



# AIM: Towards an Autonomous AI Mathematician

Peng Li

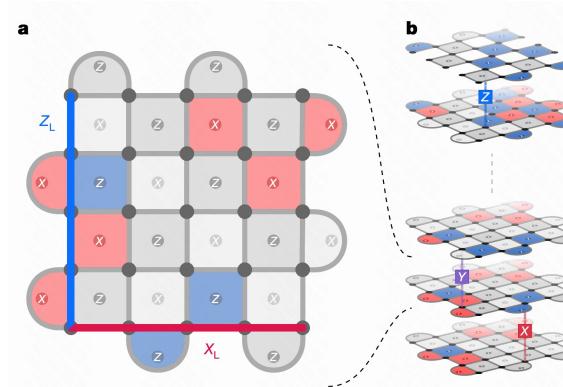
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# AI and Scientific Research



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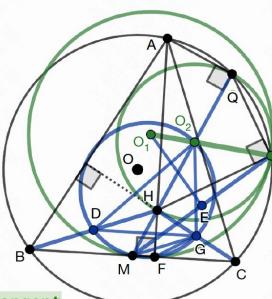
- AI has significantly accelerated scientific progress.



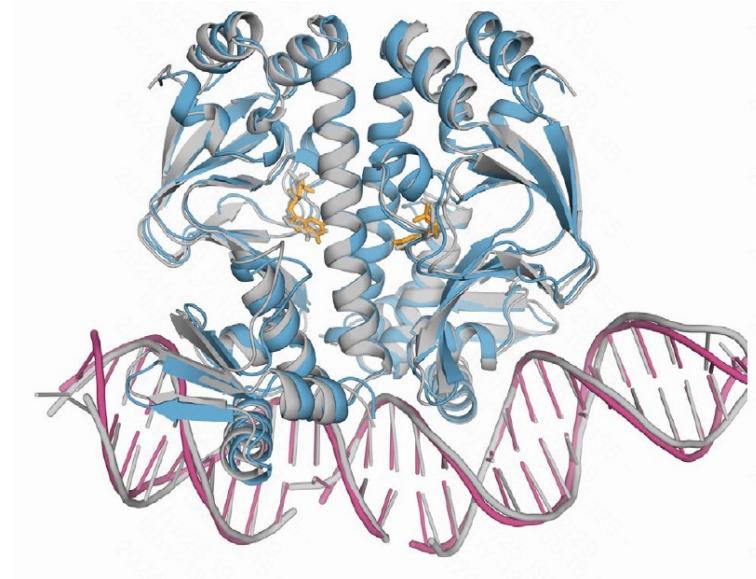
AlphaQuant

Solution

**Construct D: midpoint BH [a]**  
[a],  $O_2$  midpoint HQ  $\Rightarrow BQ \parallel O_2D$  [20]  
...  
**Construct G: midpoint HC [b]** ...  
 $\angle GMD = \angle GO_2D \Rightarrow M O_2 G D$  cyclic [26]  
...  
[a], [b]  $\Rightarrow BC \parallel DG$  [30]  
...  
**Construct E: midpoint MK [c]**  
..., [c]  $\Rightarrow \angle KFC = \angle KO_1E$  [104]  
...  
 $\angle FKO_1 = \angle FKO_2 \Rightarrow K_1 \parallel K_2$  [109]  
[109]  $\Rightarrow O_0K$  collinear  $\Rightarrow (O_1)(O_2)$  tangent



AlphaGeometry



AlphaFold

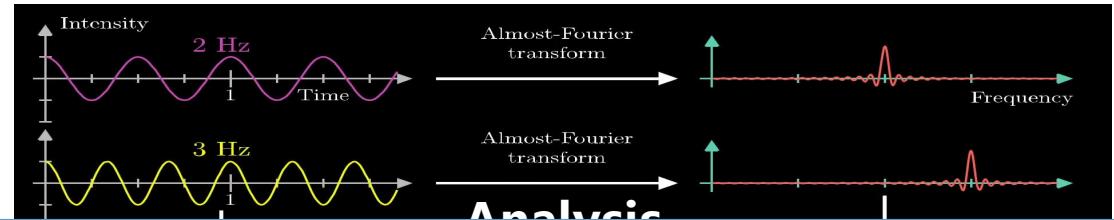
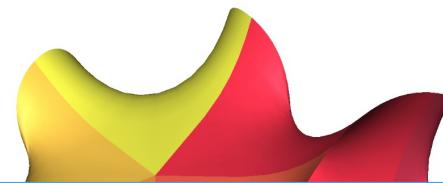
<https://www.nobelprize.org/all-nobel-prizes-2024/>  
<https://www.nature.com/articles/s41586-024-07487-w>  
<https://www.nature.com/articles/s41586-024-08148-8>  
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# The Power of Math Research

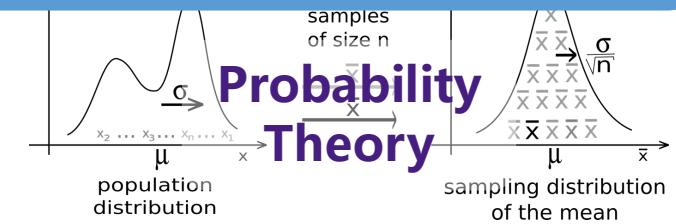
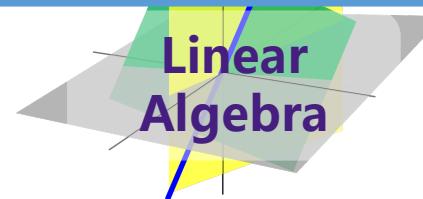
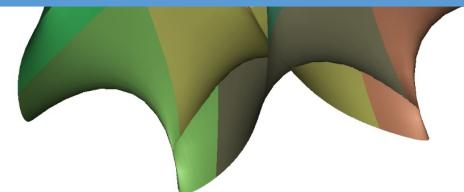


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- Mathematical research embodies both profound theoretical and practical value, representing the pinnacle of human intellect.



## What sparks when AI meets mathematics?



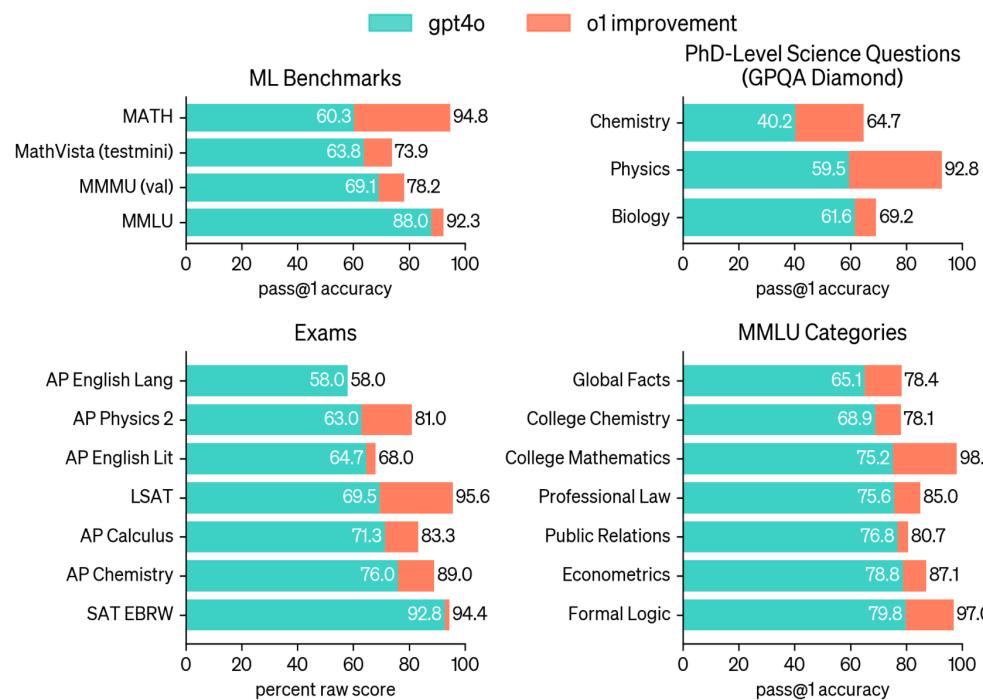
In pursuit of truth and elegance  
in nature.

The theoretical foundation  
for science and engineering.

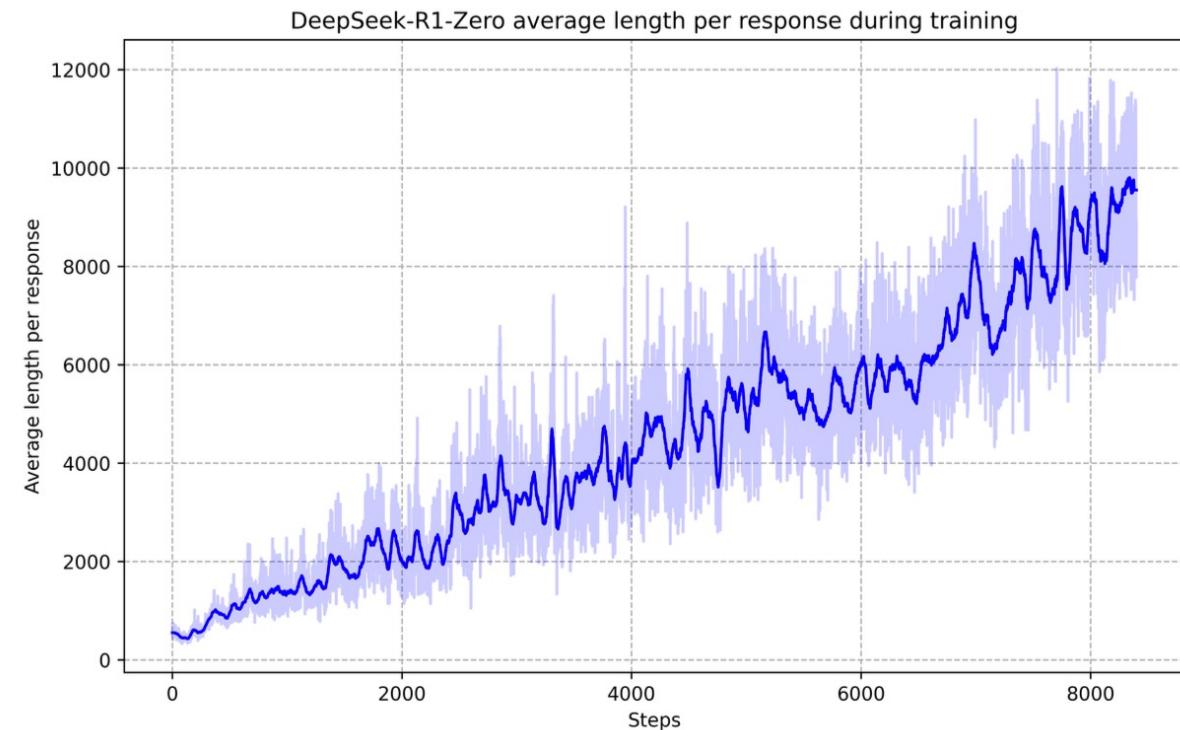
# Math4AI: A Critical Factor



- Mathematics and code are now key to advancing large models' reasoning capabilities.



**o1: The first reasoning model trained on math/code tasks, showing across-the-board improvements.**



**DeepSeek-R1 gains deep reasoning via verifiable math-focused RL training.**

# AI4Math: Approaching the Peak



- By 2025, top models are projected to score 145/150 on Gaokao.

Lack of sufficient image understanding capabilities leads to point loss  
↓

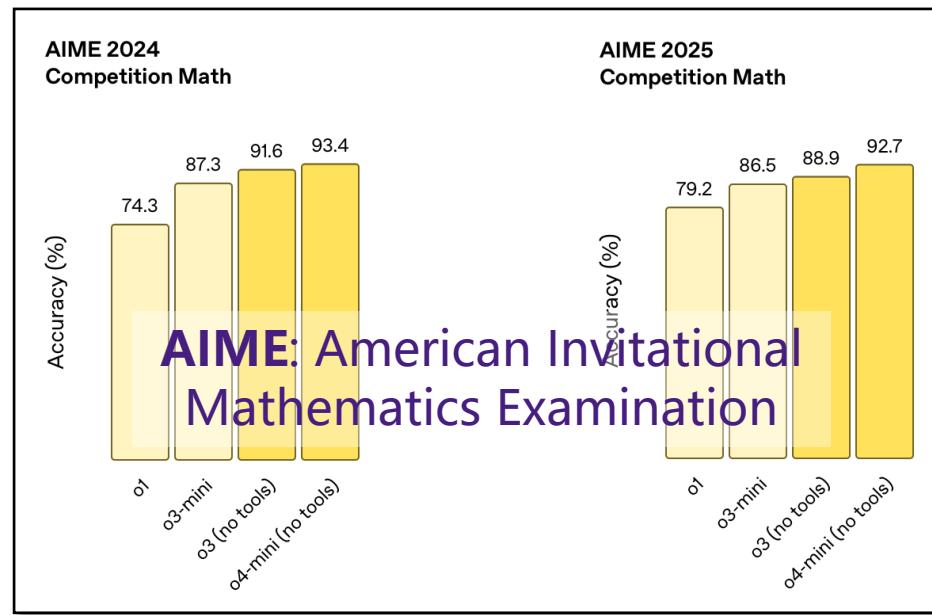
Model	Objective Questions (Text Input)	Single-choice Image Questions	Subjective Questions	Total
Gemini 2.5 pro	68	0	77	145
Doubao-1.5-thinking-vision-pro	68	0	76	144
DeepSeek R1	68	/	76	144
o3	65	0	75	140
Qwen3-235b	68	/	71	139
hunyuan-t1-latest	68	/	68	136
Wenxin X1 Turbo	68	/	66	134

**Note:** This evaluation consists of three parts: objective questions (text input), Question 6 which is an image-based single-choice question, and subjective questions. The objective questions (text input) section accounts for a total of 68 points, the image-based single-choice question is worth 5 points, and the subjective questions total 77 points. The overall score is 150 points.

