

**Start today:**

**Load:** [Chemcompute.org](https://chemcompute.org)

**Clone:** [https://github.com/scottmreed/Code\\_withGPT\\_tutorial.git](https://github.com/scottmreed/Code_withGPT_tutorial.git)

**Open:** <https://tinyurl.com/3srfte8s>

**Open:** <https://labs.perplexity.ai>

**Open:** <https://chatgpt.com/>

Hold off on using these GPTs until we start since they cap usage

# Goals for Today

- **Cement basic python skills**
- Learn capabilities of Large Language Model (LLM) based Generative Pre-Trained Transformers (GPTs)
- **Learn strategies to integrate GPTs into your learning process**
- Continue work on MolSSI curriculum

# Shared Work Space

- <https://tinyurl.com/3srfte8s>

## Instructions

Download



Home

Token

9433aa6b22a2dae3b82939362185d845

Logout

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Instructions on how to run a simulation.

1. First log in to the site at the top right. You can create an account, but logging in with Google (Gmail) or your University is probably faster
2. Click the next button to begin!

Survey

Next

## Server Options

ChemCompute has two options for your notebook. It can run on a regular node (CPU node) or a GPU node. A GPU node has access to a graphics card, which can be used to make certain calculations run faster.

If you know that you need access to a GPU, choose GPU node and image  $\geq 1.10$ . If you're not sure, choose CPU node.

GPU nodes take a few minutes to start up. CPU nodes should be immediately available

Select an instance for your notebook CPU node (default)

Select between Jupyter Notebook and Jupyter Lab

Jupyter Lab

Select how to provide the image:

☒ Select a Premade Image (default)

☐ Use a custom repository. These must be [preapproved](#)

Select between Images

1.10 (July 2024) -- GPU capable (ubuntu 24.04)

Start

# A Little Beyond the scope

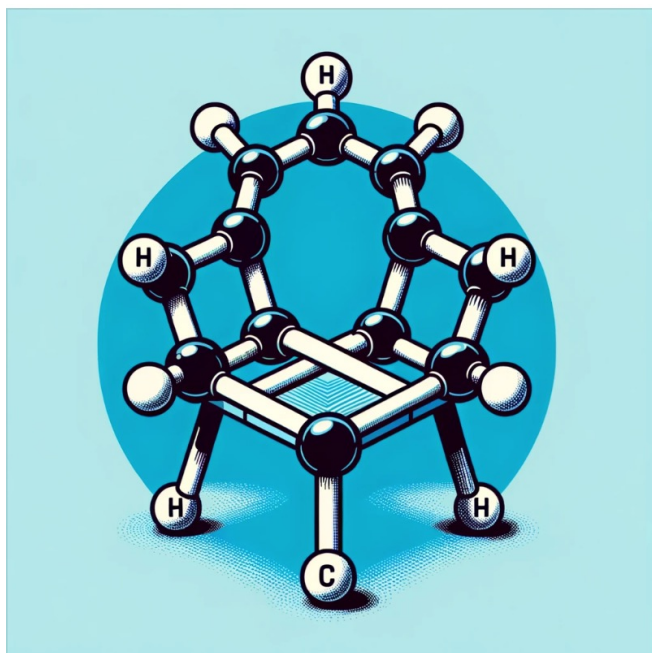
Things that are interesting but not our focus. **Everything we do today will work with free sites.** Sites and services that cost \$ might be mentioned but aren't necessary for getting started. For example:

- GPT plus, team or enterprise
- AI based plugins for Visual Studio Code, PyCharm, etc.
- Co-pilot
- Other paid services

