

Introduction to Programming with LLM Coding Assistants

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Micro Nano Technology
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My Background

My research interests

- PhD candidate, Purdue University
- Thesis topic: *simulations and machine learning to study graphene-like materials*

Outside of research

- My hobbies are reading, coffee, and coding
- I enjoy spending time with my partner and her cat, Augustus!



Outline

- 1 Introduction to Large Language Models (LLMs)
- 2 Web-Based LLM Chatbots
- 3 Editor-Integrated LLM Chatbots
- 4 Demonstration of LLMs for Programming

What is a Large Language Model?¹

Let's break it down word by word:

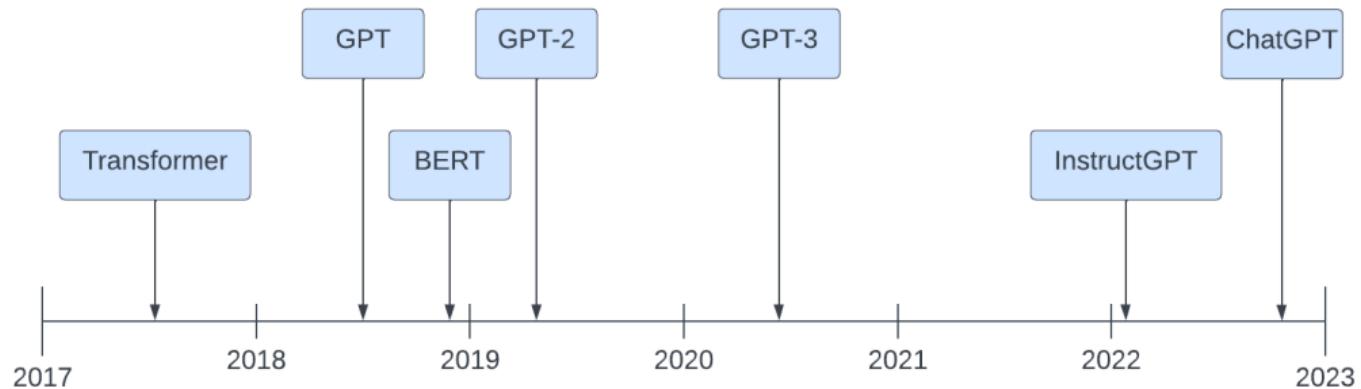
- A **model** is an algorithm that has been trained to perform a specific task.
- A **language** model is a model that has been trained to predict and generate text.
- A **large** language model contains billions of parameters learned during training.

So, what is a *large language model*?

- A *large language model*? (LLM) is a model that has been trained to predict and generate text using billions of parameters.
- "LLM" has expanded to include models that use images, audio, etc.

