Computational Biology Helpers

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Agenda

01 Problem Description

02 Our Solution Architecture

03 Use Cases

04 Interactive Demo

05 Connection to Class

06 Related & Future Work

01

Problem Description

Many software engineers want to learn about computational biology but struggle to manage projects and understand how or why different algorithms are used.

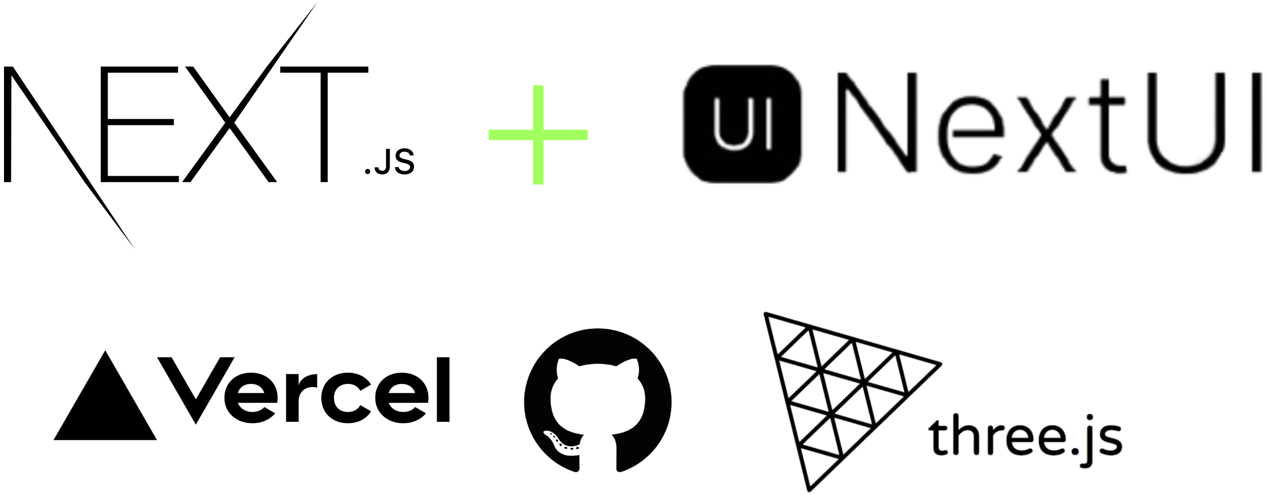
Our Motivation

Just like many other students learning computational Biology, we wanted to be able to see the algorithms in action without downloading anything to our computers

