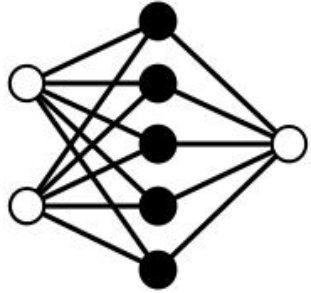


AI Workflow & Vibe Researching

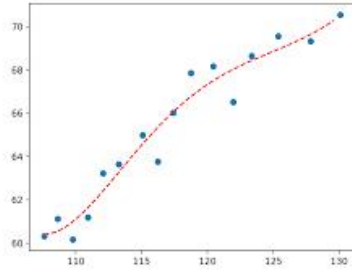
To use or not to use, that's not a question.

Yiyang Jiang

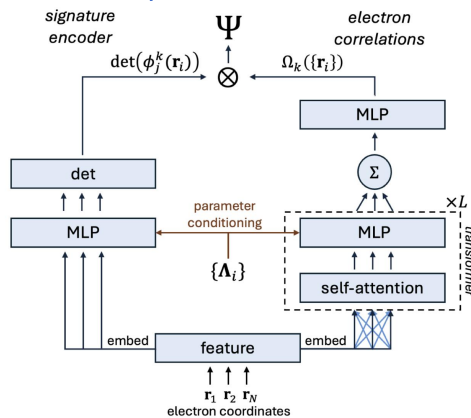
AI in Physics



Neural Network



Fitting

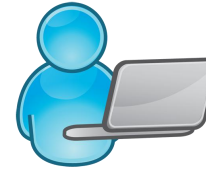


Neural Quantum State

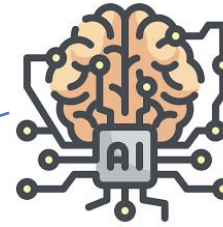


DeepH

**NN-based
(Principle)**



User



LLM



Agent Loop



Memory
(RAG, Skills)



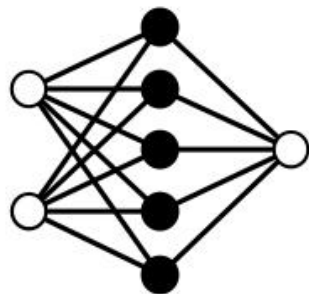
Tools
(API, MCP)



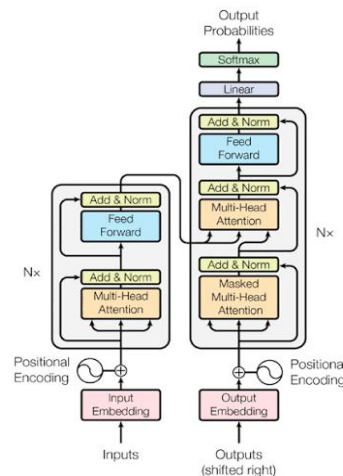
Planning

**LLM-based
(Workflow)**

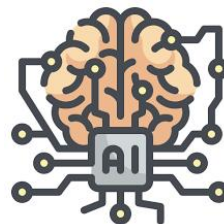
Key Concepts in AI Community



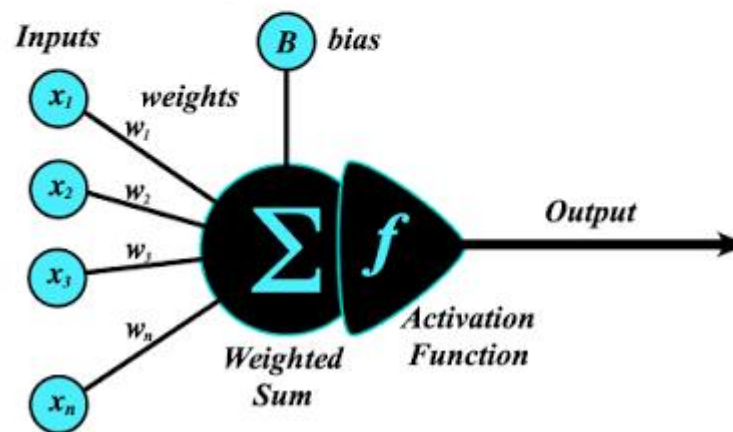
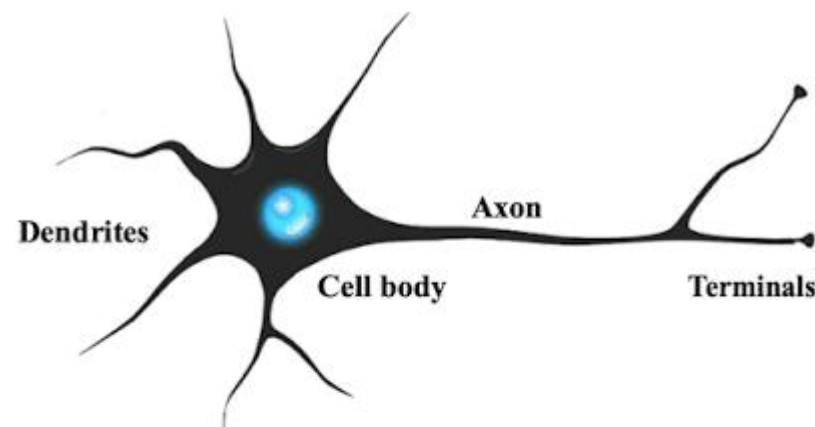
Neural Network



Transformer



LLM



1 Token
~ 0.75 words
~ 1.5 Chinese character (汉字)

Token

Key Concepts in AI Community

Context (Temporary Memory)
Context Window

Save Context

RAG (Retrieval Augmented Generation)

Prompt

User Prompt

Precise and Concise Prompt
(Prompt Engineering)

System Prompt

Tool

MCP (Model Context Protocol)

Key Concepts in AI Community

Agent

API (Application Programming Interface)