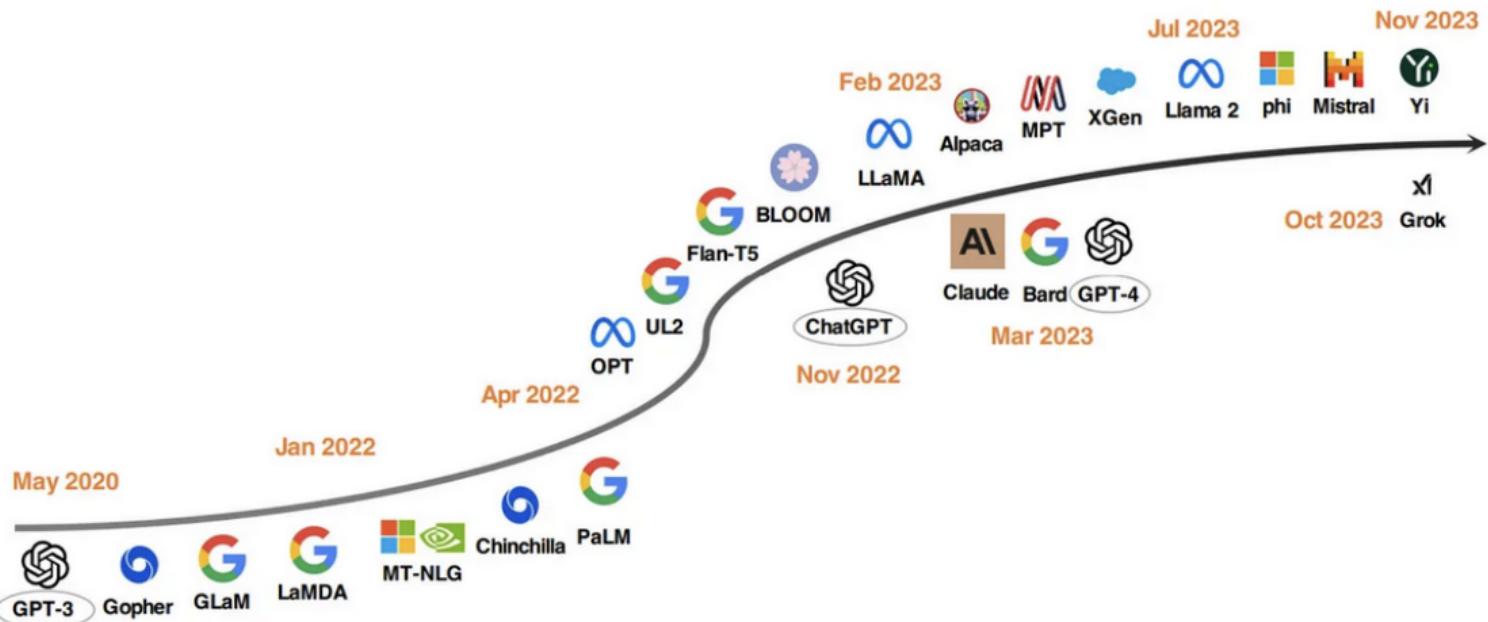
¹<https://developers.google.com/machine-learning/resources/intro-llms>

How Did We Get Here?²



²<https://www.dingran.me/from-transformer-to-l1m/>

Many LLMs Exist, not just ChatGPT³



³<https://arxiv.org/abs/2311.16989>

Which LLM Should I Use?⁴

	Average ▼	Multi-choice Qs	Reasoning ▲	Python coding	Future Capabilities	Grade school math	Math Problems
Claude 3 Opus	84.83%	86.80%	95.40%	84.90%	86.80%	95.00%	60.10%
Gemini 1.5 Pro	80.08%	81.90%	92.50%	71.90%	84%	91.70%	58.50%
Gemini Ultra	79.52%	83.70%	87.80%	74.40%	83.60%	94.40%	53.20%
GPT-4	79.45%	86.40%	95.30%	67%	83.10%	92%	52.90%
Claude 3 Sonnet	76.55%	79.00%	89.00%	73.00%	82.90%	92.30%	43.10%
Claude 3 Haiku	73.08%	75.20%	85.90%	75.90%	73.70%	88.90%	38.90%
Gemini Pro	68.28%	71.80%	84.70%	67.70%	75%	77.90%	32.60%
Palm 2-L	65.82%	78.40%	86.80%	37.60%	77.70%	80%	34.40%
GPT-3.5	65.46%	70%	85.50%	48.10%	66.60%	57.10%	34.1%
Mixtral 8x7B	59.79%	70.60%	84.40%	40.20%	60.76%	74.40%	28.40%

