



Detecting molecular and atomic convoys

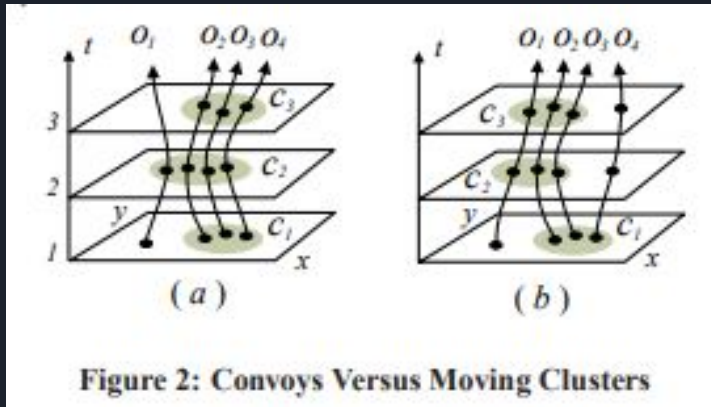
Group 33:

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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



Prior Work/Solutions

- Run algorithm manually
- No specific systems sold

Context

Area	Description	Examples
Public health, safety, and welfare	How does your project affect the general well-being of various stakeholder groups? These groups may be direct users or may be indirectly affected (e.g., solution is implemented in their communities)	Faster drug research
Global, cultural, and social	How well does your project reflect the values, practices, and aims of the cultural groups it affects? Groups may include but are not limited to specific communities, nations, professions, workplaces, and ethnic cultures.	More time efficiency for chemists
Environmental	What environmental impact might your project have? This can include indirect effects, such as deforestation or unsustainable practices related to materials manufacture or procurement.	Energy consumption from servers
Economic	What economic impact might your project have? This can include the financial viability of your product within your team or company, cost to consumers, or broader economic effects on communities, markets, nations, and other groups.	Drugs on the market quicker Replacement of someone's job

Context

Area	Considerations
Public health, safety, and welfare	Faster drug research Safer experimentation Other chemical research
Global, cultural, and social	More time efficiency for chemists Better effectiveness of products Lower barrier to entry in field
Environmental	Energy consumption from servers Uses more power than current alternatives Chemical resources for drugs
Economic	Drugs on the market quicker Replacement of someone's job Easier development means competition





Technical Complexity

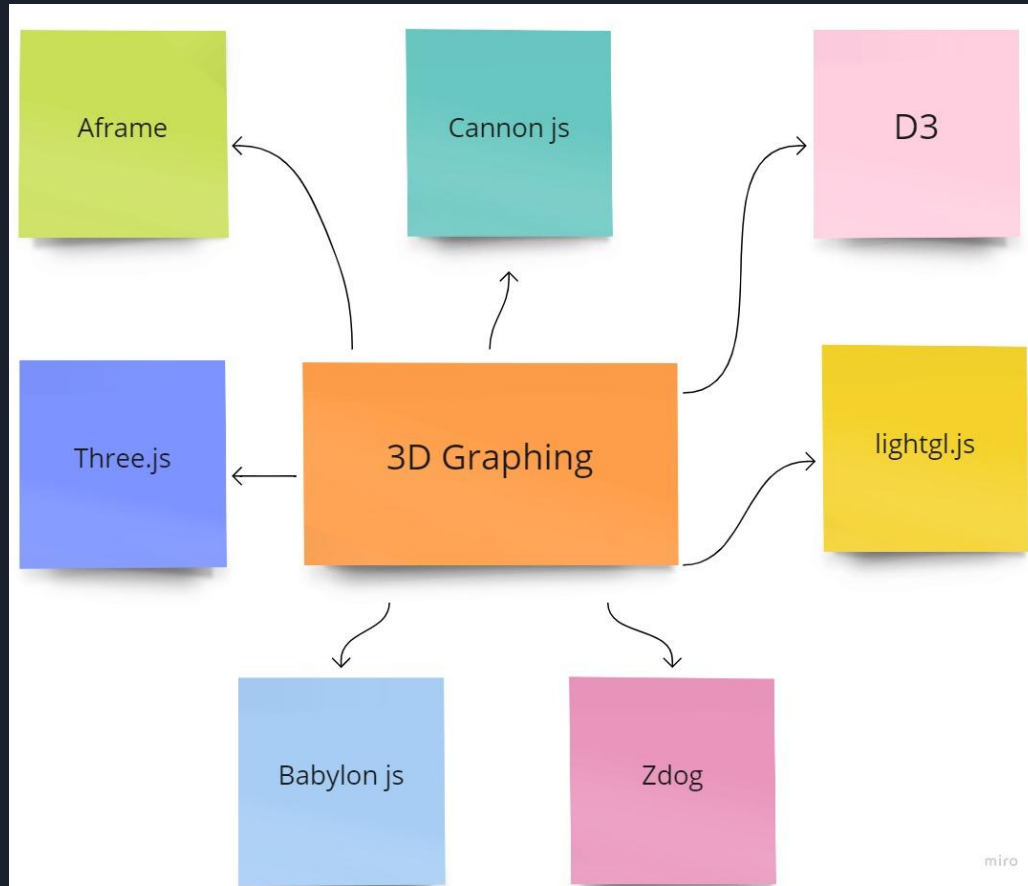
- Frontend
 - 3D graph visualization
 - Scale with users
- Backend
 - Algorithms to detect convoys
 - Server Management
 - Queues



Main Design Decisions

- Which graphing library to use
- Which frontend framework
 - React vs. Angular
- Choice of database
 - MySQL
- Use of queues on the backend

Ideation



Weighted Decision Matrix

Select Criteria	Criterion Weight	Three.js		Aframe		babylon js		canon js		lightgl.js	
		Score	total	Score	Total	Score	Total	Score	Total	Score	Total
Clean looking 3D visualization	0.3	5	1.5	5	1.5	5	1.5	3	0.9	2	0.6
Able to move through data	0.3	5	1.5	5	1.5	5	1.5	3	0.9	2	0.6
Fast load time	0.2	5	1.0	4	0.8	4	0.8	4	0.8	4	0.8
Documentation	0.2	5	1.0	5	1.0	5	1.0	5	1.0	2	0.4
Total	1	5		4.8		4.8		3.6		2.4	

Questions or
comments?

