AI for discovery in physics

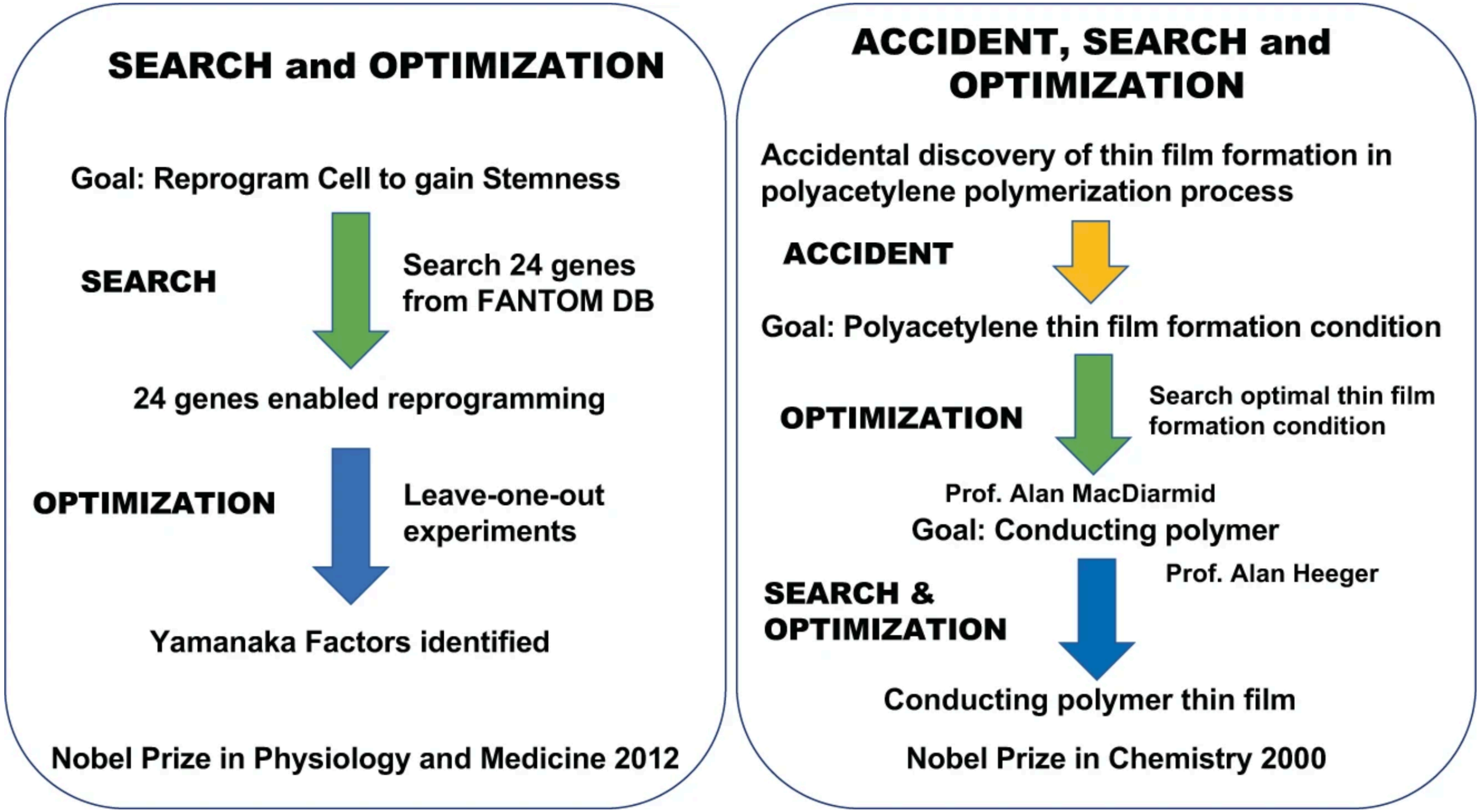
Speaker: Ziming Liu, April 2023

Overview

- AI for discovery frameworks
  - Closed loops
- Concrete things the have been (re)discovered by AI (including my works)
  - Not-yet closed loops, but still useful
- Open questions

“AI + discovery” frameworks

What makes a discovery?



nature > npj systems biology and applications > perspectives > article

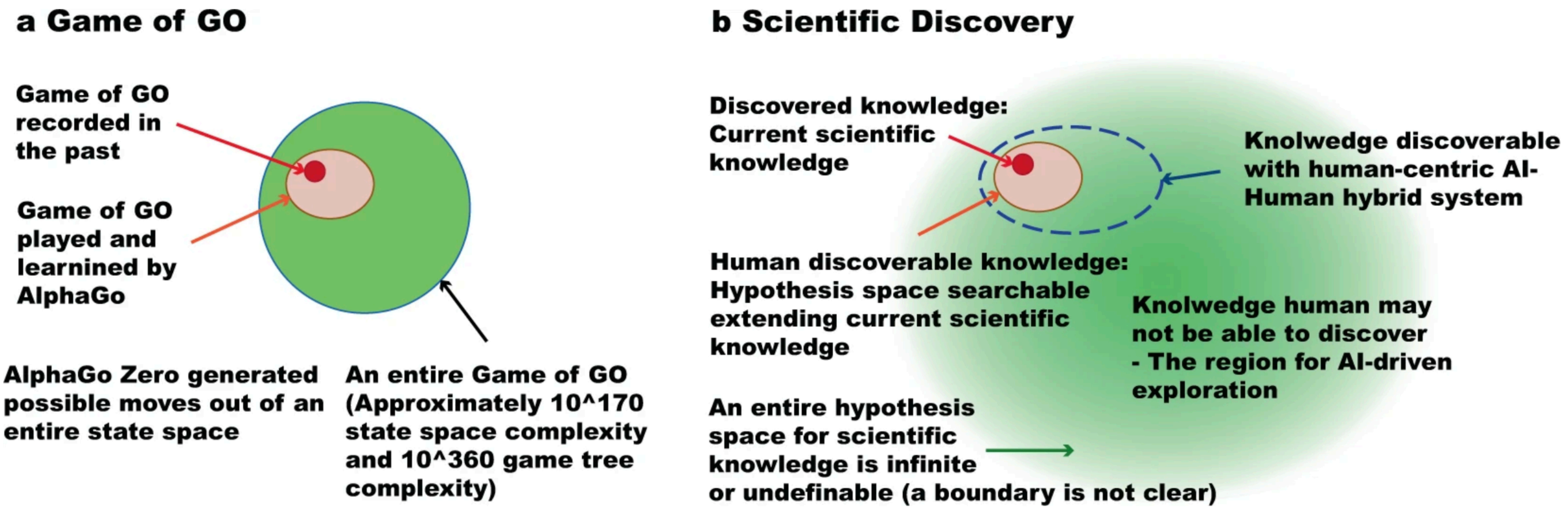
Perspective | Open Access | Published: 18 June 2021

Nobel Turing Challenge: creating the engine for scientific discovery

Hiroaki Kitano

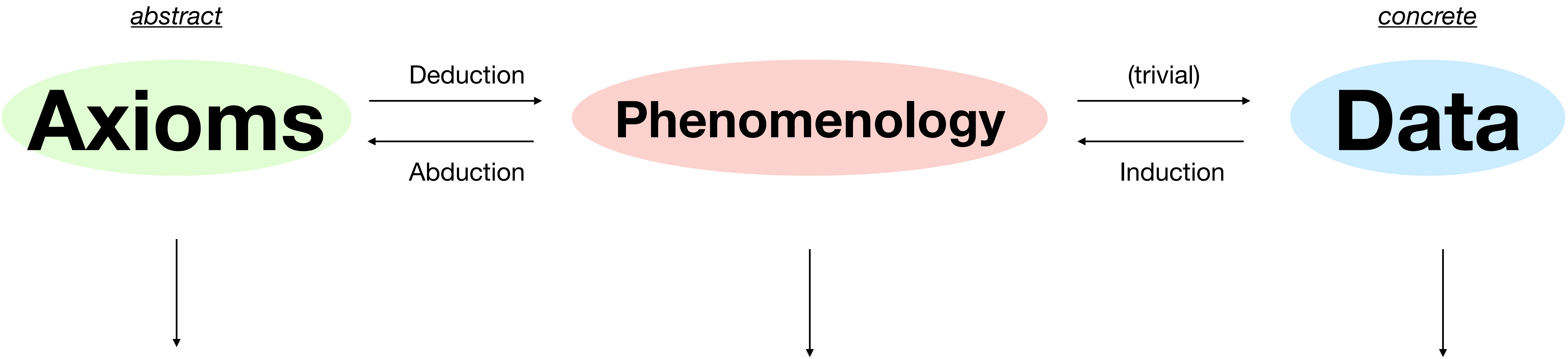
Search and optimization plays a critical role in the process of discovery. Yamanaka's case is interesting because a search was conducted in bioinformatics followed by experiment-driven optimization that may be well suited for AI Scientist in the future.

Why do we need AI for discovery



Search space structures for **a** perfect information games as represented by the Game of GO and **b** scientific discovery are illustrated with commonalities and differences. While the search space for the Game of GO is well-defined, the search space for scientific discovery is open-ended. A practical initial strategy is to augment search space based on current scientific knowledge with human-centric AI-Human Hybrid system. An extreme option is to set search space broadly into distant hypothesis spaces where AI Scientist may discover knowledge that was unlikely to be discovered by the human scientist.

Discovery types

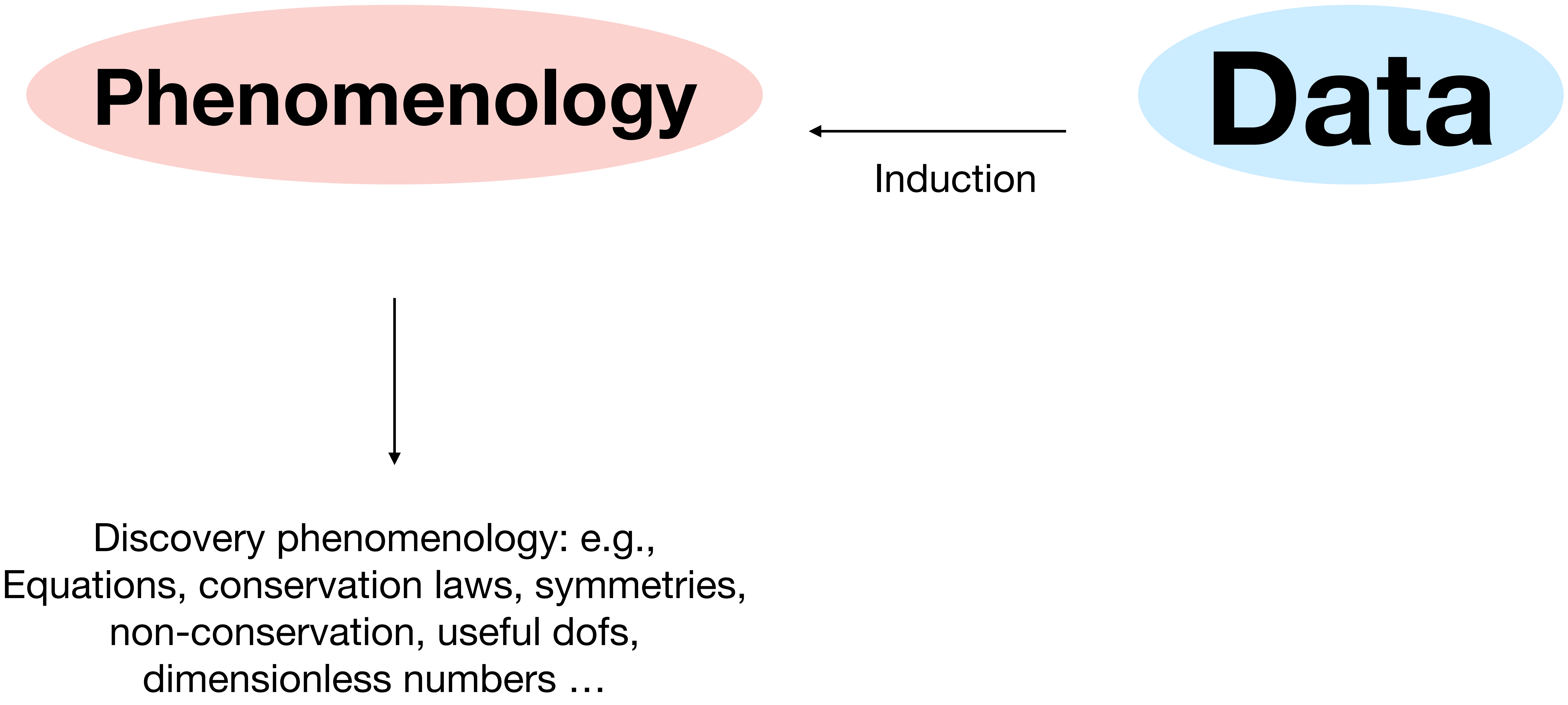


Discovering axioms: very hard!