⁴<https://www.vellum.ai/llm-leaderboard#model-comparison>

Methods to Interact with LLMs

Web-Based Chatbot

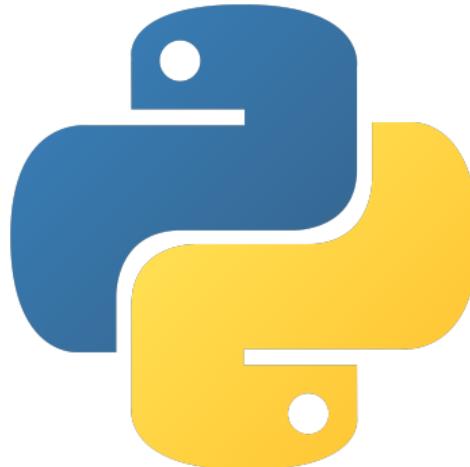
- Minimal setup required
- Generous free tier
- Paid tiers available for more features

API Calls

- Some setup required
- Pay as you go
- Wide range of models available

Run Locally

- Lots of setup required
- "Free" to run
- Limited to open source models



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Web-Based LLM Chatbot Overview

What is *web-based*?

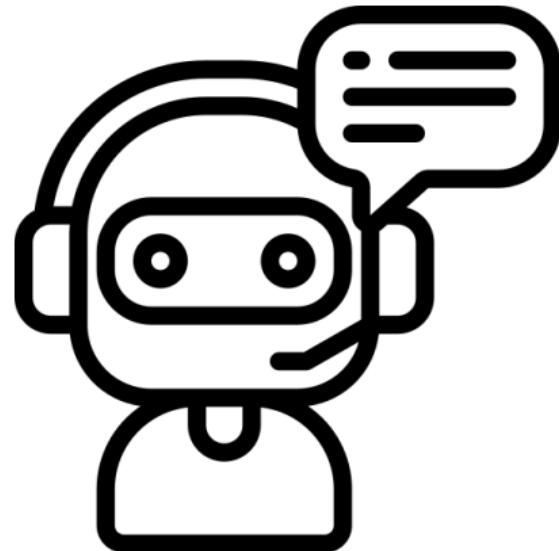
- Accessible from a web browser
- No installation required

What is a *chatbot*?