# AI4Math: Approaching the Peak

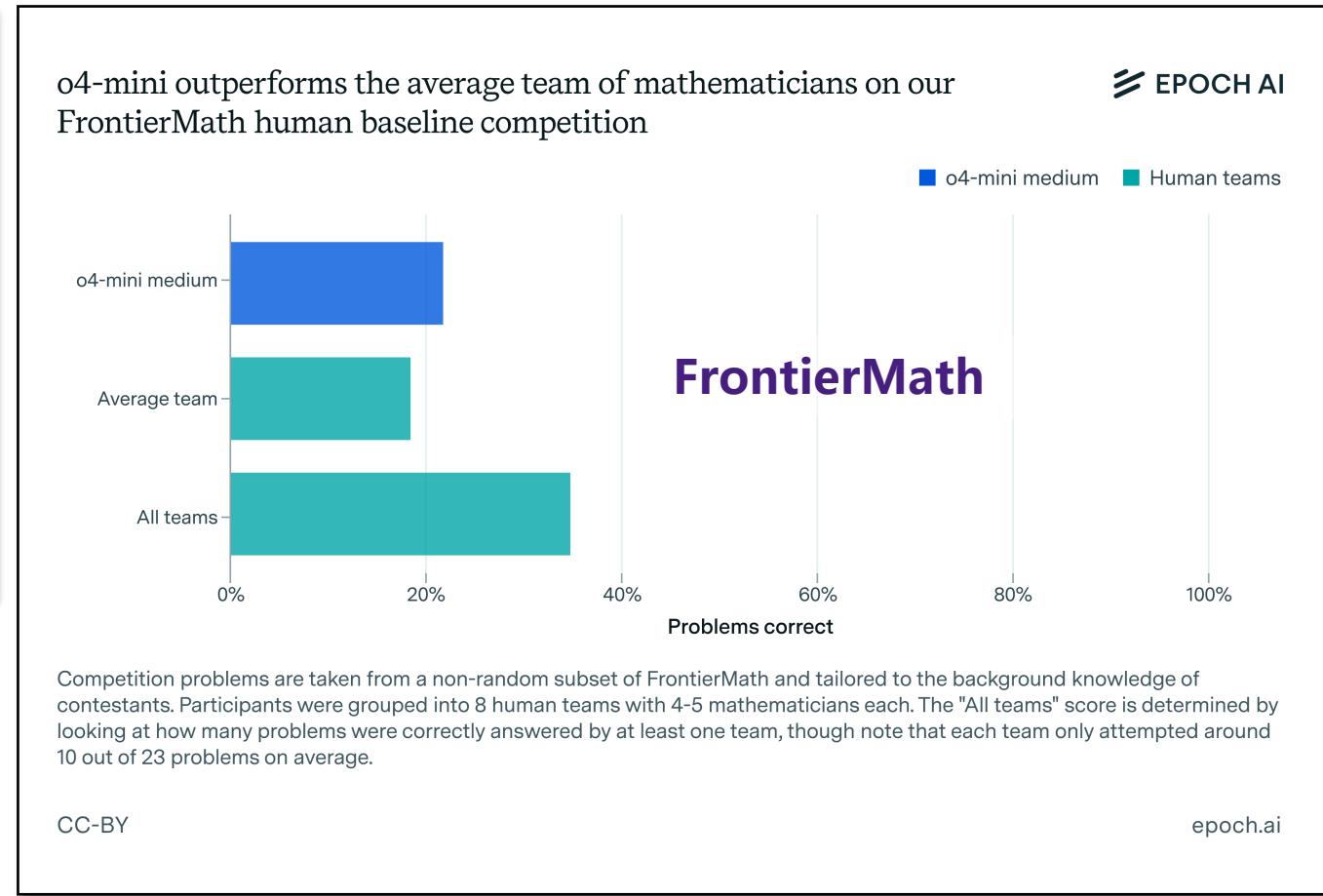


- o4-mini achieves expert-level proficiency on frontier math problems.



"I don't want to add to the hysteria, but in some ways these large language models are already outperforming most of our best graduate students in the world."

-- Ken Ono



# AIME: a High School Competition



- The AIME dataset derives from a competition (AIME) for high school students that helps select the U.S. team for the IMO.

## Problem Structure

- 15 progressively difficult problems
- Answers are integers from 0-999

## Limitations

- Predetermined unique solutions
- Focuses primarily on small techniques

### Problem

The 9 members of a baseball team went to an ice-cream parlor after their game. Each player had a single scoop cone of chocolate, vanilla, or strawberry ice cream. At least one player chose each flavor, and the number of players who chose chocolate was greater than the number of players who chose vanilla, which was greater than the number of players who chose strawberry. Let  $N$  be the number of different assignments of flavors to players that meet these conditions. Find the remainder when  $N$  is divided by 1000.

### Solution 1

Let  $c$  be the number of players who choose chocolate,  $v$  be the number of players who choose vanilla, and  $s$  be the number of players who choose strawberry ice cream. We are given two pieces of information  $c, v, s \geq 1$  and  $c + v + s = 9$ .

By inspection the only solutions for  $(c, v, s)$  are  $(2, 3, 4), (1, 2, 6), (1, 3, 5)$ .

Now we must choose which player chooses which flavor. For the general case  $(c, v, s)$ , we begin by choose  $c$  of the 9 players who eat chocolate, then we choose  $v$  of the  $9 - c$  players who eat vanilla, after this the amount of players who eat strawberry is fixed. Therefore the general formula is  $\binom{9}{c} \binom{9-c}{v}$ .

Therefore our final answer is,

$$\binom{9}{2} \binom{7}{3} + \binom{9}{1} \binom{8}{2} + \binom{9}{1} \binom{8}{3} = 2\boxed{016}.$$

# AIME: a High School Competition



- SOTA models primarily train and test on verifiable practice problems and math competition questions, similar to AIME's data distribution.

DeepSeek-R1 successfully solves the first problem in AIME 2025

- **Problem:** Find the sum of all integer bases  $b > 9$  for which  $17_b$  is a divisor of  $97_b$
- **Complexity:** Simple and no advanced concepts required
- **Reasoning Length:** Solvable within brief deductive steps
- **Assessment Focus:** Core emphasis on applied problem-solving techniques



The problem requires finding all integer bases  $b > 9$  such that  $17_b$  divides  $97_b$ , and then summing those bases.

Convert  $17_b$  and  $97_b$  to base 10:

- $17_b = 1 \cdot b + 7 = b + 7$
- $97_b = 9 \cdot b + 7$

The condition that  $17_b$  divides  $97_b$  means that  $b + 7$  divides  $9b + 7$ , or  $(b + 7) \mid (9b + 7)$ .

Set  $d = b + 7$ , so  $b = d - 7$ . Substitute into  $9b + 7$ :

$$9b + 7 = 9(d - 7) + 7 = 9d - 63 + 7 = 9d - 56$$

The condition becomes  $d \mid (9d - 56)$ . Since  $d \mid 9d$ , it follows that  $d \mid (9d - (9d - 56)) = d \mid 56$ .

Given  $b > 9$ , it follows that  $d = b + 7 > 16$ . Thus,  $d$  must be a positive divisor of 56 greater than 16.

The positive divisors of 56 are 1, 2, 4, 7, 8, 14, 28, and 56. The divisors greater than 16 are 28 and 56.

- If  $d = 28$ , then  $b = 28 - 7 = 21$ .
- If  $d = 56$ , then  $b = 56 - 7 = 49$ .

Both bases satisfy  $b > 9$ . Verify the division condition:

- For  $b = 21$ :
  - $17_{21} = 1 \cdot 21 + 7 = 28$
  - $97_{21} = 9 \cdot 21 + 7 = 189 + 7 = 196$
  - $196 \div 28 = 7$ , which is an integer.
- For  $b = 49$ :
  - $17_{49} = 1 \cdot 49 + 7 = 56$
  - $97_{49} = 9 \cdot 49 + 7 = 441 + 7 = 448$
  - $448 \div 56 = 8$ , which is an integer.

Both bases are valid, and there are no other bases  $b > 9$  that satisfy the condition. The digits in both numbers are valid since  $b > 9$  implies  $b > 9$  for digit 9 in  $97_b$  and  $b > 7$  for digit 7 in both numbers.

The sum of the bases is  $21 + 49 = 70$ .

\boxed{70}

# The Challenging FrontierMath



- Authored and endorsed by professional mathematicians (including Terence Tao), FrontierMath exhibits extremely high difficulty

## Core Features

- Authored by professional mathematicians
- Spans major modern mathematical branches
- Requires hours per problem for specialists

## Limitations

- Predetermined solutions
- Complexity ceiling below research-grade problems

Construct a degree 19 polynomial  $p(x) \in \mathbb{C}[x]$  such that  $X := \{p(x) = p(y)\} \subset \mathbb{P}^1 \times \mathbb{P}^1$  has at least 3 (but not all linear) irreducible components over  $\mathbb{C}$ . Choose  $p(x)$  to be odd, monic, have real coefficients and linear coefficient -19 and calculate  $p(19)$ .

**Answer:** 1876572071974094803391179

**MSC classification:** 14 Algebraic geometry; 20 Group theory and generalizations; 11 Number theory generalizations

# Competition v.s. Research



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## Key 1: Long Reasoning

Math research requires significantly longer and deeper reasoning.

Volume estimates for unions of convex sets, and the Kakeya set conjecture in three dimensions

Hong Wang\*      Joshua Zahl †  
February 26, 2025

**Abstract**  
We study sets of  $\delta$  tubes in  $\mathbb{R}^3$ , with the property that not too many inside a common convex set  $V$ . We show that the union of tubes from almost maximal volume. As a consequence, we prove that every Kakeya and Hausdorff dimension 3.

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1.2	Unions of convex sets, and non-clustering . . . . .
1.3	From Assertions $\mathcal{D}$ and $\mathcal{E}$ to the Kakeya set conjecture . . . . .
1.4	Proof philosophy, and previous work on the Kakeya set conjecture . . . . .
1.5	A vignette of the proof . . . . .
1.6	Tube doubling and Keleti's line segment extension conjecture . . . . .
1.7	Thanks . . . . .
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2.2	A two-scale grains decomposition . . . . .
2.3	Refined induction on scales . . . . .
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# Competition v.s. Research



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## Key 2: Procedural Rigor

Zero tolerance for errors. Verification is mandatory yet exceptionally costly

Hence if  $\mathcal{W}' \subset \mathcal{W}_0$ , to compare  $\#\left(\bigcup_{W_i \in \mathcal{W}'} \mathcal{U}_0[W_i]\right)$  and  $\sum_{W_i \in \mathcal{W}'} \#\mathcal{U}_0[W_i]$ ,

$$\begin{aligned} \kappa_0 \frac{C_{KT-CW}(\mathcal{U}_0)}{|U|} \sum_{W_i \in \mathcal{W}'} |W_i| &\leq \sum_{W_i \in \mathcal{W}'} \#\mathcal{U}_{i-1}[W_i] = \#\left(\bigsqcup_{W_i \in \mathcal{W}'} \mathcal{U}_{i-1}[W_i]\right) \\ &\leq \#\left(\bigcup_{W_i \in \mathcal{W}'} \mathcal{U}_0[W_i]\right) \leq \sum_{W_i \in \mathcal{W}'} \#\mathcal{U}_0[W_i] \leq \frac{C_{KT-CW}(\mathcal{U}_0)}{|U|} \sum_{W_i \in \mathcal{W}'} |W_i|. \end{aligned} \quad (4.12)$$

A proof fragment of  
the 3D Kakeya Set  
Conjecture

The equality in (4.12) uses the critical fact that if  $i \neq i'$ , then  $\mathcal{U}_{i-1}[W_i]$  and  $\mathcal{U}_{i'-1}[W_{i'}]$  are disjoint.

