人工智能在物理学发现中的应用

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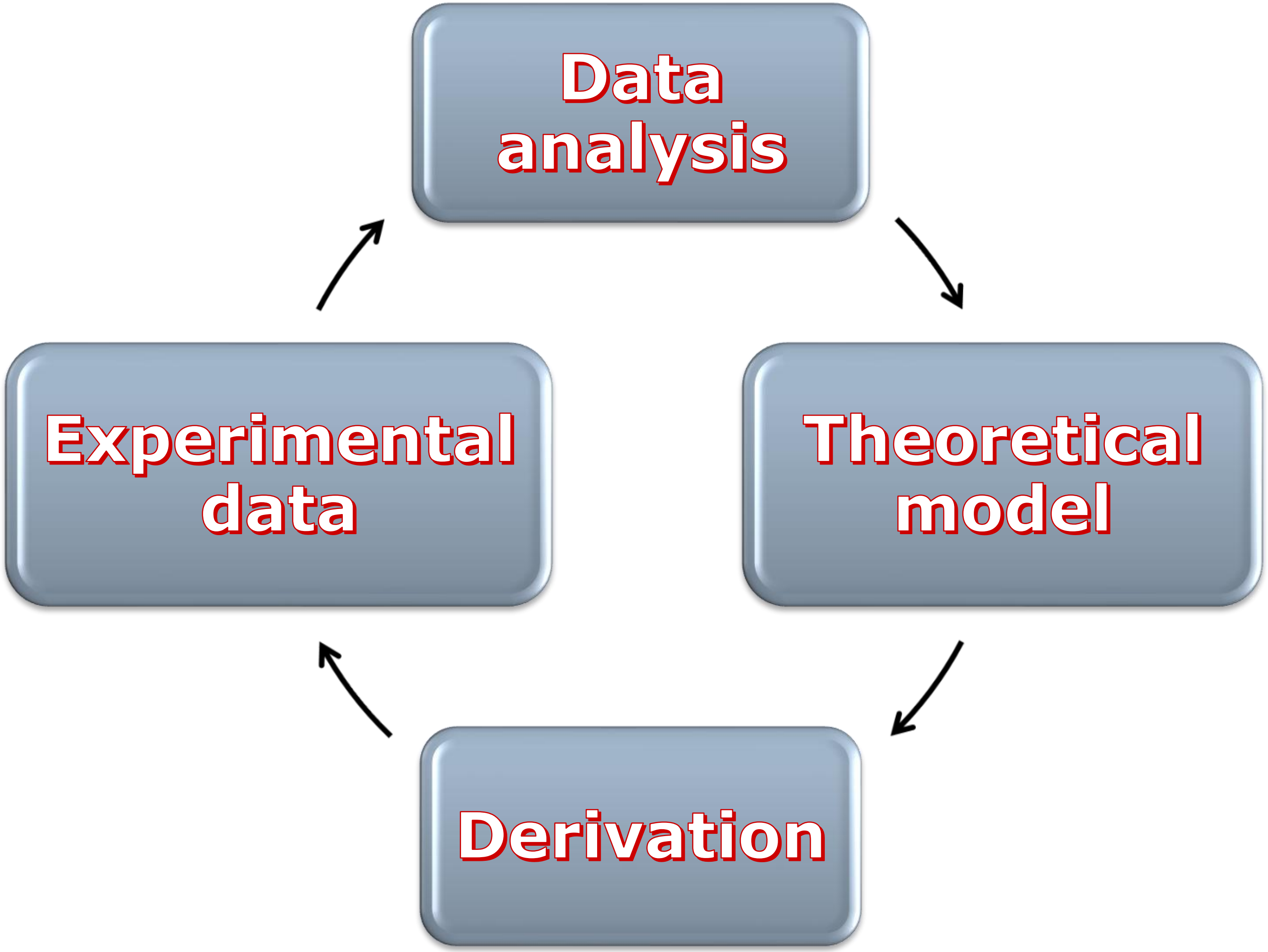
The circle of scientific discovery

From data to model



From model to data

Outline

I. From data to model

II. From model to data

III. Summary and outlook

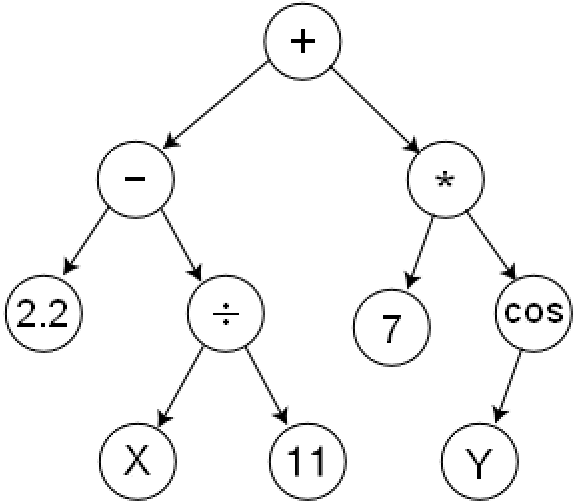
Symbolic Regression

➢ Definition

Symbolic regression (SR) is a machine learning method designed to automatically discover, through algorithms, a functional expression that effectively describes the relationships between variables in a given dataset, without prescribing the specific form of the function.

