

# Neutron Instrument Control Through Large Language Models

Jack Campbell

# Overview

1. Why we  
need an AI



2. How the  
AI works



3. Results  
and costs

# NIST Center for Neutron Research

User facility that uses neutrons to probe the structure and dynamics of materials.

1000+

Experiment Participants/Year

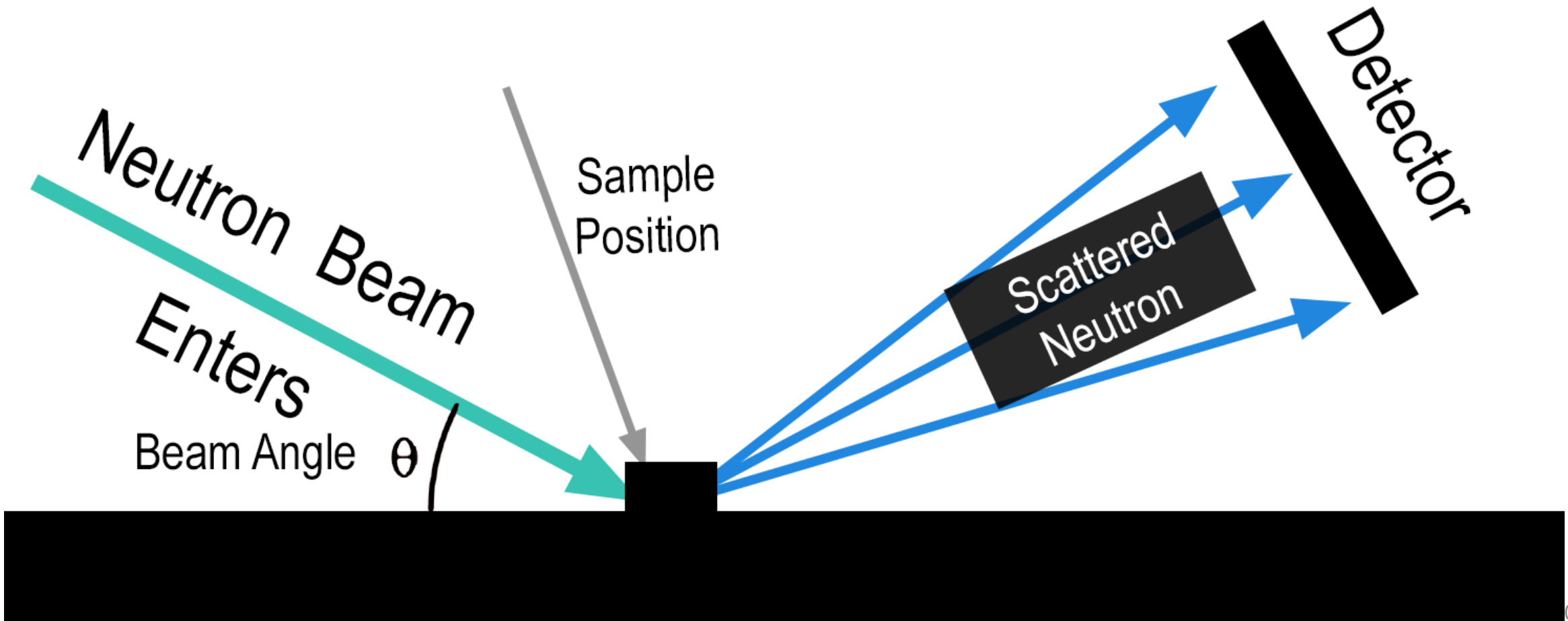
Participants from all over the world



28

Instruments

# Magik



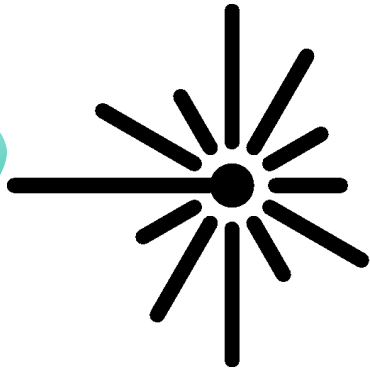


39

Parameters

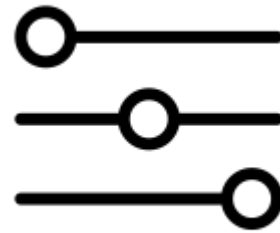
# Neutron Instrument Control Environment

15



NICE  
Instruments

585



Total  
Parameters

818



Total  
Experiments

# Move a Motor?

D3=

Drive

Dr

Rotate to

Mv

Move

?

?

?

?

?

?

?

?

?

