Scientific Equation Discovery using Modular Symbolic Regression via Vision-Language Guidance

Sepideh Fatemi[1], Abhilash Neog[1], Emma Marchisin[2], Amartya Dutta[1], Medha Sawhney[1], Paul C Hanson[2], Anuj Karpatne[1]

[1]Virginia Tech, [2]University of Wisconsin Madison

Problem Statement

- ❑ Symbolic Regression (SR) seeks explicit analytic equations that explain data.
- ❑ Traditional SR treats equations as monolithic and lacks structure.
- ❑ Can we model complex physical systems which require equations that are **interpretable**, **scientifically grounded**, and **computationally efficient?**

Motivation

❑ Why Vision-Language Models?

Vision–Language Models translate the process diagram into physics-aware seed equation.

❑ Why Large-Language Models?

LLM-powered Symbolic Regression (LLM-SR[1]) pairs the reasoning of large language models with symbolic regression to rapidly uncover physics-consistent equations.

❑ Why Modular?

A modular design breaks the final equation into reusable sub-functions, so each physical process can be inspected, a swapped with other processes.

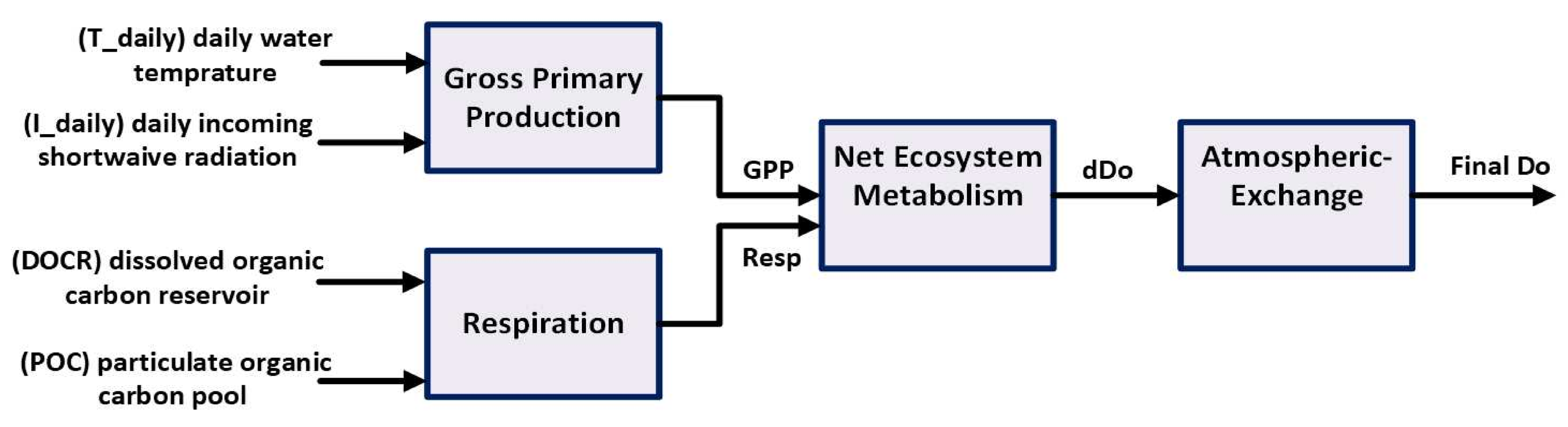
Why it matters — Accurately modeling complex physical systems demands equations that are interpretable, scientifically sound, and computationally tractable. Traditional methods rarely deliver all three.