Kepler

From Manual to Automated



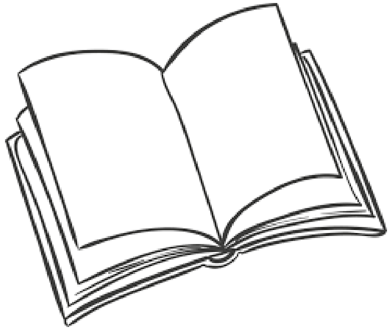
$$\left(2.2 - \left(\frac{X}{11}\right)\right) + \left(7 * \cos(Y)\right)$$

Genetic programming SR

Funsearch

➢ Funsearch--Beyond Knowledge Retrieval:

- **FunSearch's Goal: Leverage the LLM's creativity to solve complex, open scientific problems requiring rigorous discovery.**
- **FunSearch marks a paradigm shift in LLM applications: from retrieving known knowledge to creating new knowledge.**



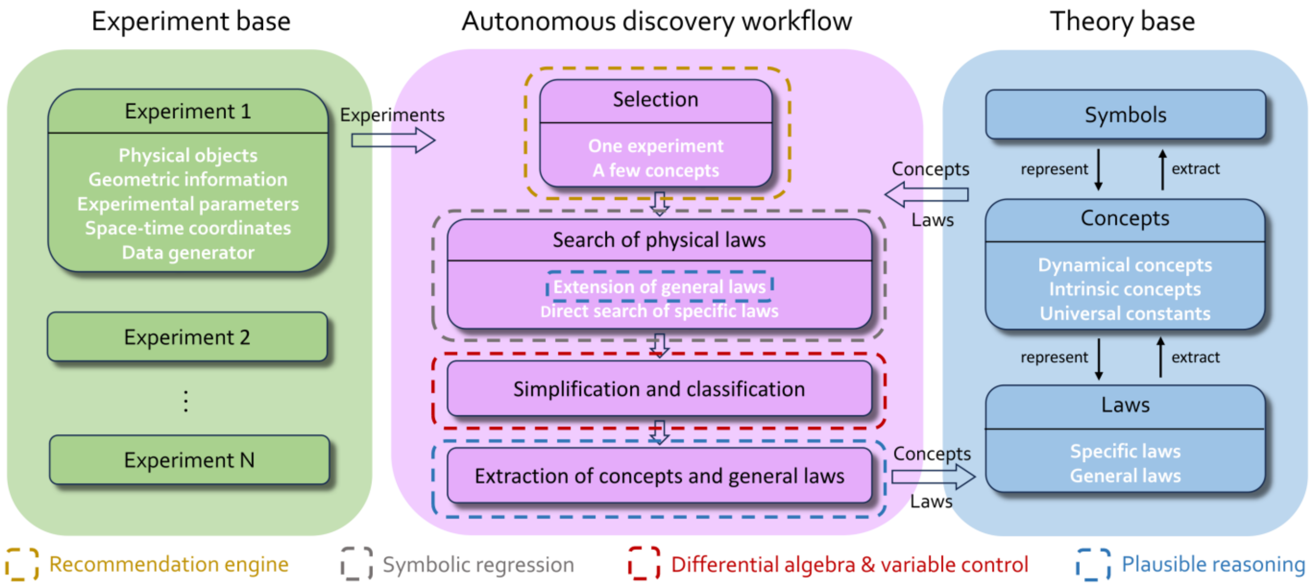
Retrieving known knowledge

Traditional LLM

Creating new knowledge

Funsearch

AI-Newton's architecture



Fang, et al., 2504.01538

- **Knowledge base** (experiment + theory):

  stores and manages structured knowledge

- **Knowledge representation**:

  employs a physical domain specific language(DSL)

- **Autonomous discovery workflow**:

  continuously explores physical laws,

  collaboratively updates both general and specific knowledge

core: physical concepts

core: plausible reasoning

1. Effectively represent knowledge;
2. Reduce search space

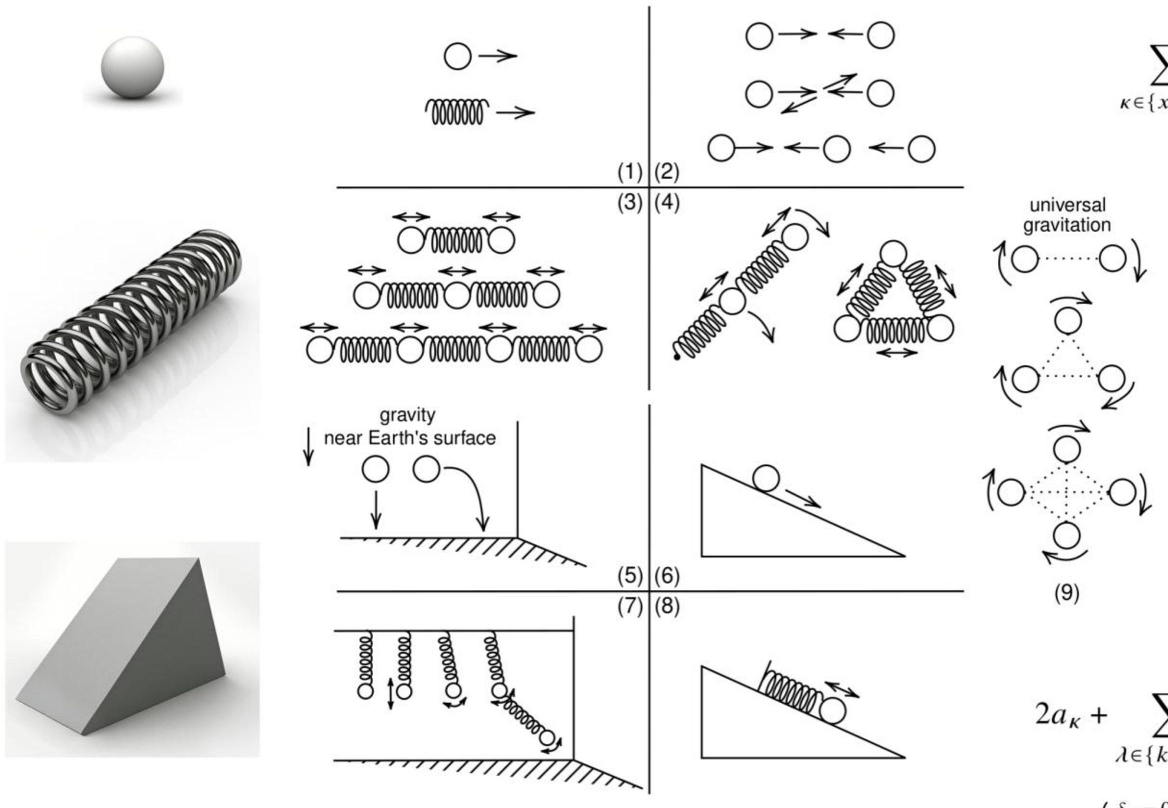
Tests and results

- ➢ **Based on noisy data, important natural laws are discovered!**
- ➢ **Unsupervised! Without prior physical knowledge!**

Fang, et al., 2504.01538

Physical objects

Schematic of experiments



Discovered important general laws

Energy conservation

$$\sum_{\kappa\in\{x,y,z\}} T_\kappa + \sum_{\lambda\in\{k,g,G\}} \delta_\lambda V_\lambda = \text{const.},$$

where T_κ and V_λ are defined as:

$$T_\kappa = \sum_{i\in\text{Particles}} m_i v_{i,\kappa}^2,$$

$$V_k = \sum_{i\in\text{Springs}} k_i (L_i - L_{0,i})^2,$$

$$V_g = \sum_{i\in\text{Particles}} 2 m_i g z_i,$$

$$V_G = \sum_{i,j\in\text{Particles}} 2\left(-\frac{G m_i m_j}{r_{ij}}\right).$$

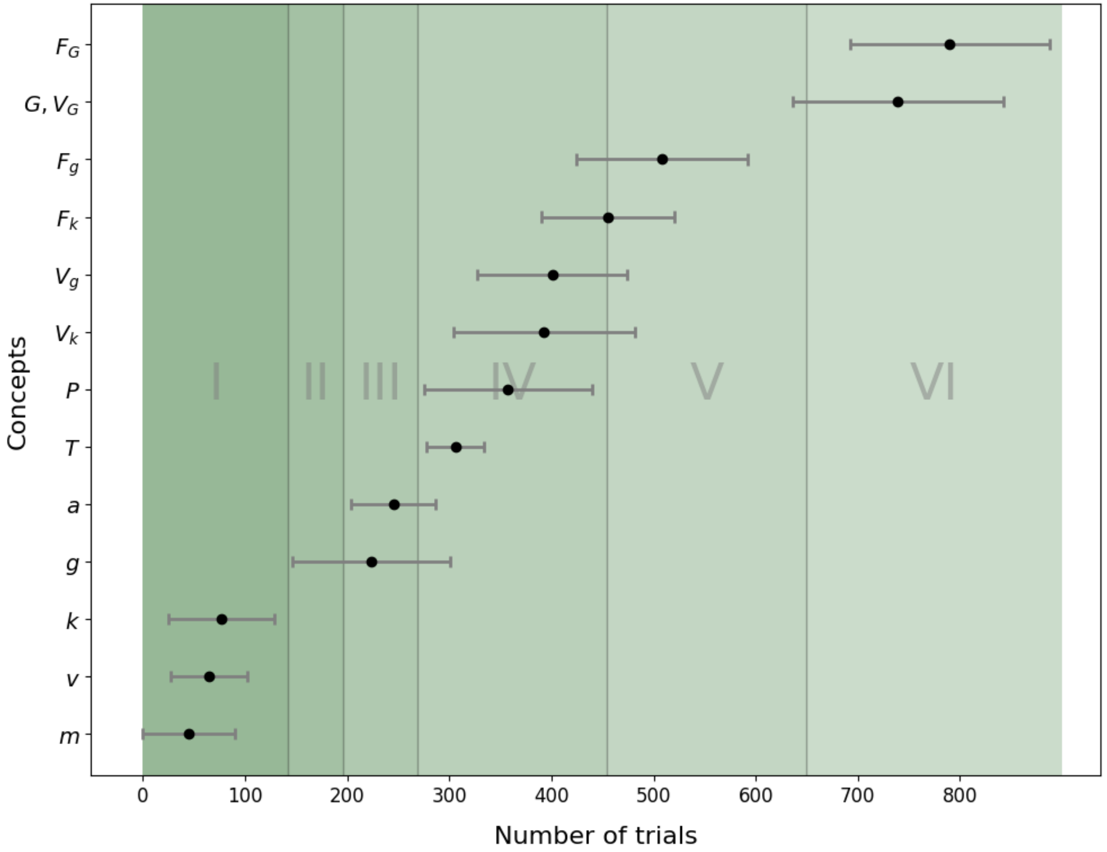
Newton's second law

$$2a_\kappa + \sum_{\lambda\in\{k,g,G\}} \delta_\lambda \left(\frac{1}{m}\frac{\partial V_\lambda}{\partial \kappa}\right) = 0, \quad \kappa\in\{x,y,z\}.$$