# VISION

Virtual Scientific Companion

Brookhaven  
National  
Laboratory



Extracted  
keywords



Managed  
x-ray  
beamlines



Low  
budget



High  
success



Large  
Language  
Model  
(LLM)



Chat GPT

# Large Language Model (LLM)

Understand/generate human language

Use a Transformer Neural Network

Process text sequentially

Predict text very well

Train on large amounts of data

# What are Trajectories?

- Simple scripts that allow for nested loops

## Why did we pick them?

Well  
documented  
format(JSON)

Large  
amounts data  
available

Middle ground  
of complexity  
and power

Can Dry Run

# Complicated Trajectory

- 17 Parameters initialized
- 3 Loops
- 9 Variables changed per loop

Properties

expression	<input type="checkbox"/> raw string
filePrefix	live.sample.name

expression  raw string

entryName	unpolarized
-----------	-------------

expression  raw string

xAxis	q.z
-------	-----

expression  raw string

description	live.sample.description
-------------	-------------------------

+Property

Init

expression  raw string

_scanType	SPEC
-----------	------

expression  raw string

_mon0	30.0
-------	------

expression  raw string

_mon1	1250.0
-------	--------

expression  raw string

_pre	1.0
------	-----

expression  raw string

_exp	2.0
------	-----

expression  raw string

_L2S	330.0
------	-------

expression  raw string

_L12	1403.0
------	--------

expression  raw string

_LS3	330.0
------	-------

expression  raw string

_L34	1193.0
------	--------

expression  raw string

_spotSize	50.0
-----------	------

expression  raw string

_thetaOffset	0.0
--------------	-----

expression  raw string

_S3Offset	1.22
-----------	------

# Background Questions

# Overarching picture

User  
Sentence



Add relevant  
data files



Processes  
and returns

**Follow up with:**

Value changes	"Change sampleAngle to 10"
Parameter additions	"When started, count against time"
Loop position changes	"Make x loop nested inside y loop"

# User Prompt

**Initial prompt contains:**

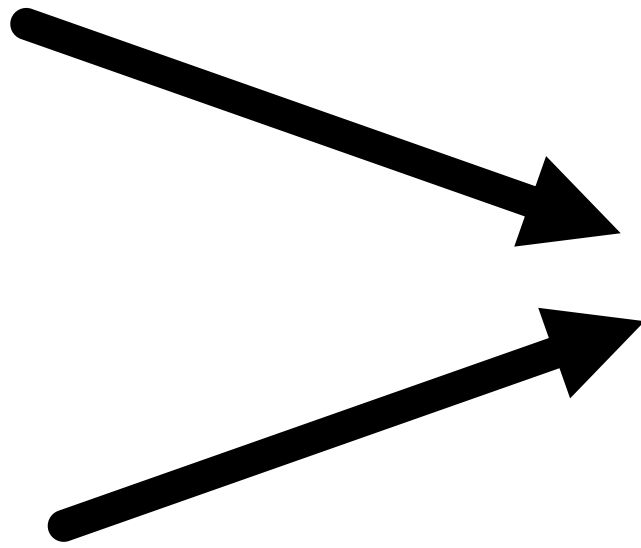
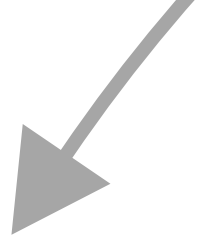
- Instrument name
- Experiment name
- Starting values
- What variables to loop

Ex: Create magik trajectory angleChecks that starts with a time of 10 and loops through sampleAngle from 2 to 10 in steps of 0.25