- LLM trained for human conversation
- Retains conversation history

Popular web-based chatbots

- GPT, Claude, Gemini



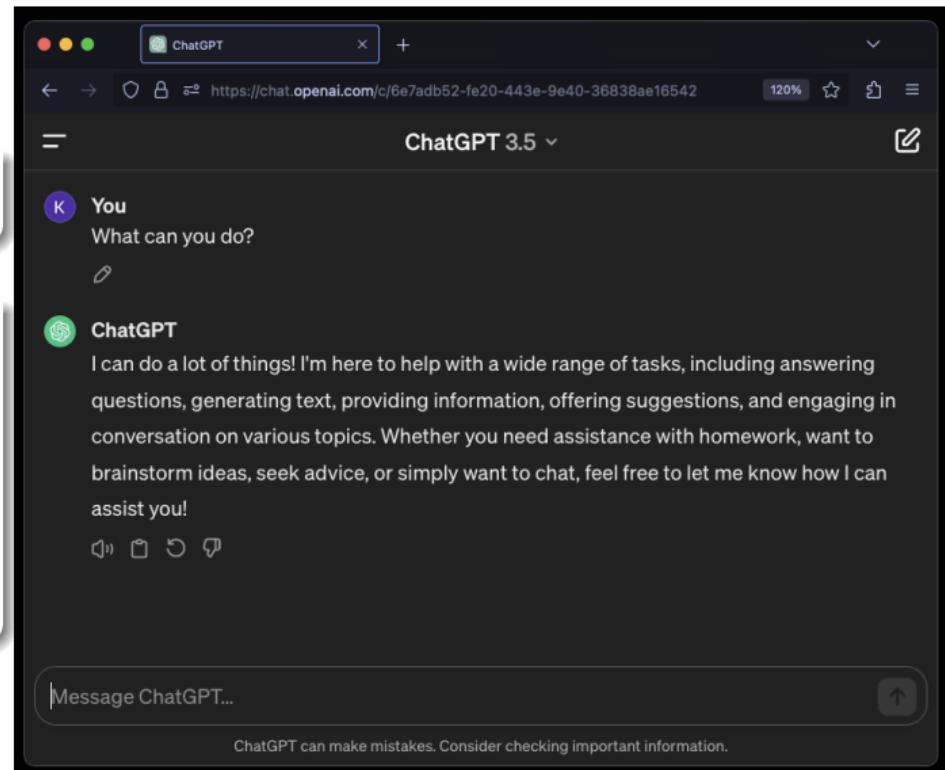
ChatGPT⁵

Free tier

- GPT-3.5

Paid tier

- \$20/month
- GPT-4
- GPT store
- DALL-E
- Browsing



⁵<https://chat.openai.com/>

Claude⁶

Free tier

- Claude 3 Haiku
- Include files in input

Paid tier

- \$20/month
- Claude 3 Sonnet
- Claude 3 Opus
- 5x usage limit

The screenshot shows a web browser window for 'Claude' at the URL <https://claude.ai/chat/92a70f59-2471-419c-b64b-44d1e45f3368>. The page title is 'AI Capabilities of an AI assistant'. A message bubble says 'What can you do?'. Below it, text states: 'As an AI assistant, I'm capable of helping with a wide variety of tasks! Some key things I can do include:' followed by two bullet points: '**Writing and Editing:** I can assist with all kinds of writing projects, from essays and articles to stories and scripts. I can help with brainstorming, outlining, drafting, revising, and polishing text.' and '**Research and Analysis:** I have access to a vast amount of information and can help conduct research, gather data, synthesize findings, and provide in-depth analysis on any topic.' At the bottom, there's a 'Subscribe to Pro' button.

⁶<https://claude.ai/chats>

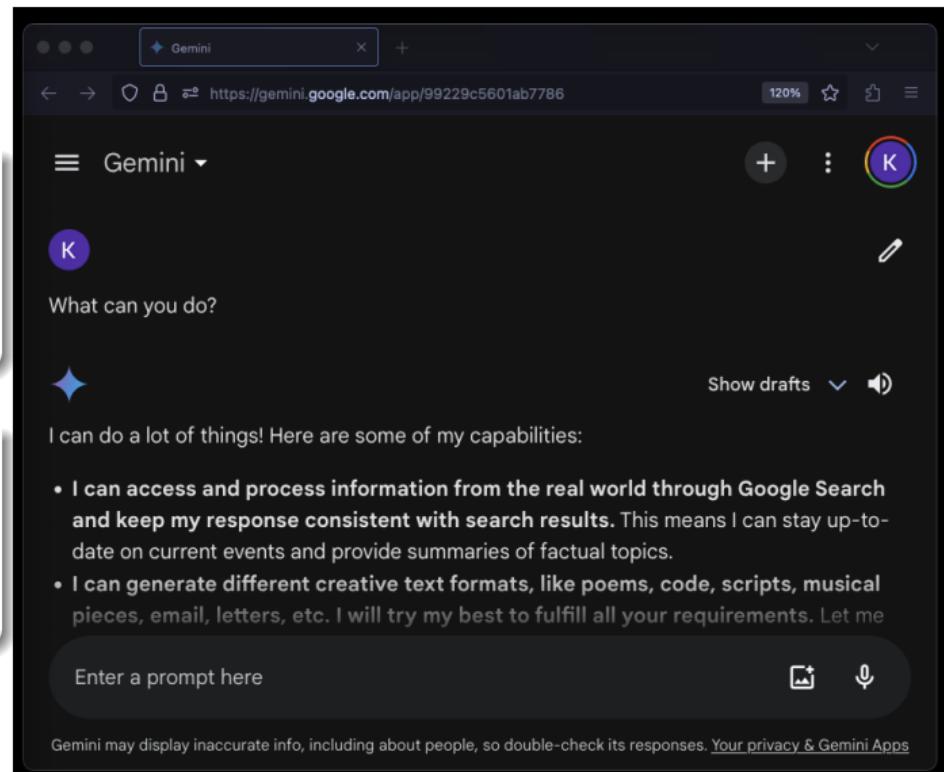
Gemini⁷

Free tier

- Gemini Pro
- Google Search
- Input and output images

Paid tier

- \$20/month
- Gemini Ultra
- Gemini in Photos, Drive, Gmail



⁷<https://gemini.google.com>

What about APIs?

