



# Detecting molecular and atomic convoys

Group 33:

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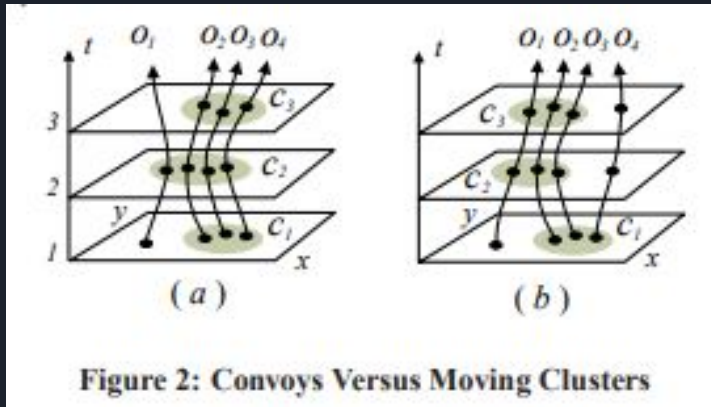
# Project Vision

- 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

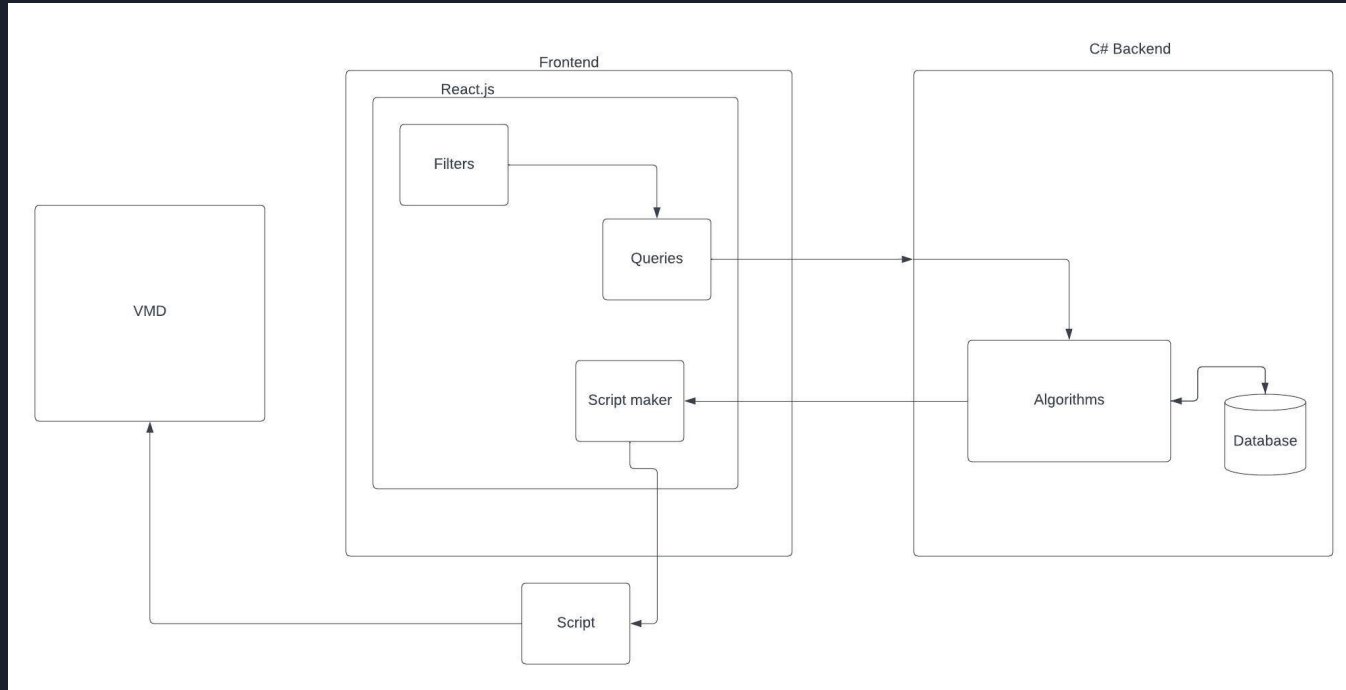
## Molecular Convoys

Groups of atoms and molecules



- Optimizing chemical research
- Simulating the molecular level
- Detecting convoys
- Finding trajectories
- Data analytics queries
- Algorithmic searching
- “Interesting Events”
- Graphical interface
- Frontend and backend design

