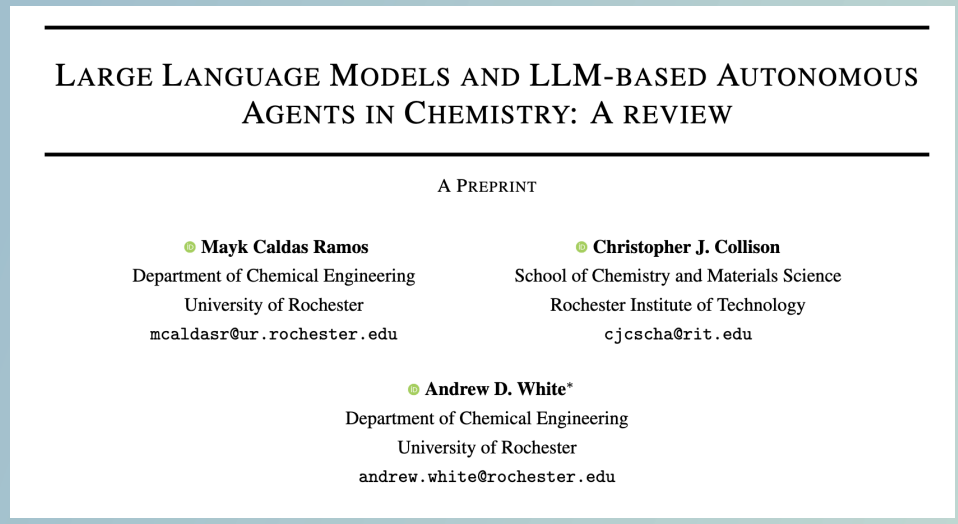
Integrating LLMs into the Science Curriculum

Chris Collison, Harris Endowed Professor, COS
Tom Fuller, Visiting Scholar, COS

Background

- Sabbatical with Andrew White/Tom Fuller
- ML in Predictive Chemistry
- Review on LLMs and Autonomous Agents in Chemistry
- AI Task Force
- Student Government/Focus Groups
- Agents in Teaching



LARGE LANGUAGE MODELS AND LLM-BASED AUTONOMOUS AGENTS IN CHEMISTRY: A REVIEW

A PREPRINT

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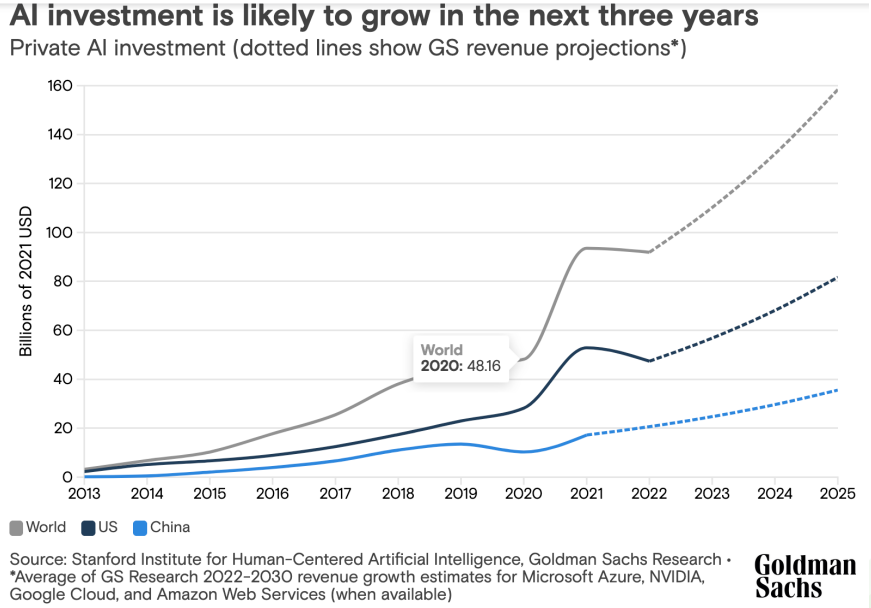
AI is unstoppable!

- AI is everywhere
- Major investment
- Need to prepare our students with managed AI experiences
- RIT: AI Task Force
- Student Focus Groups:
  - It's too easy to cheat
  - We want to learn and are curious
  - We want to use AI



"Innovations in electricity and personal computers unleashed investment booms of as much as 2% of U.S. GDP as the technologies were adopted into the broader economy. Now, investment in artificial intelligence is ramping up quickly and could eventually have an even bigger impact on GDP, according to Goldman Sachs Economics Research."