Discovering phenomenology: e.g.,
Equations, conservation laws, symmetries,
non-conservation, useful dofs,
dimensionless numbers …

Discovering instances: e.g.,
design drugs

Most AI discoveries in physics so far



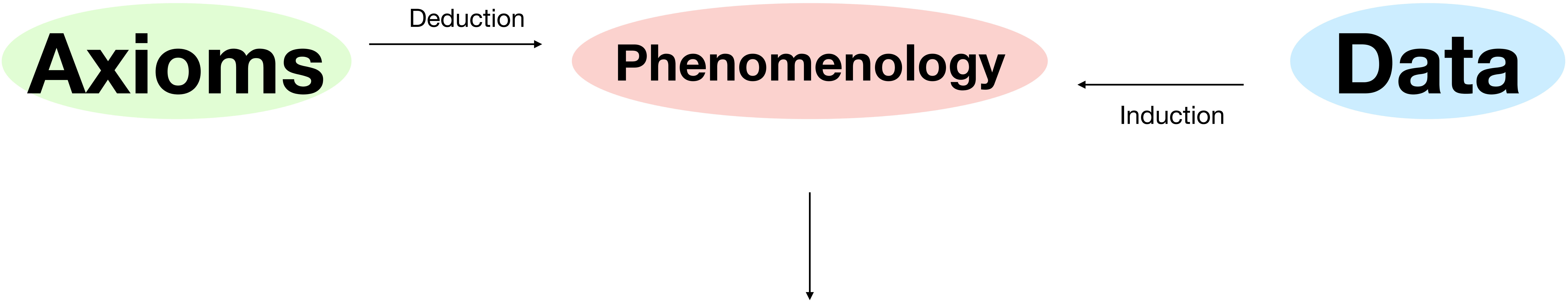
AI Des-cartes

nature › nature communications › articles › article

Article | Open Access | Published: 12 April 2023

Combining data and theory for derivable scientific discovery with AI-Descartes

Cristina Cornelio, Sanjeeb Dash, Vernon Austel, Tyler R. Josephson, Joao Goncalves, Kenneth L. Clarkson, Nimrod Megiddo, Bachir El Khadir & Lior Horesh



Discovery phenomenology: e.g.,
Equations, conservation laws, symmetries,
non-conservation, useful dofs,
dimensionless numbers …

AI Des-cartes

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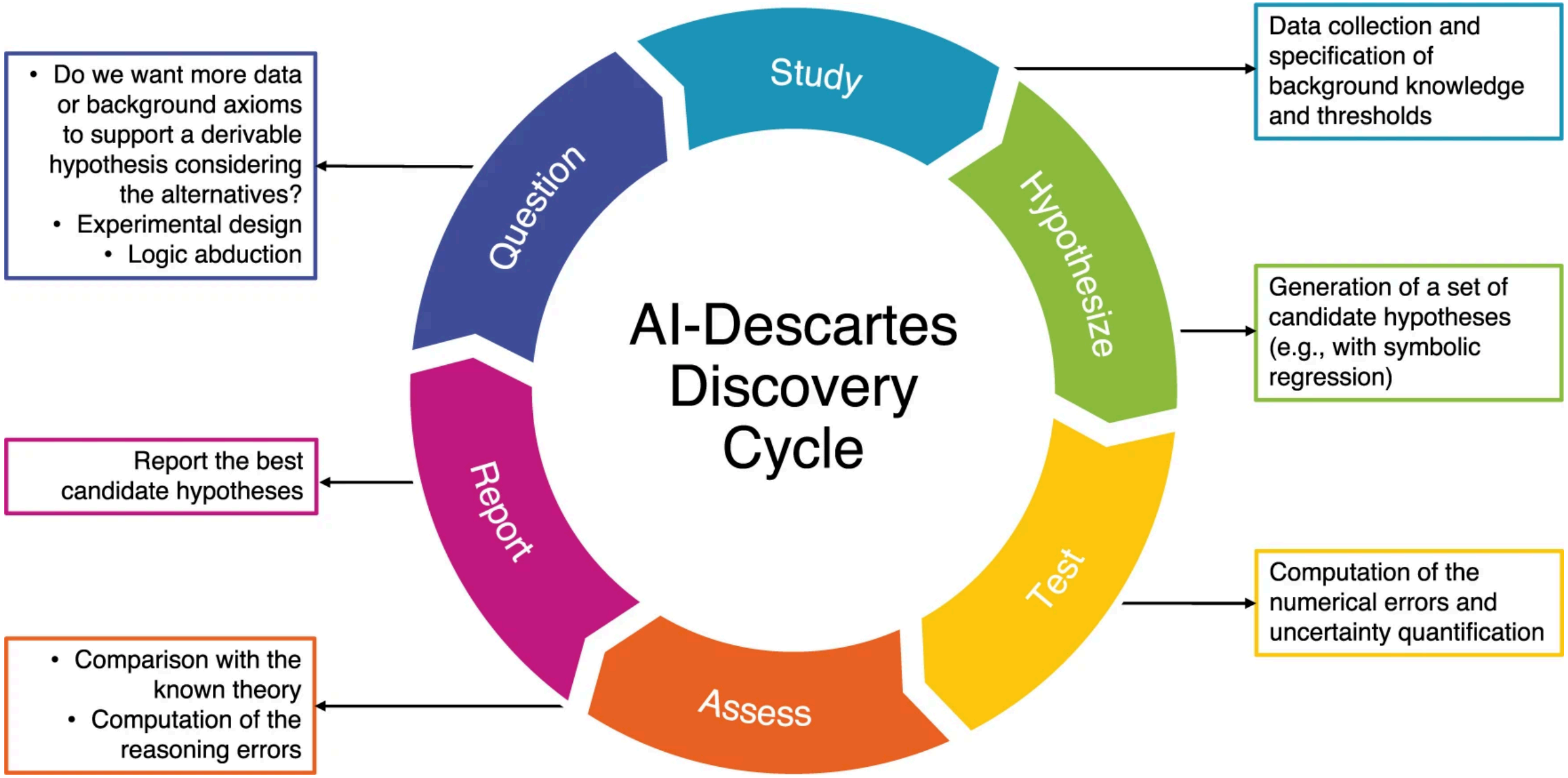

The colors match the respective components of the system in Fig. 3.

AI Des-cartes

Article | Open Access | Published: 12 April 2023

Combining data and theory for derivable scientific discovery with AI-Descartes

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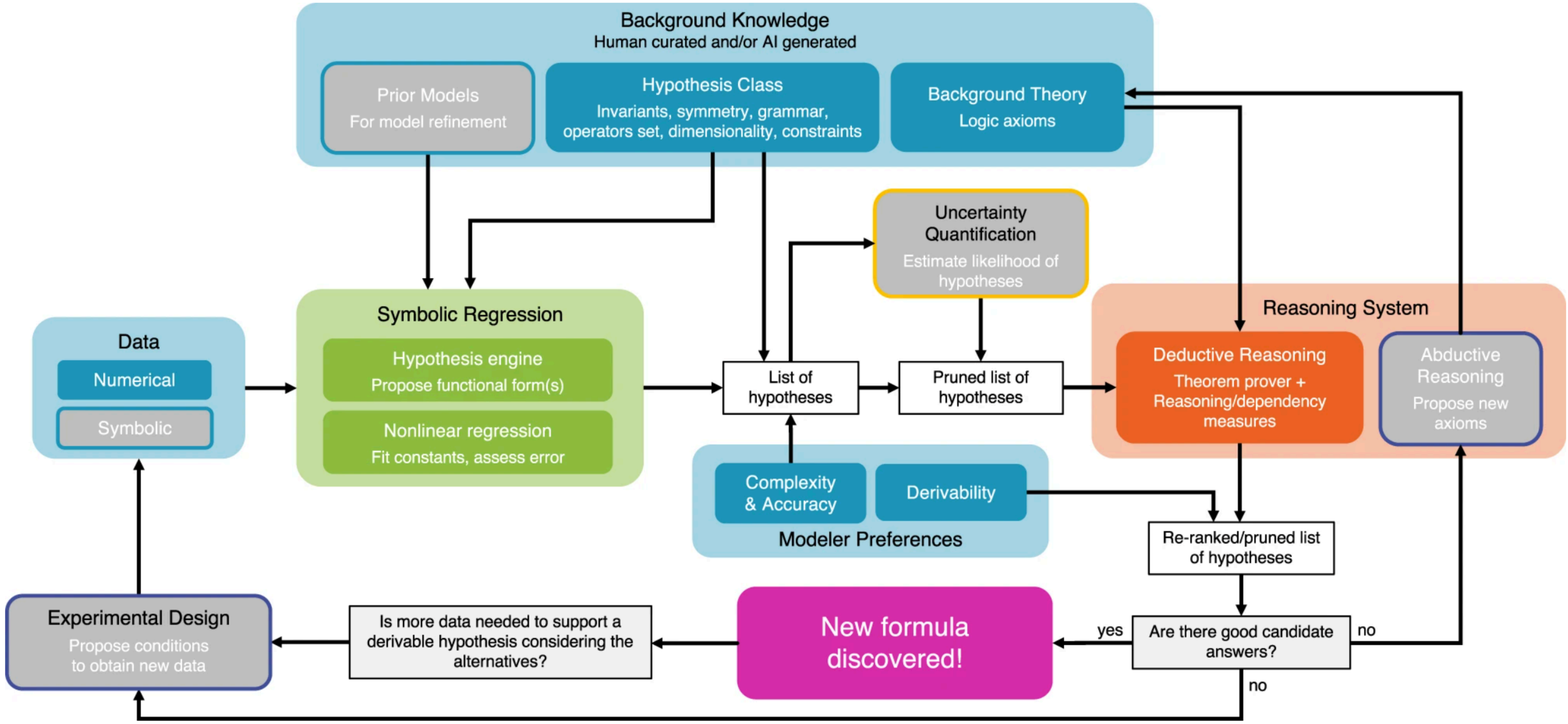

Colored components correspond to our system, and gray components indicate standard techniques for scientific discovery (human-driven or artificial) that have not been integrated into the current system. The colors match the respective components of the discovery cycle of Fig. 2. The present system generates hypotheses from data using symbolic regression, which are posed as conjectures to an automated deductive reasoning system, which proves or disproves them based on background theory or provides reasoning-based quality measures.