02

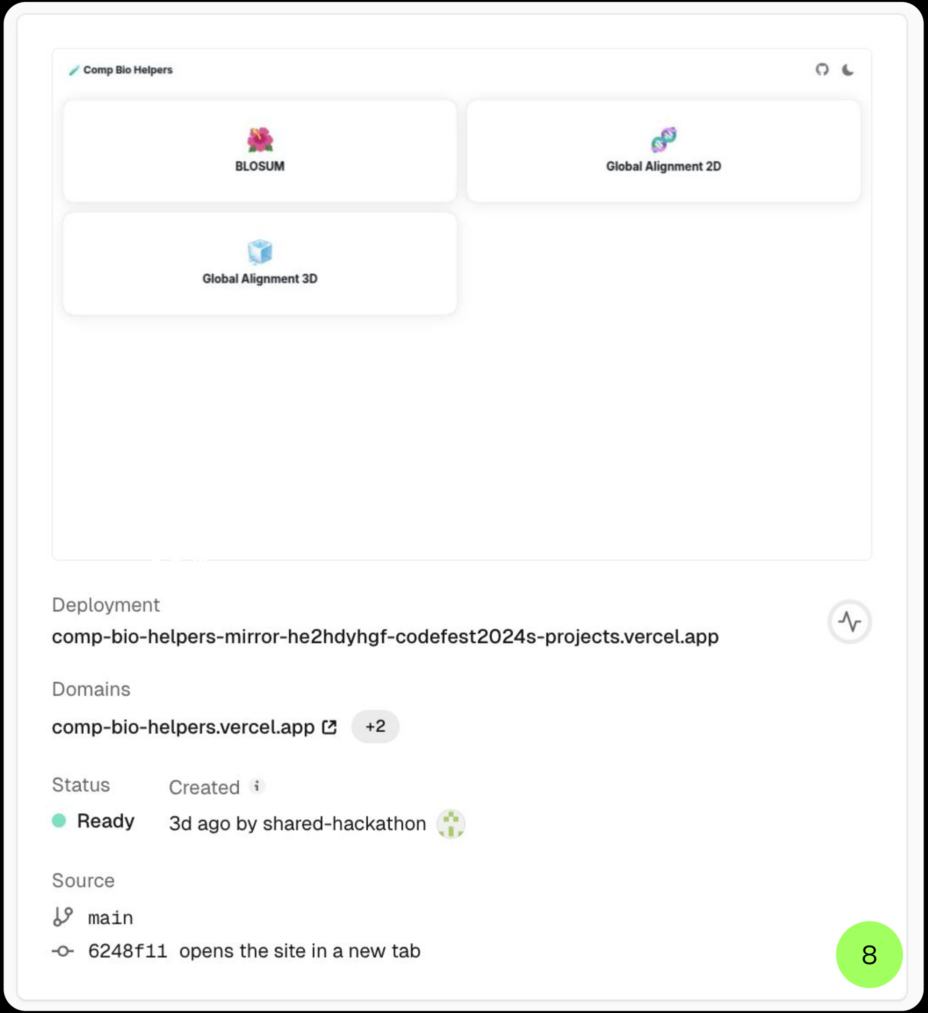
Solution Architecture

Technical Architecture



Our Deployment

1. Mirrored to a private github repository using Git Workflows
2. Hosted By Vercel
3. Custom domain purchased through Cloudflare
4. Deployment automatically updates when new code is pushed (CI/CD)



Deployment
comp-bio-helpers-mirror-he2hdyhgf-codefest2024s-projects.vercel.app

Domains
comp-bio-helpers.vercel.app +2

Status
● Ready

Created
3d ago by shared-hackathon

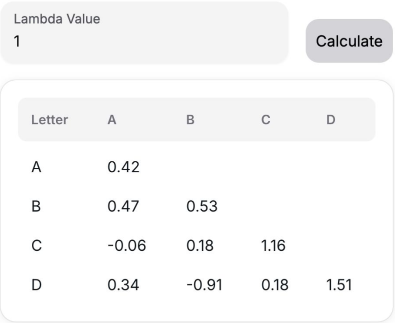
Source
main
6248f11 opens the site in a new tab