Show of hands…

- How many of you have used Generative AI as a professional aid/tool?
- How many of you have used Generative AI in your teaching?
- How many of you have encouraged students to use Generative AI?
- How many of you have discouraged students to use Generative AI?

Initial Goals

- A chatbot to help **students**:
  - Bridge gap between their answers and correct answers in an exam

Motivation

Quantum Mechanics: Complex & abstract

Students:

Incorrect exam answers

Even with answer key → gap in understanding

Don’t come to office hours

Online tutorial as practice exam

Question: Orthogonality

- Framework: electron can't be in two places at the same time!
- Quantum mechanics and probabilities
- Mathematical underpinning results in an integral over "all space" as zero

$$\int_{-\infty}^{\infty} \psi_n^* \psi_m \, d\tau = 0$$

Question: "State why two wave functions of the same system must be orthogonal."

- Answers:
  - “They must be orthonormal because of the Heisenberg uncertainty principle.”
  - “They must be orthogonal because if they had cannot equal the same thing twice.”
  - “Must describe all atoms.”
  - “The probability of an electron being in both places must be zero.”

How would I give feedback and guidance to students in office hours?
How could I help the students if they did not come to office hours?

Feedback and guidance:

Positivity, with explanation of the problem

- Your answer seems to be on the right track by recognizing the need for orthogonality, but it lacks clarity and precision in explaining why this is necessary from a quantum mechanics perspective.
- In quantum mechanics, the orthogonality of wave functions for different eigenstates of the same observable is crucial because it ensures that these states are mutually exclusive and non-overlapping. This is a mathematical requirement stemming from the postulates of quantum mechanics, particularly when dealing with Hermitian operators, which represent observables. The integral of the product of the complex conjugate of one wave function and another wave function over all space must be zero. This condition ensures that the probability of a system being in two different eigenstates simultaneously is zero, reflecting the fact that these states are distinct and the outcomes they represent do not overlap.

Specificity in the right answer

- Your response could be improved by explicitly stating that the orthogonality condition arises because the integral of the product of the complex conjugate of one wave function with another, over all space, must equal zero. This mathematical condition is what ensures that different eigenstates are indeed separate and that measurements of quantum states yield clear, distinct outcomes.

How you could improve

- For a more detailed understanding and to correct the gaps in your explanation, I recommend reviewing the following sections in the textbook "Quantum Chemistry" by Donald A. McQuarrie:
- Initially, please look at Chapter 4, Section 4.3 on "Observable Quantities Must Be Eigenvalues of Quantum-Mechanical Operators."
- Additionally, review Chapter 4, Section 4.5 on "Quantum-Mechanical Operators Must Be Hermitian Operators."
- These sections will provide a deeper insight into why orthogonality is a fundamental aspect of quantum mechanics and how it relates to the mathematical framework of the theory.

Where to get additional help

Can we do this in a Chem Bot?

Demo would appear here but see GitHub link below for cloning the Repository

Question...

- Why is this better than ChatGPT?

Agents:
What are they?