AI Physicists

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Toward an artificial intelligence physicist for unsupervised learning

Tailin Wu and Max Tegmark

Phys. Rev. E **100**, 033311 – Published 19 September 2019

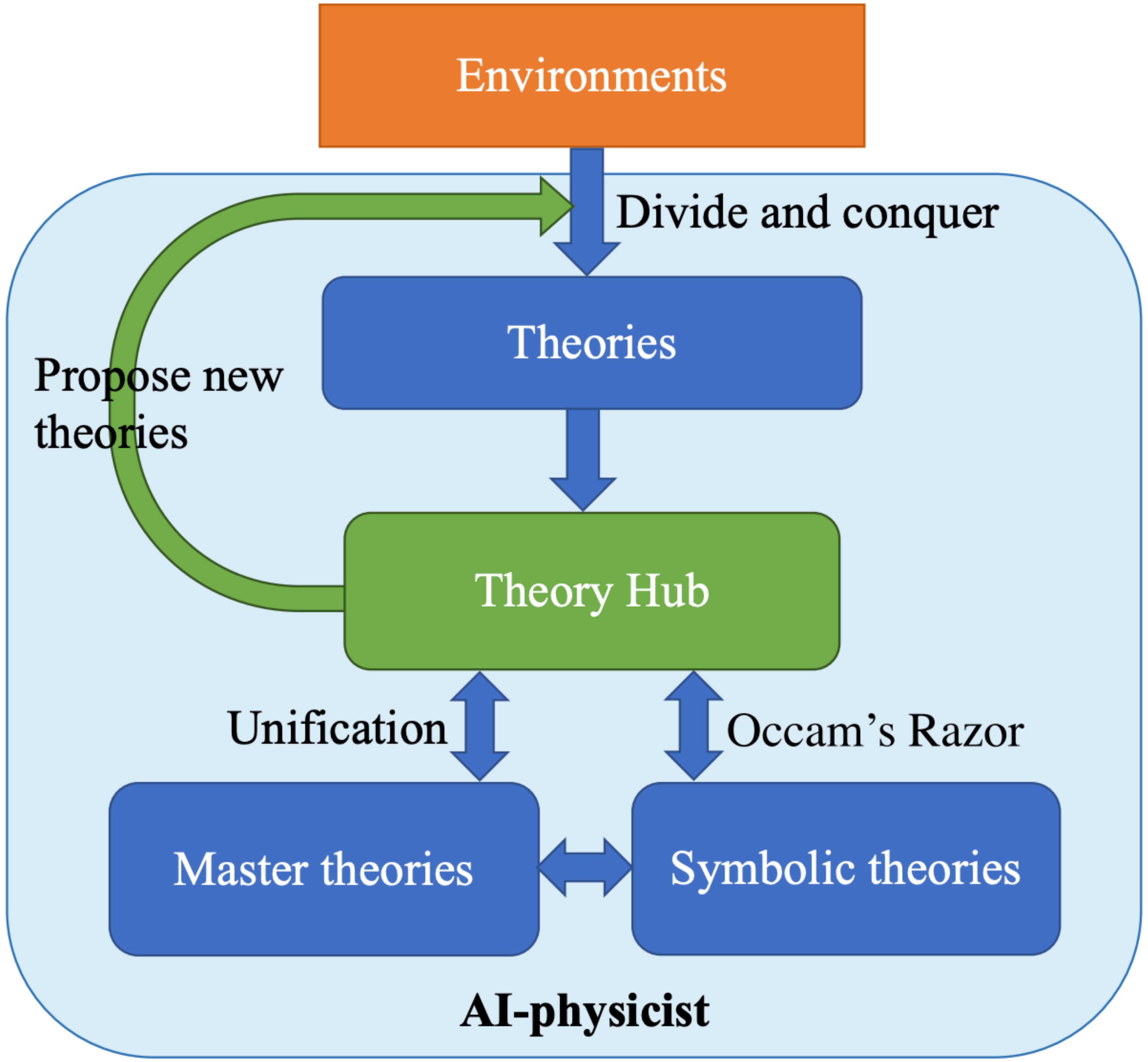


FIG. 1. AI physicist architecture.

TABLE I. AI physicist strategies tested.

Strategy	Definition
Divide and conquer	Learn multiple theories each of which specializes to fit *part* of the data very well
Occam's razor	Avoid overfitting by minimizing description length, which can include replacing fitted constants by simple integers or fractions
Unification	Try unifying learned theories by introducing parameters
Lifelong learning	Remember learned solutions and try them on future problems

AI Physicists

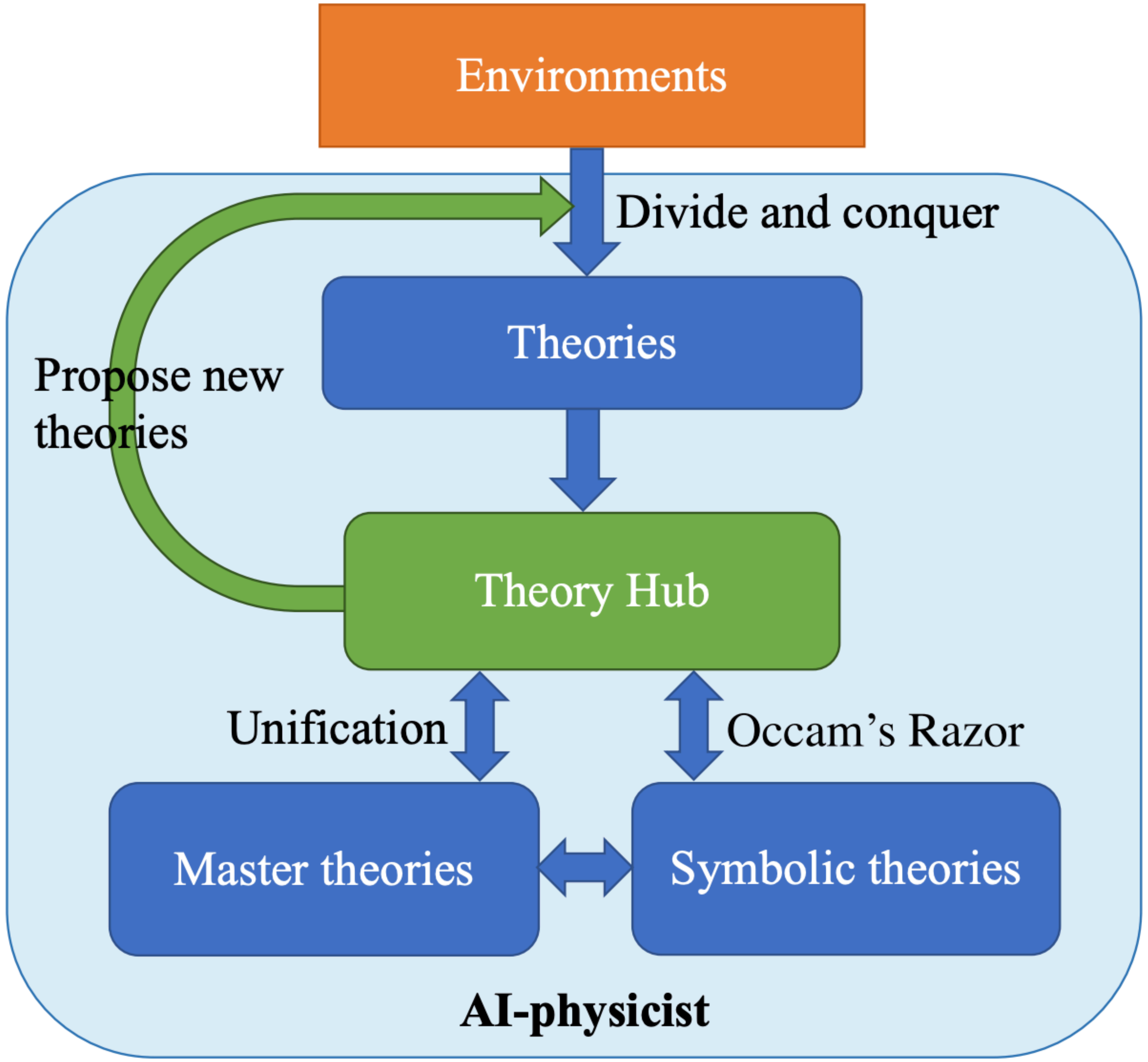
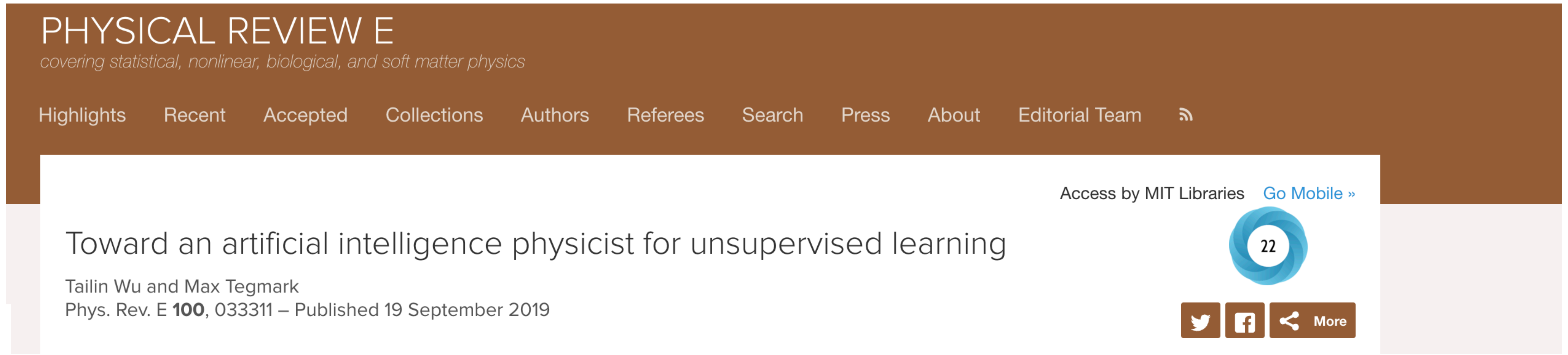


FIG. 1. AI physicist architecture.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Toward an artificial intelligence physicist for unsupervised learning

Tailin Wu and Max Tegmark
Phys. Rev. E **100**, 033311 – Published 19 September 2019