Case	Validating Process	Duration
Fermat' s Last Theorem	The initial proof was presented in 1993, and then a flaw was identified after scrutinized by top mathematicians. The revised proof was finally published in 1995.	~2 years
Poincaré Conjecture	The proof was released in three preprints, and was finally validated by the collaborative effort by geometers and topologists.	~4-5 years

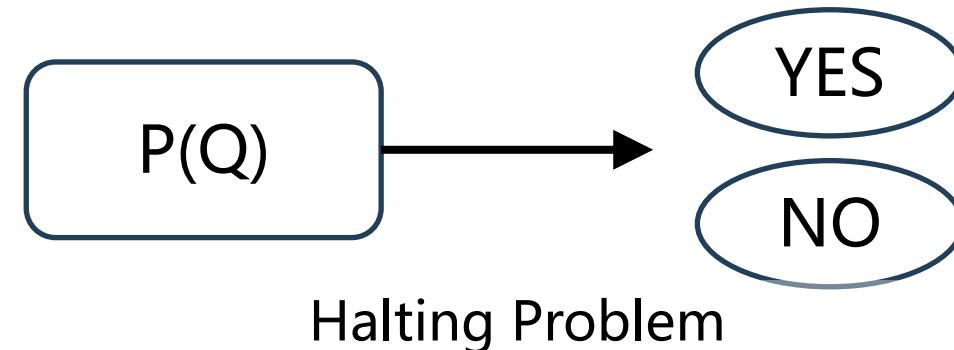
# Competition v.s. Research



## Key 3: Answer Existence

Competition problems have **known** and **determined** answers

The answers of research problems are **unknown** and **undetermined**



Kurt Gödel

### Gödel's First Incompleteness Theorem:

In any consistent formal system that is strong enough to express basic arithmetic, there will always be true statements that the system cannot prove. The system is inherently incomplete.

### Gödel's Second Incompleteness Theorem:

Such a system cannot prove its own consistency from within. To establish its consistency, we must rely on methods outside the system.

# AI4Math: Formal Proving



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- **Formal proof systems have evolved through decades of research, with institutions worldwide - including DeepSeek and ByteDance - actively advancing this field.**

## Pros

- Provides certain symbolic automation
- Guarantees absolute rigor via machine verification

## Cons

- Current formal tools faces severe performance bottlenecks
- They can not be applied to research level problems

The screenshot shows a Lean 4 Proof Assistant interface with two main sections: a left panel for the proof sketch and a right panel for the final synthesized proof.

**Left Panel (Lean 4 Proof Structure):**

- Shows the theorem: `theorem induction_ineq_nsqlefactn (n : N) (h₀ : 4 ≤ n) : n ^ 2 ≤ n ! := sorry`
- Section "Understanding the Problem":
  - We need to show that for any integer  $n \geq 4$ , the inequality  $n^2 \leq n!$  holds. Here,  $n!$  denotes the factorial of  $n$ , which is the product of all positive integers up to  $n$ .
- Section "Proof Sketch":
  - To prove this formally, we can use mathematical induction. Here's how the induction would work:
  - 1. **Base Case:** Verify the inequality for  $n = 4$ .
  - 2. **Inductive Step:** Assume the inequality holds for some  $k = 4$ , i.e.,  $k^2 \leq k!$ . Then show that it holds for  $k + 1$ , i.e.,  $(k + 1)^2 \leq (k + 1)!$ .
- Icon: chain-of-thought by DeepSeek-V3

**Right Panel (Synthesize into Complete Formal Proofs):**

- Section "Recursively Solve Subgoals by DeepSeek-Prover-V2-7B":
  - lemma `inductive_step (n : N) (h₀ : 4 ≤ n) (base_case : 4 ^ 2 ≤ 4 !) := by sorry`
- Section "Synthesize into Complete Formal Proofs":
  - theorem `induction_ineq_nsqlefactn (n : N) (h₀ : 4 ≤ n) : n ^ 2 ≤ n ! := by have base_case : 4 ^ 2 ≤ 4 ! := by simp [Nat.factorial]`
  - have `inductive_step : ∀ k ≥ 4, k ^ 2 ≤ k ! → (k + 1) ^ 2 ≤ (k + 1) ! := by intro k h₁ h₂ simp_all [Nat.factorial] nnlinarith`
  - have `final_proof : ∀ n ≥ 4, n ^ 2 ≤ n ! := by intro n hn induction' hn with k hk case refl => exact base_case case step => apply inductive_step k hk exact by assumption apply final_proof exact h₀`

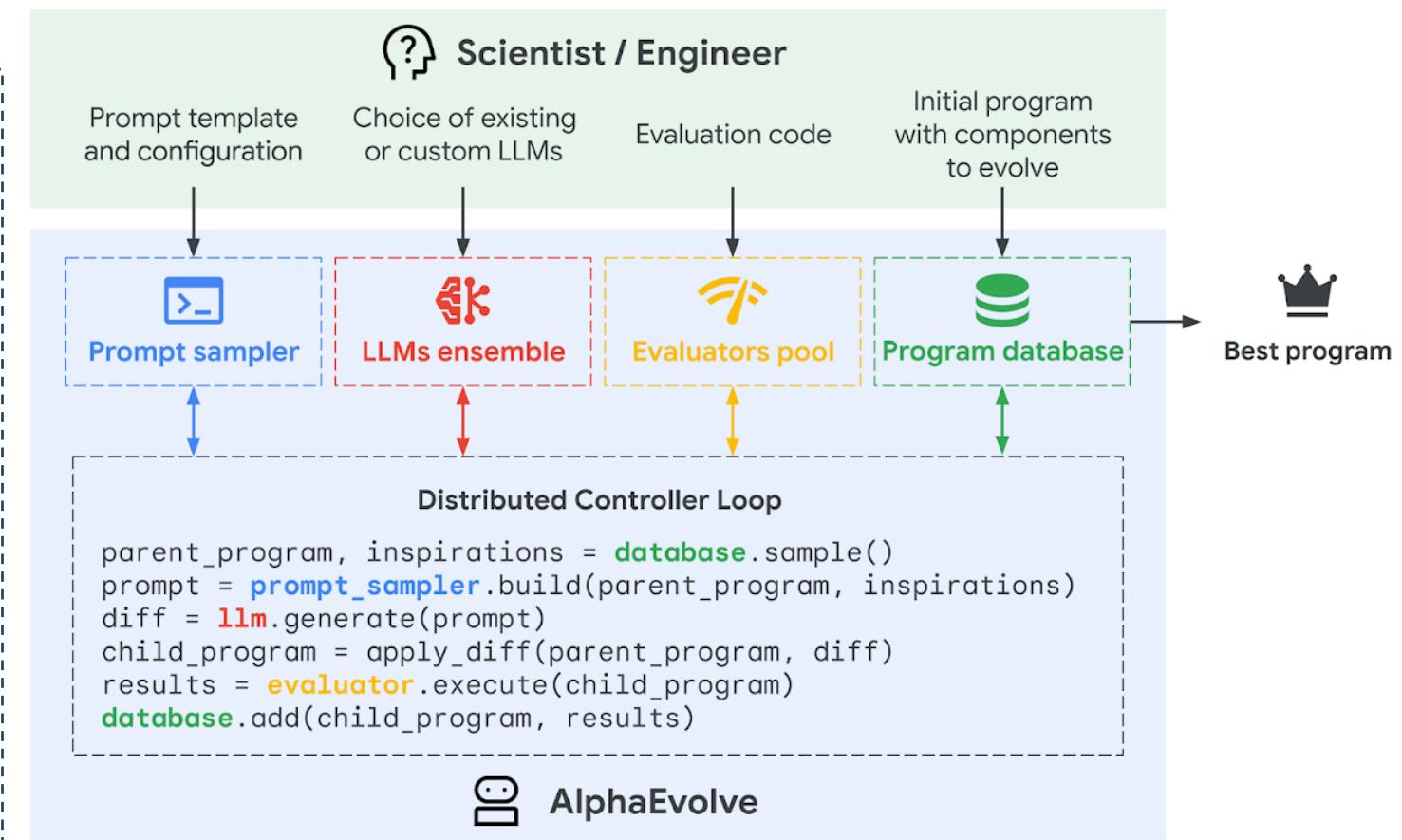
# AI4Math: Coding Agent



- Recent studies have begun exploring the potential of using large models to perform mathematical research tasks.

## AlphaEvolve

- Origin:** Launched by Google DeepMind on May 14, 2025
- Nature:** An agent system specialized in algorithmic optimization
- Achievement:** Demonstrated capacity for independent novel discoveries
- Limitation:** Limited to problems amenable to code



# AIM: AI Mathematician



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## ● AIM represents an important step towards automated math research

### Competition

- Short reasoning
- Rigor requirement is easily satisfied
- Known existence of the answer
- Deterministic

### Research

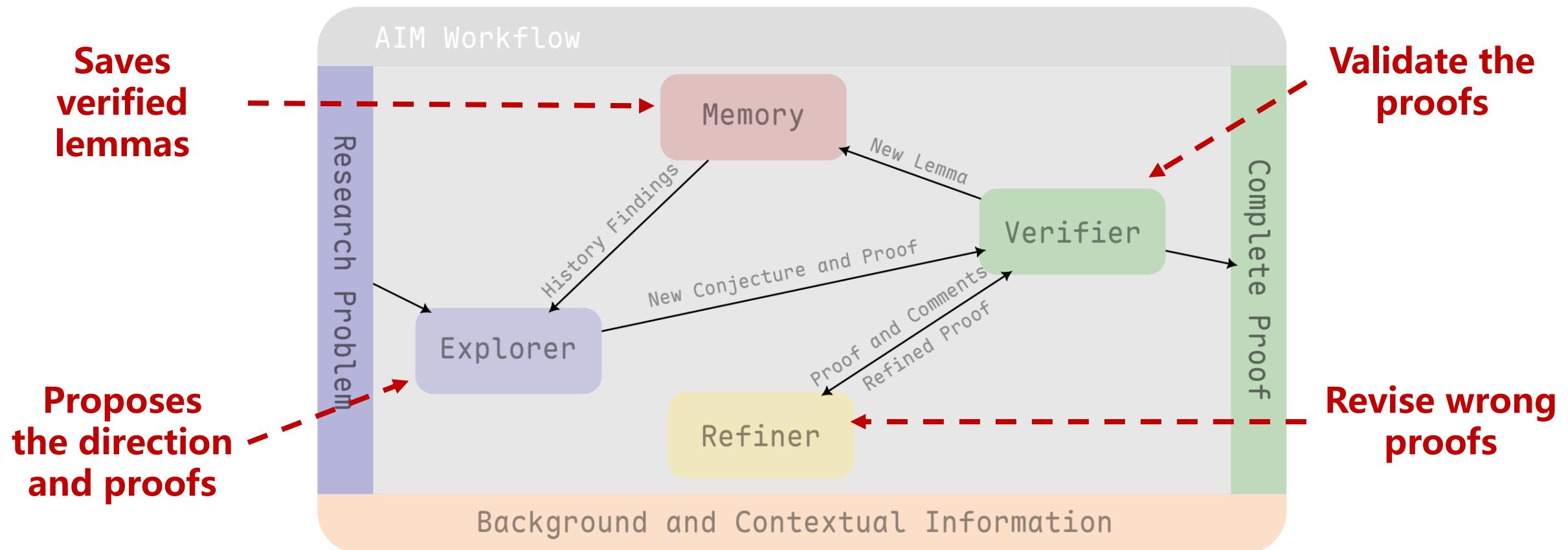
- Long reasoning
- Rigor requirement is hardly satisfied
- Unknown existence of the answer
- Indeterministic