What are APIs?

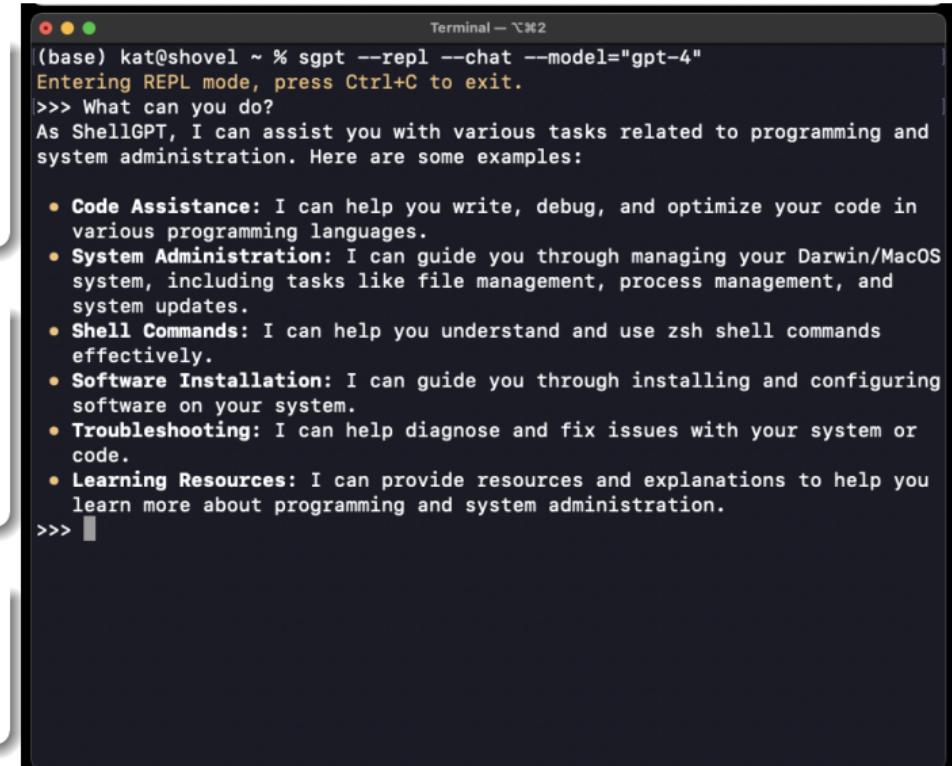
- Allow you to interact with LLMs programmatically
- Cost varies on usage

Getting API keys

- OpenAI API
- Anthropic API
- Google AI

External tools

- ShellGPT
- LangChain



The screenshot shows a Terminal window titled "Terminal - □%2". The session starts with the command `(base) kat@shovel ~ % sgpt --repl --chat --model="gpt-4"`. It then displays a welcome message: "Entering REPL mode, press Ctrl+C to exit." followed by "As ShellGPT, I can assist you with various tasks related to programming and system administration. Here are some examples:". Below this, a bulleted list of capabilities is provided:

- **Code Assistance:** I can help you write, debug, and optimize your code in various programming languages.
- **System Administration:** I can guide you through managing your Darwin/MacOS system, including tasks like file management, process management, and system updates.
- **Shell Commands:** I can help you understand and use zsh shell commands effectively.
- **Software Installation:** I can guide you through installing and configuring software on your system.
- **Troubleshooting:** I can help diagnose and fix issues with your system or code.
- **Learning Resources:** I can provide resources and explanations to help you learn more about programming and system administration.