($\delta_\lambda = 0$ or 1, determined spontaneously during instantiation as specific laws in experiments)

Tests and results

➢ **Statistical analysis of concept discovery timing:**



Fang, et al., 2504.01538

(Roman numerals for era numbering)

➢ **Incremental progression, diversity**

Laws of quantum physics

➢ Gap between classical and quantum system

- Collapse: No continuous measurement, only “in” and “out” states
- Uncertainty principle: No exact position, only distributions, eigenvalues…
- Nonlocality: Local measurement cannot provide complete information

➢ Key difficulty

- Need to construct an evolutional (continuous) theory based on discrete data, i.e., only “in” and “out” states
- Is the evolution kernel unique ?

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Challenges for scientific AI

- **LLMs' reliability often drops in scientific problem-solving**
- **Prioritize perfect performance over cost control**

- Caused from the inherent complexity of natural sciences
  - Long, multi-step and unstructured reasoning
  - Modeling of real-world scenarios
  - Understanding of fundamental laws
  - Implicit constraints
  - Deterministic & probabilistic, precise & approximate
  - …

- Hard to detect due to logical leaps in the provided answers
  - Both human and AIs alike tend to omit steps they consider "obvious"

How to address this issue?

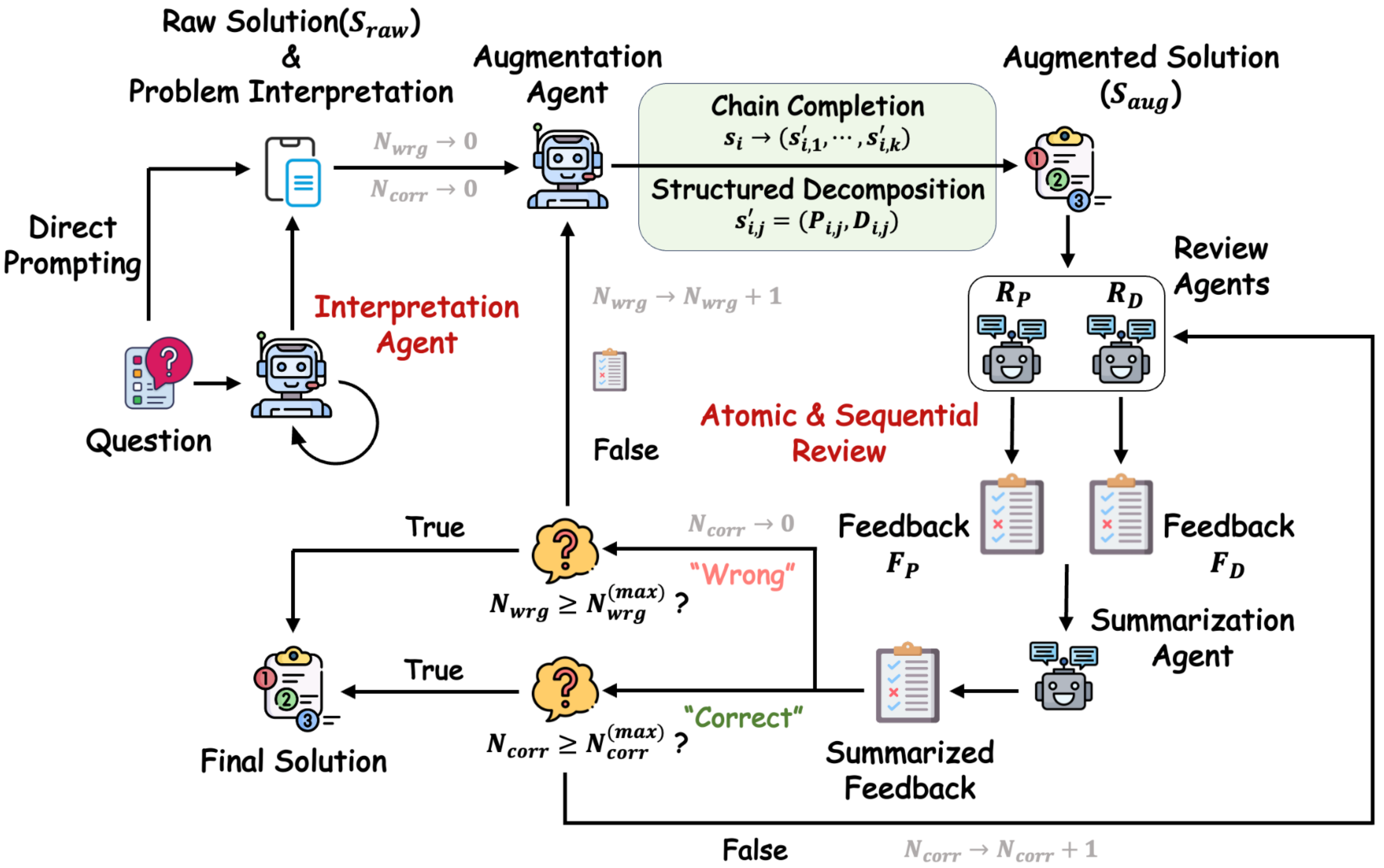
- Human expert review & refine
  - Slow and expensive, hard to scale