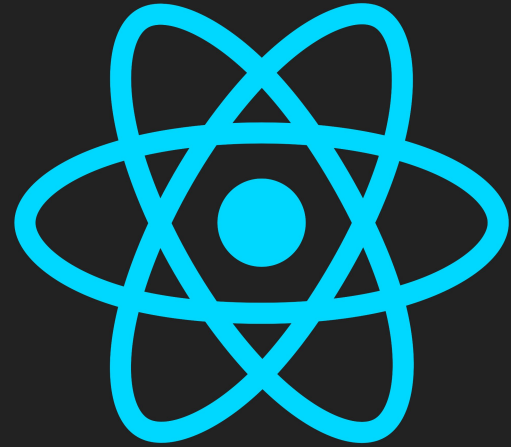
# Overview Diagram





# Frontend Implementation

- React.js
- VMD
- .TCL





# Backend Implementation

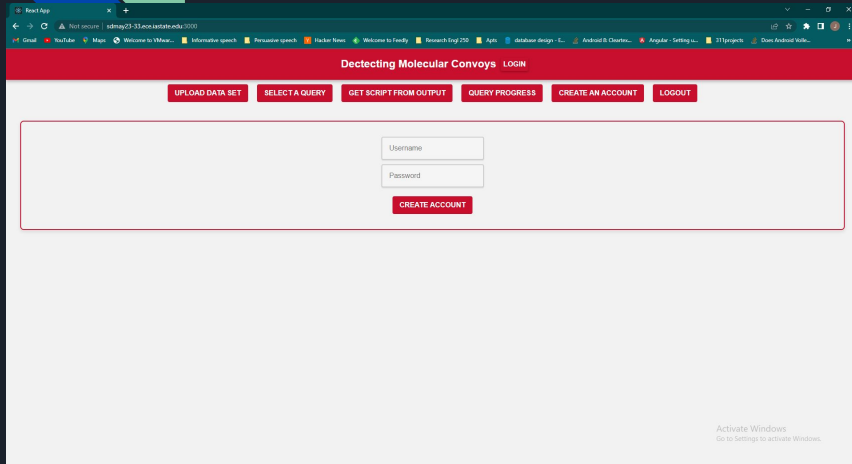
- Backend - C#/.NET
- Database - Microsoft SQL Server

## Key Points:

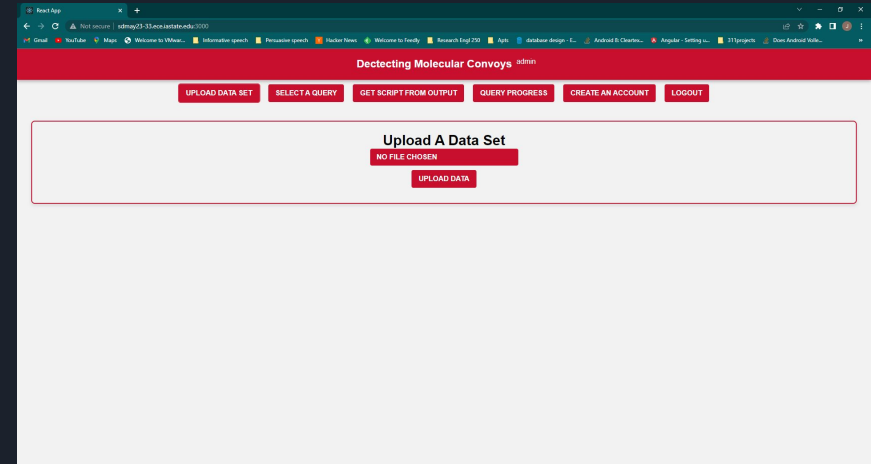
- Supporting frontend user actions
- Handling files
- Query setups
- Returning result files



# Work Accomplished



- Login system



- Upload Data

# Work Accomplished Cont.

The screenshot shows the 'Detecting Molecular Convoys' web application. The navigation bar includes buttons for 'UPLOAD DATA SET', 'SELECT A QUERY', 'GET SCRIPT FROM OUTPUT', 'QUERY PROGRESS', 'CREATE AN ACCOUNT', and 'LOGOUT'. The main content area is titled 'Select A Query' and contains a dropdown menu with the text 'Select a file...', a 'GET FILE LIST' button, and three input fields labeled 'K value', 'M value', and 'EPS value'. A 'SEND QUERY' button is positioned below the input fields.