03

Top Three Use Cases

Use Case Overview

BLOSUM Matrix

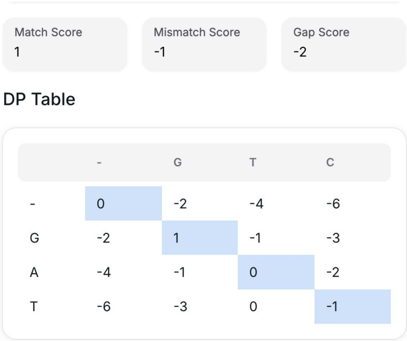


Lambda Value
1

Calculate

Letter	A	B	C	D
A	0.42			
B	0.47	0.53		
C	-0.06	0.18	1.16	
D	0.34	-0.91	0.18	1.51

2D Global Alignment



Match Score
1

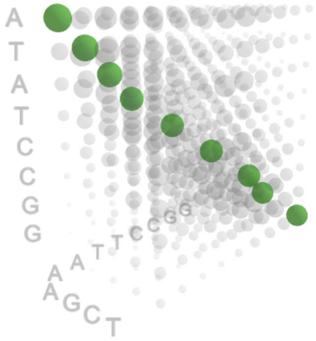
Mismatch Score
-1

Gap Score
-2

DP Table

	-	G	T	C
-	0	-2	-4	-6
G	-2	1	-1	-3
A	-4	-1	0	-2
T	-6	-3	0	-1

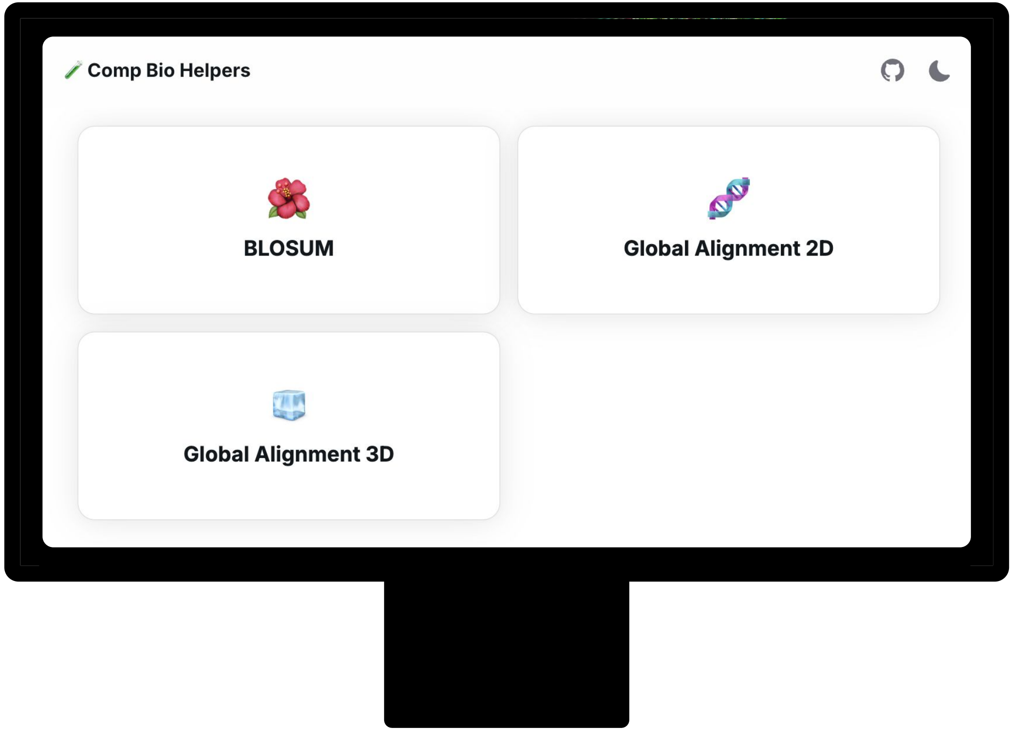
3D Global Alignment



04

Interactive Demo

comp-bio-helpers.vercel.app



05

Connection To Class

Usability Heuristics

Place User in Control