Skills

Headless mode

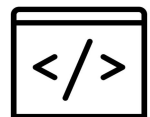
Evolution of Human-AI Collaboration



LLM



User



Code

2023



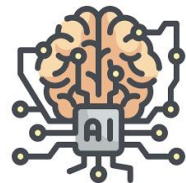
ChatGPT



Claude



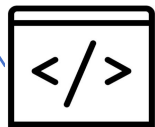
Gemini



LLM



User

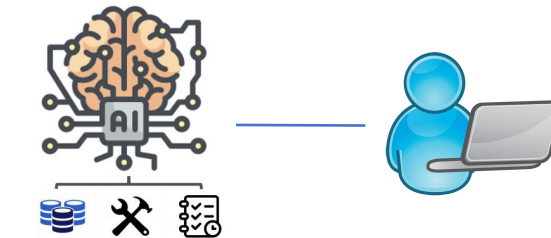


Code

2024



Cursor



Agentic AI



User



Codebase



Task 1



Task 2



Task 3

2025



Codex



Antigravity



Claude Cowork



User



Agent



Codebase



Task 1

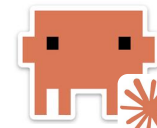


Task 2

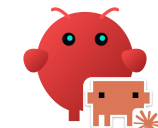


Task 3

2026

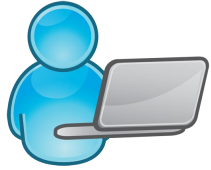


Claude Code



Openclaw

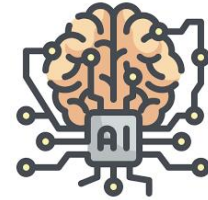
Strengths of Human / PC / AI



Human



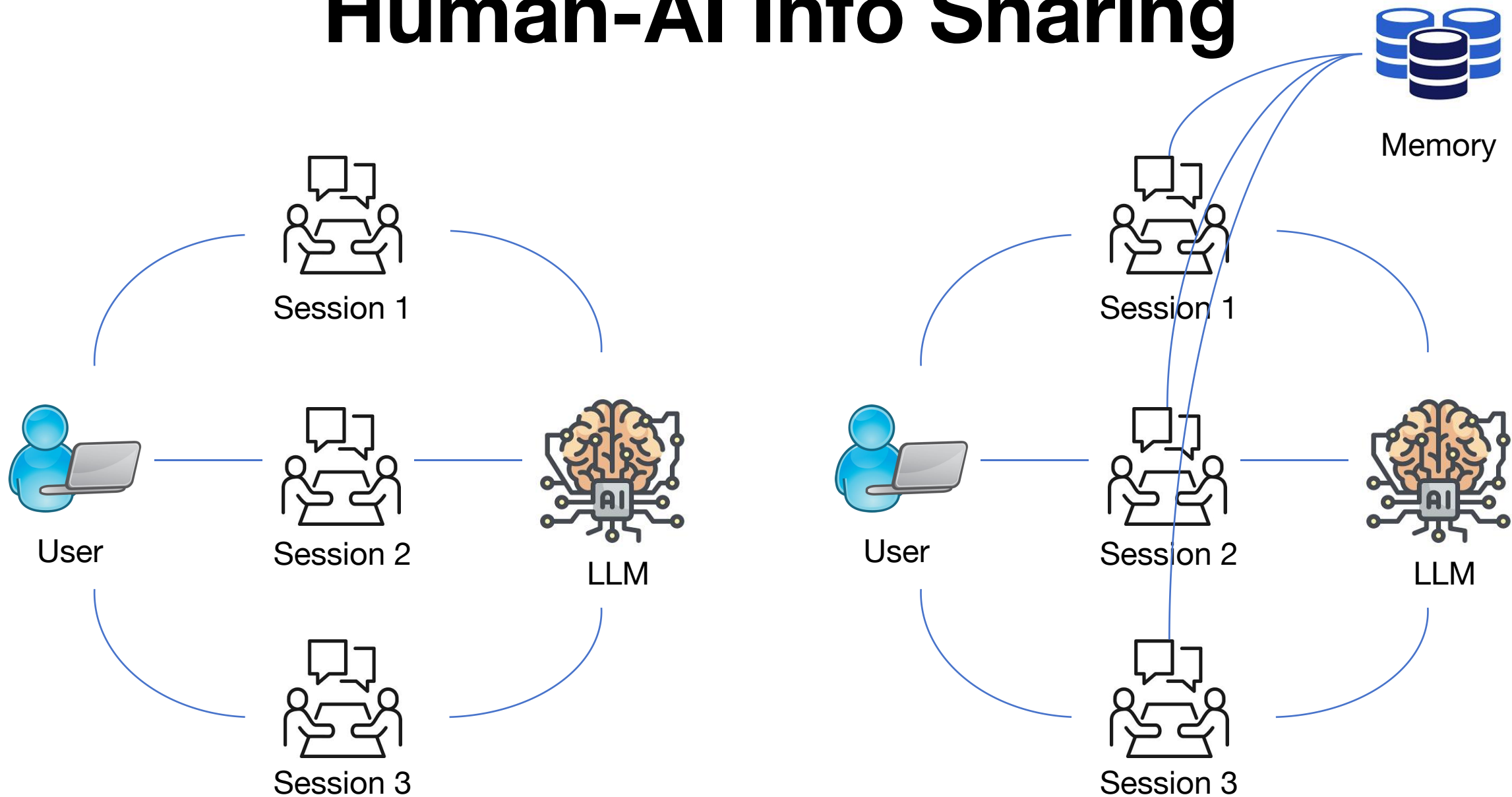
PC



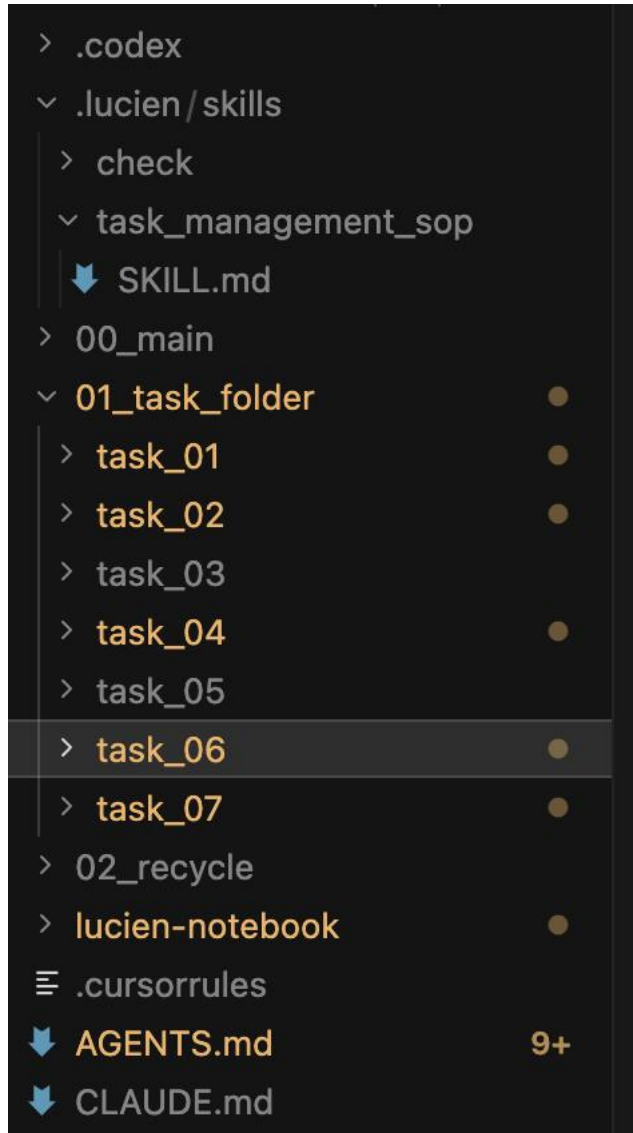
AI (LLM)

- | | | |
|--|--|--|
| <ul style="list-style-type: none">• Image Process | <ul style="list-style-type: none">• Structured Memory | <ul style="list-style-type: none">• Summary |
| <ul style="list-style-type: none">• Speaking | | <ul style="list-style-type: none">• Typing |
| <ul style="list-style-type: none">• Decision Making | | <ul style="list-style-type: none">• Coding |
| <ul style="list-style-type: none">• Longer Thinking | <ul style="list-style-type: none">• (?) | <ul style="list-style-type: none">• Literature Research |