Research Problem	AIM效果	Selected Proof Steps
Quantum Algorithm Problem (Settled Problem)	AIM effectively completes the problem with a detailed solution process	<p>Multiply through by <math>x^{(T-2)}</math>, cancel terms, and simplify:</p> $\frac{\pi^2}{2} \partial_x U = \frac{\pi^2}{2} \partial_x^2 V \Rightarrow 0 \iff \partial_x U = \partial_x^2 V.$ <p>**Step 2: Spatial Discretization**          Discritize <math>\partial_x U</math> with spacing <math>\Delta x</math>. Approximate <math>\partial_x^2 V</math> via finite differences:  <math display="block">\frac{\partial_x^2 V}{\Delta x^2} \approx \frac{V_{x+2\Delta x} - 2V_x + V_{x-2\Delta x}}{(\Delta x)^2}.</math>         Let <math>D_2</math> be the discretized second derivative matrix. Then the equation becomes:  <math display="block">U = D_2 V.</math> </p> <p>**Step 3: Positive Semi-Definite Operator**          The matrix <math>B = D_2</math> is positive semi-definite because <math>D_2</math> is a centred second derivative discretization (negative definite). This aligns with the physical nature of the heat equation.</p> <p>**Step 4: Solving the System**          While the original decomposition <math>B = L - \beta I</math> (with <math>L = -\partial_x^2</math>) is unstable due to the absence of a free term error, the operator <math>B</math> is suitable for quantum simulation methods designed for problems containing no free terms. This allows for the use of standard quantum circuitry for solving. Translating to discrete-time dissipative quantum algorithms, bypassing the need for the LCHS lemma.</p> <p>[Correct] Variable substitution and equation matching. Discritization of the spatial variable is correct. And AIM finds the required PDE iterations the LCHS lemma. It's right.</p>
Absorbing Boundary Condition (Settled Problem)	AIM provides a substantially complete proof for this problem	<p>**Revised Proof of the a priori estimate:** Define the total energy functional:</p> $E(t) = \frac{1}{2} \ u(t)\ _{H^1(\Omega)}^2 + \sum_{k=1}^{\infty} \frac{\alpha_k^2}{k^2} \ v_k(t)\ _{L^2(\Omega)}^2 + \ w(t)\ _{H^1(\Omega)}^2 + \sum_{k=1}^{\infty} \frac{\alpha_k^2}{k^2} \ z_k(t)\ _{L^2(\Omega)}^2.$ <p>[Correct] The agent consider the energy method, and derive the correct functional form.</p> <p>**Energy Estimate for <math>u(t)</math>:** Multiply the <math>t</math>-equation by <math>u</math> and integrate over <math>\Omega</math>:</p> $\frac{1}{2} \frac{d}{dt} \ u(t)\ _{L^2(\Omega)}^2 + \ \nabla u(t)\ _{L^2(\Omega)}^2 = -\ u(t)\ _{L^2(\Omega)}^2 + \sum_{k=1}^{\infty} \alpha_k^2 u_k(t) \int_{\Omega} u_k \partial_x u_k \, dx.$ <p>Apply Young's inequality to the right-hand side:</p> $\sum_{k=1}^{\infty} \alpha_k^2 u_k(t) \int_{\Omega} u_k \partial_x u_k \, dx \leq \frac{1}{2} \ u(t)\ _{L^2(\Omega)}^2 + \sum_{k=1}^{\infty} \frac{\alpha_k^2}{2} \int_{\Omega} u_k^2 \partial_x^2 u_k \, dx.$ <p>Subtract the Young's bound and integrate:</p> $\frac{1}{2} \frac{d}{dt} \ u(t)\ _{L^2(\Omega)}^2 + \ \nabla u(t)\ _{L^2(\Omega)}^2 = \frac{d}{dt} \left( \frac{1}{2} \ u(t)\ _{L^2(\Omega)}^2 + \sum_{k=1}^{\infty} \frac{\alpha_k^2}{2} \ u_k(t)\ _{L^2(\Omega)}^2 \right).$ <p>[Correct] Here, the agent gets the accurate result with the energy method and the application of inequality techniques.</p> <p>**Step 1: Estimates of the Galerkin Method:** For test functions <math>v \in V_h</math> and <math>u \in W_h</math>, the Galerkin approximation satisfy the projected weak form:</p> $\int_{\Omega} \partial_x u_h \cdot v_h \, dx + \int_{\Omega} \nabla u_h \cdot \nabla v_h \, dx = \int_{\Omega} g \cdot \nabla v_h \, dx.$ $+ \int_{\Omega} \partial_x^2 u_h \cdot v_h \, dx = \sum_{k=1}^{\infty} \int_{\Omega} u_k \partial_x^2 u_k \cdot v_k \, dx = \int_{\Omega} u_h \partial_x^2 u_h \cdot v_h \, dx.$ <p>**Step 2: Formulation of the Projected Equation:** For test functions <math>v \in V_h</math> and <math>u \in W_h</math>, the Galerkin approximation satisfy the projected weak form:</p> $\int_{\Omega} \partial_x u_h \cdot v_h \, dx + \int_{\Omega} \nabla u_h \cdot \nabla v_h \, dx = \int_{\Omega} g \cdot \nabla v_h \, dx = \int_{\Omega} u_h \partial_x^2 u_h \cdot v_h \, dx = \int_{\Omega} u_h^2 \partial_x^2 u_h \, dx.$ <p>**Step 3: Solves the Galerkin Equation:** Substituting <math>v = \sum_{k=1}^{\infty} u_k \phi_k</math> and <math>u = \sum_{k=1}^{\infty} u_k \psi_k</math>, one the projected equations yields linear ODE system for <math>u_k</math>'s. While adaptive grids are used in eigenfunctions are <math>C^1</math>, ensuring continuity. By the Cauchy-Lipchitz theorem, unique solution exists on <math>[0, T]</math>.</p> <p>[Correct] The agent gets the accurate solution with the Galerkin method.</p> <p>[Agent] It is better to have more detailed process.</p>
High Contrast Limit (Settled Problem)	AIM completes main proof of the conclusion and produces other correct results	<p>**Step 1: Corrected Test with <math>v = \nabla \phi_j</math>:** Substituting <math>v</math> into the variational equation:</p> $-\int_{\Omega} f \cdot \nabla \phi_j \, dx + \int_{\Omega} \mu(x) \partial_x \phi_j \, dx - \int_{\Omega} D(\nabla \phi_j) \cdot \nabla \phi_j \, dx = \int_{\Omega} g \cdot \nabla \phi_j \, dx.$ <p>**Step 2: Corrected Test with <math>v = \nabla \phi_j</math>:** Substituting <math>v</math> into the variational equation:</p> $-\int_{\Omega} f \cdot \nabla \phi_j \, dx + \int_{\Omega} \mu(x) \partial_x \phi_j \, dx - \int_{\Omega} D(\nabla \phi_j) \cdot \nabla \phi_j \, dx = \int_{\Omega} g \cdot \nabla \phi_j \, dx.$ <p>Rearranging and adding absolute value:</p> $ \lambda  \int_{\Omega} \mu(x) \partial_x \phi_j \, dx \leq C \int_{\Omega}  \nabla \phi_j ^2 \, dx + \int_{\Omega}  \nabla \phi_j   \nabla \phi_j  \, dx.$ <p>Using Hölder's inequality and Young's inequality:</p> $ \lambda  \int_{\Omega} \mu(x) \partial_x \phi_j \, dx \leq C \int_{\Omega}  \nabla \phi_j ^2 \, dx + \int_{\Omega}  \nabla \phi_j   \nabla \phi_j  \, dx \leq C \int_{\Omega}  \nabla \phi_j ^2 \, dx + \lambda^{-1} \int_{\Omega} \mu(x)  \nabla \phi_j ^2 \, dx.$ <p>**Step 4: Final Estimate:** Combining these bounds:</p> $\lambda \int_{\Omega} \mu(x) \partial_x \phi_j \, dx \leq 2C \int_{\Omega}  \nabla \phi_j ^2 \, dx + \lambda^{-1} \int_{\Omega} \mu(x)  \nabla \phi_j ^2 \, dx.$ <p>Dividing by <math> \lambda  \int_{\Omega} \mu(x) \partial_x \phi_j \, dx</math> yields:</p> $ \phi_j  \int_{\Omega} \mu(x)  \partial_x \phi_j  \, dx \leq \frac{2C}{ \lambda } \int_{\Omega}  \nabla \phi_j ^2 \, dx,$ <p>completing the proof with modest constant <math>C</math>.</p> <p>[Correct] Use inequality techniques to derive the correct key conclusions from variational equations.</p> <p>The limit problem (10) is a saddle point problem: Find <math>(u_{\infty}, p_{\infty}) \in H^1(\Omega) \times L^2(\Omega)</math> such that for all <math>\psi \in H^1(\Omega)</math> and <math>q \in L^2(\Omega)</math>,</p> $\int_{\Omega} b(x) \cdot \nabla u_{\infty} \cdot \nabla \psi + 2u_{\infty} D(p_{\infty}) : D(\psi) \, dx + \int_{\Omega} q D(D(u_{\infty})) : D(\psi) \, dx = \int_{\Omega} g \cdot \nabla \psi \, dx.$ <p>[Correct] Consider the weak form of this equation.</p>
Homogenization Problem (Open Problem)	AIM provides partially correct conclusions and reasoning, offering instructive guidance	<p>1. Cauchy-Schwarz with uniform constant: Since <math>Y_T = Y</math>, <math>\omega</math> is a bounded Lipschitz set, the classical Korn inequality holds in <math>H^1(Y_T)</math>: <math>\ u\ _{H^1(Y_T)} \leq C \ u\ _{L^2(Y_T)} + \ u\ _{W^{1,1}(Y_T)}</math>, where <math>u \in \text{sub}(H^1(Y_T))</math> is the unique solution of the homogenized Lamé system <math>\lambda \Delta u + \mu \nabla \cdot (\nabla u) = f</math> in <math>L^2(Y_T)</math>. The unique solution of the homogenized first-order system <math>\lambda \Delta u + \mu \nabla \cdot (\nabla u) = f</math> is given by the following particular solution: <math>u_h = \frac{1}{2} \int_{Y_T} f(x) \, dx</math>, which is the solution for the first boundary condition <math>u_h = 0</math> on <math>\partial Y_T</math>.</p> <p>(1) In the first place, <math>\lambda \Delta u_h + \mu \nabla \cdot (\nabla u_h) = f</math> in <math>L^2(Y_T)</math>.</p> <p>(2) Then the final result <math>\lambda \Delta u_h + \mu \nabla \cdot (\nabla u_h) = f</math> in <math>L^2(Y_T)</math>.</p> <p>(3) On the material interface <math>\Gamma = \partial Y_T \setminus Y</math>, <math>\lambda \Delta u_h + \mu \nabla \cdot (\nabla u_h) = f</math> in <math>L^2(Y_T \setminus Y)</math>.</p> <p>(4) <math>(\delta y + x) \cdot n</math> is <math>T</math>-periodic, with zero-mean normalizations on <math>\chi_T^2</math> and <math>X_T^2</math>.</p> <p>The <math>C^{0,1}</math> norm: <math>E := \int_{Y_T} (E \cdot D_x D_y \chi_T^2) : C(Y_T \setminus Y, D_x D_y \chi_T^2) \, dy + \int_{Y_T} 2u_h D_x u_h : D_y u_h^2 \, dy</math>.</p> <p>[Correct] The accurate convergence of the function space.</p>

# Overview of AIM



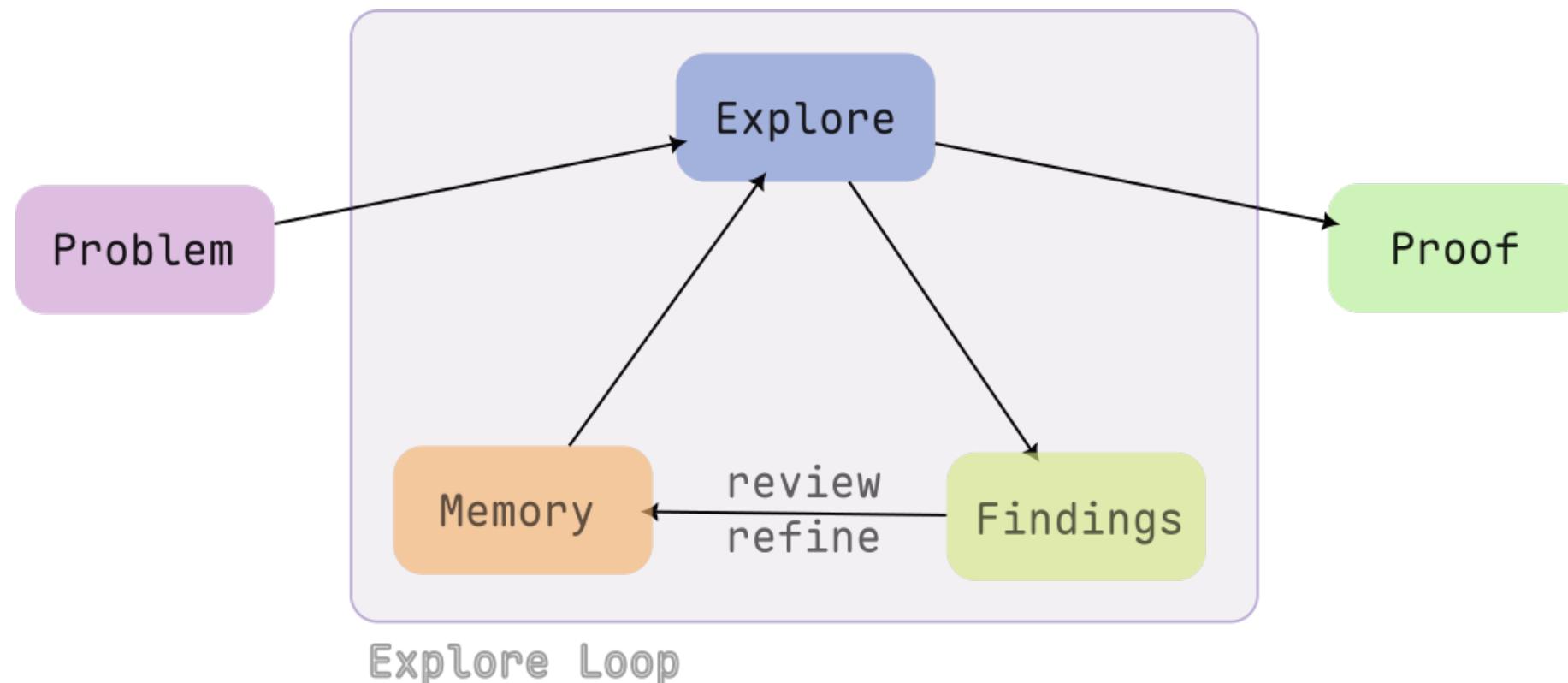
- An LLM-powered agent system specially designed for math research, consisting of three agents (Explorer, Verifier, Refiner) and a Memory.



# Long Reasoning: Explore & Memory



- The agents within AIM are tasked with exploring the original problem and documenting their discoveries as lemmas during the process. By iterating this procedure, the exploration progresses further, ultimately achieving problem resolution.