# System Message

**System Message**

<p><b>System Message Goals</b></p> <ul style="list-style-type: none"> <li>• Provide the JSON format</li> <li>• Ask follow up questions</li> <li>• Add @#@#@#@ before and after trajectory</li> <li>• Only use data from our sources</li> </ul>	<p><b>Format required:</b></p> <pre> @*01010* {   "fileRef": "",   "description": "",   "set": [{"paramName": "paramValue"}],   "loop": [{"paramName": "range": 0}]} } @*01010* </pre>
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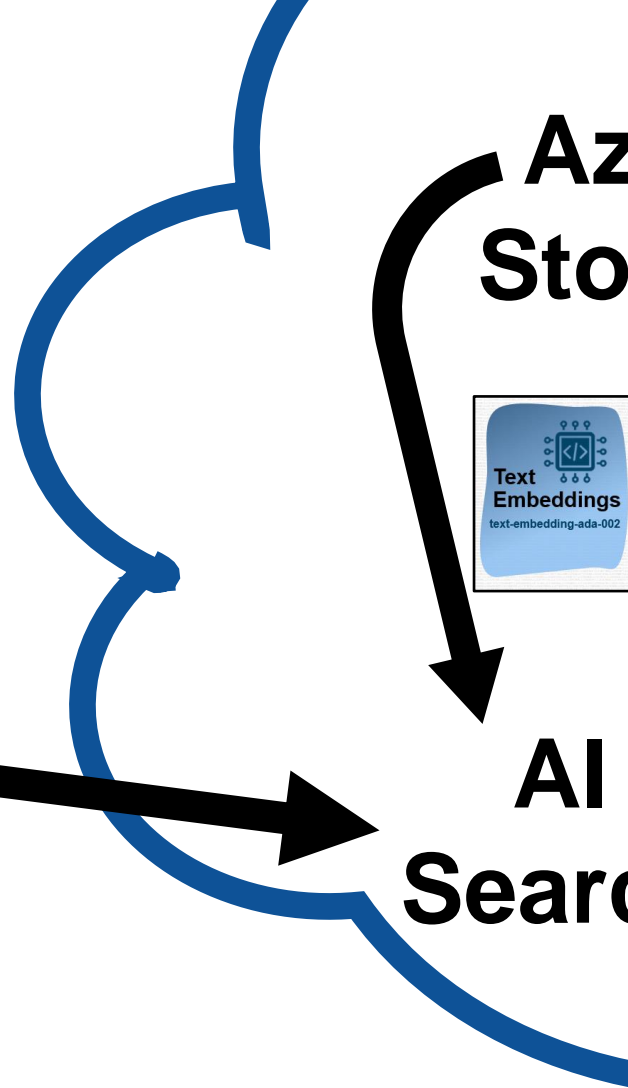
# Code

**Our code**

- Combines:
  - User Message
  - System Prompt
  - Previous messages

~500 lines

Communicates with Azure



# AI Search

**Text Embeddings**  
text-embedding-ada-002

# Azure Storage

# Initial prompt contains:

- Instrument name
- Experiment name
- Starting values
- What variables to loop

Ex: Create **magik** trajectory **angleChecks** that starts with a **time of 10** and **loops through sampleAngle from 2 to 10 in steps of 0.25**



# System Message

## System Message Goals:

- Provide the JSON format
- Ask follow up questions
- Add @#\$@%@^@ before and after trajectory
- Only use data from our sources

## Format required:

```
@#$@%@^@
{
  "filePrefix": "",
  "description": "",
  "init": [["paramName", "paramValue"]],
  "loops": [{
    "vary": [{"paramName", {"range":
    {}}}]
  }],
}
@#$@%@^@
```

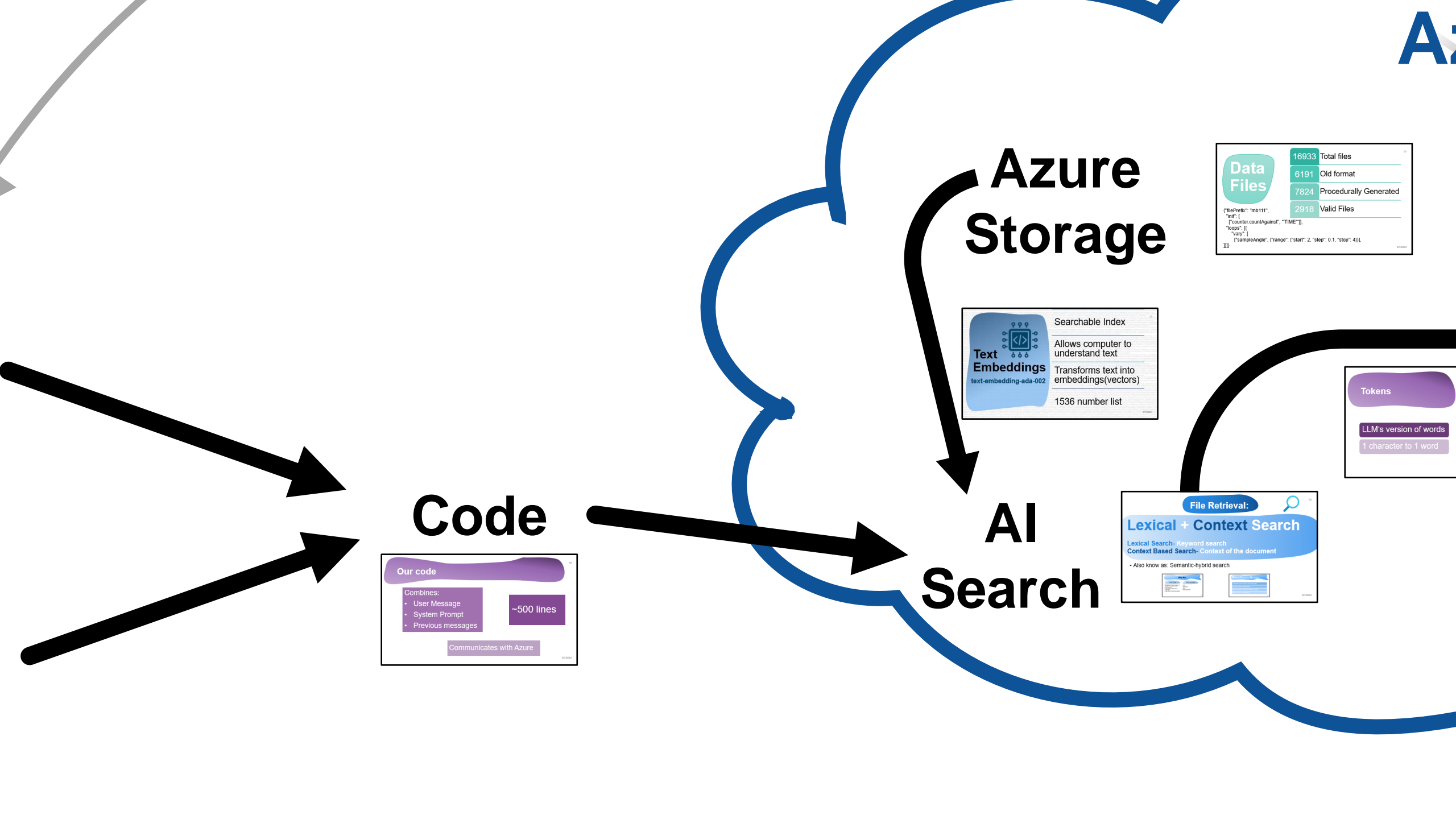
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# Code