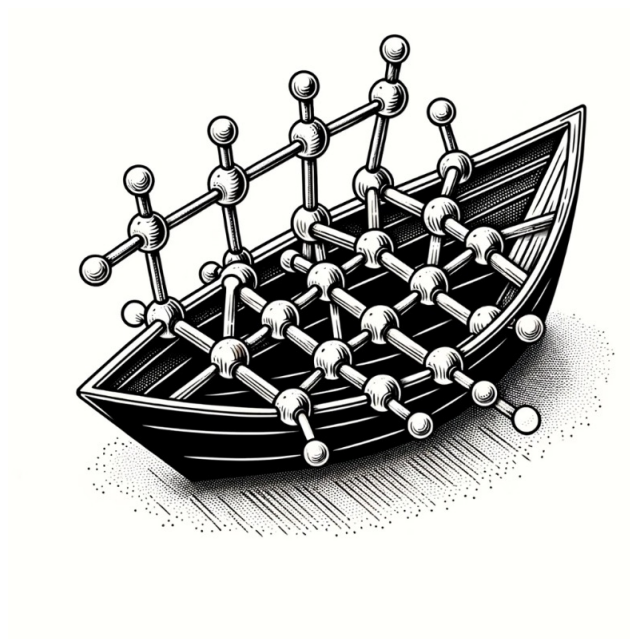
**Feel free to use these services today if you have them.** Or ask questions about them. If you were thinking of trying a one-month subscription to ChatGPT, doing it today means you don't have to be as careful about how many prompts you submit.

## GPT Hallucinations and how to avoid them:

Draw the cyclohexane chair conformation



Draw the cyclohexane boat conformation



## Try my hallucination-avoiding informatics GPT:

<https://chat.openai.com/g/g-jGpmTZnqM-molecular-informatics-code-helper>



### Molecular Informatics Code Helper

By Scott M Reed 8

Writes and executes Python code for bioinformatics and cheminformatics

Install the provided rdkit wheel and use rdkit to draw the...

Install the provided Biopython wheel and draw the...

Use pyscf and pyberny and to perform a...

Create a curl command that retrieves the InCh...