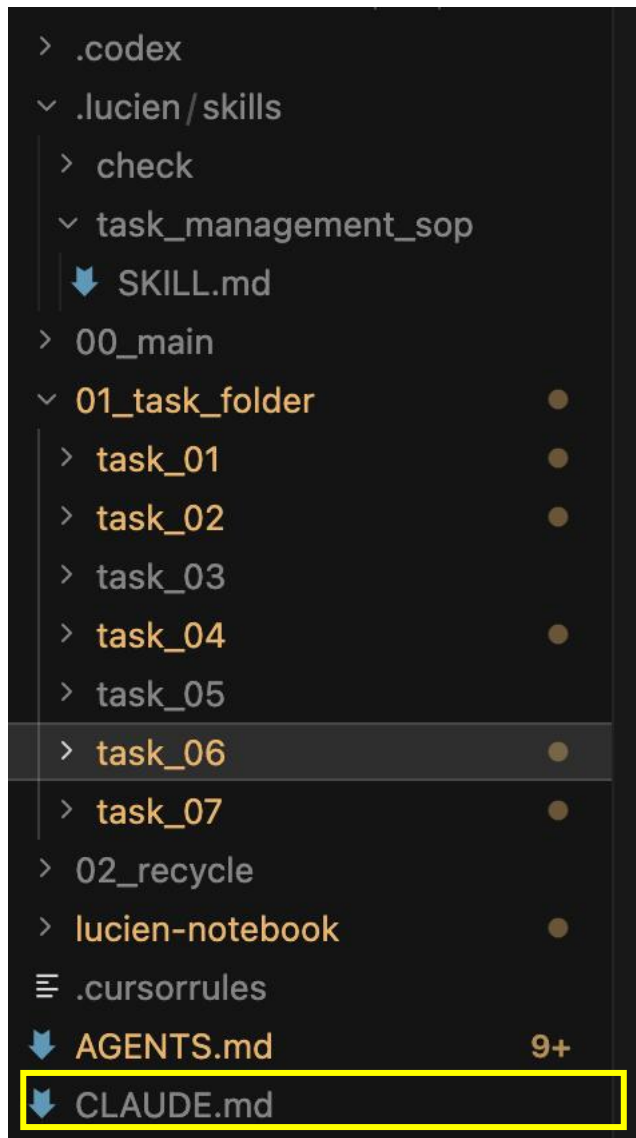
Human-AI Info Sharing



Project Folder Structure



Project Folder Structure



Preview CLAUDE.md

3. Workspace Architecture

The repository default workspace layout is strictly restricted to the following directories.

Anti-proliferation rule: do not create `02_execution`, `03_scripts`, or any other legacy top-level folders. Do not operate outside of the allowed directories unless the human explicitly changes the architecture.

00_main/ (Global State)

Strictly contains only:

- `main_dashboard.md`: the global ledger; read this first every session.
- `system_prompt.md`: the master operating instructions.
- `history/`: historic, timestamped versions of `main_dashboard.md` and prompt files.
- Other optional files only if explicitly requested by the human.

01_task_folder/ (Execution Zone)

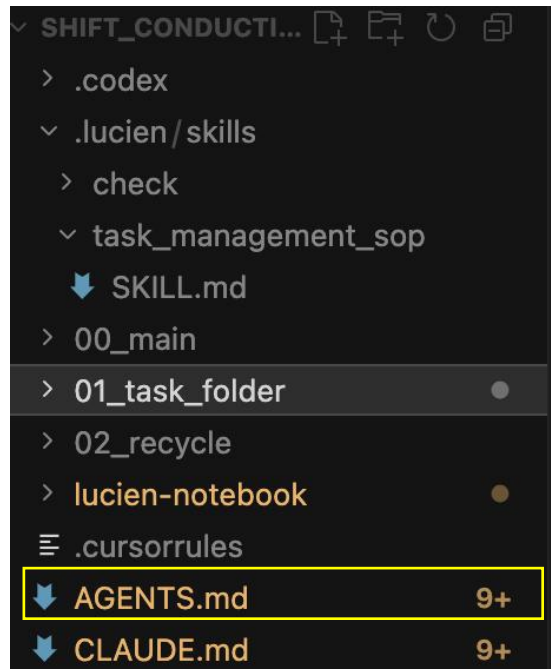
Contains self-contained task folders such as `task_11/`. Every task or subtask should contain:

- `task_X_dashboard.md`
- `script/`
- `script/output/`
- `history/`
- Task-local generated outputs written under `script/output/` by default

02_recycle/ (Archive / Graveyard)

Contains failed, deprecated, or archived task folders moved out of the active workspace.

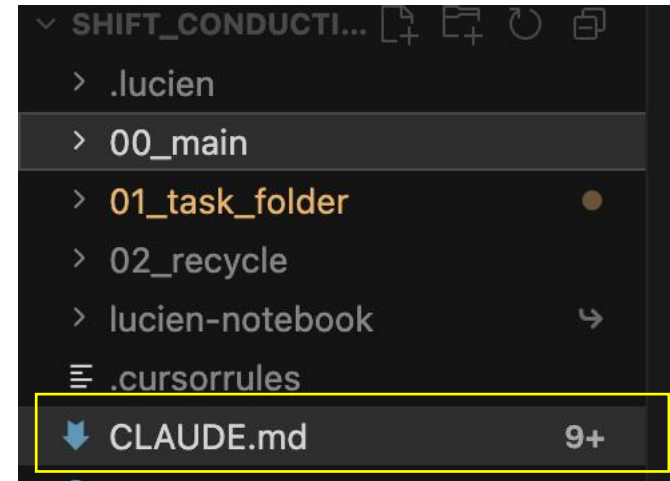
System Prompt



Setup Prompt

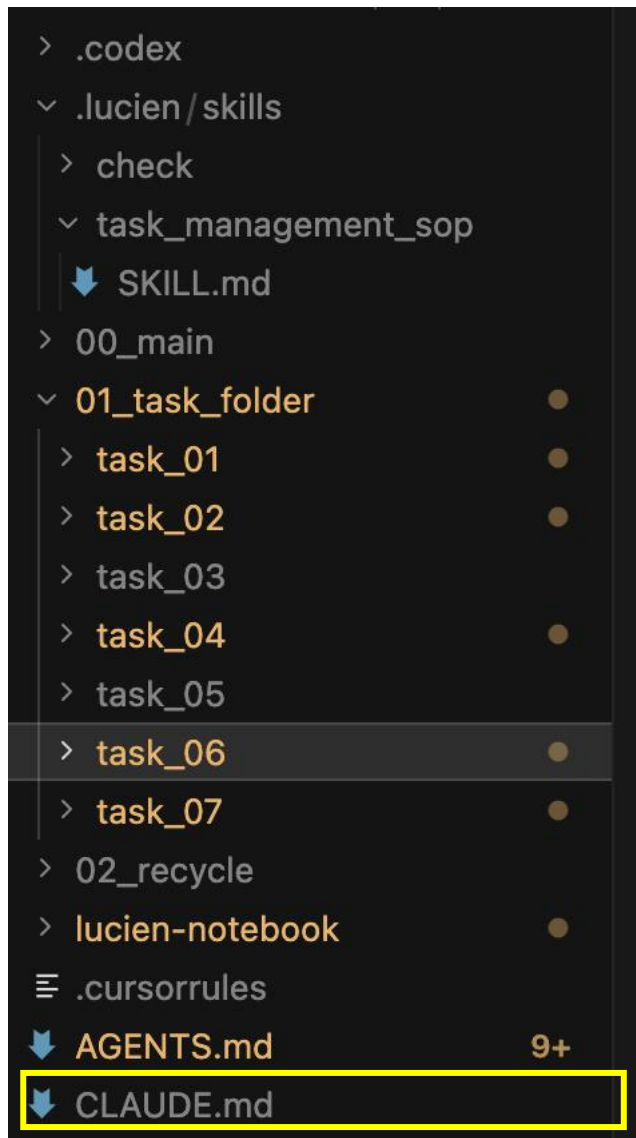


Claude Cowork



CLAUDE.md

Project Folder Structure



Preview CLAUDE.md

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01_task_folder/ (Execution Zone)