**Our code**

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~500 lines

Communicates with Azure

# Azure Storage

**Data Files**

16933	Total files
6191	Old format
7824	Procedurally Generated
2918	Valid Files

```
["filePrefix": "mb111", "url": [{"counter": countAgainst, "TIME": [{"loops": 0, "vary": [{"sampleAngle": {"range": {"start": 2, "step": 0.1, "stop": 4}}]}]}]]
```

**Text Embeddings**  
text-embedding-ada-002

Searchable Index

- Allows computer to understand text
- Transforms text into embeddings(vectors)

1536 number list

# AI Search

**File Retrieval:**

**Lexical + Context Search**

- Lexical Search- Keyword search
- Context Based Search- Context of the document

• Also know as: Semantic-hybrid search

**Tokens**

- LLM's version of words
- 1 character to 1 word

# Azure Cloud



## Azure Storage

Data Files	Count	Description
	16933	Total files
	6191	Old format
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	2918	Valid Files

```
["filePrefix": "mb111",  
 "url": "  
  ["counter":countAgainst", "TIME"],  
 "loops": [  
   "vary": [  
    ["sampleAngle", {"range": {"start": 2, "step": 0.1, "stop": 4}}]
```

**Text Embeddings**  
text-embedding-ada-002

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Allows computer to understand text  
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1536 number list

## GPT 4o

**Model: GPT 4o**

**Advantages:**

- Faster and cheaper than GPT3.5 turbo
- Large token count
- Less system message needed
- Asks follow up questions

**Disadvantages:**

- Includes information not provided by the user
- Misses information clearly provided

**Tokens**

LLM's version of words  
1 character to 1 word

Characters: 386  
Tokens: 112

## AI Search

**File Retrieval:**

**Lexical + Context Search**

Lexical Search - Keyword search  
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Also know as: Semantic-hybrid search