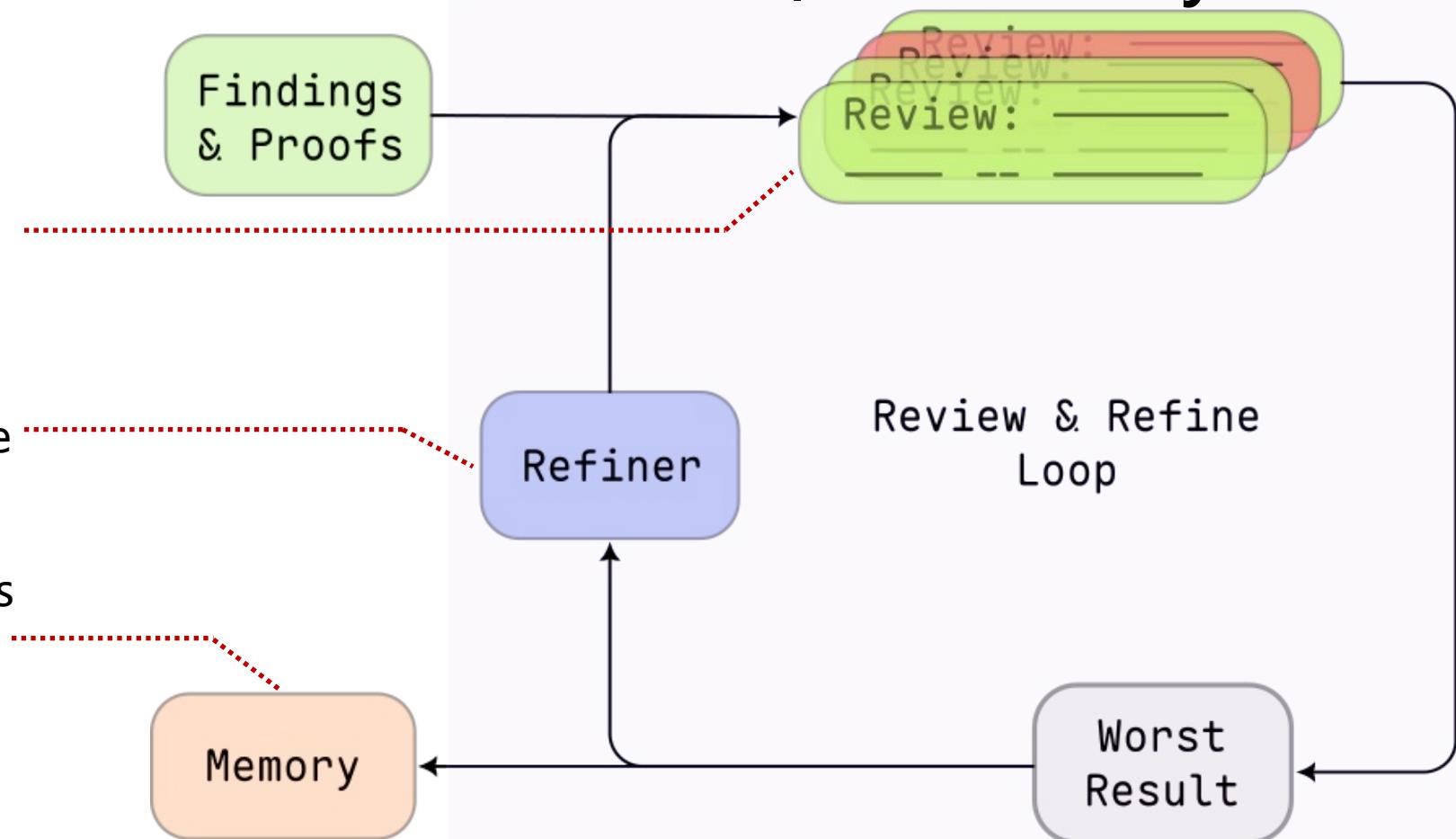


# Validation: Pessimistic Verification



- Each new discovery during exploration is repeatedly verified multiple times; if any single verification detects an error, the discovery is deemed incorrect.

- Conducting multiple rounds of self-checking can effectively identify issues
- Erroneous proofs can be analyzed and corrected
- Correct proof conclusions are eventually stored in memory



# Agent Design in AIM



- All three agents are guided by meticulously designed prompts, supported by logical processing methods to facilitate collaboration.

Prompt Structure
### Instruct _____, _____. _____. 1. _____. 2. _____. 3. _____.
### Problem Description ◊_____, _____. _____. _____. </> ◊_____, _____, _____. _____. _____, _____. </>
### Memories _____, _____. _____.
#### Mem ID: 0 _____. _____.
#### Mem ID: 1 _____. _____, _____, _____. _____, _____. .....

←--- Define behavior of an agent

## Prompt Example

Including task goal, reasoning direction, output format, etc.

You are an expert that is knowledgeable across all domains in math. This time you are asked to help with our frontier math research. Its statement is as follows:

This problem could be difficult and not able to be directly solved, but you can make your contribution with the following instructions:

1. You are required to explore different approaches or directions that might help with our final goal, and write down one interesting finding in your explorations as a new conjecture in your response. DO NOT claim that you can not do this job.

2. Your conjecture must contain the complete definitions required within it, such that it is able to stand alone as an independent lemma, unless it is declared in memory. Do not propose any existing lemmas as your new conjectures. You can directly use them in your explorations.

3. You should wrap your finding inside a latex environment: \begin{conjecture}\end{conjecture}. This conjecture should be equipped with a detailed, complete and rigorous proof. You should explicitly write down every intermediate derivation step in the proof. The corresponding proof should be wrapped in \begin{proof}\end{proof} directly followed by the conjecture.

4. After these components you should also provide the dependency of this conjecture. You need to write down the memory IDs of lemmas used in this conjecture in a JSON array format, and wrap them inside \begin{dependency}\end{dependency}. For example, a dependency of a new conjecture could be \begin{dependency}[0, 3, 4]\end{dependency}. You can use an empty array "[]" when this conjecture does not depend on other lemmas.

More accurately, your response should obey the following format:

```
\begin{conjecture}Your new findings here\end{conjecture}  
\begin{proof}Your proof of the conjecture above\end{proof}  
\begin{dependency}A json array of related memory IDs of this conjecture\end{dependency}  
Moreover, when you think the time is right that you are able to prove the original problem, you can simply state your proof inside \begin{final_proof}\end{final_proof} and explain
```

# Agent Design in AIM



- All three agents are guided by meticulously designed prompts, supported by logical processing methods to facilitate collaboration.

Prompt Structure
### Instruct _____, _____. 1. _____. 2. _____, _____. 3. _____.
### Problem Description ◊_____, _____. _____. _____. </> ◊_____, _____, _____. _____. _____, _____. </>
### Memories _____, _____. _____. ##### Mem ID: 0 _____. _____. ##### Mem ID: 1 _____. _____, _____, _____. _____, _____. .....

Define behavior of an agent  
←---  
Description of the problem  
←---

## Prompt Example

Information directly related to the task, for each agent it could be:

- Explorer: The statement of the final goal
- Verifier: a conjecture and its proof
- Refiner: a flawed conjecture, proof, and the feedback from the verifier

```
\begin{problem}Question:  
Can we prove: for any  $\delta > 0$ ,  
[  
 \mathbb{P}[n^{-\delta} \mathbb{E}[Y_n] \leq Y_n \leq n^{\delta}] \geq 1 - O(d^{-n})  
 ]  
  
If the second claim is not true, can we prove: for any  $\delta > 0$ ,  
[  
 \mathbb{P}[Y_n \leq n^{2+\delta}] \geq 1 - O(d^{-n})  
 ]  
\end{problem}  
This problem could be difficult and not able to be directly solved, but you can make your contribution with the following instructions:
```

# Agent Design in AIM



- All three agents are guided by meticulously designed prompts, supported by logical processing methods to facilitate collaboration.

Prompt Structure
### Instruct _____, _____. _____. 1. _____. 2. _____, _____. 3. _____.
### Problem Description ◊_____, _____. _____. _____. </> ◊_____, _____, _____. _____. _____, _____. </>
### Memories _____, _____. _____. ##### Mem ID: 0 _____. _____. ##### Mem ID: 1 _____. _____, _____, _____. _____, _____. .....

Define behavior of an agent  
←--- Description of the problem  
←--- Information in memory

## Prompt Example

Formatted exploration history in memory

```
### Context and History Explorations

Here is a list of context that we have collected for this problem or our history finding
s during exploration. They serve as the background of the conjecture and proof and can be ac
cepted without controversy as correct.

#### Memory **ID: 1**

\begin{lemma}

There exists a constant  $(A>0)$  and a nonnegative random variable  $(Y)$  such that
\[
\forall k \geq 1: \quad \mathbb{E}[Y^k] \leq k! \cdot A^k,
\]
yet for some  $(t>0)$ ,
\[
\mathbb{P}(Y \geq t) > \exp(-\frac{t}{2A}).
\]
In other words, the bound
\[
\mathbb{P}(Y \geq t) \leq \exp(-\frac{t}{2A})
\]
cannot hold for all  $(t>0)$  under only the moment hypothesis.

**DEPENDENCY**: []
\end{lemma}

#### Memory **ID: 2**
```

# Memory Design in AIM



- AIM parses and logs four categories of data from the model's outputs, with a portion of it being structured and fed into later agents' inputs.

Memory type, e.g.,  
context, lemma,  
conjecture, etc

Textual description  
of the memory  
content

A complete proof  
to this lemma

```
struct MemoryBlock {  
    Memory Type  
  
    Content Description  
  
    Proof: _____.  
    _____, _____.  
  
    MetaData  
};
```

Visible to all these  
agents

Saved and discarded  
in explorations

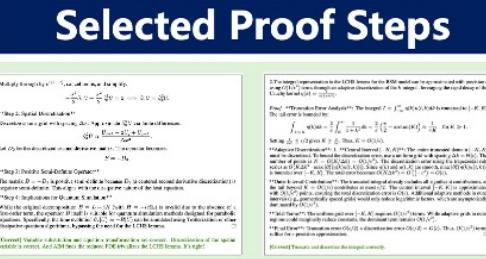
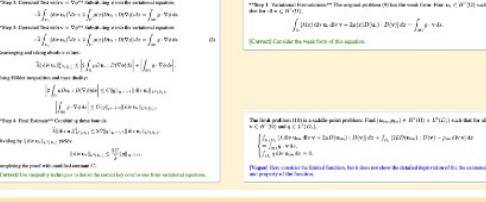
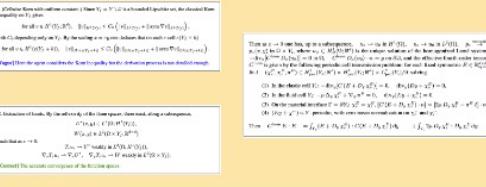
All components in the  
memory blocks will be  
visible in the output

Other metadata of this memory,  
e.g., solved tag, num reviews, etc

# Overview of Experiments



- AIM is applied to address four mathematical theory problems, including three settled problems and one open problem.

Research Problem	AIM效果	Selected Proof Steps
Quantum Algorithm Problem (Settled Problem)	AIM effectively completes the problem with a detailed solution process	
Absorbing Boundary Condition (Settled Problem)	AIM provides a substantially complete proof for this problem	
High Contrast Limit (Settled Problem)	AIM completes main proof of the conclusion and produces other correct results	
Homogenization Problem (Open Problem)	AIM provides partially correct conclusions and reasoning, offering instructive guidance	

Settled Problem

Open Problem

---- DeepSeek-R1

---- DeepSeek-R1

DeepSeek-R1  
and o4-mini,  
each conducted  
one experiment

---- o4-mini

# Direct Use of LLMs Fails



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- Directly using large language models (LLMs) fails to produce effective mathematical proofs.

## Existence and uniqueness:

A fixed-point argument is used on the boundary trace space  $L^2([0, T] \times \mathcal{S})$ . Define the mapping  $T : g \mapsto u|_{\mathcal{S}}$  as follows:

1. Given  $g \in L^2([0, T] \times \mathcal{S})$ , solve for each  $k$ :

$$\partial_t \varphi_k - \Delta_{\mathcal{S}} \varphi_k + d_k \varphi_k = g, \quad \varphi_k(0) = 0.$$

This parabolic equation on  $\mathcal{S}$  (a compact Riemannian manifold) has a unique solution  $\varphi_k \in C([0, T]; L^2(\mathcal{S})) \cap L^2([0, T]; H^1(\mathcal{S})) \cap H^1([0, T]; H^{-1}(\mathcal{S}))$  if  $d_k > 0$ .

2. Define  $h = \sum_{k=1}^m c_k \varphi_k$ .

3. Solve the heat equation with Robin-type boundary condition:

$$\partial_t u - \Delta u = 0, \quad u(0) = u_0, \quad \frac{\partial u}{\partial \nu} + au = h \quad \text{on } \mathcal{S}.$$

For  $u_0 \in L^2(\Omega)$  and  $h \in L^2([0, T] \times \mathcal{S})$ , this has a unique solution  $u \in C([0, T]; L^2(\Omega)) \cap L^2([0, T]; H^1(\Omega)) \cap H^1([0, T]; H^{-1}(\Omega))$ .

4. Set  $T(g) = u|_{\mathcal{S}}$ .

## 4. Quantum Algorithm

The algorithm computes  $u(\tau)$  for  $\tau = T$ :

### 1. Initial state preparation:

- Prepare  $|u(0)\rangle \propto u(x, 0) = K \max(e^x - 1, 0)$  using an oracle  $\mathcal{O}_{\text{init}}$ . Assume  $\|u(0)\| = 1$ .