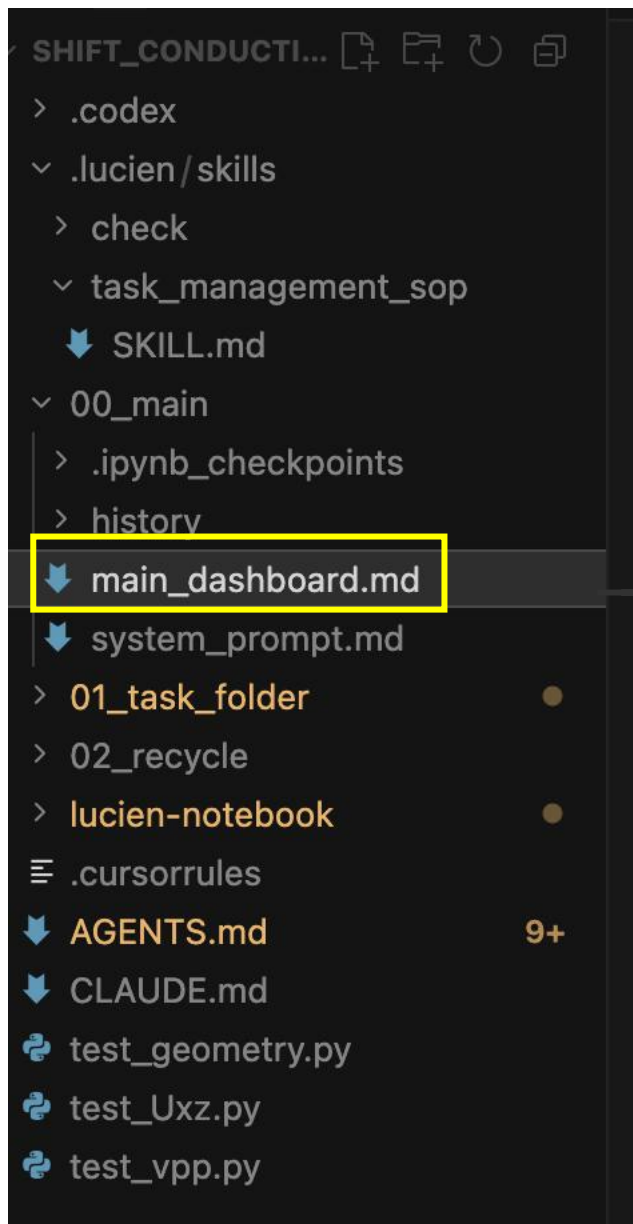
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- `history/`
- Task-local generated outputs written under `script/output/` by default

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Contains failed, deprecated, or archived task folders moved out of the active workspace.

Main Dashboard



```

9_dashboardboard × 2025-04-02 15:00 EDT × task_dashboardboard × 2025-04-02 15:00 EDT × system_prompt 9+
00_main → main_dashboard → Main Dashboard → ## Global Log

1 # Main Dashboard
2
3 - Last Updated: 2026-04-02 15:00 EDT
4 - Workspace Status: Ready
5 - Active Task: task_00
6 - Repository Objective: Calculate shift conductivity
7
8 ## Task Ledger
9
10 | Task | Objective | Status | Last Updated |
11 | --- | --- | --- | --- |
12 | task_00 | Literature research on paper focusing on building MoS2 tight-binding models | ● Finished | 2026-04-02 |
13 | task_01 | Reproduce Rice-Mele 1D  $\sigma(\omega)$  with physical units (analytic/sum-rule/Wilson loop,  $e^3/h$  prefactor) | ● Finished | 2026-03-31 |
14 | task_02 | Construct the tight-binding model of MoS2 from PhysRevB.92.205108 | ● Ongoing | 2026-03-30 23:13 EDT |
15 | task_03 | Literature Review on MoS2 Shift Conductivity via Tight-Binding models | ● Finished | 2026-03-31 |
16 | task_04 | Reproduce Fig. 2 of Phys. Rev. B 111, 125203 using the Task 2 MoS2 tight-binding model and the arXiv:2409.15673 formalism | ● Finished | 2026-03-31 |
17 | task_05 | Continue Fig. 2 Reproduction & Improvement Plan | ● Finished | 2026-03-31 |
18 | task_06 | General gauge-stable shift-conductivity engine for arbitrary tight-binding Hamiltonians | ● Ongoing | 2026-04-01 03:18 UTC |
19 | task_07 | Find paper with 1D 2D 3D toy model with calculated shift conductivity for future tasks benchmark | ● Finished | 2026-04-01 02:51 UTC |
20 | task_08 | Shift Conductivity Benchmarks for 1D, 2D, 3D Models | ● Ongoing | 2026-04-02 15:00 EDT |
21 | task_09 | Calculate MoS2 shift conductivity using the task_02 11-band model and task_06 solver in an isolated task workspace | ● Ongoing | 2026-04-02 14:22 EDT |
22 | task_10 | Extract Wannier/TB setup for bulk GaAs and monolayer GeS from PRB 97, 245143 and prepare shift-current reproduction workflow | ● Ongoing | 2026-04-02 15:00 EDT |
23
24 ## Global Log
25
26 - 2026-03-30: Initialized task-centric workspace structure and synchronized prompt files.
27 - 2026-03-30: Updated synchronized prompt family with repository-level objective to calculate shift conductivity.
28 - 2026-03-30 22:07 EDT: Created task_01 for reproducing the Rice-Mele benchmarks from arXiv:2206.04560 and initialized the task dashboard and script workspace.
29 - 2026-03-31: Created task_02 to construct the tight-binding model of MoS2 from Fang et al. (PhysRevB.92.205108). Replicated band structure.
30 - 2026-03-31: Created task_03 to compile a list of literature that calculated MoS2's shift conductivity using tight-binding models. Found papers and logged arXiv links.
31 - 2026-03-30 23:59 EDT: Reopened task_02 and set it as the active task for the current session per user instruction.
32 - 2026-03-31 00:10 EDT: Extended task_02 with a generalized TMDC script and documented the WSe2 band-structure reproduction workflow in the task canvas.
33 - 2026-03-30 23:13 EDT: Generated WSe2 and refreshed MoS2 'v2' band figures for task_02, embedded the WSe2 figure in the task canvas, updated the synchronized prompt rule to always place the most important output figure in the canvas, and added the strict audit skill 'Lucien/skills/check/SKILL.md'.
34 - 2026-03-31: Verified and completed task_01 (session 1). Shift vector benchmarks in reduced units confirmed.