- AI: e.g., Logical Chain Augmentation (LOCA)
  - Enforcing logical completeness and structurally decomposing reasoning steps into verifiable principles and derivations, within an augment-and-review loop

Fang et al., 2510.01249
Jian et al., 2511.10515

Overview of LOCA-R's pipeline

Jian et al., 2511.10515



Example: raw answer with logical leaps

➢ For the following question

Question

There is now an electrolyte with thickness L in the z direction, infinite in the x direction, and infinite in the y direction. The region where $y > 0$ is electrolyte 1, and the region where $y < 0$ is electrolyte 2. The conductivities of the two dielectrics are σ_1, σ_2, and the dielectric constants are $\varepsilon_1, \varepsilon_2$, respectively. On the xOz interface of the two dielectrics, two cylindrical holes with a radius R are drilled in the z direction, spaced $2D$ ($D > R, R, D \ll L$) apart, with centers located on the interface as long straight cylindrical holes. Two cylindrical bodies $\pm$ are inserted into the holes, with the type of the cylinders given by the problem text below.

The cylindrical bodies $\pm$ are metal electrodes filling the entire cylinder. Initially, the system is uncharged, and at $t = 0$, a power source with an electromotive force U and internal resistance r_0 is used to connect the electrodes. Find the relationship between the current through the power source and time, denoted as $i(t)$.

- Non-atomicity
- Implicit justification

➢ The raw answer is

Raw Answer

Given the potential difference u, it can be seen:

$$\varphi_+ = u/2, \varphi_- = -u/2, \lambda = \frac{2\pi(\varepsilon_1+\varepsilon_2)\varphi_+}{2\xi_+} = \frac{\pi(\varepsilon_1+\varepsilon_2)u}{\text{arccosh(D/R)}}$$

Select a surface encapsulating the cylindrical surface and examine Gauss's theorem. For the positive electrode, it is easy to see:

$$\iint \vec{E}\cdot d\vec{S} = L\oint \vec{E}\cdot\hat{n}dl = \frac{\lambda L}{(\varepsilon_1+\varepsilon_2)/2} = \frac{2\pi uL}{2\text{arccosh}(D/R)}$$

Since the above potential distribution is deemed directly applicable for the calculation of current, the total current flowing out of the positive electrode is:

$$I = \iint \sigma\vec{E}\cdot d\vec{S} = \frac{\sigma_1+\sigma_2}{2}\times\frac{2\pi uL}{2\text{arccosh}(D/R)}$$

Given the current i passing through the power source, this current changes the net charge:

$$\frac{d(\lambda L)}{dt} = i - I = i - \frac{2\pi uL}{2\text{arccosh}(D/R)} = \frac{\pi(\varepsilon_1+\varepsilon_2)L}{2\text{arccosh}(D/R)}\frac{du}{dt}$$

According to the loop voltage drop equation:

$$U = r_0 i + u \to u = U - r_0 i$$

$$\to i - \frac{\pi(\sigma_1+\sigma_2)L}{2\text{arccosh}(D/R)}(U - r_0 i) = -\frac{\pi(\varepsilon_1+\varepsilon_2)L}{2\text{arccosh}(D/R)}r_0\frac{di}{dt}$$

$$\to \frac{di}{dt} = \frac{(\sigma_1+\sigma_2)U}{r_0(\varepsilon_1+\varepsilon_2)} - \left(\frac{\sigma_1+\sigma_2}{\varepsilon_1+\varepsilon_2} + \frac{2\text{arccosh}(D/R)}{\pi r_0 L(\varepsilon_1+\varepsilon_2)}\right)i$$

At time $t = 0$, all current should preferentially enter the capacitor. At this time, the initial current is U/r_0, and this differential equation yields:

$$i(t) = \frac{U}{r_0\left(1+\frac{2\text{arccosh}(D/R)}{\pi r_0 L(\sigma_1+\sigma_2)}\right)}\left\{2 + \frac{2\text{arccosh}(D/R)}{\pi r_0 L(\sigma_1+\sigma_2)} - \exp\left[-\left(\frac{\sigma_1+\sigma_2}{\varepsilon_1+\varepsilon_2} + \frac{2\text{arccosh}(D/R)}{\pi r_0 L(\varepsilon_1+\varepsilon_2)}\right)\right]\right\}$$

Example: complete and structured answer

➢ The complete and structured answer with logical rigor

Refined Answer 1

Problem Statement Explanation

The problem describes a physical system composed of two semi-infinite electrolytes, separated by the xOz plane.
- **Electrolyte 1**: Occupies the region $y > 0$, with electrical conductivity σ_1 and dielectric constant (permittivity) ε_1.

- **Electrolyte 2**: Occupies the region $y < 0$, with conductivity σ_2 and permittivity ε_2.

Two long, parallel cylindrical metal electrodes, denoted as $+$ and $-$, are placed within this system.

- **Geometry**: The electrodes are of radius R and length L. They are oriented parallel to the z-axis. Their centers lie on the xOz interface and are separated by a distance of $2D$.

- **Assumptions**: The geometry satisfies the conditions $D > R$ and $\{R, D\} \ll L$. The latter condition allows us to neglect end effects and treat the problem as two-dimensional in the xy-plane, with total quantities (like capacitance and resistance) being proportional to the length L.

At time $t = 0$, this system is connected to a power source.

- **Power Source**: An ideal electromotive force (EMF) U with a constant internal resistance r_0.

- **Initial Condition**: The system is initially uncharged, meaning the potential difference across the electrodes is zero at $t = 0$.