Personality

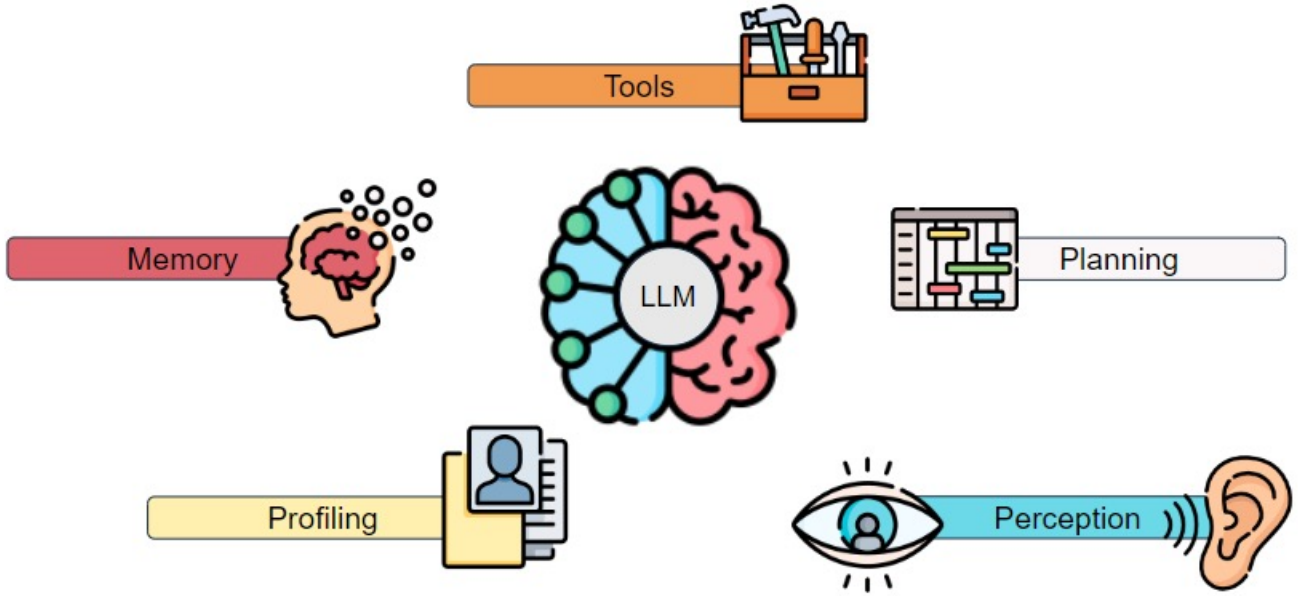
Brains

Knowledge

Tools

Agentic AI

- Andrew Ng, presenting to Sequoia Venture Capital
- “Agentic AI is the exciting trend that I think everyone building in AI should pay attention to.



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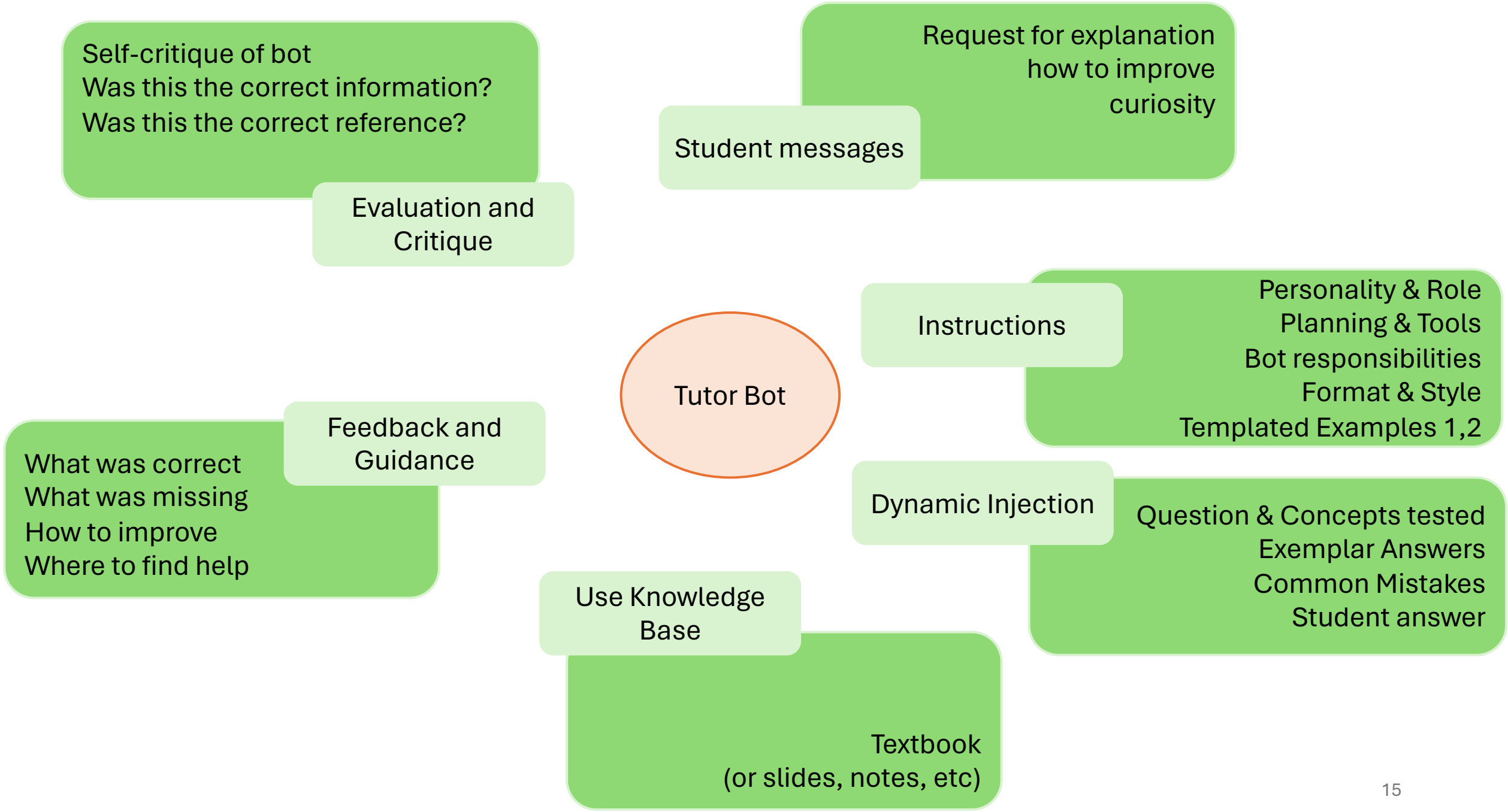
What are Agents in ***our*** case?