```

- Repository Objective: Calculate shift conductivity

Task Ledger

Task	Objective	Status	Last Updated
task_00	Literature research on paper focusing on building MoS2 tight-binding models	Finished	2026-04-02
task_01	Reproduce Rice-Mele 1D $\sigma(\omega)$ with physical units (analytic/sum-rule/Wilson loop, e^2/h prefactor)	Finished	2026-03-31
task_02	Construct the tight-binding model of MoS2 from PhysRevB.92.205108	Ongoing	2026-03-30 23:13 EDT
task_03	Literature Review on MoS2 Shift Conductivity via Tight-Binding models	Finished	2026-03-31
task_04	Reproduce Fig. 2 of Phys. Rev. B 111, 125203 using the Task 2 MoS2 tight-binding model and the arXiv:2409.15673 formalism	Finished	2026-03-31
task_05	Continue Fig. 2 Reproduction & Improvement Plan	Finished	2026-03-31
task_06	General gauge-stable shift-conductivity engine for arbitrary tight-binding Hamiltonians	Ongoing	2026-04-01 03:18 UTC
task_07	Find paper with 1D 2D 3D toy model with calculated shift conductivity for future tasks benchmark	Finished	2026-04-01 02:51 UTC
task_08	Shift Conductivity Benchmarks for 1D, 2D, 3D Models	Ongoing	2026-04-02 15:00 EDT
task_09	Calculate MoS2 shift conductivity using the task_02 11-band model and task_06 solver in an isolated task workspace	Ongoing	2026-04-02 14:22 EDT
task_10	Extract Wannier/TB setup for bulk GaAs and monolayer GeS from PRB 97, 245143 and prepare shift-current reproduction workflow	Ongoing	2026-04-02 15:00 EDT

10 min read

main_dashboard.md

preview

Task Dashboard

SHIFT_CONDUCTI...

> .codex

> .lucien/ skills

> check

> task_management_sop

SKILL.md

> 00_main

> 01_task_folder

> task_01

> task_02

> history

> paper

> script

task_02_dashboard.md 5

> task_03

> task_04

> task_05

> task_06

> task_07

> 02_recycle

> lucien-notebook

.cursorrules

AGENTS.md 9+

CLAUDE.md 9+

test_geometry.py

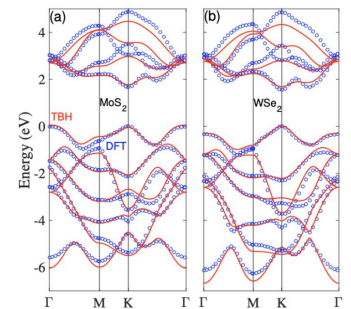
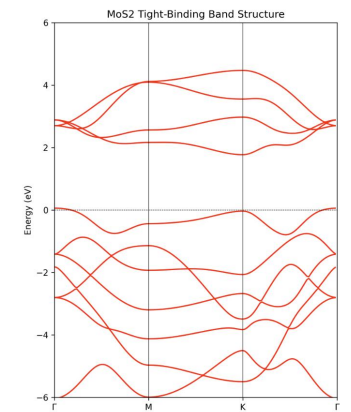
test_Uxz.py

test_vpp.py

```
1 # Task 02: Construct Tight-Binding Model for MoS2
2 - **Main Outputs:** '01_task_folder/task_02/script/output/band_structure_soc.png', '01_task_folder/task_02/script/output/spin_splitting_v2.png'
3
4 ## Objective
5 Construct the tight-binding model of MoS2 from the paper PhysRevB.92.205108 (arXiv:1506.08860). Specifically, reproduce the paper's band structure and spin
6 splitting due to spin-orbit coupling (SOC), and provide a side-by-side comparison.
7
8 ## Version Log
9 - **2026-03-31:** Initialized task 2.
10 - **2026-03-31:** Extracted tight-binding parameters and constructed the 11-band spinless tight-binding Hamiltonian ('mos2_tb.py'). Replicated the spinless
11 band structure.
12 - **2026-03-31:** Extended the script to include the spin-orbit coupling terms ('mos2_tb_soc.py') based on the angular momentum operations and lambda
13 coefficients ($\lambda_{Mo}=0.0836$, $\lambda_{S}=0.0556$).
14 - **2026-03-31:** Computed the spin splitting for the highest valence band along the $\Gamma$-K path to reproduce Figure 4(a) from the paper.
15 - **2026-03-31:** Diagnosed "kink" artefact in the original spin-splitting plot. Root cause: 50 k-points too coarse to resolve the smooth sigmoid profile. Full
16 audit confirmed: (a) $H_{SOC}$ is exactly Hermitian; (b) no band crossings - band indices 12 and 13 are verified as the correct HOMO pair throughout the path via
17 $\angle S_z$ expectation values; (c) splitting at K = 145 meV vs paper 148 meV (2%); (d) $L_x/L_y$ terms contribute $\le 5$ meV and are not the source of any
18 discrepancy. Rewrote the plotting script with 500 k-points ('plot_soc_splitting_v2.py'); the curve is now smooth and the sigmoid shape is confirmed to be
19 intrinsic physics (spin character evolves from zero at $\Gamma$ to pure $\pm \frac{1}{2}$ at K).
20
21 ## Canvas
22
23 ### 1. Spinless Band Structure
24 Code output vs Paper Figure 3a
25
26 ![Reproduced Band Structure](script/output/band_structure.png)
27 ![Paper Fig 3a](script/output/paper_fig3.png)
28
29 ### 2. Band Structure with SOC
30 ![Reproduced SOC Band Structure](script/output/band_structure_soc.png)
31
32 ### 3. Spin Splitting along $\Gamma$ - K$ (corrected, 500 k-points)
33
34 Code output vs Paper Figure 4a (the spin splitting of the highest valence band pair)
35
36 ![Reproduced Spin Splitting - corrected v2](script/output/spin_splitting_v2.png)
37 ![Paper Fig 4](script/output/paper_fig4.png)
38
39 **Audit findings (2026-03-31):**
40
41 The original 50-point plot showed an apparent "kink" near $k_x/k_y \approx 0.4$. Investigation showed this was a sampling artefact, not a band-crossing or SOC
42 error. Key verified facts:
43
44 - **Band tracking:** indices 12 and 13 are unambiguously the HOMO pair throughout the path. The gap between bands 11 and 12 is always > 200 meV; no crossing
45 occurs. Confirmed by $\angle S_z$ expectation values: band 13 transitions from 0 at $\Gamma$ to $\frac{1}{2}$ at K, band 12 from 0 to $-\frac{1}{2}$ at K.
46 - **Hermiticity:** $H_{SOC}^\dagger = H_{SOC}$ exactly.
47 - **Magnitude:** 145 meV at K vs. paper's $\sim 148$ meV (2% agreement).
48 - **Shape:** The smooth sigmoid (slow start, fast middle, levelling near K) is intrinsic - it reflects the gradual development of spin character from the
49 time-reversal-degenerate $\Gamma$ point to the spin-split K valley. The $L_x/L_y$ terms contribute $\le 5$ meV and are not responsible for the shape.
50
51 The 500-point corrected plot (left panel below) and the $\angle S_z$ diagnostic (right panel) are the canonical outputs for this task.
52
53 ![50 vs 500 k-point comparison](script/output/spin_splitting_comparison.png)
```

