished Cont.

● Query Creation and Posting

● Progress System

Work Accomplished Cont.

- Dynamic Script Creation

Work Accomplished Cont.
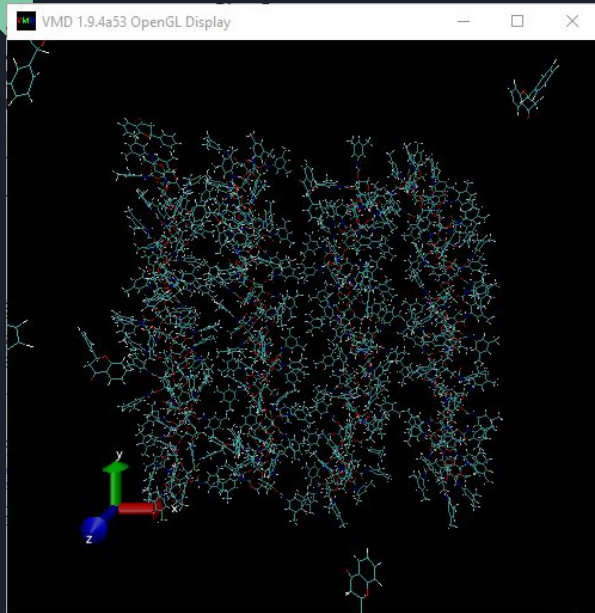
- Unfiltered Molecule

- Filtered Molecule

Work Accomplished Example

Key Contributions

- Jeremy Lewis
  - React Application
  - VMD Scripting
- Daryl Kay
  - API
  - Database
- Claira Springer
  - Testing
- Jason Guo
  -

Future Work

- Work with optimization
  - Parallel processing
- Further detail
  - Hydrogen bonds rather than convoys
- More security
  - Encryption
- Cloud computing
- Better handling of large files

Conclusion

- Achieved proof of concept vision of the application tool
- React
- VMD
- Backend
- Future work