Self-critique of bot
Was this the correct information?
Was this the correct reference?
Evaluation and Critique
Request for explanation
how to improve
curiosity
Student messages
Instructions
Personality & Role
Planning & Tools
Bot responsibilities
Format & Style
Templated Examples 1,2
Tutor Bot
Feedback and Guidance
What was correct
What was missing
How to improve
Where to find help
Dynamic Injection
Question & Concepts tested
Exemplar Answers
Common Mistakes
Student answer
Use Knowledge Base
Textbook
(or slides, notes, etc)

Pedagogy Reflection

- How are your students struggling?
- For which concepts do they need more help?
- The question sheet is helpful for Pedagogy
  - Question
  - Concepts Tested
  - Good answer
  - Common mistakes

How can I do this?

Premade Solutions
e.g. OpenAI

Python Code
Jupyter Notebook

Beginner Coding Experience

Pedagogy
What are the concepts we are testing?
How do we address common mistakes?

Domain Expert

How can RIT do this?

Premade Solutions
e.g. OpenAI

Buy-in
Commitment of Resources
IT/Infrastructure
Integration into
cybersecurity
Access services

Pedagogy
What are the concepts we are testing?
How do we address common mistakes?

Domain Experts

But let's test this on prototypes!
PLIG Grant testing

Frequently asked questions

Critique

- Hallucinations?
- Response too long?
  - Student reading more than interacting
  - Change the prompt to maintain shorter “text messaging” style
- Text-based or Math-based?
- Points to wrong part of text book?
  - Chunk the book differently…
  - Hmmm… Fair use???

- Text books & Fair use
- Legal grey area
- Localized system
- Recommend generating personal course material