1. Spinless Band Structure

Code output vs Paper Figure 3a

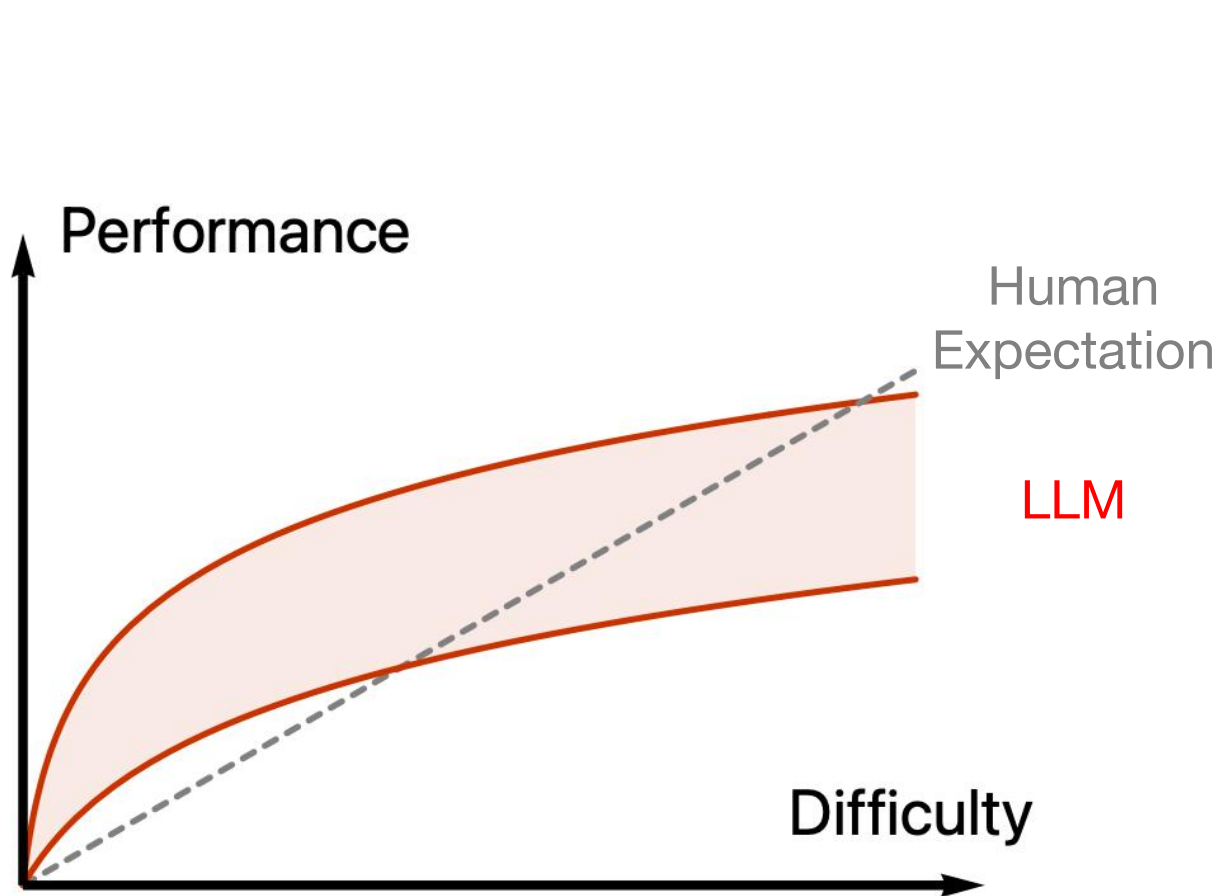


3 min read

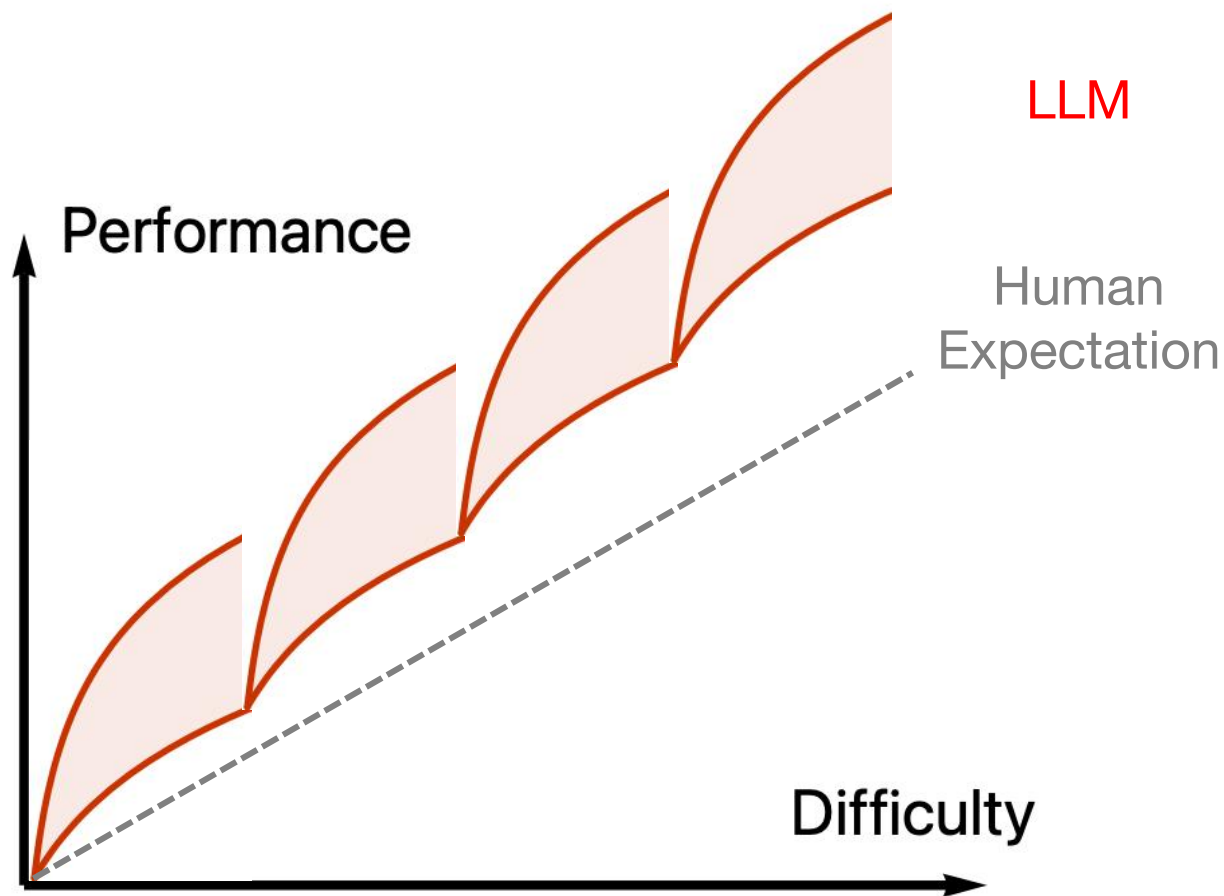
task_XX_dashboard.md

preview

1 Difficult Step → 4 Easy Steps

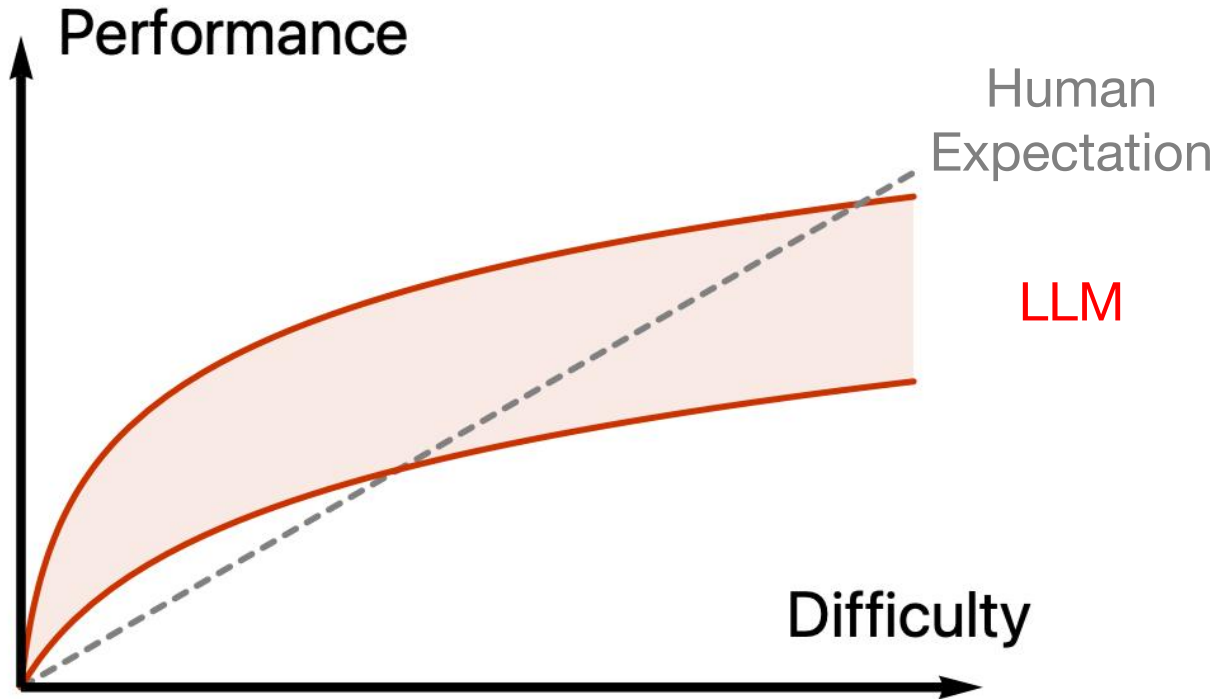


Single Step

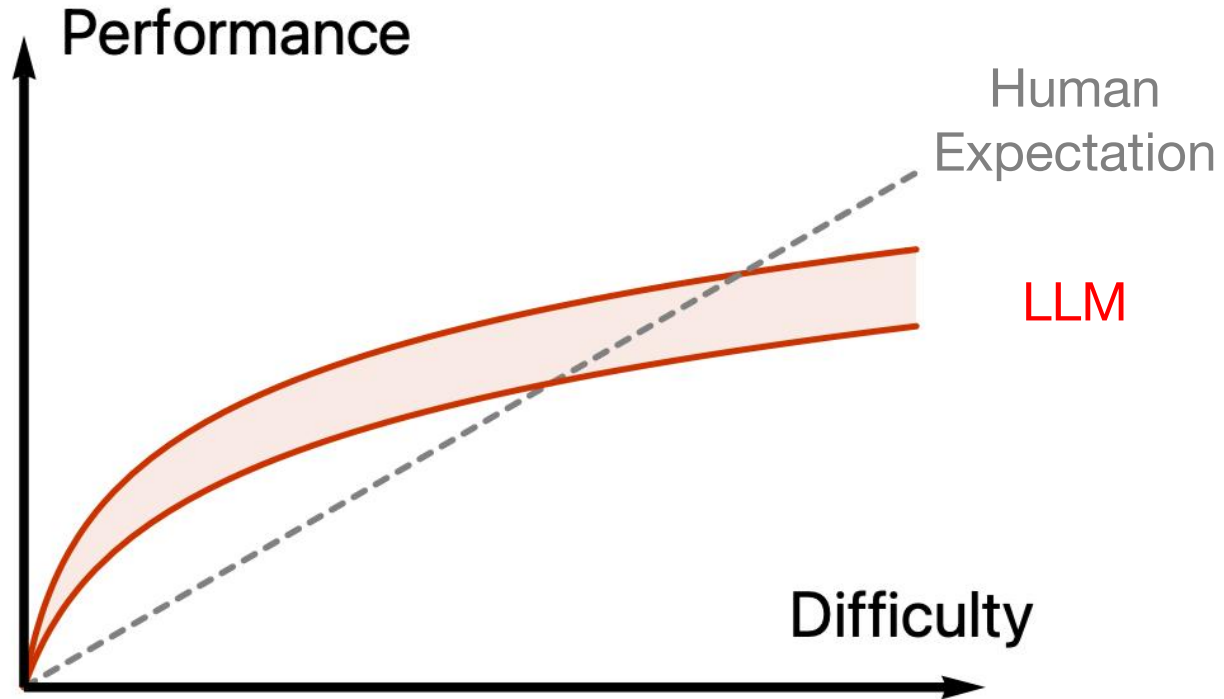


Multiple Steps

Art of Prompt: Precise & Concise



Vague Prompt



Precise Prompt

Coding v.s. Prompting

```
def get_k_path():
    Gamma = np.array([0.0, 0.0])
    M = np.array([np.pi, np.pi/np.sqrt(3)])
    K = np.array([4*np.pi/3, 0.0])