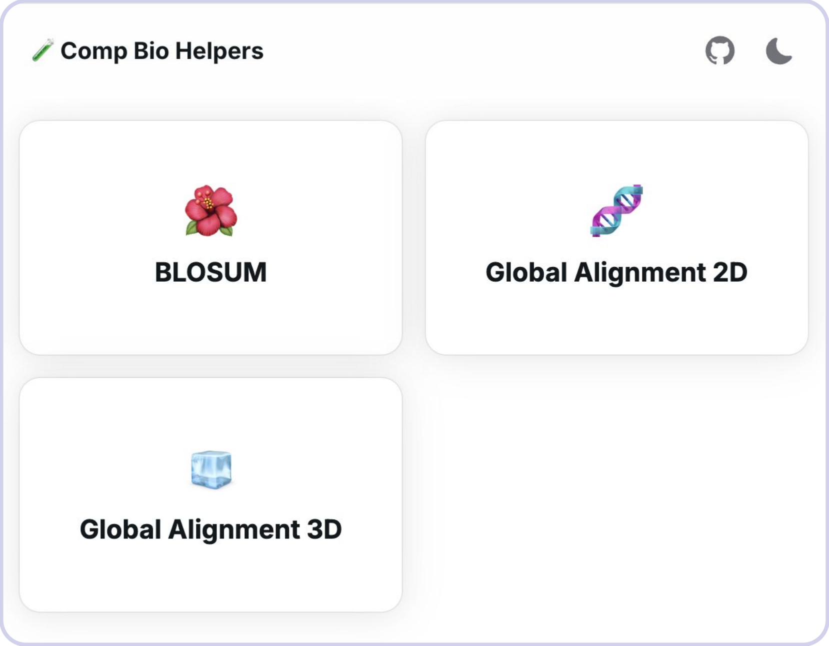
Reduce User’s Memory

Make Interface Consistent

Place User in Control

Home page has 3 tabs for quick, **easy access**

Light/Dark mode toggle for more **customization**

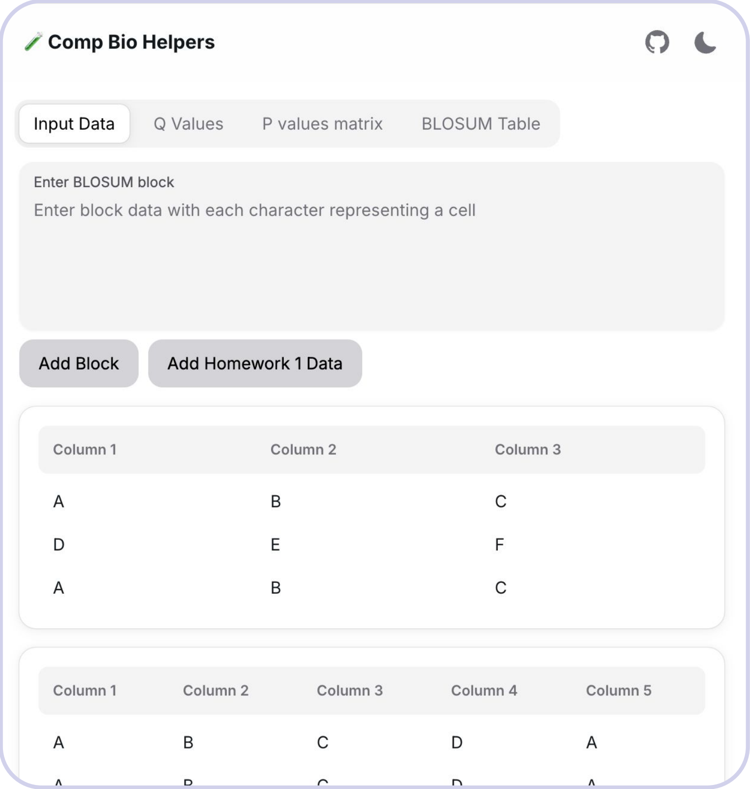


🧪 Comp Bio Helpers

Reduce User’s Memory

The user **doesn’t have to remember** the intermediate values of the BLOSUM Matrix calculation

Values are **automatically saved** when switching tabs



Comp Bio Helpers

Enter BLOSUM block

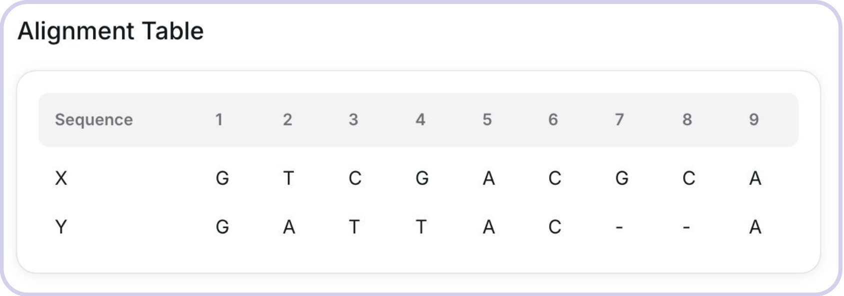
Enter block data with each character representing a cell