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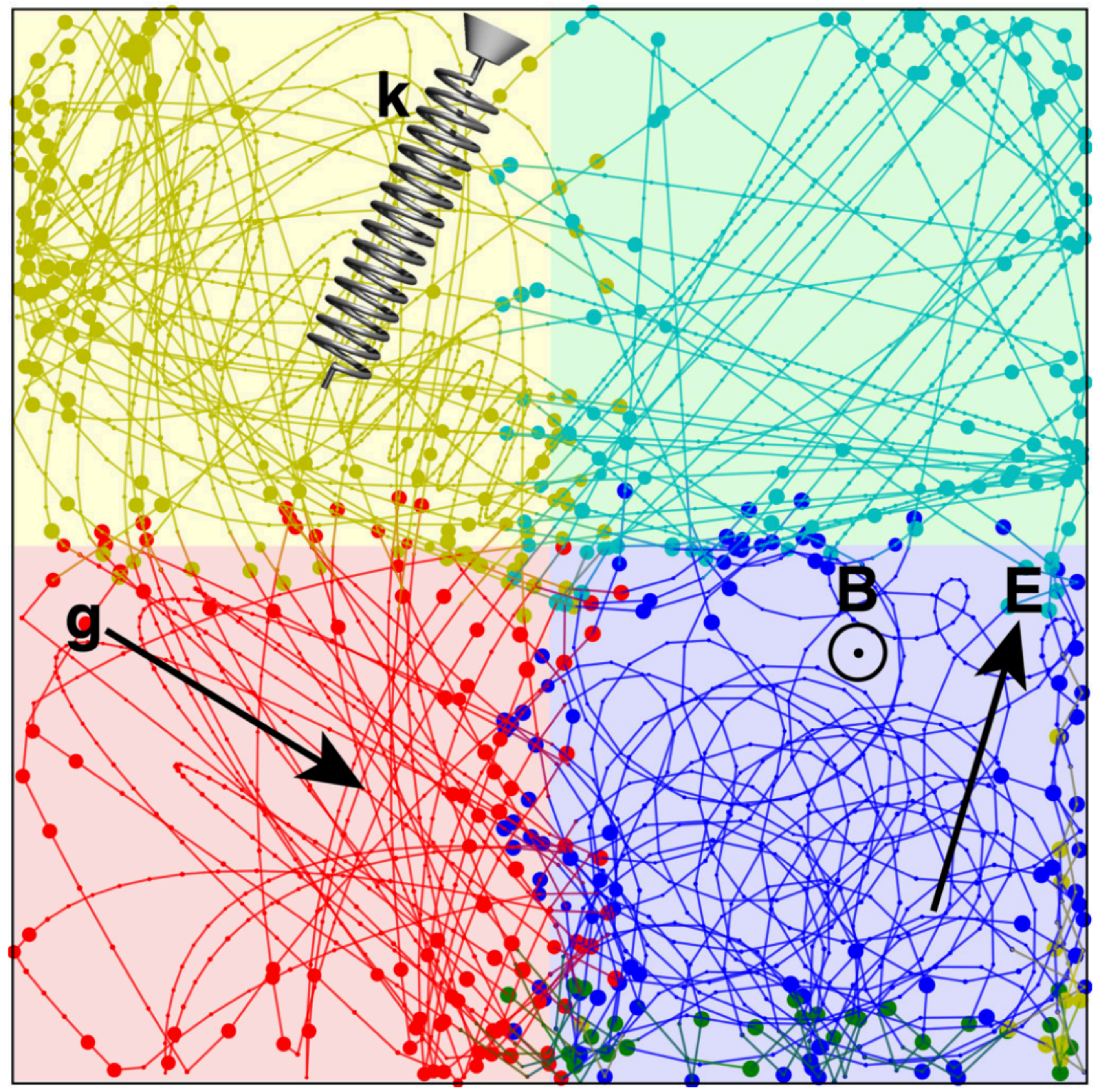


Concrete things (re)discovered by AI

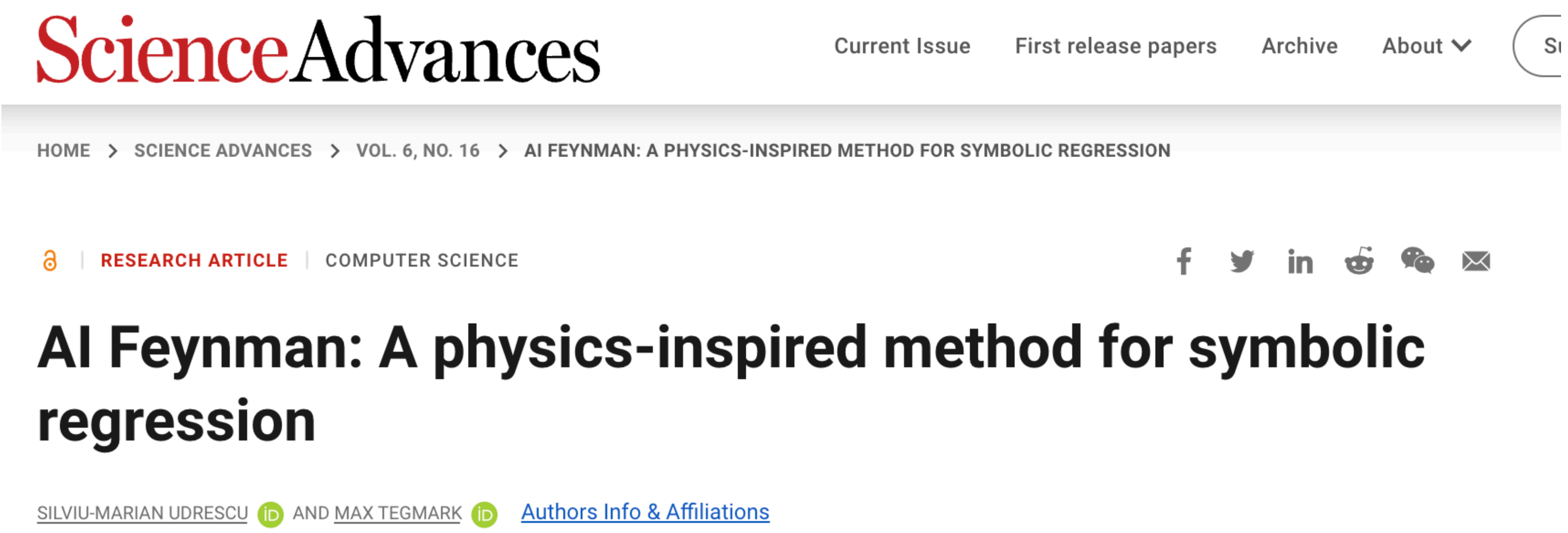
Concrete things (re)discovered by AI

- (Symbolic) Equations: symbolic regression
- Conservation Laws
- Symmetries
- Useful degrees of freedom
- Dimensionless numbers

Symbolic regression

Data Formula

$$\{x_i, y_i\} \rightarrow y = f(x)$$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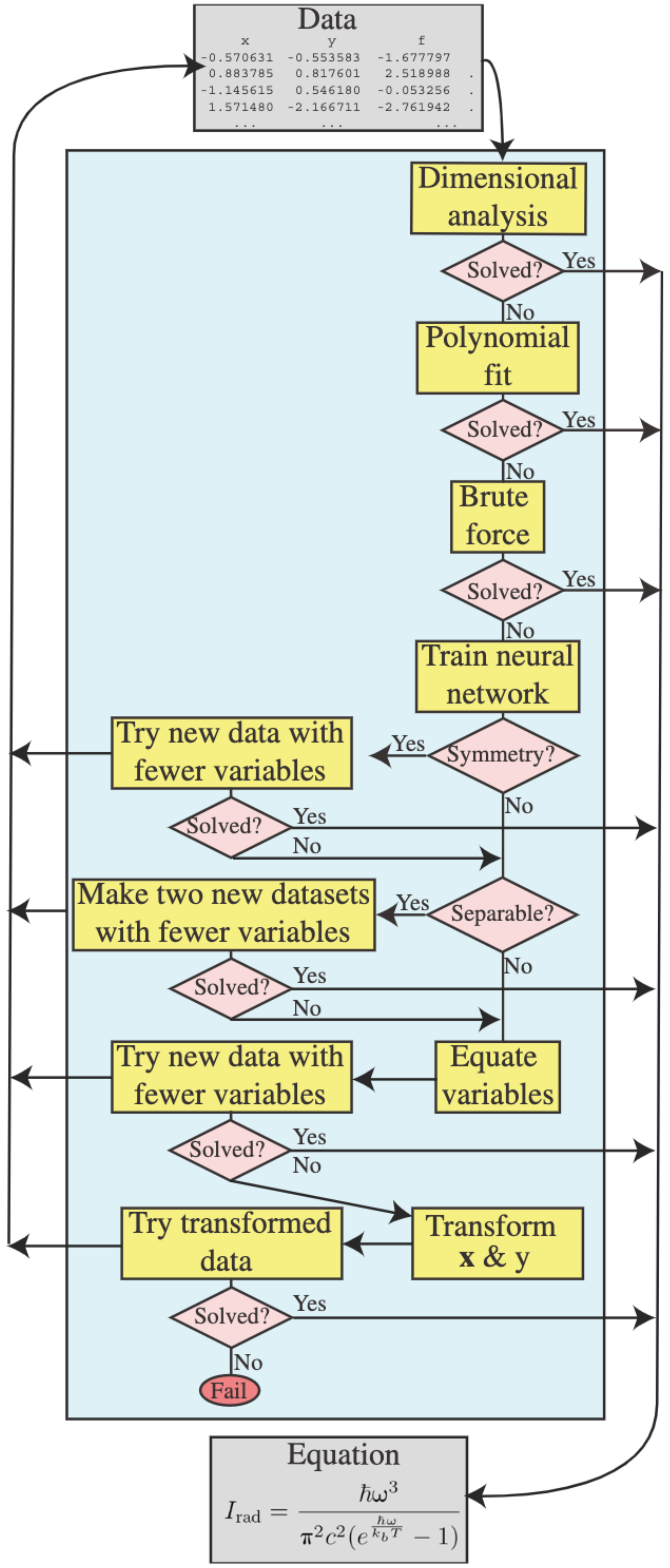
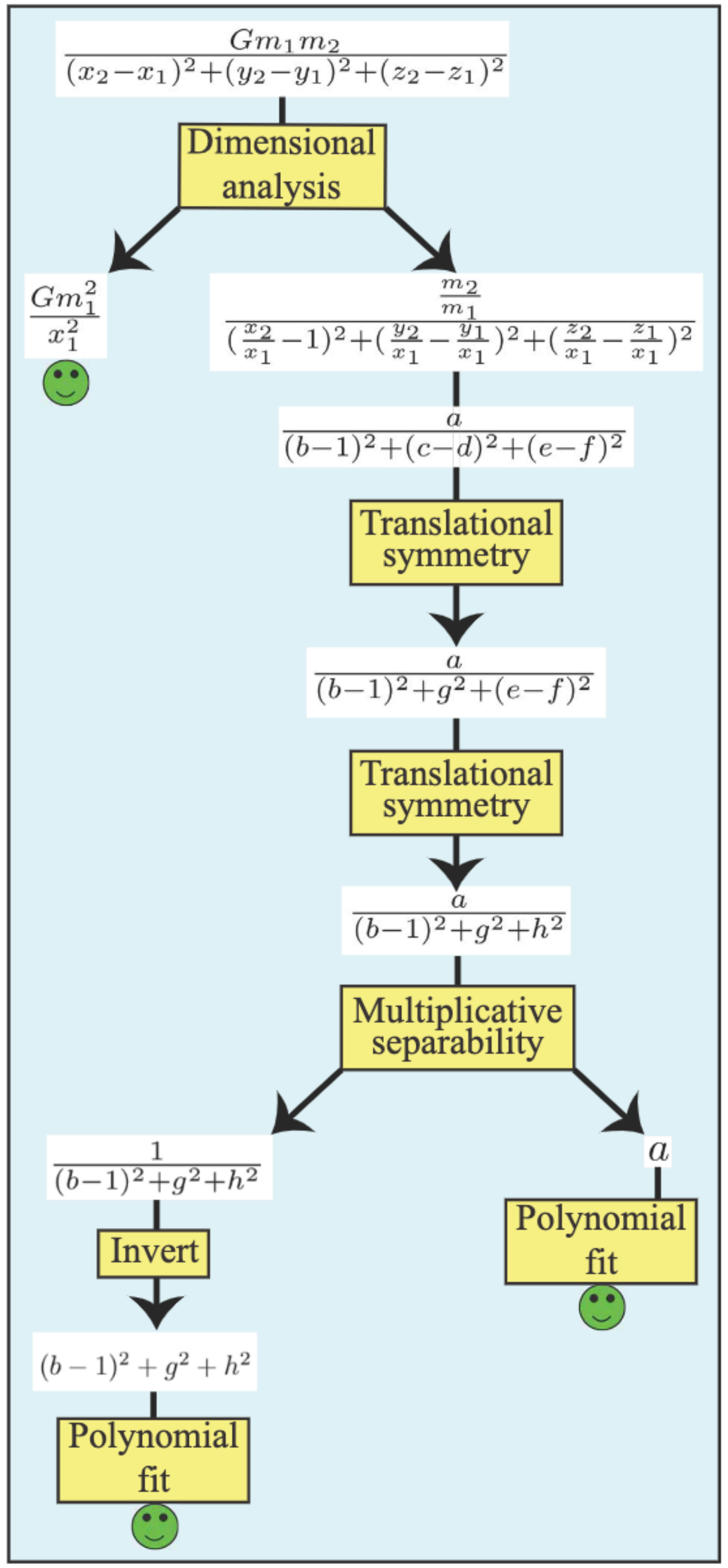
RESEARCH ARTICLE | COMPUTER SCIENCE

AI Feynman: A physics-inspired method for symbolic regression

SILVIU-MARIAN UDRESCU AND MAX TEGMARK Authors Info & Affiliations





Main idea:
Test whether data have desirable/simplifying properties.
If yes, can simplify the original problem to subproblems by leveraging the property.
Divide-and conquer.