# Data Files

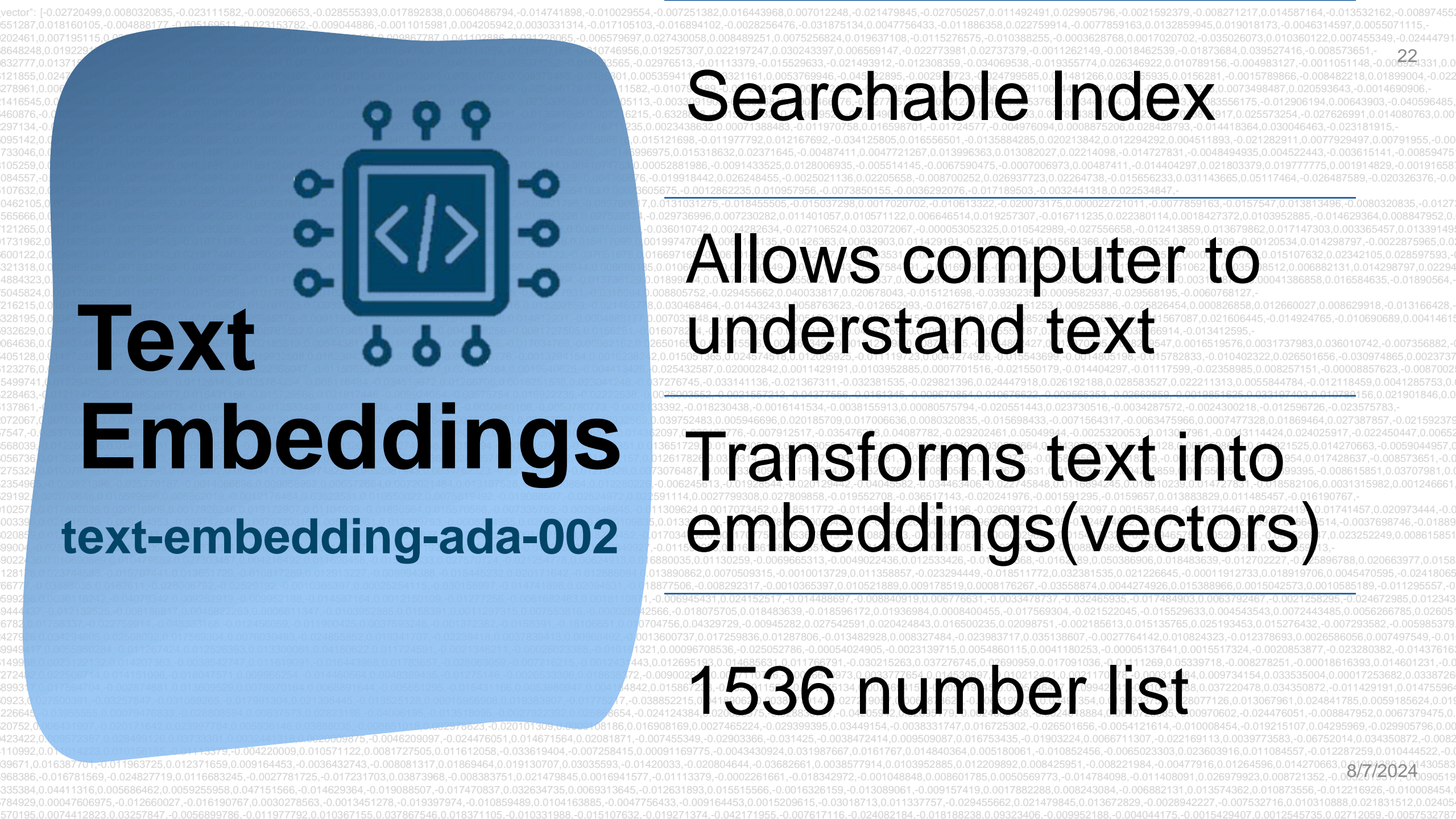
```
{"filePrefix": "mb111",  
  "init": [  
    ["counter.countAgainst", "'TIME'"]],  
  "loops": [{  
    "vary": [  
      ["sampleAngle", {"range": {"start": 2, "step": 0.1, "stop": 4}}],  
    ]}]}
```

16933 Total files

6191 Old format

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**Text Embeddings**  
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## File Retrieval:

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**Lexical Search-** Keyword search

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**Why Not..**

<p><b>Fine Tune</b></p> <ul style="list-style-type: none"> <li>• <b>Definition</b>- Provide examples of prompt and output to model</li> <li>• Time and cost</li> <li>• Large data set required per instrument</li> <li>• High effort to expand knowledge</li> </ul>	<p><b>Train our own</b></p> <ul style="list-style-type: none"> <li>• Cost</li> <li>• Resources</li> <li>• Time</li> <li>• Not enough data</li> </ul>
---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	------------------------------------------------------------------------------------------------------------------------------------------------------

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**Retrieval-Augmented Generation**

- Integrating documents into AI prompt
- Breaking down documents
- Most relevant 5 files for specific prompt
- Best way to use ChatGPT

©7/2024

# Why Not..

## Fine Tune

- **Definition-** Provide examples of prompt and output to model
- Time and cost
- Large data set required per instrument
- High effort to expand knowledge

## Train our own

- Cost
- Resources
- Time
- Not enough data



# Retrieval-Augmented Generation

Integrating documents into AI prompt

Breaking down documents

Most relevant 5 files for specific prompt

Best way to use ChatGPT

# Tokens

LLM's version of words

1 character to 1 word

```

{
  "loops": [
    {
      "vary": [
        [
          "trajectory angle",
          "circle that starts",
          "with a time of 10",
          "and loops through",
          "sampleAngle from 2",
          "to 10 in steps of",
          "0.25",
          "counter.countAgainst",
          "counter.timePreset",
          "30.0"
        ]
      ]
    }
  ]
}