The goal is to find the current $i(t)$ flowing from the power source as a function of time.

Step 1: Equivalent Circuit Model

The physical system can be modeled as a simple electrical circuit. The two electrodes immersed in the electrolytes act as a capacitor, storing charge, and simultaneously as a resistor, allowing a leakage current to flow between them through the conductive medium.

- The capacitive nature is due to the storage of electric charge on the electrodes when a potential difference is applied, with the electrolytes acting as the dielectric material. Let's denote the equivalent capacitance as C.

- The resistive nature is due to the flow of charge (ions) through the electrolytes under the influence of the electric field, from the positive to the negative electrode. Let's denote the equivalent resistance of the electrolytes as R_{elec}.

Since charge can be stored on the electrodes while simultaneously leaking through the medium, the capacitor C and the resistor R_{elec} are in parallel. This parallel combination is connected in series with the internal resistance r_0 of the power source with EMF U.

Step 2: Derivation of the System's Capacitance

The total capacitance is the sum of the capacitances of the upper and lower halves of the system, which are connected in parallel.

First, we state the standard formula for the capacitance per unit length, C', between two parallel cylindrical conductors of radius R with centers separated by a distance $2D$ in a uniform dielectric medium with permittivity ε.

$$\boxed{C' = \frac{\pi\varepsilon}{\operatorname{arccosh}(D/R)}}$$

In our problem, the upper half-space ($y > 0$) is filled with electrolyte 1 (ε_1), and the lower half-space ($y < 0$) is filled with electrolyte 2 (ε_2). Due to the symmetry of the electric field about the $y = 0$ plane, we can consider this as two capacitors in parallel.

- C_1: Capacitance of the upper half, in a medium with permittivity ε_1.

- C_2: Capacitance of the lower half, in a medium with permittivity ε_2.

The capacitance per unit length for each half is:

$$C'_1 = \frac{\pi\varepsilon_1}{\operatorname{arccosh}(D/R)} \quad (1)$$

$$C'_2 = \frac{\pi\varepsilon_2}{\operatorname{arccosh}(D/R)} \quad (2)$$

The total capacitance per unit length, C'_{total}, is the sum of the parallel contributions.

$$\boxed{C'_{total} = C'_1 + C'_2}$$

The total capacitance C for the electrode length L is then derived.

$$C'_{total} = \frac{\pi\varepsilon_1}{\operatorname{arccosh}(D/R)} + \frac{\pi\varepsilon_2}{\operatorname{arccosh}(D/R)} = \frac{\pi(\varepsilon_1+\varepsilon_2)}{\operatorname{arccosh}(D/R)} \quad (3)$$

$$C = C'_{total} \cdot L = \frac{\pi(\varepsilon_1+\varepsilon_2)L}{\operatorname{arccosh}(D/R)} \quad (4)$$

Step 3: Derivation of the System's Resistance Similarly, the total resistance of the electrolyte is determined by the two parallel paths for current flow through the upper and lower electrolytes.

For a system with a given geometry, the resistance R and capacitance C in a homogeneous medium are related.

$$\boxed{RC = \frac{\varepsilon}{\sigma}}$$

We can apply this relation to each half of our system. - R_1: Resistance of the upper electrolyte with conductivity σ_1. - R_2: Resistance of the lower electrolyte with conductivity σ_2.

$$R_1 = \frac{\varepsilon_1}{\sigma_1 C_1} = \frac{\varepsilon_1}{\sigma_1(C'_1 L)} = \frac{\varepsilon_1}{\sigma_1 L}\frac{\operatorname{arccosh}(D/R)}{\pi\varepsilon_1} = \frac{\operatorname{arccosh}(D/R)}{\pi\sigma_1 L} \quad (5)$$

$$R_2 = \frac{\varepsilon_2}{\sigma_2 C_2} = \frac{\varepsilon_2}{\sigma_2(C'_2 L)} = \frac{\varepsilon_2}{\sigma_2 L}\frac{\operatorname{arccosh}(D/R)}{\pi\varepsilon_2} = \frac{\operatorname{arccosh}(D/R)}{\pi\sigma_2 L} \quad (6)$$

Since the current can flow through both electrolytes simultaneously, these two resistances are in parallel. The total equivalent resistance of the electrolyte, R_{elec}, is given by:

$$\boxed{\frac{1}{R_{elec}} = \frac{1}{R_1} + \frac{1}{R_2}}$$

Example: complete and structured answer

➢ The complete and structured answer with logical rigor

$$\frac{1}{R_{elec}} = \frac{\pi\sigma_1 L}{\operatorname{arccosh}(D/R)} + \frac{\pi\sigma_2 L}{\operatorname{arccosh}(D/R)} = \frac{\pi(\sigma_1+\sigma_2)L}{\operatorname{arccosh}(D/R)} \tag{7}$$

$$R_{elec} = \frac{\operatorname{arccosh}(D/R)}{\pi(\sigma_1+\sigma_2)L} \tag{8}$$

Step 4: Formulation of the Governing Differential Equation

Let $i(t)$ be the current from the source and $u(t)$ be the potential difference across the electrodes. Applying Kirchhoff's Voltage Law to the circuit loop:

$$\boxed{U = i(t)r_0 + u(t)}$$

The current $i(t)$ from the source splits into two paths in the parallel combination: a charging current $i_C(t)$ for the capacitor and a leakage current $i_R(t)$ through the resistor.