Column 1	Column 2	Column 3
A	B	C
D	E	F
A	B	C

Column 1	Column 2	Column 3	Column 4	Column 5
A	B	C	D	A
A	B	C	D	A

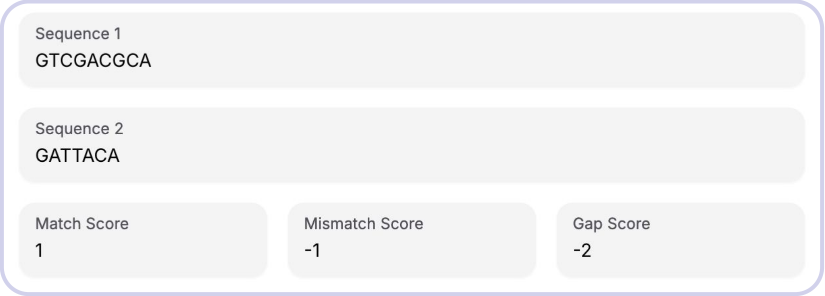
Make Interface Consistent

The Alignment Table and Sequence Input user interface **remain consistent** between both 2D and 3D Global Alignment



Alignment Table

Sequence	1	2	3	4	5	6	7	8	9
X	G	T	C	G	A	C	G	C	A
Y	G	A	T	T	A	C	-	-	A



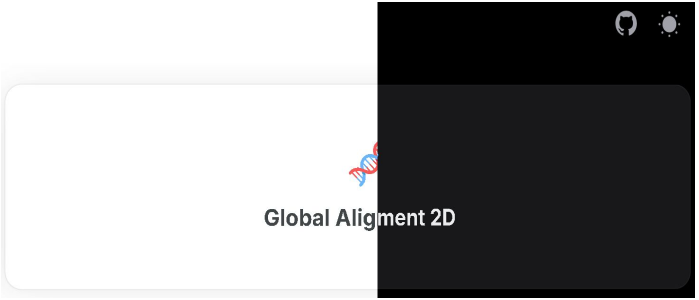
Sequence 1
GTCGACGCA

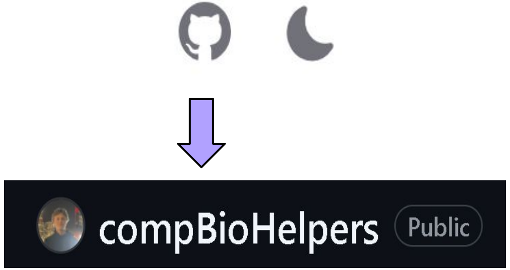
Sequence 2
GATTACA

Match Score
1

Mismatch Score
-1

Gap Score
-2





HCI Design Principles | Part 2

Visibility of system status (1)

- Visual cues for toggling mode
- Action is instant and reversible
- Light/dark mode have different images

Flexibility and Efficiency of use (7)

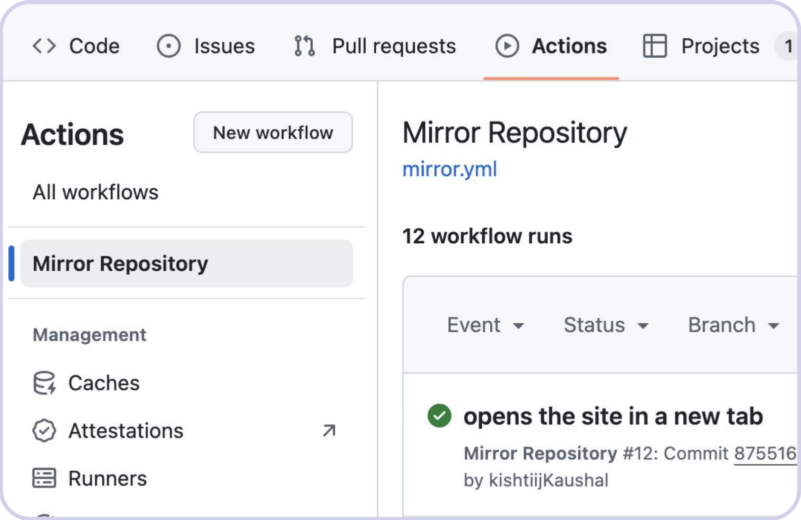
- Supports 2D and 3D visualizations
- More use cases for more user's needs, improving experience