- Query Creation and Posting

The screenshot shows the 'Detecting Molecular Convoys' web application displaying a 'Previous Queries' section. A 'SEARCH FOR PROGRESS' button is at the top. Below it, three query entries are listed, each with a 'DOWNLOAD RESULTS IF FINISHED' button. The entries are:

- Query ID: 1  
Parameters: [K:2, M:2, eps:2]  
File ID: 1  
Status: Complete  
FilePath: queries/1/output.txt
- Query ID: 2  
Parameters: [K:3, M:3, eps:3.2]  
File ID: 1  
Status: Complete  
FilePath: queries/1/output.txt
- Query ID: 3  
Parameters: [K:3, M:3, eps:3.5]  
File ID: 1  
Status: Complete  
FilePath: queries/1/output.txt

- Progress System



# Work Accomplished Cont.

The screenshot shows a web browser window displaying a web application titled "Detecting Molecular Convoys". The interface features a red header with the application name and a navigation bar with buttons for "UPLOAD DATA SET", "SELECT A QUERY", "GET SCRIPT FROM OUTPUT", "QUERY PROGRESS", "CREATE AN ACCOUNT", and "LOGOUT". The main content area is a white box with a red border containing a form. The form has a red header "OUTPUT.TXT" and a red button "IMPORT OUTPUT FILE". Below this are five input fields: a text field with "0", a text field with "E:/Downloads/traj1.dcd", a text field with "E:/Downloads/4csp\_no\_sol.prm1op", a text field with "55000", and a text field with "traj1". At the bottom of the form are two red buttons: "MAKE SCRIPT" and "DOWNLOAD SETUP SCRIPT".

OUTPUT.TXT

IMPORT OUTPUT FILE

0

E:/Downloads/traj1.dcd

E:/Downloads/4csp\_no\_sol.prm1op

55000

traj1

MAKE SCRIPT

DOWNLOAD SETUP SCRIPT

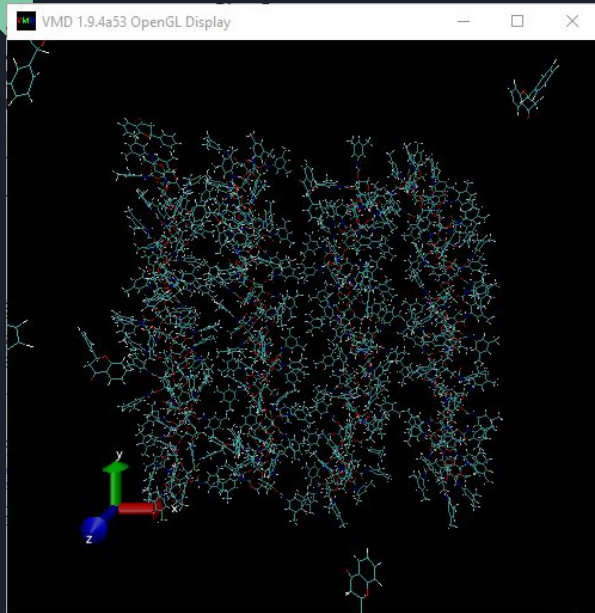
Welcome!

Text

Activate Windows  
Go to Settings to activate Windows.

- Dynamic Script Creation

# Work Accomplished Cont.



- Unfiltered Molecule



- Filtered Molecule

# Work Accomplished Example

The screenshot shows a web browser window displaying a React App. The browser's address bar shows the URL `sdmay23-33.ece.iastate.edu:3000`. The application's header is red and contains the title "Detecting Molecular Convoys" and the user role "admin". Below the header is a navigation bar with six buttons: "UPLOAD DATA SET", "SELECT A QUERY", "GET SCRIPT FROM OUTPUT", "QUERY PROGRESS", "CREATE AN ACCOUNT", and "LOGOUT".

The main content area is titled "Previous Queries" and contains a "SEARCH FOR PROGRESS" button. Below this, there are three query entries, each in a white box with a red border. Each entry displays the following information:

- Query ID: 1
- Parameters: {"k":2,"m":2,"eps":2}
- File ID: 1
- Status: Complete
- FilePath: queries\1\output.txt
- A red button labeled "DOWNLOAD RESULTS IF FINISHED"

The second query entry shows:

- Query ID: 2
- Parameters: {"k":3,"m":3,"eps":3.2}
- File ID: 1
- Status: Complete
- FilePath: queries\1\output.txt
- A red button labeled "DOWNLOAD RESULTS IF FINISHED"

The third query entry shows:

- Query ID: 3
- Parameters: {"k":3,"m":3,"eps":3.5}
- File ID: 1
- Status: Complete
- FilePath: queries\1\output.txt
- A red button labeled "DOWNLOAD RESULTS IF FINISHED"

The Windows taskbar is visible at the bottom of the screen, showing the time as 1:26 PM on 5/2/2023.



# 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