$$\boxed{i(t) = i_C(t) + i_R(t)}$$

The currents $i_C(t)$ and $i_R(t)$ are defined by the properties of the capacitor and resistor:

$$\boxed{i_C(t) = C\frac{du}{dt}}$$

$$\boxed{i_R(t) = \frac{u(t)}{R_{elec}}}$$

Combining these, we get a differential equation relating $i(t)$ and $u(t)$.

$$i(t) = C\frac{du}{dt} + \frac{u(t)}{R_{elec}} \tag{9}$$

To find an equation solely for $i(t)$, we eliminate $u(t)$. From the loop law, $u(t) = U - i(t)r_0$. Differentiating with respect to time gives $\frac{du}{dt} = -r_0\frac{di}{dt}$. Substituting these into Eq. equation 9:

$$\begin{aligned} i &= C\left(-r_0\frac{di}{dt}\right) + \frac{U - ir_0}{R_{elec}} \\ i &= -Cr_0\frac{di}{dt} + \frac{U}{R_{elec}} - \frac{r_0}{R_{elec}}i \\ Cr_0\frac{di}{dt} &= \frac{U}{R_{elec}} - i\left(1 + \frac{r_0}{R_{elec}}\right) \\ \frac{di}{dt} &= \frac{U}{Cr_0R_{elec}} - \left(\frac{1}{Cr_0} + \frac{1}{CR_{elec}}\right)i \end{aligned} \tag{10}$$

This is a first-order linear ordinary differential equation for $i(t)$.

Step 5: Solving the Differential Equation The differential equation equation 10 is of the form $\frac{di}{dt} + Bi = A$.

$$\boxed{\frac{dy}{dt} + P(t)y = Q(t) \implies y(t) = e^{-\int P(t)dt}\left(\int Q(t)e^{\int P(t)dt}dt + K\right)}$$

For our constant-coefficient case, the general solution is $i(t) = i_{ss} + i_h(t) = A/B + Ke^{-Bt}$, where i_{ss} is the steady-state current and K is a constant determined by the initial condition.

$$B = \frac{1}{Cr_0} + \frac{1}{CR_{elec}} = \frac{r_0 + R_{elec}}{Cr_0R_{elec}} \tag{11}$$

$$i_{ss} = \frac{A}{B} = \frac{U/(Cr_0R_{elec})}{(r_0+R_{elec})/(Cr_0R_{elec})} = \frac{U}{r_0+R_{elec}} \tag{12}$$

The initial condition at $t = 0$ is that the system is uncharged, so $u(0) = 0$. From the loop law, $U = i(0)r_0 + u(0)$, which gives the initial current:

$$i(0) = \frac{U}{r_0} \tag{13}$$

Applying this to the general solution at $t = 0$:

$$\begin{aligned} i(0) &= i_{ss} + Ke^0 \\ \frac{U}{r_0} &= \frac{U}{r_0+R_{elec}} + K \\ K &= \frac{U}{r_0} - \frac{U}{r_0+R_{elec}} = U\frac{(r_0+R_{elec}) - r_0}{r_0(r_0+R_{elec})} = \frac{UR_{elec}}{r_0(r_0+R_{elec})} \end{aligned} \tag{14}$$

Substituting i_{ss}, K, and B back into the solution gives $i(t)$:

$$i(t) = \frac{U}{r_0+R_{elec}} + \frac{UR_{elec}}{r_0(r_0+R_{elec})}\exp\left(-\frac{r_0+R_{elec}}{Cr_0R_{elec}}t\right) \tag{15}$$

Final Answer

The relationship between the current through the power source and time, $i(t)$, is found by substituting the expressions for the equivalent capacitance C (Eq. equation 4) and resistance R_{elec} (Eq. equation 8) into the general solution (Eq. equation 15).

The steady-state current is:

$$i_{ss} = \frac{U}{r_0+R_{elec}} = \frac{U}{r_0 + \frac{\operatorname{arccosh}(D/R)}{\pi(\sigma_1+\sigma_2)L}}$$

The decay constant in the exponent is:

$$B = \frac{1}{CR_{elec}} + \frac{1}{Cr_0} = \frac{\sigma_1+\sigma_2}{\varepsilon_1+\varepsilon_2} + \frac{\operatorname{arccosh}(D/R)}{\pi r_0(\varepsilon_1+\varepsilon_2)L}$$

The final expression for the current $i(t)$ is:

$$\boxed{i(t) = \frac{U}{r_0 + \frac{\operatorname{arccosh}(D/R)}{\pi(\sigma_1+\sigma_2)L}} + \left(\frac{U}{r_0} - \frac{U}{r_0 + \frac{\operatorname{arccosh}(D/R)}{\pi(\sigma_1+\sigma_2)L}}\right)\exp\left[-\left(\frac{\sigma_1+\sigma_2}{\varepsilon_1+\varepsilon_2} + \frac{\operatorname{arccosh}(D/R)}{\pi r_0(\varepsilon_1+\varepsilon_2)L}\right)t\right]} \tag{8}$$

The CPhO: a challenging testbed

- **The Chinese Physics Olympiad (CPhO): a premier national physics competition organized annually in China**