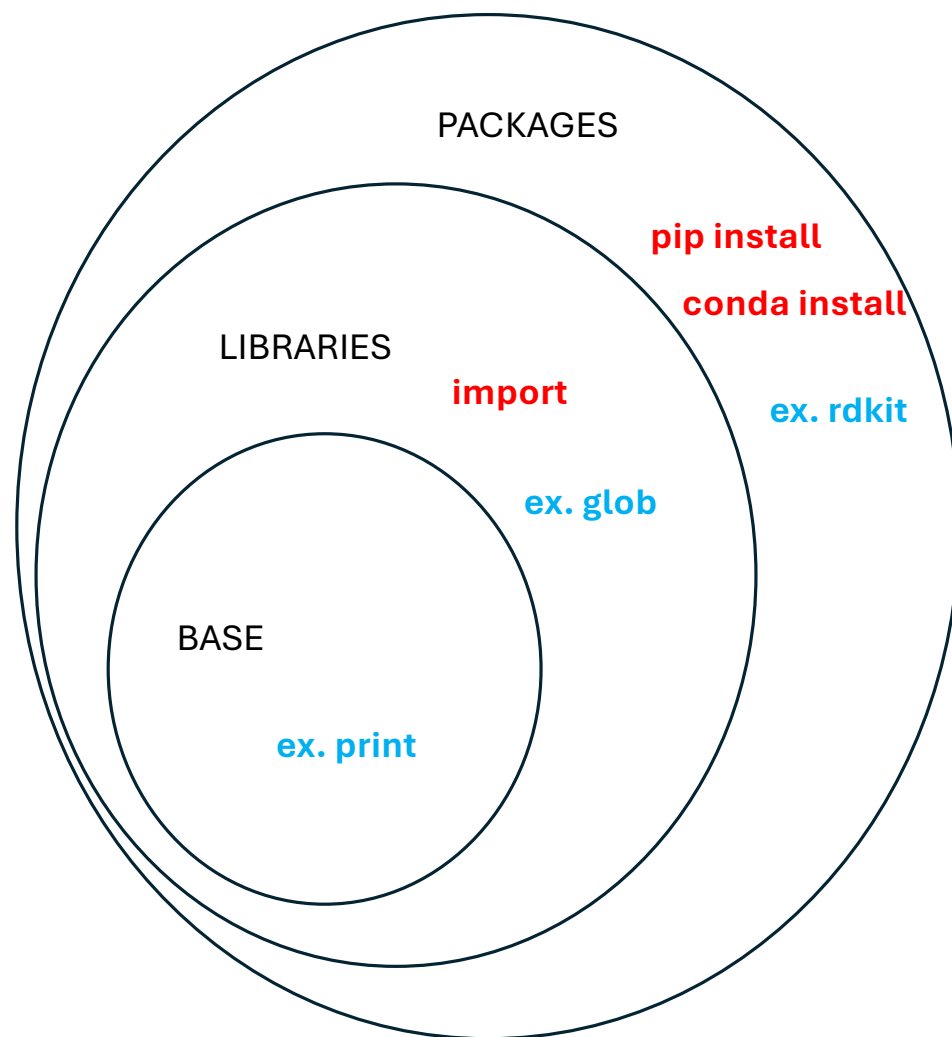


Message Molecular Informatics Code Helper









# Contextual and combinatorial structure in sperm whale vocalisations

Received: 23 January 2024

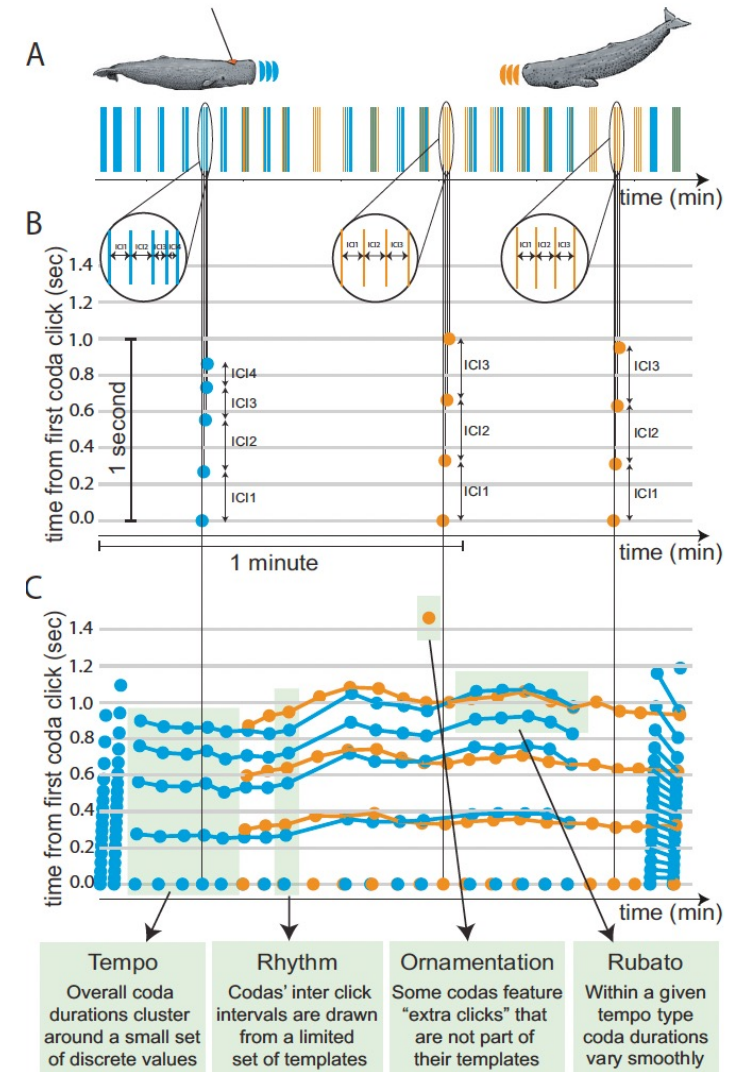
Accepted: 25 March 2024

Published online: 07 May 2024



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Sperm whales (*Physeter macrocephalus*) are highly social mammals that communicate using sequences of clicks called codas. While a subset of codas have been shown to encode information about caller identity, almost everything else about the sperm whale communication system, including its structure and information-carrying capacity, remains unknown. We show that codas exhibit contextual and combinatorial structure. First, we report previously undescribed features of codas that are sensitive to the conversational context in which they occur, and systematically controlled and imitated across whales. We call these rubato and ornamentation. Second, we show that codas form a combinatorial coding system in which rubato and ornamentation combine with two context-independent features we call rhythm and tempo to produce a large inventory of distinguishable codas. Sperm whale vocalisations are more expressive and structured than previously believed, and built from a repertoire comprising nearly an order of magnitude more distinguishable codas. These results show context-sensitive and combinatorial vocalisation can appear in organisms with divergent evolutionary lineage and vocal apparatus.



try running that python script to get the mw of benzene



Since I can't execute code directly, I'll guide you through running the Python script on your local machine to calculate the molecular weight of benzene using RDKit.

### Instructions

#### 1. Ensure RDKit is Installed:

Make sure RDKit is installed in your Python environment. If not, you can install it using conda:

```
bash
```

Copy code

```
conda install -c conda-forge rdkit
```

#### 2. Write the Python Script:

Create a Python script file, for example, `calculate_benzene_weight.py`, with the following content:

```
python
```

Copy code

```
from rdkit import Chem
from rdkit.Chem import Descriptors