Symbolic regression

AI Feynman 2.0: Pareto-optimal symbolic regression exploiting graph modularity

Silviu-Marian Udrescu[1], **Andrew Tan**[1], **Jiahai Feng**[1], **Orisvaldo Neto**[1], **Tailin Wu**[2] **& Max Tegmark**[1,3]
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NeurIPS 2020

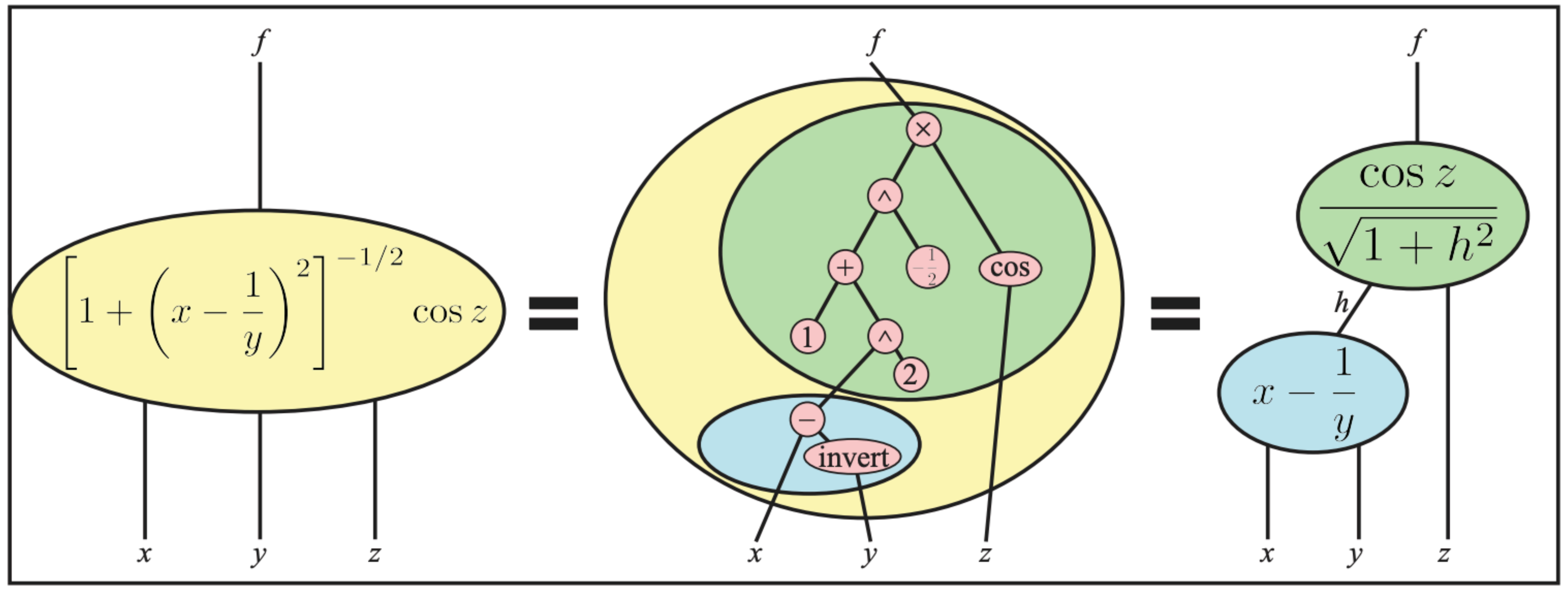


Figure 2: All functions can be represented as tree graphs whose nodes represent a set of basic functions (middle panel). Using a neural network trained to fit a mystery function (left panel), our algorithm seeks a decomposition of this function into others with fewer input variables (right panel), in this case of the form $f(x, y, z) = g[h(x, y), z]$.

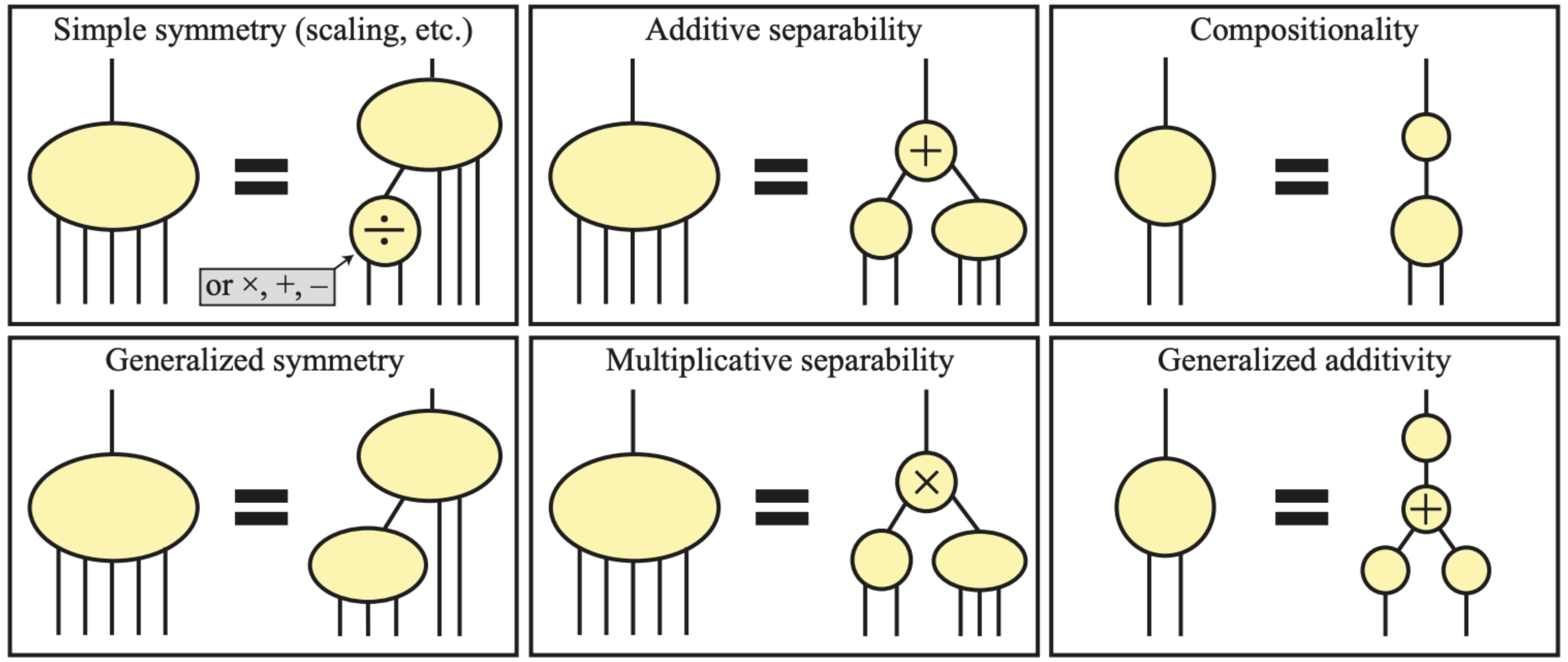


Figure 3: Examples of graph modularity that our algorithm can auto-discover. Lines denote real-valued variables and ovals denote functions, with larger ones being more complex.

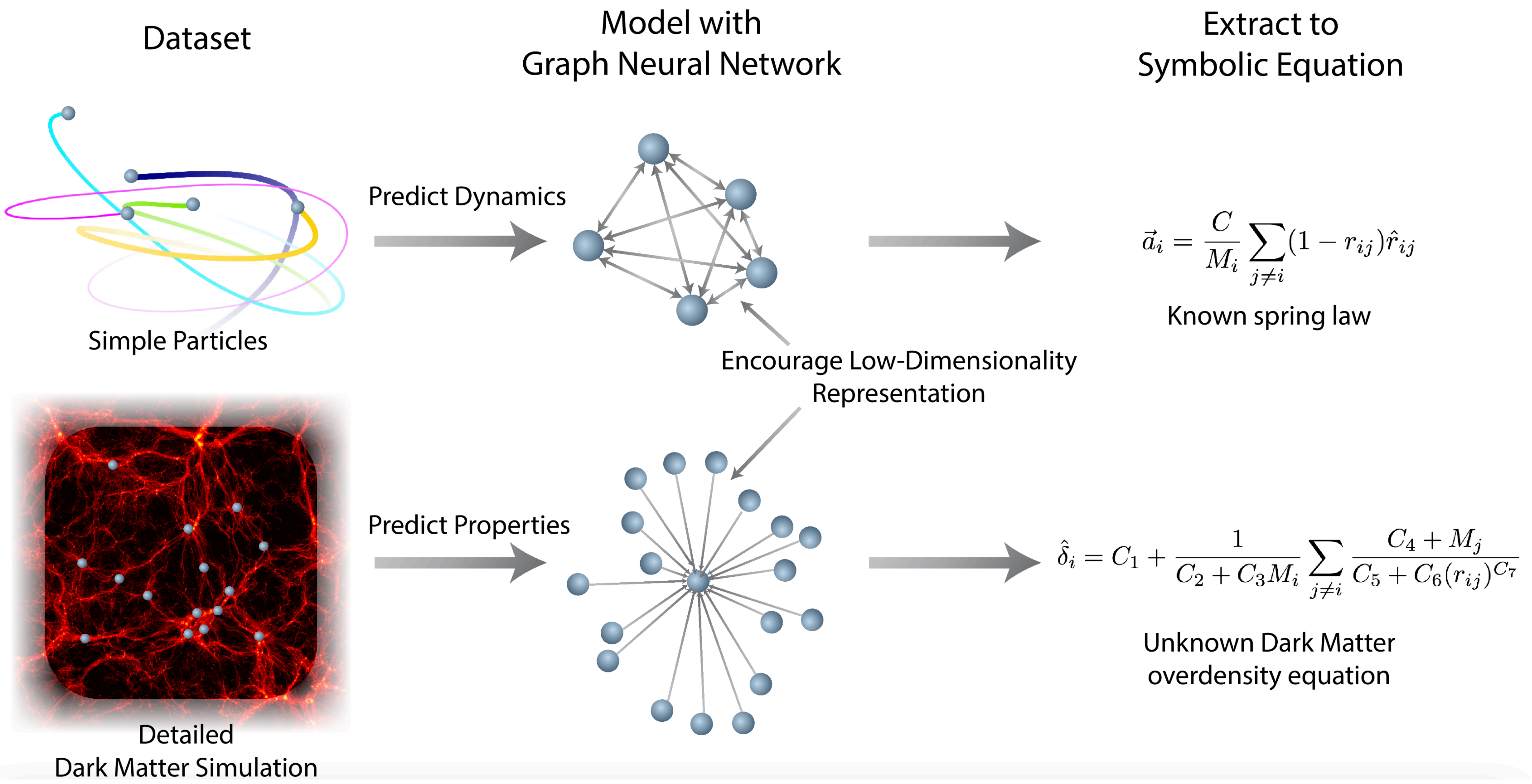
Symbolic regression

Discovering Symbolic Models from Deep Learning with Inductive Biases

Miles Cranmer[1] Alvaro Sanchez-Gonzalez[2] Peter Battaglia[2] Rui Xu[1]
Kyle Cranmer[3] David Spergel[4,1] Shirley Ho[4,3,1,5]