The prompt "`>>> █`" is visible at the bottom of the terminal window.

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What is an Editor-Integrated LLM?⁸

An editor-integrated LLM works directly from your editor, without needing to switch between applications.



⁸<https://fengyuan-yap.medium.com/what-are-code-editors-ide-37727d6b8060>

GitHub Copilot

GitHub Copilot

- GitHub Copilot is an AI-powered coding assistant developed by GitHub

GitHub Student Developer Pack

- GitHub Copilot is included in the free GitHub Student Developer Pack
- To be eligible, you must be enrolled in a degree or diploma granting course of study



GitHub Copilot: Chat Conversation Feature

- GitHub Copilot can generate responses in a chat-like format.
- This feature allows developers to interact with the AI in a more conversational manner.
- It can provide code suggestions, answer programming questions, and more.

The screenshot shows a LaTeX editor interface with two tabs: 'presentation.tex — grave' and 'TEX presentation.tex 2'. The right pane displays the LaTeX code:

```
\section{Editor-Integrated LLM Chatbots}
\begin{frame}
\frametitle{GitHub Copilot: Chat Conversation Feature}
\begin{columns}
\begin{column}{0.5\textwidth}
\begin{itemize}
- GitHub Copilot can generate responses in a chat-like format.
- This feature allows developers to interact with the AI in a more conversational manner.
- It can provide code suggestions, answer programming questions, and more.



\begin{column}{0.5\textwidth}
\begin{itemize}
- How can I customize the appearance of the Beamer slide generated by GitHub Copilot?



\end{columns}
\end{frame}
```

The left pane shows a 'CHAT' window with a message from user 'katnykiel' and a response from 'GitHub Copilot'. The 'GitHub Copilot' response includes a LaTeX snippet and a question about customizing the Beamer slide appearance.

GitHub Copilot: Tab Completion Feature

- GitHub Copilot can provide code suggestions as you type.
- This feature is similar to tab completion in other editors.
- It can help you write code faster and more accurately.

The screenshot shows a LaTeX editor window titled "presentation.tex — grave". The file content is as follows:

```
\section{Editor—Integrated LLM Chatbots}
\begin{frame}
    \begin{columns}
        \begin{column}{0.5\textwidth}
            \includegraphics[width=\textwidth]{chat-conversation.png}
        \end{column}
    \end{columns}
\end{frame}

\begin{frame}
    \frametitle{GitHub Copilot: Tab Completion Feature}
    \begin{itemize}
        \begin{columns}
            \begin{column}{0.5\textwidth}
                \begin{itemize}
                    \item GitHub Copilot can provide code suggestions as you type.
                    \item This feature is similar to tab completion in other editors.
                    \item It can help you write code faster and more accurately.
                \end{itemize}
            \end{column}
        \end{columns}
        \begin{column}{0.5\textwidth}
            \includegraphics[width=\textwidth]{tab-completion.png}
        \end{column}
    \end{itemize}
\end{frame}

\begin{frame}
    \frametitle{GitHub Copilot: Inline Chat}

```

The "GitHub Copilot: Tab Completion Feature" frame contains an itemized list with three items. The first item is expanded, showing its own list items. The "tab-completion.png" image is visible in the right column of the frame. The "GitHub Copilot: Inline Chat" frame is partially visible at the bottom.

GitHub Copilot: Inline Chat

- GitHub Copilot can provide inline chat within your code.
- It can assist you in writing code by providing suggestions and answering questions directly in your editor.