```

Characters: 386  
 Tokens: 33

# Model: GPT 4o

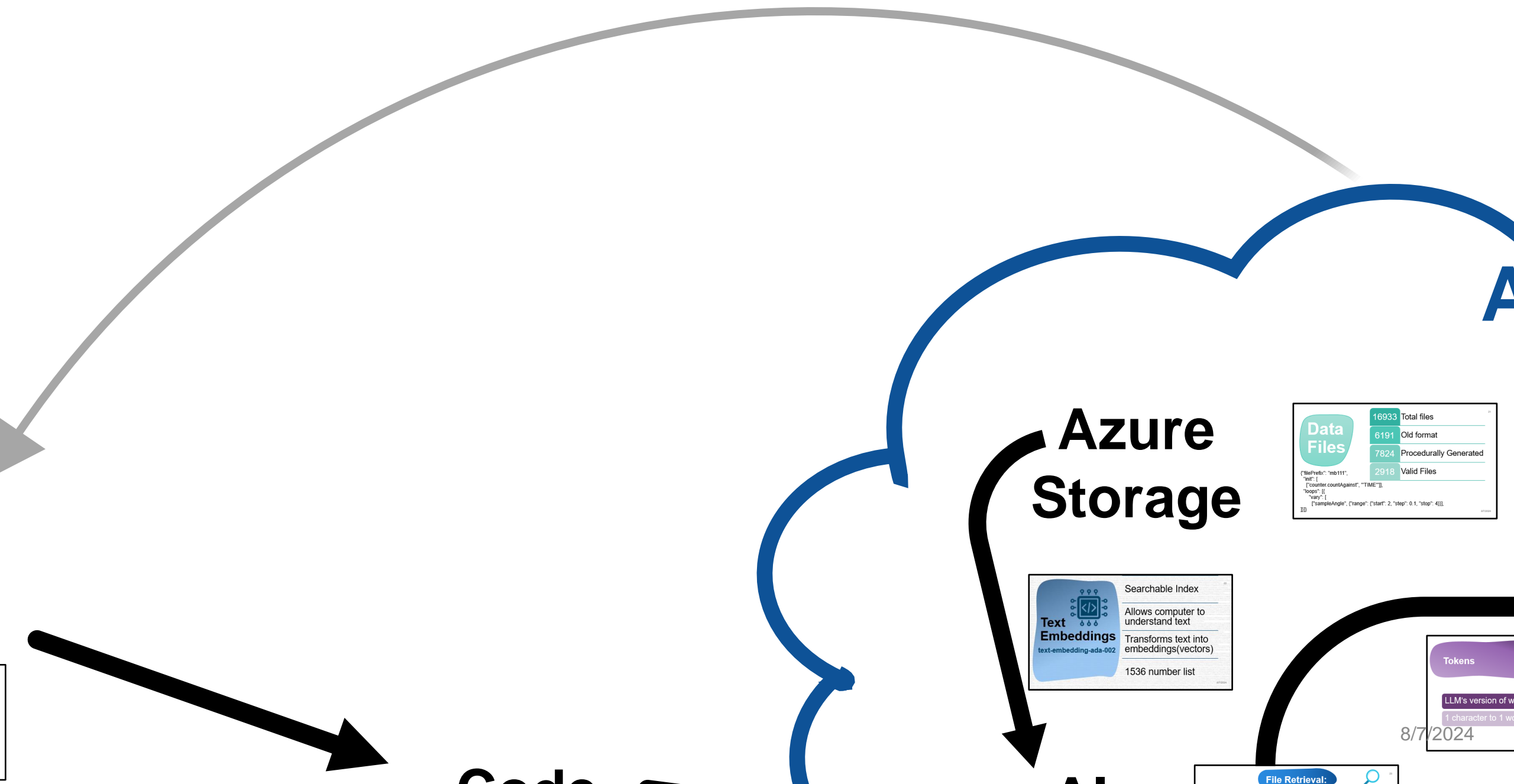
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# Azure Storage