    nodes = [Gamma, M, K, Gamma]
    labels = [r'$\Gamma$', r'$M$', r'$K$', r'$\Gamma$']

    n_points = 100
    k_path = []
    k_dist = []
    ticks = [0]
    current_dist = 0

    for i in range(len(nodes)-1):
        start = nodes[i]
        end = nodes[i+1]
        length = np.linalg.norm(end - start)

        for t in np.linspace(0, 1, n_points, endpoint=True):
```

Coding

Precise

- “**Get** {Bi2Se3} band structure from arXiv: XXXX.XXXXXX”

“Band structure in Fig. X (x)” -

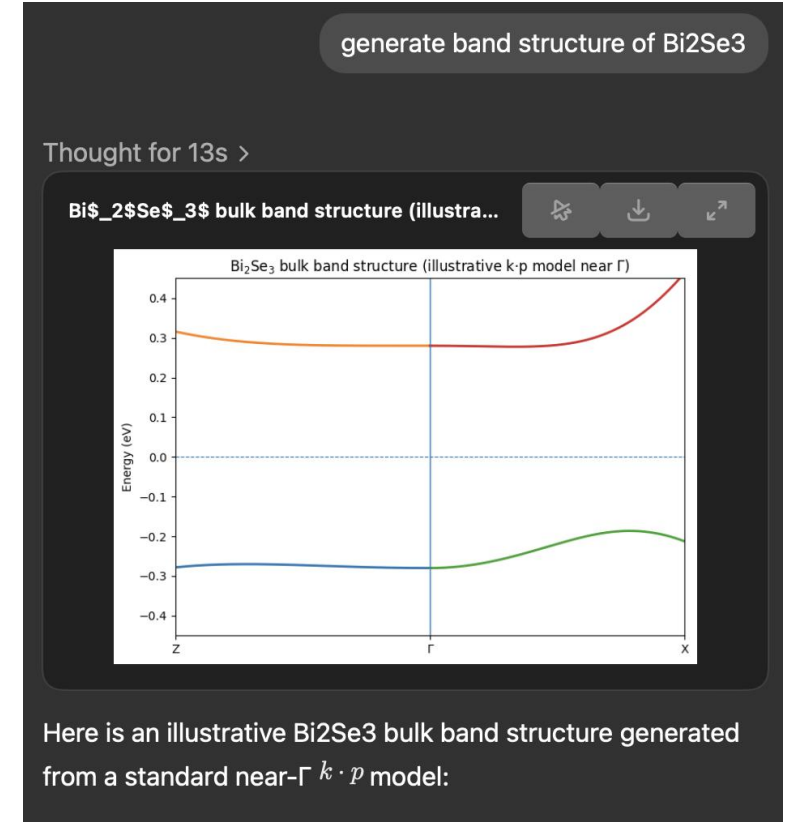
- “**Generate** {Bi2Se3} band structure with code”