Ethics

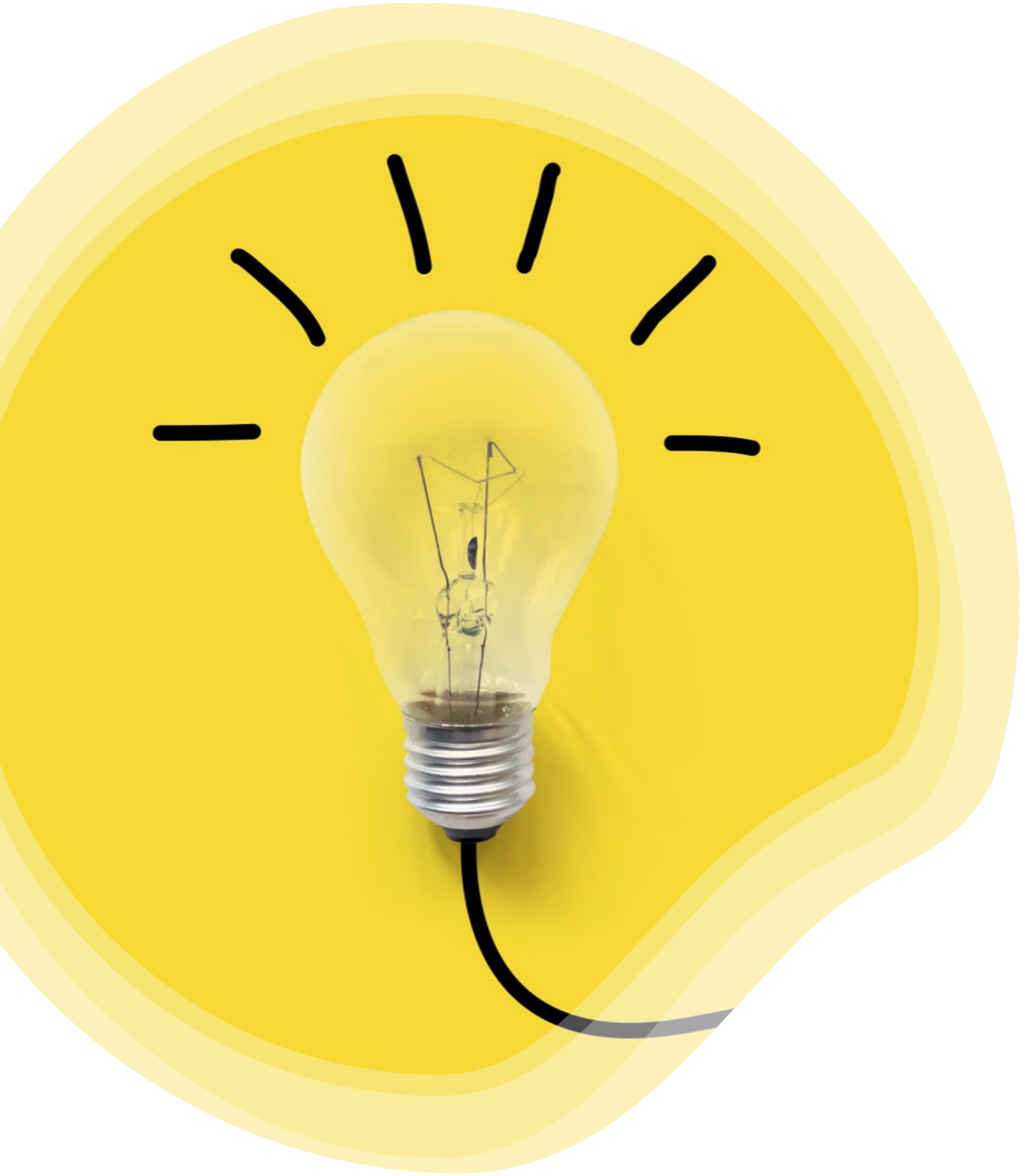
Governance and Oversight

- Instructors must be responsible
- This is a pilot; not ready for primetime
- Demonstrate capability
- Expect Academic Affairs/Faculty Senate oversight in future

- learn
- practice curiosity
- Access to “tutors”
- May prefer a bot to a social interaction
- AI personalized to course
- Connection to tomorrow’s technology

Students - what do they want?

Degree of Hallucination?
Model selection & $$?



Use Agent Architecture to write questions!

Other plans

Exam Bot

Instructions

Personality & Role
Planning & Tools
Bot responsibilities
Format & Style
Templated Examples 1,2

Dynamic Injection

Concepts tested
Exemplar Questions
Complexity
Number of layers
Type of answer sought

Use Knowledge Base

Textbook
(or slides, notes, etc)

Question Generation

This is the question
These are the concepts
How the student would answer
References to relevant course material

Evaluation and Critique

Self-critique of bot
Was this the correct information?
Was this the correct reference?

Instructor-led critique & iteration

Simulated student response

Your Turn… We can implement it!

- Choosing a domain
  - A topic that's conceptually challenging?
  - A topic to test the Chatbot's limits?
  - A topic to build trust with the chatbot?
  - A custom topic not covered in a textbook?
  - A topic from a high-level paper outside of ChatGPT's training set?
- Write an exam question
- Note the concepts to be tested
- State the correct answer
- Identify where students go wrong
- Fill out the form and we'll select a demo case for our booth

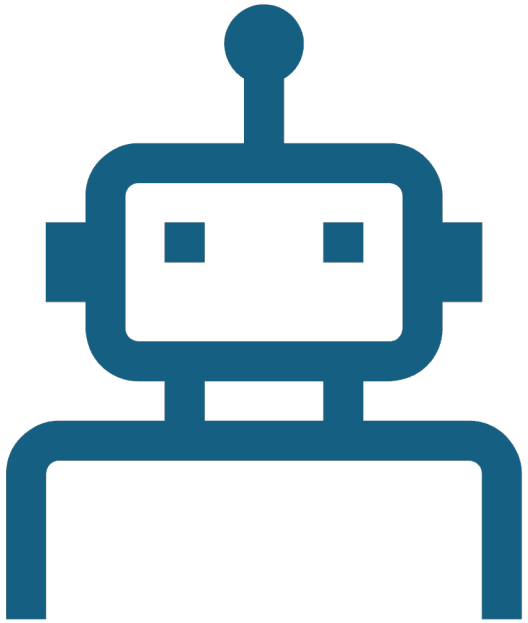
Interest in Collaborating?

Next Steps

- Testing in Fall 2024
  - Different questions
  - Initial Feedback
- Deploy as full pilot in Spring
- Measure utility & feedback
- Expansion opportunities

Conclusions

- AI is here to stay and will soon be ubiquitous
- AI Experts and bing companies are backing Agentic AI
- Students will value exposure in a curated mode
- Instructor improvements through review of pedagogy
- Moves RIT forward with working prototype
  - If we don’t do it…someone else will!



Thank you for your attention!

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GitHub:
https://github.com/tomfuller71/RIT_QMBot