Data Files	
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```
["filePrefix": "mb111",  
"file":  
  [{"counter": "countAgainst", "time": "TIME"},  
  {"loops": 1,  
   "sampleAngle": [{"range": {"start": 2, "step": 0.1, "stop": 4}}]}]
```

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text-embedding-ada-002

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**Tokens**

LLM's version of w  
1 character to 1 w

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**File Retrieval:**

**Follow up with:**

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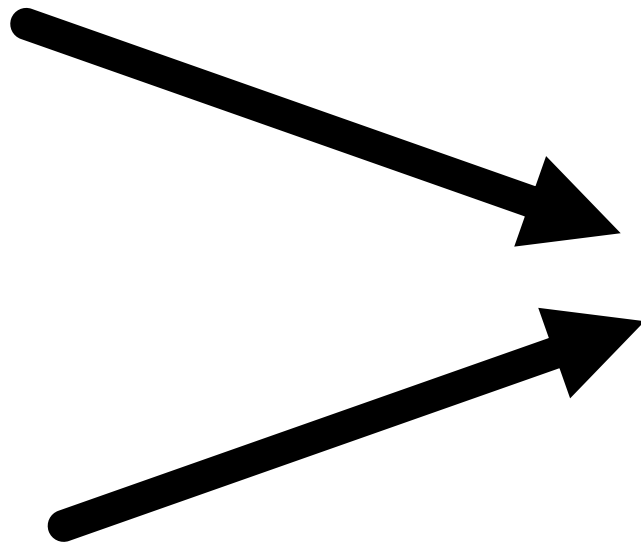
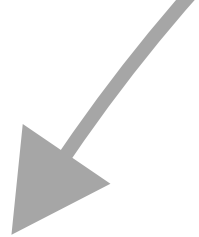
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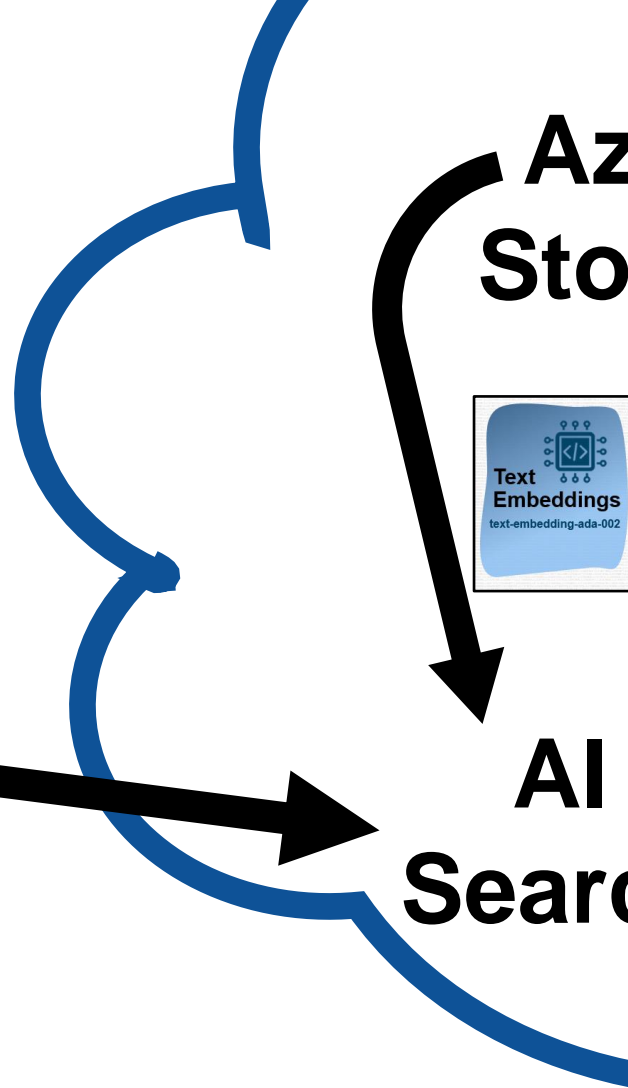
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Communicates with Azure



# AI Search

**Text Embeddings**  
text-embedding-ada-002

# Azure Storage

# Follow up with:

Value changes

“Change sampleAngle to 10”

Parameter additions

“When started, count against time”

Loop position changes

“Make x loop nested inside y loop”

# Costs

\$6.20

To create searchable database

Per Message

\$0.02

Per Month

\$96.09

\$0.14

Per Conversation

\$1,153

Per Year

# Breakdown

	\$/Month
Azure Open AI	\$14
Azure Storage	\$0.25
Azure AI Search	\$81.84
Total	\$96.09

**100**  
Conversations

**\$15.00**  
Second AI



# How we decide success rate

## Current

- Trajectory format is valid
- Parameter are correct
- Correct after conversation

**2,918**

Training Data Files

## Future

- Harder prompts
- More instruments

**100%**

Trajectories Correctly  
Generated

Sample Size: 250

# Current progress

Writes trajectories for all instruments

Generates a trajectory in the correct format

Asks follow up questions

Added NICE editor

User:

Create a json trajectory that loops x from 1 to 10 in steps of 1 and at each point loops y from x to x\*2 over 20 points

AI:

Which instrument would you like to use for this JSON trajectory? Additionally, please provide the values for "filePrefix" and "init" sections.

User:

What can you put in the init section

AI:

The "init" section in a JSON trajectory file for neutron instruments typically contains initial parameter settings required for the experiment. Here are some examples from the retrieved documents: 1. `**For the 'ng7sans' instrument**` `json [{"counter.countAgainst": "TIME"}, {"counter.timePreset": 0.5}]` 2. `**For the 'bt4' instrument**` `json [{"counter.countAgainst": "TIME"}, {"counter.timePreset": 1}]` 3. `**For the 'pbr' instrument**` `json [{"POLXS": ["A", "B", "C", "D"]}, {"down": 0}, {"up": 1}, {"counter": {"countAgainst": "TIME", "timePreset": 1}}, {"vertSlitAperture1": 0.2}, {"vertSlitAperture2": 0.2}, {"vertSlitAperture3": 0.2}, {"vertSlitAperture4": 0.2}, {"slitAperture3": 4.0}, {"slitAperture4": 4.0}]` Please specify which instrument you are using and any specific initial parameters you would like to include in the "init" section.

User:

I would like to put in the init section to count for a constant time of one second. This is for the magik instrument and the filePrefix is hi

AI:

User:

Can you please make the y loop nested

AI:

User:

Actually can you make the y loop 30 points

AI:

# Live Demo

## Properties

expression	<input type="checkbox"/> raw string	
filePrefix	hi	X

expression	<input type="checkbox"/> raw string	
description		X

+Property

## Init

expression	<input checked="" type="checkbox"/> raw string	
counter.countAgainst	TIME	X

expression	<input type="checkbox"/> raw string	
counter.timePreset	1.0	X

+Initial Value

range (double-click text fields to enlarge)	start	end	step	range	center	#points	<input type="checkbox"/> log	X
x	1.0	10.0	1.0					X

+Range +Expression +List +Surround with Loop

Loop	range (double-click text fields to enlarge)	start	end	step	range	center	#points	<input type="checkbox"/> log	X
	y	x	x*2				30	X	

+Range +Expression +List +Surround with Loop

+Loop

+Loop

+Loop

# Future Goals

Add the 6191 broken files

Create trajectories with less specific names

Allow LLM to assume parameters

**Moonshot goal:** Suggested trajectories based on experiment details

# Acknowledgements

## My Mentors

Alan Munter

William Ratcliff

Stephen Pheiffer

## NIST Staff

Brian Maranville  
Magik

Sean Dwyer  
NICE

Fawaz Joseph  
NICE

Julie Borchers  
Core

Leland Harriger  
Core

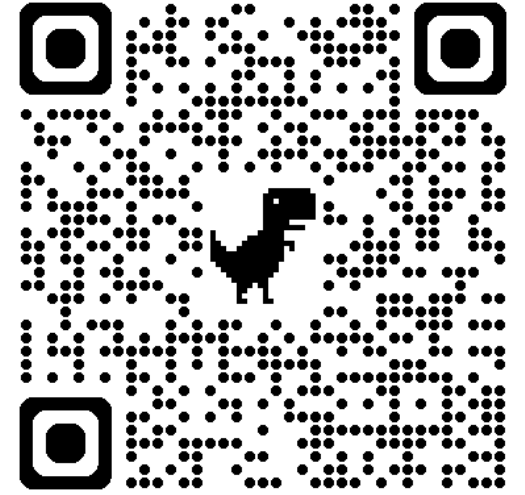
Olufisan Epebinu  
OSIM

Lisa Ho  
OSIM

NICE Team

Shark Tank

# Thank You!



Slides

## Contact Me!

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*GitHub:* [@JackCampbell5](https://github.com/JackCampbell5)

*LinkedIn:* [/JackCampbell5](https://www.linkedin.com/in/JackCampbell5)



# Where Creation Happens

## Code

- Contact Azure
- User prompt
- System Message

## Azure

- Creating model
- Organizing data(Vectorize)

## Short Scripts

- Moving training data
- Adding meta data



# Our system Message

You are artificial intelligence for the National Institute Of Technology's Center for Neutron Research program Neutron Instrument Control Environment (NICE) that controls neutron instruments via programming. You should output a single block of text in the following JSON format with "@#@\$@\$@^@" characters at the top and bottom of the file, not ````json:

```
@#@$@$@^@
{
"filePrefix": "",
"description": "",
"init": [{"paramName", "paramValue"}],
"loops": [{
"vary": [{"paramName", {"range": {}}]}
}],
}
@#@$@$@^@
```

If the user does not specify ask to create a json trajectory for (name) instrument , ask them which instrument they would like to use. Furthermore, if the user does not specify what the "init" (initialization), "filePrefix" (name), or "loops" sections should contain, please ask the user what they would like to put if they did not provide any information relating to these sections before printing the JSON output. You should only use data from your sources. If you cannot find the answer, just say "I cannot do that yet."