Datasets

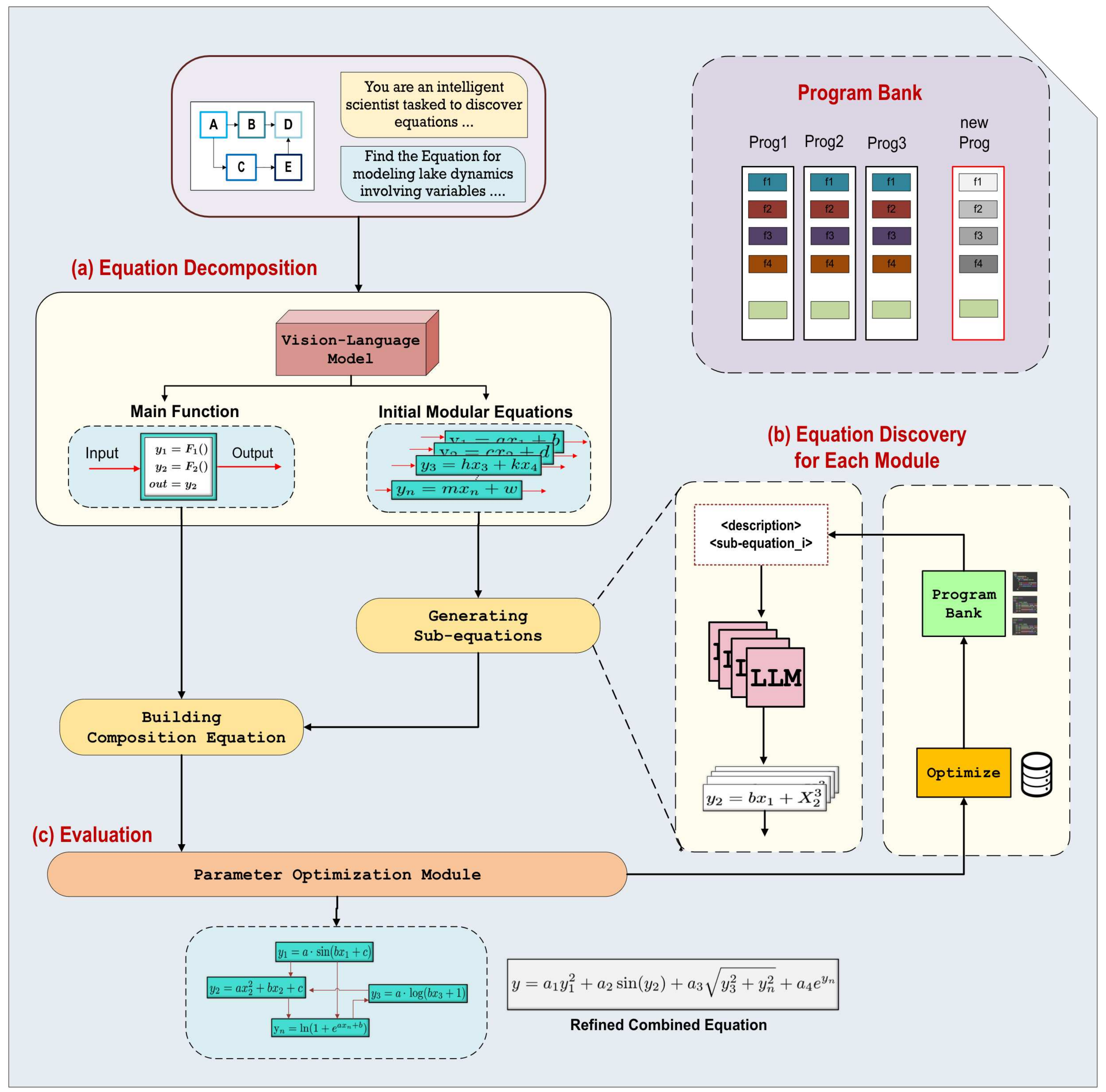
Synthetic:
Math logic

Real-world:
Lake DO simulation (environmental dynamics)

Expert-provided box and arrow diagram:



Proposed Approach



Key Contribution:

- ❑ **Modular Structure:** Decompose equations into interpretable components.
- ❑ **Integration of Domain Knowledge:** Enhance interpretability and accuracy with scientific insights.
- ❑ **Scalable Discovery:** Handle larger solution spaces via modular decomposition.
- ❑ **Vision-Language Guidance:** Multimodal models aid equation discovery and validation.