[Generated Figure.jpg] -

- “**Compare** your band structure with Bi2Se3 band structure”

“Similarity 99.9%” -

LLM Workflow

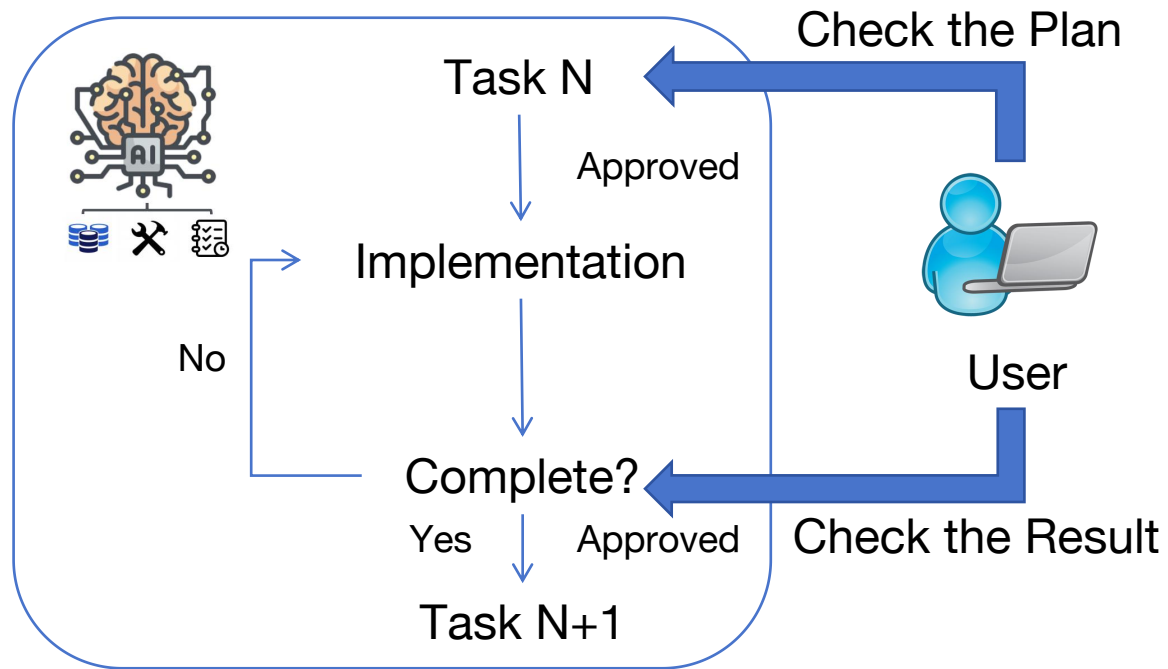


Prompt

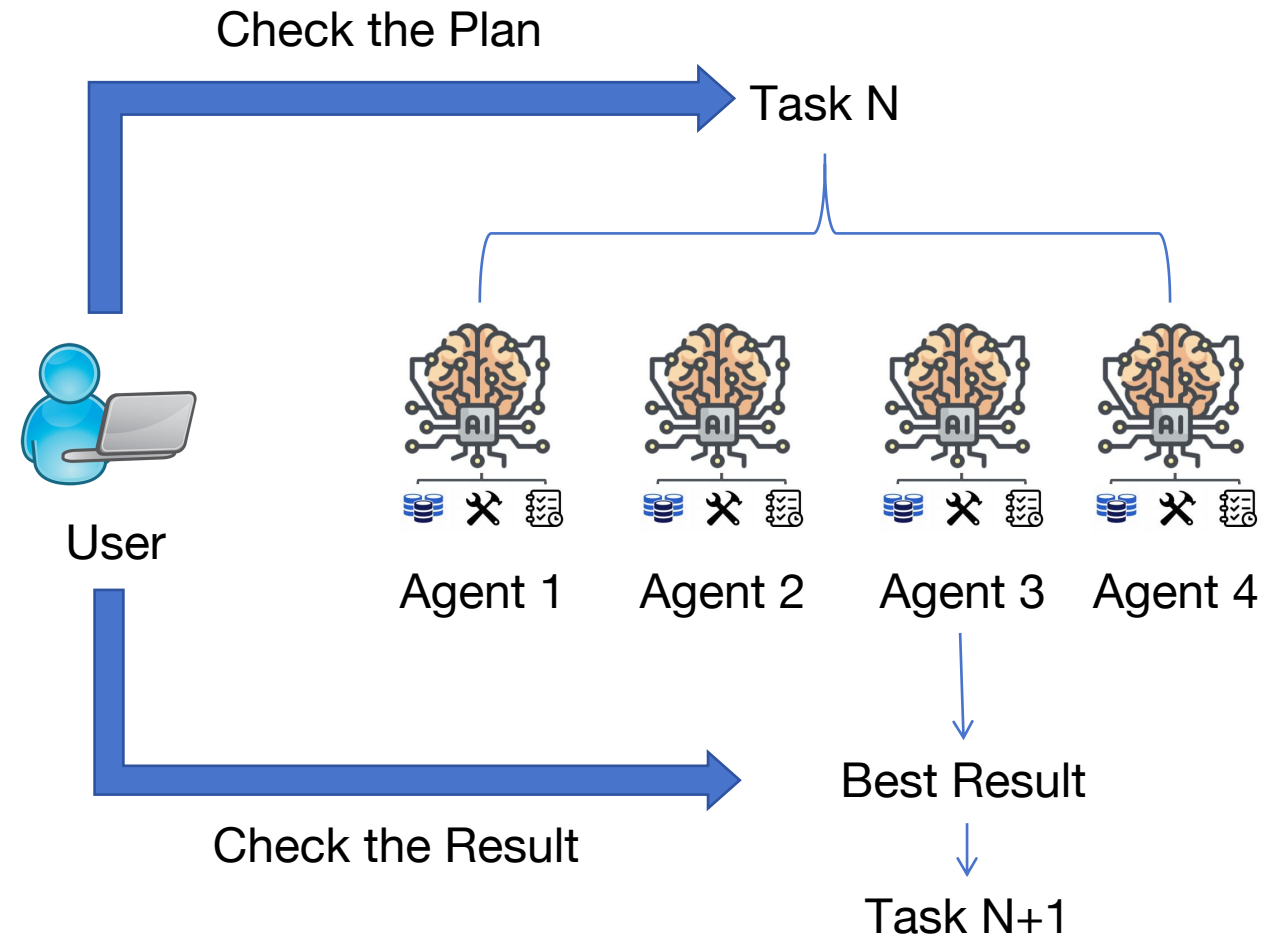
Vague

Further Automization

Automized Workflow



Massive Test



Further Automization