The screenshot shows a LaTeX editor window titled "presentation.tex — grave". The code editor displays a frame containing two columns. The left column contains a list item about GitHub Copilot's inline chat capability. The right column contains a list item about GitHub Copilot assisting in writing code. A floating GitHub Copilot interface is overlaid on the editor, asking if it can generate the slide and include a disclaimer. The Copilot interface shows a "Made changes." message and "Accept" and "Discard" buttons. Below the code editor, a LaTeX logo and the word "LaTeX" are visible.

```
\begin{frame}
\frametitle{GitHub Copilot: Inline Chat}
\begin{columns}
\begin{column}{0.5\textwidth}
\begin{itemize}
\item GitHub Copilot can provide inline chat within your code.
\end{itemize}

\begin{column}{0.5\textwidth}
\begin{itemize}
\item It can assist you in writing code by providing suggestions and answering questions directly in your editor.
\end{itemize}

\end{columns}
\end{frame}
```

Can you generate this slide for me? Include a disclaimer that this, and the last two slides, have all been written by Copilot

GitHub Copilot
Made changes.
Accept Discard

Accept or Discard 2 changes.

Disclaimer

The content of this slide, as well as the previous two slides, has been generated by GitHub Copilot.

GitHub Copilot Alternatives

GitHub Copilot API

- Use the GitHub Copilot API to integrate Copilot anywhere
- Works in editors other than VSCode

Other Editor-Integrated LLMs

- Tabnine, Kite, Ponicode, DeepCode
- Cursor is a VSCode fork with extended features



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Large Language Models (LLMs) as Research Tools

How can we use LLMs to accelerate research?

```
units metal
dimension 3
boundary p p p

atom.style atomic
lattice fcc 4.05

region box 0 5 0 5 0 5 units lattice
create_box 1 box
create_atoms 1 box

replicate 5 5 5

pair.style <eam/fs> or <eam/alloy>
pair.coeff * * <potential file name> Al
mass 1 26.9815

neighbor 2.0 bin
neigh.modify delay 10

velocity all create 300 <random seed> mon yes rot yes dist <uniform> or <gaussian>

fix 1 all npt temp 300 300 0.1 iso 1 1 1
thermo <thermo steps>
thermo.style <custom step temp pe etotal press vol>

timestep 0.001
run 500000
unfix 1

dump, print, write_data, ...
```

GPT for simulation design

ChatGPT OpenAI API Key

Sure, the LAMMPS script for a simple molecular dynamics (MD) simulation of Aluminum (Al) at 1000 K using a NPT ensemble could look something like this.

```
#box
# Initialization
units metal
boundary p p p
atom_style atomic

# Atomic Configuration
lattice fcc 4.05
region box block 0 10 0 10 0 10
create_box 1 box
create_atoms 1 box

# Potential
pair_style eam
pair_coeff * * Al.eam

All thermo modify statements will be overwritten
```

Run a MD simulation of Al at 1000 K, NPT

Write a script

Researcher Chat example

Structure (S) Potential (P)

GPT Methods

In the computational study, molecular dynamics simulations were performed using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). An atomic configuration of face-centered cubic (fcc) Aluminum with a lattice constant of 4.05 Å was generated within a periodic cubic box sizing 10x10x10 unit cells, summing up to 4000 atoms. The atomic interactions were described using the Embedded Atom Method (EAM) potential for Aluminum provided in the Al.eam file.

The initial velocities were assigned to the atoms such that the system temperature was approximately 1000 K, followed by equilibration under a NPT (constant Number of particles, Pressure, and Temperature) ensemble for 5000 steps maintaining a constant temperature and isotropic pressure conditions. The temperature and pressure were controlled using a Nose-Hoover thermostat and barostat with a damping parameter of 0.01.

Thermodynamic status of the system was periodically outputted every 100 steps during the entire course of the simulation run. Please note that the Aluminum potential file (Al.eam) should be present in the working directory.

Clear all

GPT to write methodology

Example Use Case: Python Programming

Sample Problem: Board Game Dice

- Simulating a dice roll
- Performing statistics
- Generating static plots



Gemini-generated image... notice anything off?

nanoHUB Tool

Check out the nanoHUB tool for this demonstration here!

<https://nanohub.org/tools/l1m4code>