### 2. Hamiltonian simulation:

- For each  $k_j$ , simulate  $U_j = \exp(-iT[H + k_j L])$ , where  $H$  and  $L$  are discretized Hermitian matrices (sparsity  $d = O(1)$ ).
- Use sparse Hamiltonian simulation (e.g., QSP) with oracle access to  $H$  and  $L$ .

### 3. Linear combination of unitaries (LCU):

- Prepare ancilla state  $|\psi_{\text{anc}}\rangle = \frac{1}{\sqrt{s}} \sum_{j=1}^M \sqrt{w_j} |j\rangle$  with  $s = \sum_j w_j \approx 1$ .
- Apply controlled- $U_j$ :  $\sum_j \sqrt{w_j/s} |j\rangle \otimes U_j |u(0)\rangle$ .
- Use amplitude amplification to extract the state with  $O(1)$  iterations (success probability  $\Theta(1)$ ).

Incorrect application of the fixed-point theorem, lacking a derivation process.

The derivation process is missing, and the positive semi-definiteness of  $L$  is not verified.

# Quantum Algorithm Problem



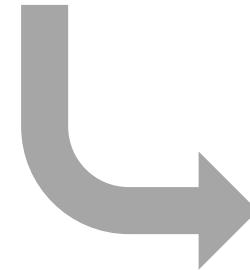
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The Linear Combination of Hamiltonian Simulation (LCHS) method is an efficient approach in scientific computing. Its main idea is to transform non-unitary dynamical problems into linear combinations of Hamiltonian simulation.

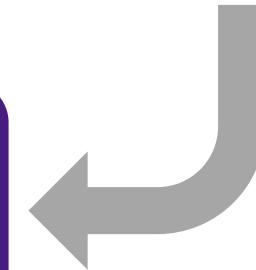
$$\mathcal{T}e^{-\int_0^t A(s) ds} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T}e^{-i \int_0^t (H(s) + kL(s)) ds} dk$$

The Black-Scholes-Merton (BSM) model is the fundamental mathematical framework used for pricing European options in finance.

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0$$



**Objective:** To simulate the BSM model using the LCHS method, design corresponding quantum algorithms, and analyze the complexity of the algorithms.



**AIM correctly applies this method, providing a detailed proof and basically solving this problem**

# Quantum Algorithm Problem



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## Explanation of the LCHS lemma

Lemma (Linear combination of Hamiltonian simulation, LCHS): For  $t \in [0, T]$ , let  $A(t) \in \mathbb{C}^{N \times N}$  be decomposed into Hermitian and anti-Hermitian parts such that  $A(t) = L(t) + iH(t)$ , where  $L(t) = \frac{1}{2}[A(t) + A^\dagger(t)]$  and  $H(t) = \frac{1}{2i}[A(t) - A^\dagger(t)]$ . Assume that  $L(t)$  is positive semi-definite for all  $t \in [0, T]$ . Denoting the time ordering operator by  $\mathcal{T}$ , we have  $\mathcal{T} \exp \left\{ - \int_0^t A(s) ds \right\} = \int_{\mathbb{R}} \eta(k) u(t, k) dk$ , where  $u(t, k)$  is the propagator for a time-dependent Hamiltonian simulation problem such that  $u(t, k) = \mathcal{T} \exp \left\{ -i \int_0^t [H(s) + kL(s)] ds \right\}$ , and  $\eta(k) = \frac{1}{\pi(1+k^2)}$  is the kernel function with respect to  $k$ .

## System input

BSM model: The PDE in the BSM model is given by

$$\frac{\partial V(S, t)}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0.$$

Boundary conditions are characterized by:  $V(0, t) = 0$  for all  $0 < t \leq T$ ;  $V(S, t) \rightarrow S - Ke^{-r(T-t)}$  for  $S \rightarrow \infty$ ;  $V(S, T) = \max\{S - K, 0\}$ .

## Explanation of the BSM model

Your tasks are to: Use the idea of LCHS to deal with the BSM model. Design a quantum algorithm to solve the equation. And compute the complexity (query complexity to state preparation oracle and operator oracles, gate complexity, ancilla qubits, (parameters: norm of boundary and initial, T, approximation error  $\epsilon$ , etc)).

## Objective

# Quantum Algorithm Problem



- AIM solves the problem by transforming the BSM equation into a heat equation, applying the LCHS lemma to reformulate the problem, and proposing a quantum algorithm. The core steps are as follows:

1	PDE transformation and spatial discretization	Transform the BSM equation into the standard heat equation using variable substitution, and discretize the spatial variables.
2	Operator decomposition and integral discretization	Apply the LCHS lemma to decompose the solution operator of the heat equation into a continuous linear combination of unitary operators. Then, truncate and approximate the continuous integral and discretize it.
3	Quantum algorithm implementation and complexity analysis	Design quantum algorithms using the linear combination of unitaries (LCU) and Hamiltonian simulation techniques, and calculate the complexity.

# Quantum Algorithm Problem



**AIM explores step by step through a seq. of progressively built lemmas.**

**Lemma 1:** First, AIM transforms the BSM equation into a heat equation, then discretizes the spatial variables, and verifies semi-definiteness. Further, AIM converts it into a form that can utilize the LCHS lemma, with a detailed proof.

1. The Black-Scholes-Merton (BSM) partial differential equation (PDE) can be transformed into the standard heat equation via a logarithmic substitution. Specifically, under the transformation  $x = \ln(S/K) + (r - \sigma^2/2)(T - t)$ ,  $\tau = \sigma^2(T - t)/2$ , and  $V(S, t) = e^{-r(T-t)}U(x, \tau)$ , the BSM PDE reduces to:

$$\frac{\partial U}{\partial \tau} = \frac{\partial^2 U}{\partial x^2}.$$

Discretizing this PDE spatially yields a matrix equation  $\partial_\tau|U\rangle = -B|U\rangle$ , where  $B = -\partial_x^2$ . The operator  $B$  is positive semi-definite and can be directly interpreted as  $B = L$ , where  $L = -\partial_x^2$ . While the original Hermitian decomposition  $B = L + iH$  (with  $H = 0$ ) trivializes the LCHS lemma, the dissipative nature of  $B$  permits alternative quantum simulation methods.

## Transform the BSM equation into a heat equation

*Proof.* \*\*Step 1: Transform BSM to the Heat Equation

Start with the BSM PDE:

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0.$$

Apply the substitution  $V(S, t) = e^{-r(T-t)}U(x, \tau)$ ,  $x = \ln(S/K) + (r - \sigma^2/2)(T - t)$ , and  $\tau = \sigma^2(T - t)/2$ . Compute derivatives rigorously:  $-\partial_t V = e^{-r(T-t)} \left( rU - \frac{\sigma^2}{2} \partial_\tau U - (r - \sigma^2/2) \partial_x U \right)$ ,  $-\partial_S V = e^{-r(T-t)} \partial_x U \cdot \frac{1}{S}$ ,  $-\partial_S^2 V = e^{-r(T-t)} (\partial_x^2 U - \partial_x U) \cdot \frac{1}{S^2}$ .

Substitute into the BSM PDE:

$$e^{-r(T-t)} \left[ rU - \frac{\sigma^2}{2} \partial_\tau U - (r - \sigma^2/2) \partial_x U + \frac{1}{2} \sigma^2 (\partial_x^2 U - \partial_x U) + r \partial_x U - rU \right] = 0.$$

Multiply through by  $e^{r(T-t)}$ , cancel terms, and simplify:

$$-\frac{\sigma^2}{2} \partial_\tau U + \frac{\sigma^2}{2} \partial_x^2 U = 0 \implies \partial_\tau U = \partial_x^2 U.$$

\*\*Step 2: Spatial Discretization\*\*

Discretize  $x$  on a grid with spacing  $\Delta x$ . Approximate  $\partial_x^2 U$  via finite differences:

$$\partial_x^2 U \approx \frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2}.$$

Let  $D_2$  be the discretized second derivative matrix. The operator becomes:

$$B = -D_2.$$

\*\*Step 3: Positive Semi-Definite Operator\*\*

The matrix  $B = -D_2$  is positive semi-definite because  $D_2$  (a centered second derivative discretization) is negative semi-definite. This aligns with the dissipative nature of the heat equation.

\*\*Step 4: Implications for Quantum Simulation\*\*

While the original decomposition  $B = L + iH$  (with  $H = -ic\partial_x$ ) is invalid due to the absence of a first-order term, the operator  $B$  itself is suitable for quantum simulation methods designed for parabolic equations. Specifically, the time evolution  $\partial_\tau|U\rangle = -B|U\rangle$  can be simulated using Trotterization or other dissipative quantum algorithms, bypassing the need for the LCHS lemma. □

**Discretize spatial variables**

**[Correct]** Variable substitution and equation transformation are correct. Discretization of the spatial variable is correct. And AIM finds the reduced PDE trivializes the LCHS lemma. It's right!

# Quantum Algorithm Problem



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**AIM explores step by step through a seq. of progressively built lemmas.**

**Lemma 2:** AIM analyzes truncation errors and determines discrete intervals, laying the foundation for constructing quantum algorithms.

2. The integral representation in the LCHS lemma for the BSM model can be approximated with precision  $\epsilon$  using  $O(1/\epsilon^2)$  terms through an adaptive discretization of the  $k$ -integral, leveraging the rapid decay of the Cauchy kernel  $\eta(k) = \frac{1}{\pi(1+k^2)}$ .

*Proof.* **\*\*Truncation Error Analysis\*\*:** The integral  $I = \int_{-\infty}^{\infty} \eta(k)u(t, k)dk$  is truncated to  $[-K, K]$ . The tail error is bounded by:

$$\int_{|k|>K} \eta(k)dk = \frac{2}{\pi} \int_K^{\infty} \frac{1}{1+k^2} dk = \frac{2}{\pi} \left( \frac{\pi}{2} - \arctan(K) \right) \approx \frac{1}{\pi K} \quad \text{for } K \gg 1.$$

Setting  $\frac{1}{\pi K} \leq \epsilon/2$  gives  $K \geq \frac{2}{\pi\epsilon}$ . Thus,  $K = O(1/\epsilon)$ .

**\*\*Adaptive Discretization\*\*:** 1. **\*\*Central Interval  $[-K, K]$ \*\*:** The entire truncated domain  $[-K, K]$  must be discretized. To bound the discretization error, use a uniform grid with spacing  $\Delta k = \Theta(\epsilon)$ . The number of points is  $N = O(K/\Delta k) = O(1/\epsilon^2)$ . The discretization error using the trapezoidal rule scales as  $O(K\Delta k^2 \cdot \max |\partial_k^2(\eta(k)u(t, k))|)$ . Since  $\eta(k)$  and  $u(t, k)$  are smooth,  $\max |\partial_k^2(\eta(k)u(t, k))|$  is bounded over  $[-K, K]$ . The total error becomes  $O(K\Delta k^2) = O(\frac{1}{\epsilon} \cdot \epsilon^2) = O(\epsilon)$ .

**\*\*Outer Interval Contribution\*\*:** The truncated integral already includes all significant contributions, as the tail beyond  $K = O(1/\epsilon)$  contributes at most  $\epsilon/2$ . The central interval  $[-K, K]$  is approximated with  $O(1/\epsilon^2)$  points, ensuring the total discretization error is  $O(\epsilon)$ . Additional adaptive methods in outer intervals (e.g., geometrically spaced grids) would only reduce logarithmic factors, which are asymptotically dominated by  $O(1/\epsilon^2)$ .

**\*\*Total Terms\*\*:** The uniform grid over  $[-K, K]$  requires  $O(1/\epsilon^2)$  terms. While adaptive grids in outer regions could marginally reduce constants, the dominant term remains  $O(1/\epsilon^2)$ .

**\*\*Final Error\*\*:** Truncation error  $O(\epsilon/2) +$  discretization error  $O(\epsilon/2) = O(\epsilon)$ . Thus,  $O(1/\epsilon^2)$  terms suffice for  $\epsilon$ -precision approximation.  $\square$

Analyze truncation error

Determine discrete intervals

Overall error analysis

[Correct] Truncate and discretize the integral correctly.

# Quantum Algorithm Problem



**AIM explores step by step through a seq. of progressively built lemmas.**

AIM combines previous lemmas to construct a quantum algorithm using Hamiltonian simulation and the linear combination of unitary operators (LCU), then calculates its complexity. There are some errors in the complexity calculation, but the core methods are correct.

3. The solution operator for the heat equation derived from the BSM model,  $U(\tau) = e^{\tau B}$ , can be approximated via the LCHS lemma as a linear combination of Hamiltonian simulations. Specifically, the integral representation  $\int_{\mathbb{R}} \eta(k) e^{-ikL\tau} dk$  (where  $L = -B$ ) can be discretized into  $M = O(1/\epsilon^2)$  terms with quadrature weights  $\eta(k_j)\Delta k$ . The total query complexity to the  $L$ -oracle is  $\tilde{O}(\|L\|\tau/\epsilon^3)$ , where  $T = \frac{2\tau}{\sigma^2}$  and the gate complexity scales polynomially with  $\|L\|$ ,  $T$ ,  $1/\epsilon$ , and logarithmic factors.