[1] Princeton University, Princeton, USA [2] DeepMind, London, UK
[3] New York University, New York City, USA [4] Flatiron Institute, New York City, USA
[5] Carnegie Mellon University, Pittsburgh, USA

PySR:
Symbolic regression using genetic programming



Symbolic regression

Published as a conference paper at ICLR 2021

DEEP SYMBOLIC REGRESSION: RECOVERING MATHEMATICAL EXPRESSIONS FROM DATA VIA RISK-SEEKING POLICY GRADIENTS

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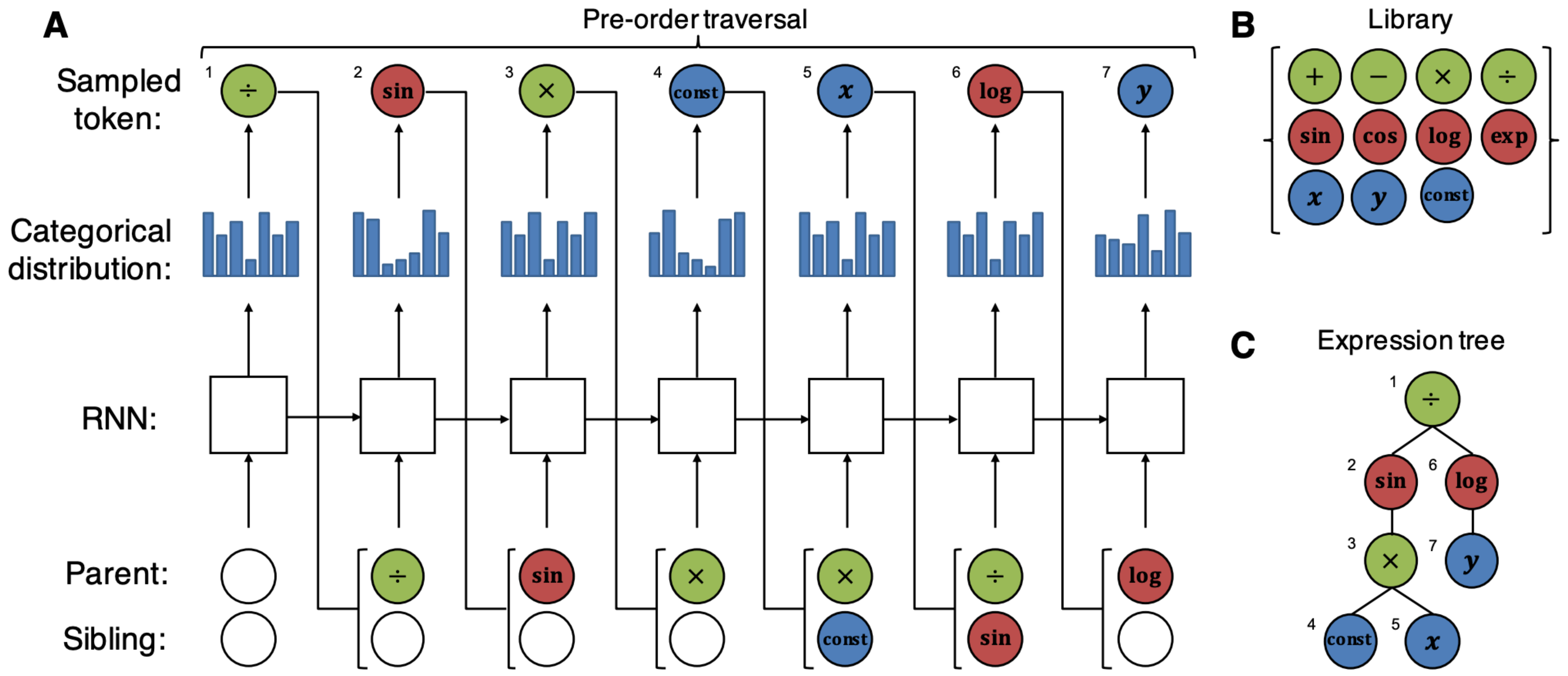
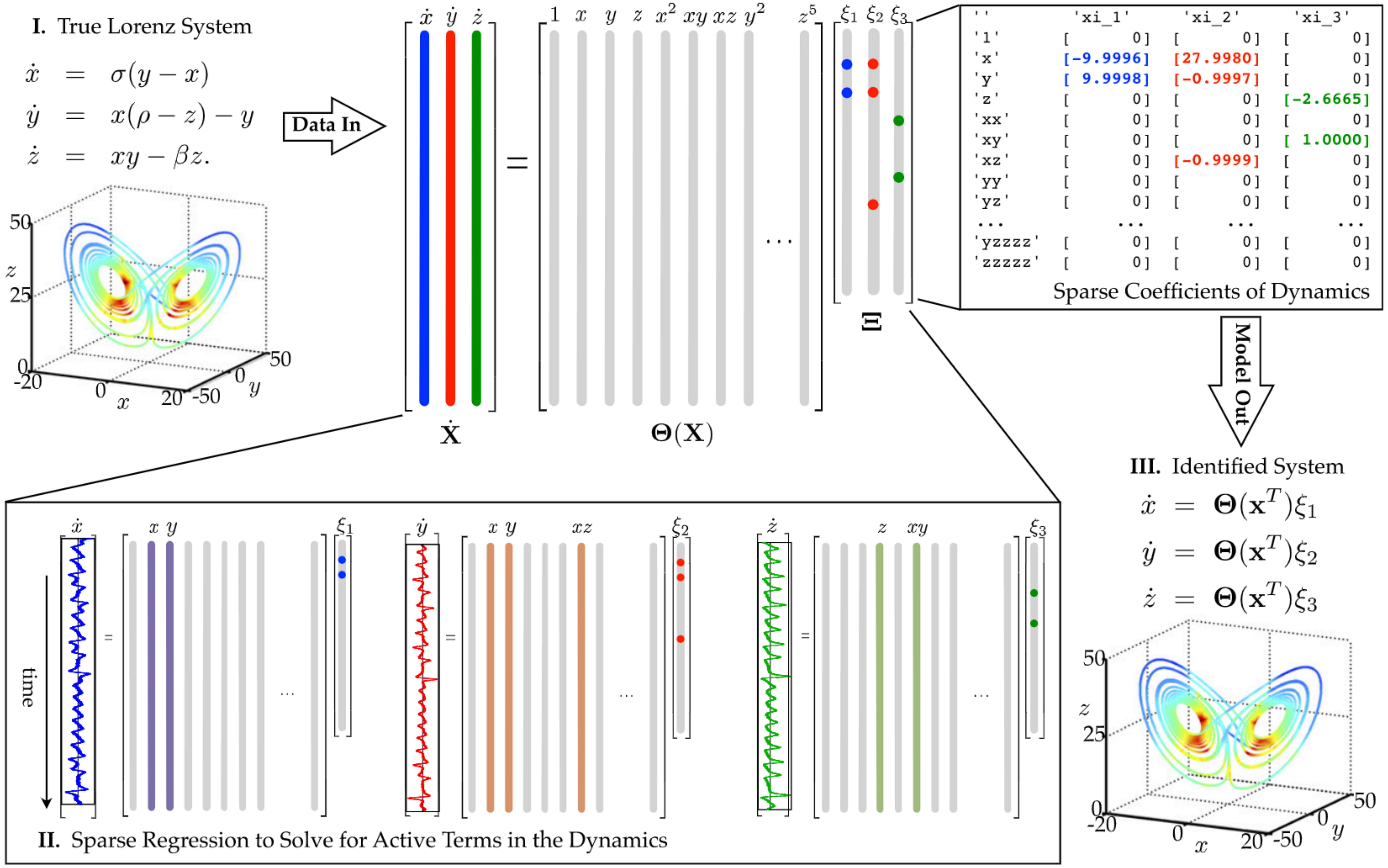


Deep reinforcement learning

SINDY



PNAS

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RESEARCH ARTICLE | APPLIED MATHEMATICS

Discovering governing equations from data by sparse identification of nonlinear dynamical systems

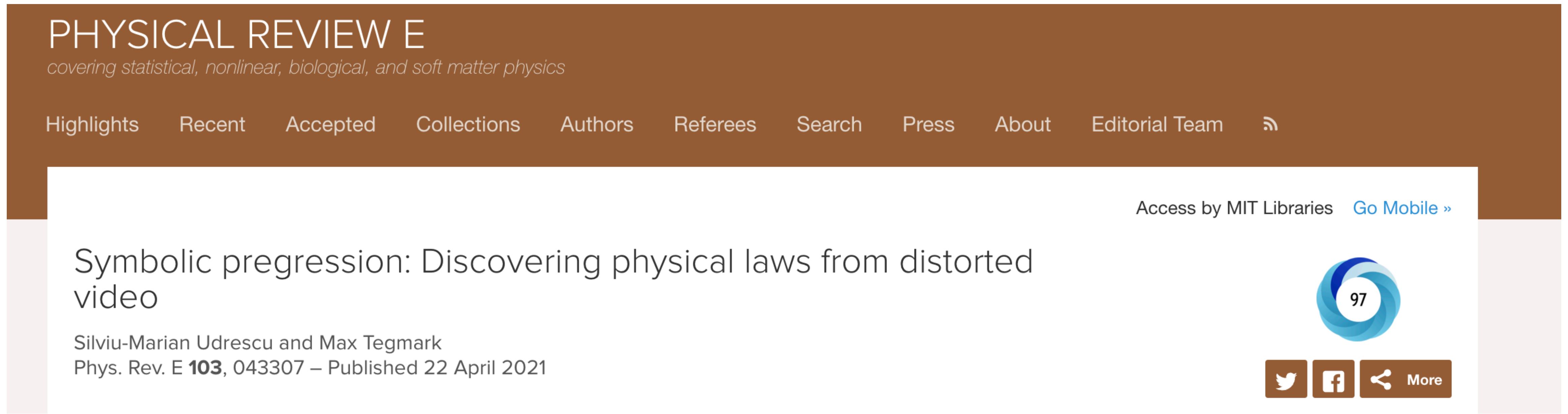
Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz Authors Info & Affiliations

Edited by William Bialek, Princeton University, Princeton, NJ, and approved March 1, 2016 (received for review August 31, 2015)

March 28, 2016 | 113 (15) 3932-3937 | https://doi.org/10.1073/pnas.1517384113

Discover (determine) coefficients

Useful degrees of freedom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Symbolic pregression: Discovering physical laws from distorted video
Silviu-Marian Udrescu and Max Tegmark
Phys. Rev. E **103**, 043307 – Published 22 April 2021
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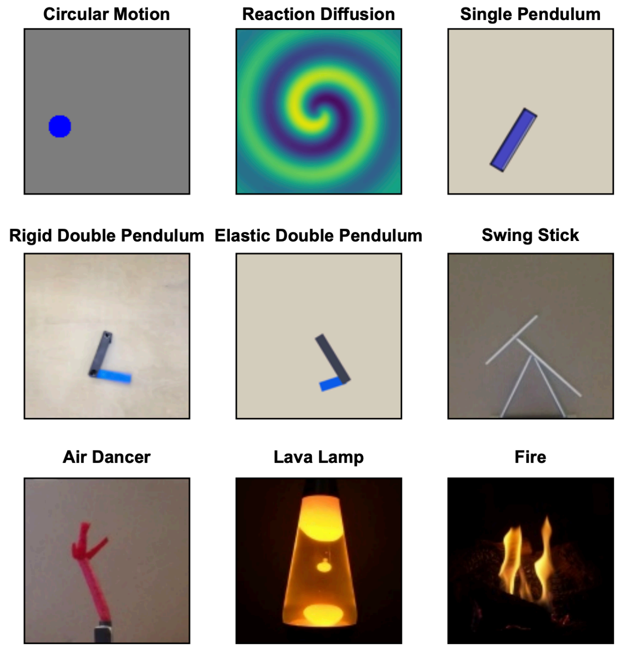
Pregression