Help and documentation (10)

- GitHub icon links to repository
- Entry point for documentation
- One spot for all relevant information

CI/CD Part 1

Continuous Integration and Deployment helped us to quickly iterate on new features and see their resulting changes without tedious processes



Mirror Repository

mirror.yml

12 workflow runs

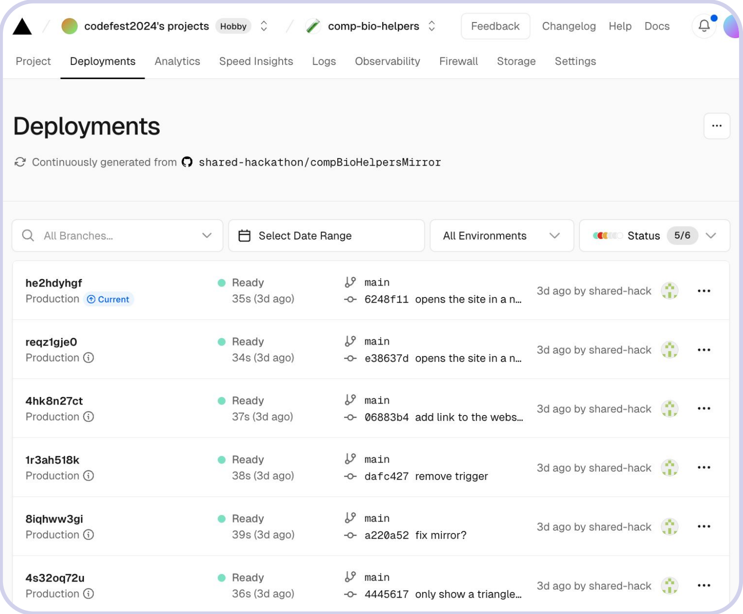
opens the site in a new tab

Mirror Repository #12: Commit 875516 by kishtiijKaushal

Github Action to mirror the repository in preparation for Vercel

CI/CD Part 2

Once our infrastructure was set up, anyone could push a change to Github and see the live website update in <3 minutes with **no extra work needed**.



Deployments

Continuously generated from shared-hackathon/compBioHelpersMirror

he2hdyhgf Production Current	Ready 35s (3d ago)	main 6248f11 opens the site in a n...	3d ago by shared-hack
reqz1gje0 Production	Ready 34s (3d ago)	main e38637d opens the site in a n...	3d ago by shared-hack
4hk8n27ct Production	Ready 37s (3d ago)	main 06883b4 add link to the webs...	3d ago by shared-hack
1r3ah518k Production	Ready 38s (3d ago)	main dafc427 remove trigger	3d ago by shared-hack
8iqhww3gi Production	Ready 39s (3d ago)	main a220a52 fix mirror?	3d ago by shared-hack
4s32oq72u Production	Ready 36s (3d ago)	main 4445617 only show a triangle...	3d ago by shared-hack

Continuously Generated Deployments from our Github on Vercel

01

Related & Future Work

Related Work

3D Alignment

A Github Repository for a python script that extends the Needleman–Wunsch algorithm to 3 sequences

BLOSUM Matrix

A Wikipedia Page for how to calculate the matrix. There was no other published code or websites for how to implement the algorithm.

2D Alignment

An interactive Github Pages website for doing Global Alignment. Very useful but the interface is cluttered and confusing.

Future of our project

Use multithreading to compute the alignments quickly

Make the user interface nicer and easier to navigate

Incorporate more computational biology algorithms and general Software Engineering Algorithms

Share solutions with team members and other users of the website

Any Questions?