Results

Interpretability: Each equation module corresponds to a real-world scientific process, making the final model easy to interpret and validate.

Step-by-Step Reasoning: The system builds equations incrementally, reasoning one sub-process at a time, just like how scientists break down complex systems.

VLM generated output

Gross Primary Production

```
def gross_primary_production(T_daily, I_daily, params):
    return params[0] * T_daily + params[1] * I_daily +
    params[2]
```

Respiration

```
def respiration(DOCR, POC, params):
    return params[0] * DOCR + params[1] * POC + params[2]
```

Net Ecosystem Metabolism

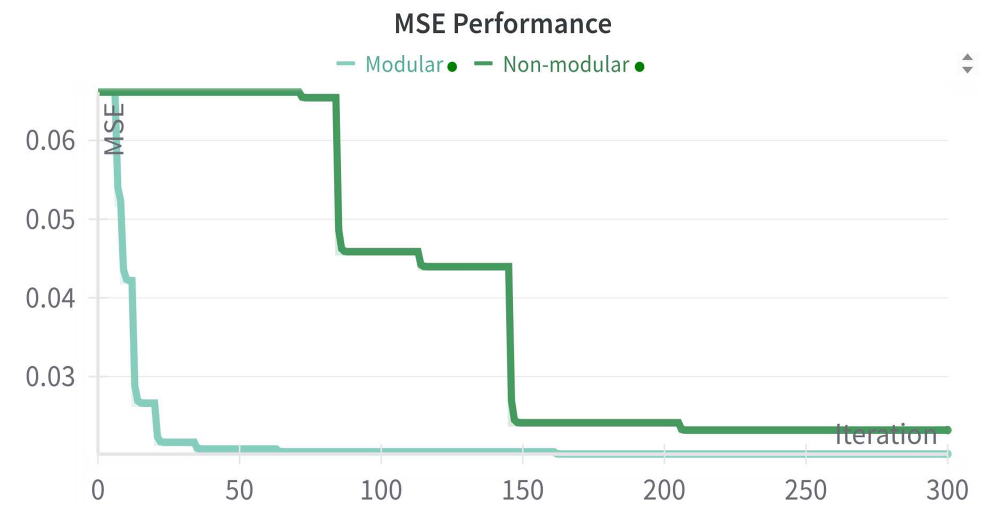
```
def net_ecosystem_metabolism(GPP, Resp, params):
    return params[0] * GPP - params[1] * Resp + params[2]
```

Atmospheric Exchange

```
def atmospheric_exchange(dDO, params):
    return params[0] * dDO + params[1]
```

Main Equation

```
def main_equation(I_daily, T_daily, POC, DOCR, params):
    GPP = gross_primary_production(T_daily, I_daily,
    params[0])
    Resp = respiration(DOCR, POC, params[1])
    dDO = net_ecosystem_metabolism(GPP, Resp, params[2])
    DO_exchange = atmospheric_exchange(dDO, params[3])
    return DO_exchange
```



Comparing Modular vs Non-modular on different datasets.

Model	Lake Modeling	Math Logic
VLM(gpt-4o)	0.0661	0.1885
Modular-SR w/o modules	0.0241	0.01560
Modular-SR	**0.0201**	**2.8e10-12**

Future Work & Discussion

- ✓ Extend to other equations and domains
- ✓ Evaluate and refine individual modules
- ✓ Improve explainability and scientific alignment
- ✓ Benchmark across diverse LLMs and VLMs
- ✓ Optimize for time and computational efficiency

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Refrences: [1] Shojaee, Parshin, Kazem Meidani, Shashank Gupta, Amir Barati Farimani, and Chandan K. Reddy. "Llm-sr: Scientific equation discovery via programming with large language models." arXiv preprint arXiv:2404.18400 (2024).