**Based on the first lemma, use the LCHS lemma to transform into a continuous integral of unitary operators**

Proof:  
\*\*Step 1: Integral Representation via LCHS\*\* From Lemma-0, the solution operator for the heat equation is  $U(\tau) = e^{\tau B}$ . Let  $L = -B$ , a positive semi-definite operator. By the LCHS lemma with  $H = 0$ , we express:

$$e^{\tau B} = \int_{\mathbb{R}} \eta(k) e^{-ikL\tau} dk, \quad \eta(k) = \frac{1}{\pi(1+k^2)}.$$

\*\*Step 2: Quadrature Discretization\*\* Lemma-1 guarantees the integral can be discretized into  $M = O(1/\epsilon^2)$  terms with weights  $\eta(k_j)\Delta k$ , yielding:

$$e^{\tau B} \approx \sum_{j=1}^M \eta(k_j)\Delta k \cdot e^{-ik_j L\tau}.$$

The truncation and discretization error is  $O(\epsilon)$  due to the  $O(1/k^2)$  decay of  $\eta(k)$ .

[Correct] Properly utilizing the LCHS lemma and memory lemmas for problem transformation.

**Transform the solution of the equation into a linear combination of unitary operators**

## Utilize Hamiltonian simulation algorithms

\*\*Step 3: Hamiltonian Simulation Costs\*\* Each term  $e^{-ik_j L\tau}$  requires simulating  $L$  for time  $t_j = k_j\tau$ . Using optimal Hamiltonian simulation algorithms (e.g., quantum signal processing or Taylor series) with query complexity  $O(\|L\|t_j + \log(1/\epsilon_{\text{sim}}))$ , set  $\epsilon_{\text{sim}} = \epsilon/M$  to bound the total simulation error by  $\epsilon$ . Since  $k_j = O(1/\epsilon)$  dominates the quadrature,  $t_j = O(\tau/\epsilon)$ . The per-term complexity becomes:

$$O(\|L\|\tau/\epsilon + \log(M/\epsilon)) = \tilde{O}(\|L\|\tau/\epsilon).$$

\*\*Step 4: Total Query Complexity\*\* Summing over  $M = O(1/\epsilon^2)$  terms, the total queries to the  $L$ -oracle are:

$$\tilde{O}\left(M \cdot \frac{\|L\|\tau}{\epsilon}\right) = \tilde{O}\left(\frac{\|L\|\tau}{\epsilon^3}\right).$$

Expressing in terms of  $T = \frac{2\tau}{\sigma^2}$  and absorbing constants:

$$\tilde{O}\left(\frac{\|L\|T}{\epsilon^3}\right).$$

## Complexity analysis

\*\*Step 5: Ancilla and Gate Complexity\*\* The LCU framework requires  $\log M = O(\log(1/\epsilon))$  ancilla qubits. Gate complexity inherits  $\tilde{O}(M)$ -scaling from the superposition state, augmented by  $O(\text{poly}(\log(\|L\|T/\epsilon)))$  factors from simulation subroutines. The dominant terms remain polynomial in  $\|L\|$ ,  $T$ , and  $1/\epsilon$ , with polylogarithmic corrections.

[Error] There are some mistakes about complexity computing. And the calculation process lacks detail.

# Absorbing Boundary Condition Problem



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- **Problem Description:** Prove the well-posedness and uniqueness of the solution to the heat conduction equation under specifically designed absorbing boundary condition constraints.

$$\begin{cases} \mathcal{L}u = 0, & [0, \infty) \times \Omega \\ \frac{\partial u}{\partial \nu} = -\beta u - \sum_{k=1}^m \alpha_k (\partial_t - \Delta_S) \varphi_k = \mathcal{F}_1 u, & [0, \infty) \times \mathcal{S} \\ u = u_0, & t = 0 \\ (\partial_t - \Delta_S + d_k) \varphi_k = u, & t \geq 0 \\ \varphi_k = 0, & t = 0 \end{cases} \quad u \in C([0, T]; L^2(\Omega)) \cap H^1([0, T]; H^{-1}(\Omega)) \cap L^2([0, T]; H^1(\Omega)),$$
$$\varphi_k \in C([0, T]; L^2(\mathcal{S})) \cap H^1([0, T]; H^{-1}(\mathcal{S})) \cap L^2([0, T]; H^1(\mathcal{S}))$$

AIM correctly applied the approach and methods for analyzing such problems, providing a highly complete proof process.

\*\*A priori energy estimate for the coupled system\*\* Let  $u$  and  $\varphi_k$  ( $k = 1, \dots, m$ ) satisfy the system (2.10) with  $u_0 \in L^2(\Omega)$  and  $\varphi_k(0) = 0$ . Then, there exists a constant  $C > 0$  depending on  $T, \beta, \alpha_k, d_k$ , but independent of  $u_0$ , such that:

$$\begin{aligned} & \sup_{t \in [0, T]} \|u(t)\|_{L^2(\Omega)}^2 + \int_0^T \|\nabla u(t)\|_{L^2(\Omega)}^2 dt + \int_0^T \|u(t)\|_{L^2(\mathcal{S})}^2 dt \\ & + \sum_{k=1}^m \left( \sup_{t \in [0, T]} \|\varphi_k(t)\|_{L^2(\mathcal{S})}^2 + \int_0^T \|\nabla_S \varphi_k(t)\|_{L^2(\mathcal{S})}^2 dt \right) \leq C \|u_0\|_{L^2(\Omega)}^2. \end{aligned}$$

Here is the core norm control inequality provided by AIM, which is a key intermediate conclusion for this problem.

# High Contrast Limit Problem



- **Problem Description:** Consider a special case of a transmission system under a certain parameter limit. Analyze and prove the error estimation between the limit solution and the original solution.

$$\begin{cases} \mathcal{L}_{\lambda,\mu}\mathbf{u}_\epsilon = 0 & \text{in } \Omega \setminus \overline{D_\epsilon}, \\ \mathcal{L}_{\tilde{\lambda},\tilde{\mu}}\mathbf{u}_\epsilon = 0 & \text{in } D_\epsilon, \\ \mathbf{u}_\epsilon|_- = \mathbf{u}|_+ \text{ and } \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\tilde{\lambda},\tilde{\mu})}}|_- = \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda,\mu)}}|_+ & \text{on } \partial D_\epsilon, \\ \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda,\mu)}}|_{\partial \Omega} = g \in H_{\mathbb{R}}^{-\frac{1}{2}}(\partial \Omega) \text{ and } \mathbf{u}_\epsilon|_{\partial \Omega} \in H_{\mathbb{R}}^{\frac{1}{2}}(\partial \Omega). & \end{cases}$$

$$\begin{cases} \mathcal{L}_{\lambda,\mu}\mathbf{u}_\epsilon = 0 & \text{in } \Omega \setminus \overline{D_\epsilon}, \\ \mathcal{L}_{\tilde{\mu}}(\mathbf{u}_\epsilon, p_\epsilon) = 0 \text{ and } \operatorname{div} \mathbf{u}_\epsilon = 0 & \text{in } D_\epsilon, \\ \mathbf{u}_\epsilon|_- = \mathbf{u}_\epsilon|_+ \text{ and } \frac{\partial (\mathbf{u}_\epsilon, p_\epsilon)}{\partial \nu_{(\infty, \tilde{\mu})}}|_- = \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda,\mu)}}|_+ & \text{on } \partial D_\epsilon, \\ \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda,\mu)}}|_{\partial \Omega} = g \in H_{\mathbb{R}}^{-\frac{1}{2}}(\partial \Omega) \text{ and } \mathbf{u}_\epsilon|_{\partial \Omega} \in H_{\mathbb{R}}^{\frac{1}{2}}(\partial \Omega), & \end{cases}$$

**AIM provided the main derivation process and proof of the core conclusion and proactively explored to obtain other correct conclusions.**

Under the given assumptions, the difference  $\mathbf{w}_\epsilon = \mathbf{u}_{\lim} - \mathbf{u}_\epsilon$  between the solutions of the limit problem (10) and the original problem (9) satisfies the homogenized error estimate in the energy norm weighted by the Lamé parameters:

$$\left( \int_{\Omega} [\lambda(x)|\operatorname{div} \mathbf{w}_\epsilon|^2 + 2\mu(x)|\mathcal{D}(\mathbf{w}_\epsilon)|^2] dx \right)^{1/2} \leq \frac{C}{\sqrt{\tilde{\lambda}}} \|g\|_{H_{\mathbb{R}}^{-\frac{1}{2}}(\partial \Omega)},$$

where  $C$  is independent of  $\tilde{\lambda}$ . This implies that the error in the energy norm decays proportionally to  $\tilde{\lambda}^{-\frac{1}{2}}$ .

**correctness:** True

**AIM explored and obtained control results over the global space.**

# Homogenization Problem



- **Problem Description:** The homogenization problem for transmission systems requires analyzing the properties of equations and their corresponding solutions under specific physical scale limits. The goal is to ultimately prove the error estimation of solutions, which remains **an open problem**.

$$\begin{cases} \mathcal{L}_{\lambda,\mu} \mathbf{u}_\epsilon = 0 \\ \mathcal{L}_{\tilde{\mu}}(\mathbf{u}_\epsilon, p_\epsilon) = 0 \text{ and } \operatorname{div} \mathbf{u}_\epsilon = 0 \\ \mathbf{u}_\epsilon|_- = \mathbf{u}_\epsilon|_+ \text{ and } \left. \frac{\partial(\mathbf{u}_\epsilon, p_\epsilon)}{\partial \nu_{(\infty, \tilde{\mu})}} \right|_- = \left. \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda, \mu)}} \right|_+ \\ \left. \frac{\partial \mathbf{u}_\epsilon}{\partial \nu_{(\lambda, \mu)}} \right|_{\partial \Omega} = g \in H_{\mathbb{R}}^{-\frac{1}{2}}(\partial \Omega) \quad \text{and} \quad \mathbf{u}_\epsilon|_{\partial \Omega} \in H_{\mathbb{R}}^{\frac{1}{2}}(\partial \Omega), \end{cases}$$

in  $\Omega \setminus \overline{D_\epsilon}$ , where  $\mathcal{L}_{\tilde{\mu}}(\mathbf{u}_\epsilon, p_\epsilon) = \tilde{\mu} \Delta \mathbf{u}_\epsilon + \nabla p_\epsilon$  denotes the Stokes operator with viscosity constant  $\tilde{\mu}$  and  $p_\epsilon$  is the pressure field. Its exterior derivative is defined as  $\left. \frac{\partial(u, p)}{\partial \nu_{(\infty, \mu)}} \right|_- := pN + 2\mu D(u)N$ .

Now we let  $\epsilon \rightarrow 0$ , so that the scale of the cell is tend to be zero. We wonder what homogenization equation does the limited solution  $\mathbf{u}_{lim}$  satisfies. At the same time, whether the estimate between the original solution and the limited solution has the form  $C\epsilon^\alpha \|g\|_{H_{\mathbb{R}}^{-\frac{1}{2}}(\partial \Omega)}$  for some  $\alpha \in (0, 1)$ .

- AIM correctly applied mathematical theorems and analytical derivations, providing some accurate conclusions and approaches.
- The results are of guiding significance for human mathematicians conducting this research.

## 6. Error estimate and strong convergence Define the two-scale corrector

$$u_\epsilon^{\text{app}}(x) = u_0(x) + \varepsilon \chi^{D_x u_0(x)}(x/\varepsilon) \text{ in } \Omega_\varepsilon,$$

extended in each  $D_\varepsilon$  by  $Ey + \chi_i^E(y)$ . A Céa-lemma-type argument in the perforated domain (again relying on uniform Korn and Stokes inf-sup, Lemma A.1-A.2) yields for some  $\alpha \in (0, 1)$

$$\|u_\varepsilon - u_\varepsilon^{\text{app}}\|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^\alpha \|g\|_{H_R^{-1/2}(\partial \Omega)}.$$

From this one deduces  $u_\varepsilon \rightarrow u_0$  strongly in  $L^2(\Omega)$  (and even in  $H^1(\Omega_\varepsilon)$  up to the corrector).

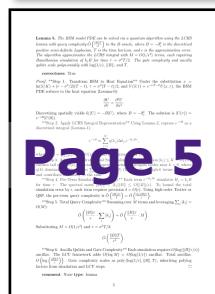
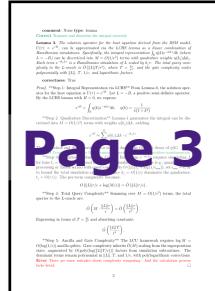
This completes a fully rigorous derivation of the homogenized elastic limit and the explicit formula for  $C^{\text{hom}}$ .

**Correct asymptotic expansion approaches and exploration of conclusions.**

# Limitation 1: Redundant Exploration



- Currently, AIM often explores in the same direction, presenting a series of similar conjectures and identical lemmas, which increases costs, reduces efficiency, and limits the performance ceiling.