Symbolic regression

$$\ddot{x} = -(x^2+y^2)x$$
$$\ddot{y} = -(x^2+y^2)y$$

Useful degrees of freedom



arXiv > math > arXiv:2112.10755

Mathematics > Dynamical Systems

[Submitted on 20 Dec 2021]

Discovering State Variables Hidden in Experimental Data

Boyuan Chen, Kuang Huang, Sunand Raghupathi, Ishaan Chandratreya, Qiang Du, Hod Lipson

NEWS RELEASE 26-JUL-2022

Columbia Engineering roboticists discover alternative physics

A new AI program observed physical phenomena and uncovered relevant variables–a necessary precursor to any physics theory. But the variables it discovered were unexpected

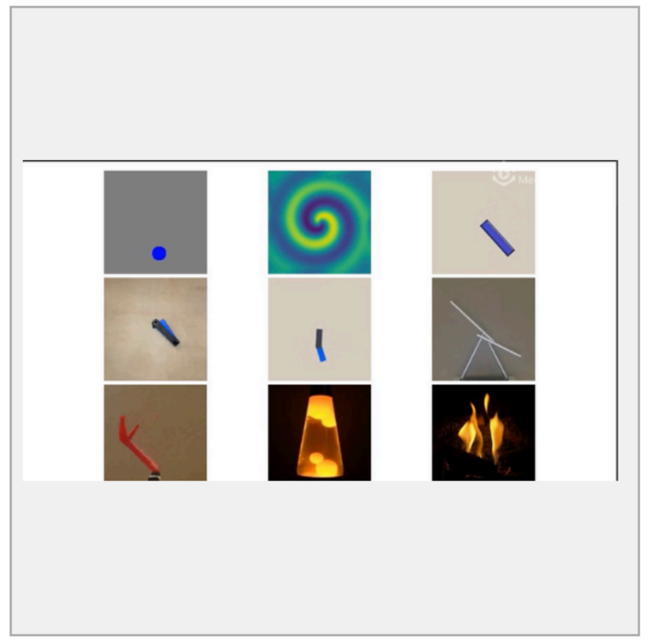
Peer-Reviewed Publication

COLUMBIA UNIVERSITY SCHOOL OF ENGINEERING AND APPLIED SCIENCE

Print Email App

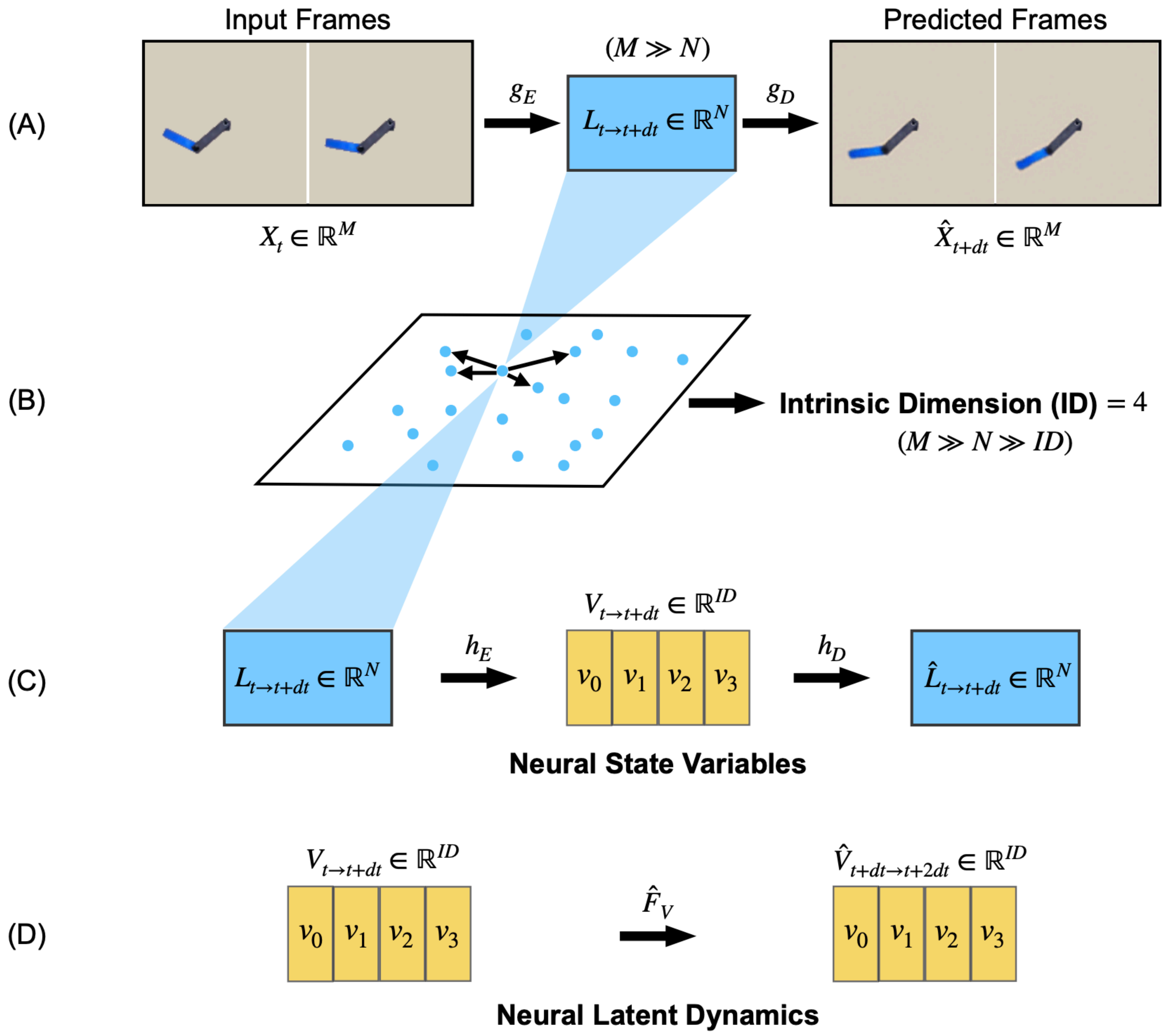
New York, NY—July 25, 2022— Energy, Mass, Velocity. These three variables make up Einstein's iconic equation $E=MC^2$. But how did Einstein know about these concepts in the first place? A precursor step to understanding physics is identifying relevant variables. Without the concept of energy, mass, and velocity, not even Einstein could discover relativity. But can such variables be discovered automatically? Doing so could greatly accelerate scientific discovery.

This is the question that researchers at Columbia Engineering posed to a new AI program. The program was designed to observe physical phenomena through a video camera, then try to search for the minimal set of fundamental variables that fully describe the observed dynamics. The study was published on July 25 in *Nature Computational Science.*



VIDEO: THE IMAGE SHOWS A CHAOTIC SWING STICK DYNAMICAL SYSTEM IN MOTION. OUR WORK AIMS AT IDENTIFYING AND EXTRACTING THE MINIMUM NUMBER OF STATE VARIABLES NEEDED TO DESCRIBE SUCH SYSTEM FROM HIGH DIMENSIONAL VIDEO FOOTAGE DIRECTLY. view more ›

CREDIT: CREDIT AS YINUO QIN/COLUMBIA ENGINEERING



Useful degrees of freedom

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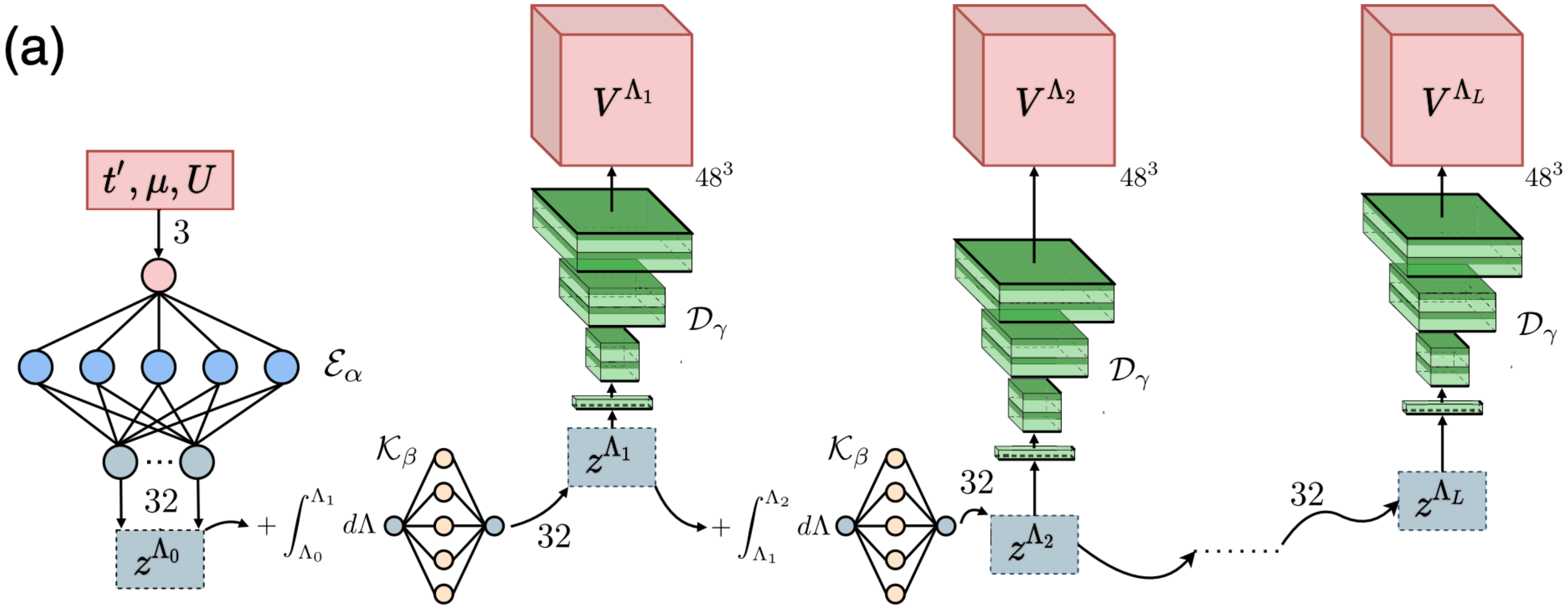
Deep Learning the Functional Renormalization Group

Domenico Di Sante, Matija Medvidović, Alessandro Toschi, Giorgio Sangiovanni, Cesare Franchini, Anirvan M. Sengupta, and Andrew J. Millis

Phys. Rev. Lett. **129**, 136402 – Published 21 September 2022



NEWS RELEASE 26-SEP-2022

Artificial intelligence reduces a 100,000-equation quantum physics problem to only four equations

Researchers at the Flatiron Institute and their colleagues trained a machine learning tool to capture the physics of electrons moving on a lattice using far fewer equations than would typically be required, all without sacrificing accuracy

Peer-Reviewed Publication

SIMONS FOUNDATION

Using artificial intelligence, physicists have compressed a daunting quantum problem that until now required 100,000 equations into a bite-size task of as few as four equations — all without sacrificing accuracy. The work, published in the September 23 issue of *Physical Review Letters*, could revolutionize how scientists investigate systems containing many interacting electrons. Moreover, if scalable to other problems, the approach could potentially aid in the design of materials with sought-after properties such as superconductivity or utility for clean energy generation.