```



Message ChatGPT



LLM served by Perplexity Labs  
Hello! How can I help you?

📄 Copy

Spell Pennsylvania backwards

LLM served by Perplexity Labs  
The word "Pennsylvania" spelled backwards is "ainiYlnnep".

📄 Copy   ➞ Ask Perplexity



0.21 SEC TO FIRST TOKEN

175 TOKENS/SEC

16 TOKENS

0.09 SEC

llama-3-8b-instruct



LLM served by Perplexity Labs

Here's a step-by-step process to spell a word backwards:

1. Write the word out in its normal spelling: Start by writing the word out in its correct spelling. For example, let's use the word "hello".
2. Separate the word into individual letters: Take the word and separate it into individual letters. For the word "hello", this would be:
  - h
  - e
  - l
  - l
  - o
3. Reverse the order of the letters: Now, reverse the order of the letters. Start with the last letter and move backwards to the first letter. For the word "hello", this would be:
  - o
  - l



0.22 SEC TO FIRST TOKEN

120 TOKENS/SEC

208 TOKENS

1.73 SEC

llama-3-8b-instruct

- l
- l
- o

3. Reverse the order of the letters: Now, reverse the order of the letters. Start with the last letter and move backwards to the first letter. For the word "hello", this would be:

- o
- l
- l
- e
- h

4. Combine the reversed letters: Finally, combine the reversed letters to form the word spelled backwards. For the word "hello", this would be:

- olleh

And that's it! By following these steps, you can correctly spell a word backwards.



0.22 SEC TO FIRST TOKEN

120 TOKENS/SEC

208 TOKENS

1.73 SEC

llama-3-8b-instruct

LLM served by Perplexity Labs

Let's follow the process to spell the word "Pennsylvania" backwards:

1. Write the word out in its normal spelling: Pennsylvania
2. Separate the word into individual letters:
  - P
  - E
  - N
  - N
  - S
  - Y
  - L
  - V
  - A
  - N



0.21 SEC TO FIRST TOKEN

124 TOKENS/SEC

200 TOK

- A
- V
- L
- Y
- S
- N
- N
- E
- P

4. Combine the reversed letters: The word "Pennsylvania" spelled backwards is:

- A-I-N-A-V-L-Y-S-N-N-E-P

So, the correct spelling of "Pennsylvania" backwards is indeed A-I-N-A-V-L-Y-S-N-N-E-P.



Copy Ask Perplexity



0.21 SEC TO FIRST TOKEN

124 TOKENS/SEC

200 TOKENS

1.60 SEC

llama-3-8b-instruct