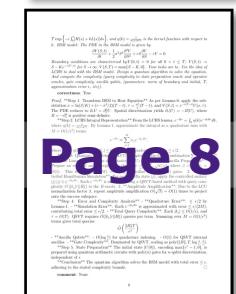
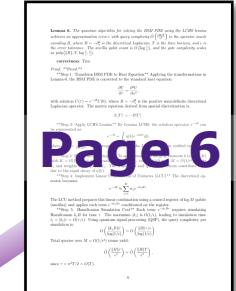


**Lemma 4.** The solution operator  $e^{-\tau B}$  for the heat equation derived from the BSM model can be approximated with error  $\epsilon$  using a quantum algorithm that implements a discretized version of the LCHS lemma. This algorithm requires  $M = O(\frac{1}{\epsilon^2})$  terms in the quadrature approximation, and the total query complexity to the  $B$ -oracle (encoding the discretized Laplacian) is  $\tilde{O}\left(\frac{\|B\|T}{\epsilon^3}\right)$ , where  $T = \frac{2\tau}{\sigma^2}$ . The gate complexity and ancilla qubits scale polynomially with  $\log(1/\epsilon)$ ,  $\|B\|$ , and  $T$ .

**Lemma 6.** The quantum algorithm for solving the BSM PDE using the LCHS lemma achieves an approximation error  $\epsilon$  with query complexity  $\tilde{O}\left(\frac{\|B\|T}{\epsilon^3}\right)$  to the operator oracle encoding  $B$ , where  $B = -\partial_x^2$  is the discretized laplacian,  $T$  is the simulation time, and  $\epsilon$  is the error tolerance. The ancilla qubit count is  $O(\log \frac{1}{\epsilon})$ , and the gate complexity scales as  $\text{poly}(\|B\|, T, \log \frac{1}{\epsilon}, \frac{1}{\epsilon})$ .

**Lemma 7.** The quantum algorithm for solving the BSM PDE using the LCHS lemma requires simulating the discretized Laplacian operator  $B = -\partial_x^2$  for a total time  $\tau = \frac{\sigma^2 T}{2}$ . The integral  $\int_{\mathbb{R}} \eta(k) e^{-ikB\tau} dk$  is approximated by  $M = O(\frac{1}{\epsilon^2})$  quadrature terms. Each term involves Hamiltonian simulation of  $k_j B$ , where  $|k_j| \leq O(\frac{1}{\epsilon})$ . The total query complexity to the  $B$ -oracle is  $\tilde{O}\left(\frac{\|B\|T}{\epsilon^3}\right)$ , and the gate complexity scales as  $\text{poly}(\|B\|, T, \log \frac{1}{\epsilon}, \frac{1}{\epsilon})$ , with ancilla qubit count  $O(\log \frac{1}{\epsilon})$ .

## Three Similar Lemmas



# Limitation 2: Insufficient Understanding of Mathematical Settings



- The current AIM has limited ability to understand lengthy mathematical setups and background conditions, which can lead to errors in the agent's analysis process.

Then as  $\varepsilon \rightarrow 0$  one has, up to a subsequence,  $u_\varepsilon \rightharpoonup u_0$  in  $H^1(\Omega)$ ,  $u_\varepsilon \rightarrow u_0$  in  $L^2(\Omega)$ ,  $p_\varepsilon \xrightarrow{\text{two-scale}} p_1(x, y)$  in  $\Omega \times Y_i$ , where  $u_0 \in H_R^1(\Omega; \mathbb{R}^d)$  is the unique solution of the homogenized Lamé system  $-\operatorname{div}_x [C^{\text{hom}} D_x(u_0)] = 0$  in  $\Omega$ ,  $C^{\text{hom}} D_x(u_0) \cdot n = g$  on  $\partial\Omega$ , and the effective fourth-order tensor  $C^{\text{hom}}$  is given by the following periodic cell transmission problem: for each fixed symmetric  $E \in \mathbb{R}_{\text{sym}}^{d \times d}$  find  $(\chi_e^E, \chi_i^E, \pi^E) \in H_{\text{per}}^1(Y_e; \mathbb{R}^d) \times H_{\text{per}}^1(Y_i; \mathbb{R}^d) \times L_{\text{per}}^2(Y_i)/\mathbb{R}$  solving

- (1) In the elastic cell  $Y_e$ :  $-\operatorname{div}_y [C(E + D_y \chi_e^E)] = 0$ ,  $\operatorname{div}_y(Ey + \chi_e^E) = 0$ ,
- (2) In the fluid cell  $Y_i$ :  $-\mu \Delta_y \chi_i^E + \nabla_y \pi^E = 0$ ,  $\operatorname{div}_y(Ey + \chi_i^E) = 0$ ,
- (3) On the material interface  $\Gamma = \partial Y_i$ :  $\chi_e^E = \chi_i^E$ ,  $[C(E + D_y \chi_e^E) \cdot n] = [2\mu D_y \chi_i^E - \pi^E I] \cdot n$ ,

The lack of understanding of the boundaries of the unit cell here has led to conclusions that do not align with the actual situation

# Limitation 3: Lack of Derivation Details



- AIM tends to "skip steps" , which is detrimental to both manual and automated verification of the proof and may lead to incorrect proofs.

\*\*Step 2: Formulate the Projected Equations\*\* For test functions  $v \in V_N$  and  $\psi \in W_{k,N}$ , the Galerkin approximations satisfy the projected weak form:

$$\int_{\Omega} \partial_t u^N v \, dx + \int_{\Omega} \nabla u^N \cdot \nabla v \, dx + \int_{\Omega} \rho u^N v \, dx \\ + \beta \int_S u^N v \, ds + \sum_{k=1}^m \alpha_k \int_S (\partial_t \varphi_k^N - \Delta_S \varphi_k^N) v \, ds = 0,$$

$$\int_S \partial_t \varphi_k^N \psi \, ds + \int_S \nabla_S \varphi_k^N \cdot \nabla_S \psi \, ds + d_k \int_S \varphi_k^N \psi \, ds = \int_S u^N \psi \, ds.$$

\*\*Step 3: Solve the ODE System\*\* Substituting  $u^N = \sum_{j=1}^N a_j(t)w_j$  and  $\varphi_k^N = \sum_{l=1}^N b_{k,l}(t)\theta_{k,l}$  into the projected equations yields a linear ODE system for  $a_j(t)$  and  $b_{k,l}(t)$ . The coefficients are smooth (as eigenfunctions are  $C^\infty$ ), ensuring continuity. By the Cauchy-Lipschitz theorem, unique solutions exist on  $[0, T]$ .

[Correct] The agent gets the ODE satisfied with the approximated solution.

[Vague] It is better to have more detailed process.

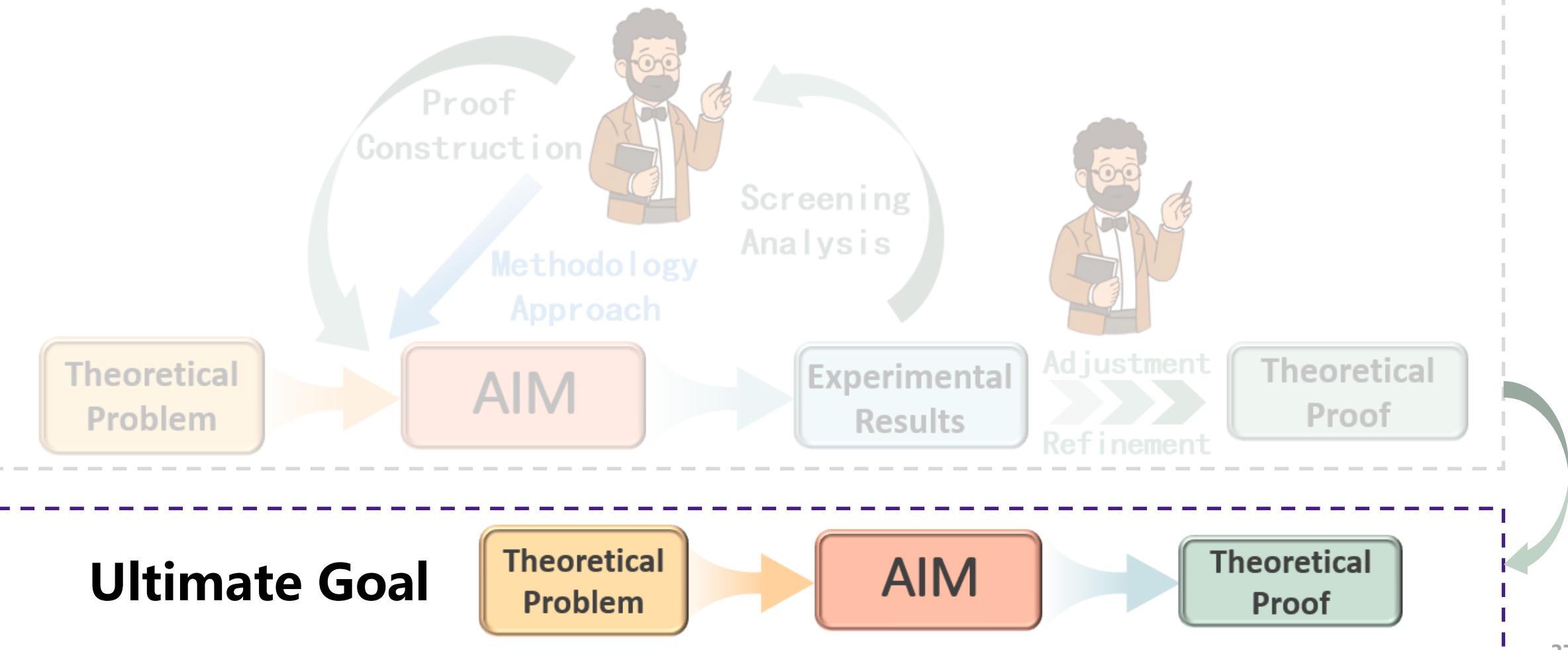
The specific derivation and analysis process of the ODE system is not provided here, but the conclusion is correct.

# Outlook: Assistive to Proactive



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## Auxiliary Proof + Idea Validation + Open Exploration



# Outlook: Enhancing Collaboration



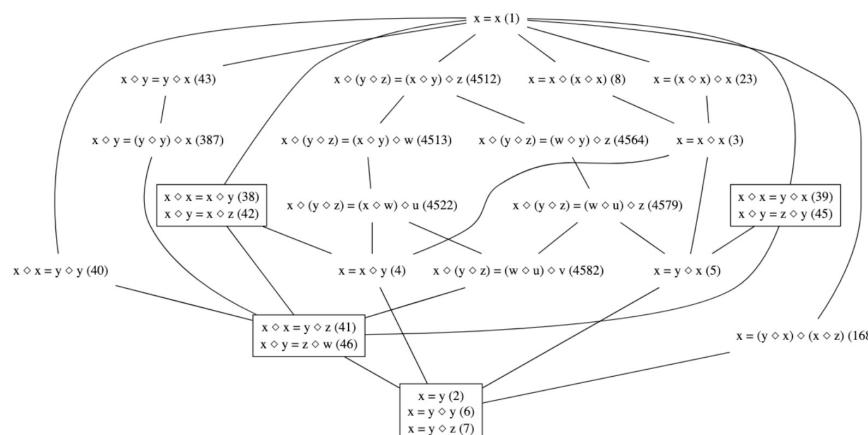
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- AI mathematicians, acting as independent entities, facilitate collaboration and accelerate the advancement of mathematics.



Terence Tao  
[@tao@mathstodon.xyz](mailto:@tao@mathstodon.xyz)

As of yesterday, the Equational Theories Project [teorth.github.io/equational\\_th...](https://teorth.github.io/equational_th...) has (provisionally) attained its aim of resolving all 22028942 implications between the 4694 equational laws of magmas involving at most four multiplication operations. We are not fully done yet - there are 52 resolutions that currently only have a human-readable proof but not a Lean-formalized proof (actually, there are a few that are not even human-readable, but are instead computer-generated by some non-Lean program) - but it should now just be a matter of time before we can declare final success in which the full implication graph is completely formalized in Lean. As such, we are now beginning the process of writing up the results. 公分是 - 最高位



## Equational Theories Project

- **57 Days:** Human and AI collaboration resolved 22,028,942 implications among 4,694 equations
- **9 Days:** Progress reached 99.866% with AI assistance

## Contributors 61



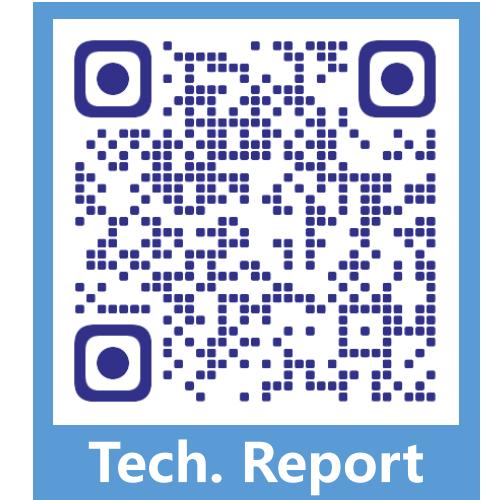
+ 47 contributors

# Summary



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- Large language models enable greater AI impact in mathematical research.
- Three key characteristics distinguish mathematical research from problem-solving, including long reasoning, procedural rigor, and answer existence.
- We propose the AI mathematician system **AIM**, which has achieved preliminary success on four research-level mathematical problems, showing promising potential.
- In the future, AI will play a more proactive and important role in mathematical research.



Our AIM is AI Mathematician!