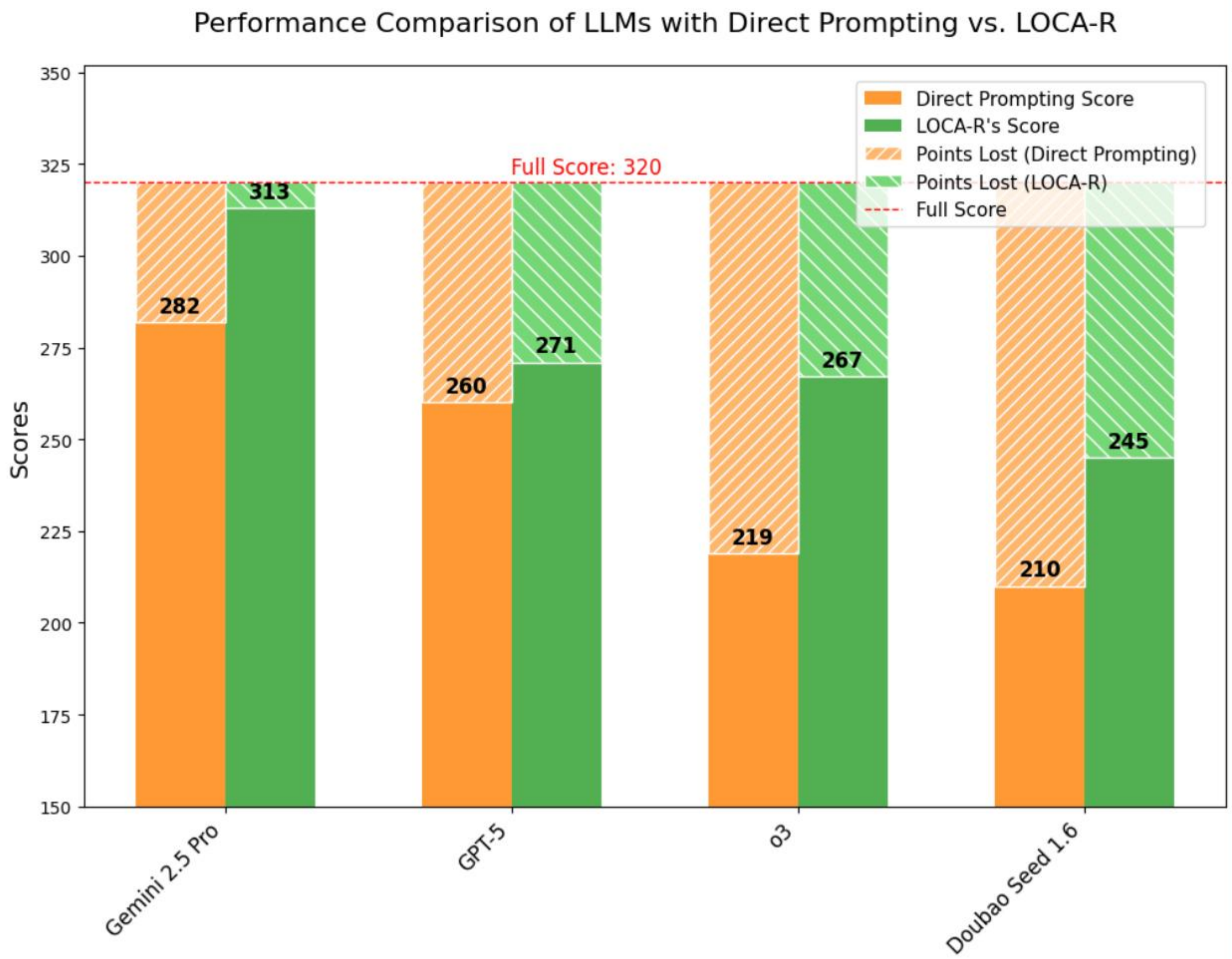
- **For our evaluation, we focus on the theory examination of the 42nd CPhO 2025 (final round held in Fuzhou at the end of October)**

  - Demands of long, multi-step reasoning
  - Multimodal problems
  - No data contamination issue

Overall performance across various base LLMs

Jian et al., 2511.10515

➢ **Overall performance of LOCA-R on four mainstream LLMs**



Comparison across more baseline methods

Jian et al., 2511.10515

➢ Comparison of LOCA-R and more baselines

Table 1: **Comparison across baseline methods.** Gemini 2.5 Pro is used for all cases, and results are presented as the score of each theory problem, the total score of all 7 theory problems and the error rate defined in Eq. 7. Bold indicates the best performance. LOCA-R consistently achieves the highest score and the lowest error rate.

Method	1	2	3	4	5	6	7	Total Score	Error Rate
Human's highest	-	-	-	-	-	-	-	204	36%
Direct Prompting	45	41	45	33	39	39	40	282	12%
Zero-Shot-CoT	45	37	45	45	45	38	40	295	7.8%
Few-Shot CoT	45	45	45	41	45	42	39	302	5.6%
ToT	45	45	45	41	45	40	39	300	6.3%
GoT	45	34	20	36	45	39	39	258	19%
MAD	45	33	42	43	45	44	40	292	8.8%
Self-refine	45	43	45	35	39	41	40	288	10%
PSN	45	32	39	43	45	43	45	292	8.8%
LOCA-R (ours)	45	45	45	45	45	43	45	**313**	**2.2%**

Summary and outlook

- Human scientific discovery necessitates a new research paradigm, AI may help

- From data to theory:
  - Plenty of ideas proposed
  - Surpasses human experts in many topics

- From theory to data:
  - AI surpasses human experts for established fields
  - AI improves fast for frontier fields

- AI for scientific discovery: remains in its nascent stage, but very promising

Thank you !