"We start with this huge object of all these coupled-together differential equations; then we're using machine learning to turn it into something so small you can count it on

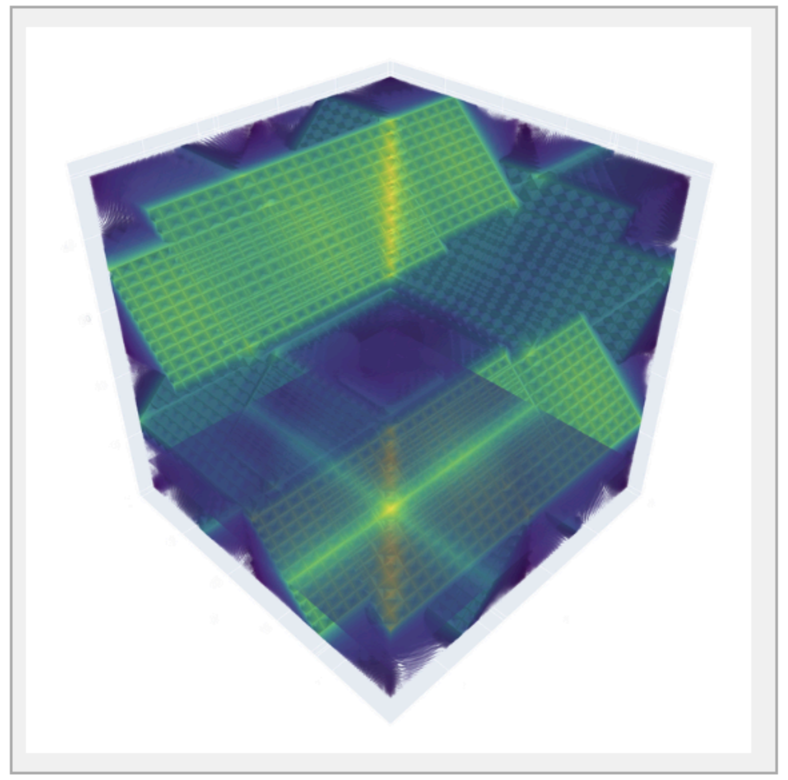
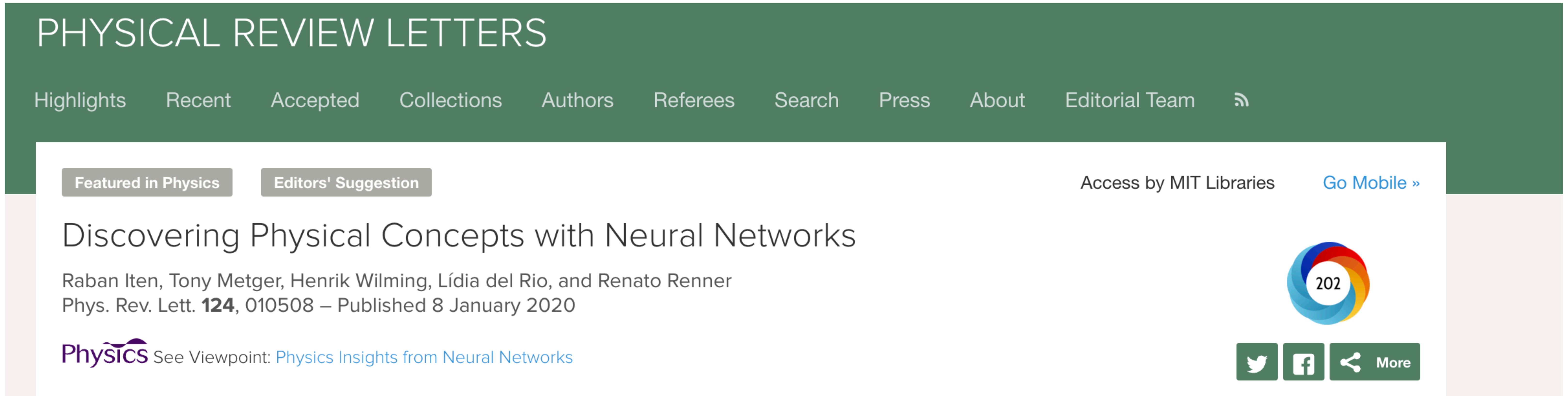
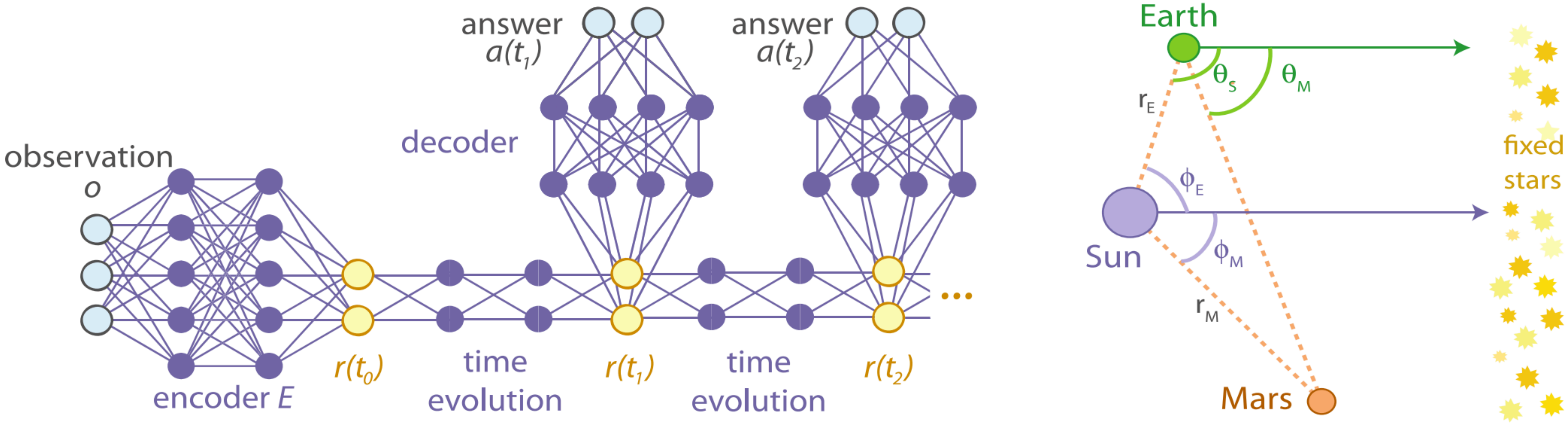


IMAGE: A VISUALIZATION OF A MATHEMATICAL APPARATUS USED TO CAPTURE THE PHYSICS AND BEHAVIOR OF ELECTRONS MOVING ON A LATTICE. EACH PIXEL REPRESENTS A SINGLE INTERACTION BETWEEN TWO ELECTRONS. UNTIL NOW, ACCURATELY CAPTURING THE SYSTEM REQUIRED AROUND 100,000 EQUATIONS — ONE FOR EACH PIXEL. USING MACHINE LEARNING, SCIENTISTS

Useful degrees of freedom





(a) (b)

Emergence of heliocentric views

Useful degrees of freedom

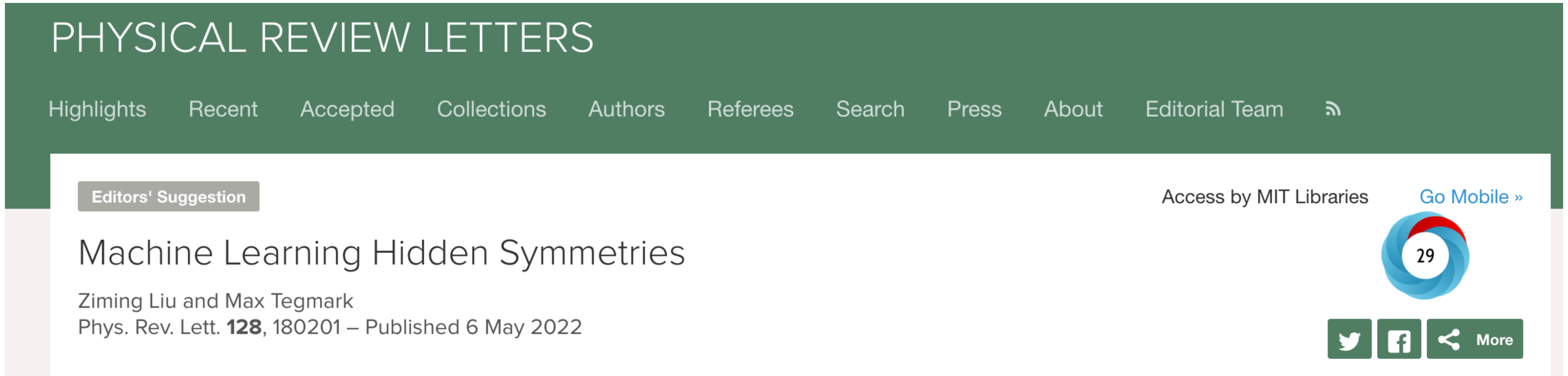
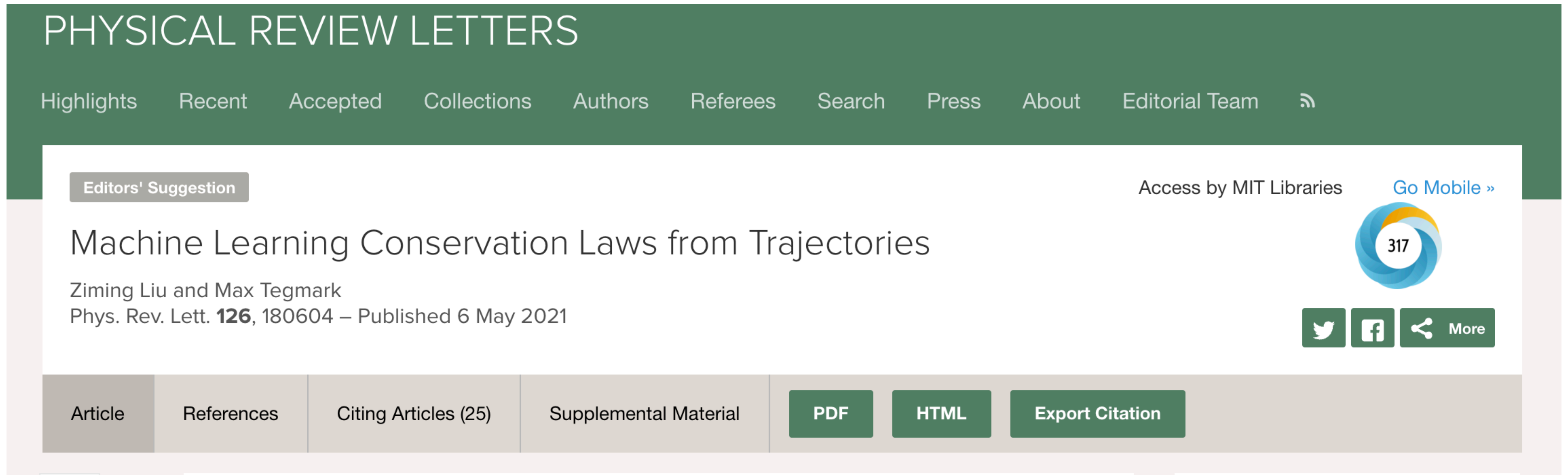


TABLE I: PDE and Losses for Generalized Symmetries

Generalized symmetry	Linear operator $\hat{L}$	Loss ℓ	Examples
Translation invariance	$\hat{L}_j = \partial_j$	ℓ_{TI}	A,E,F
Lie invariance	$\hat{L}_j = K_j\mathbf{z}\cdot\nabla$	ℓ_{INV}	E,F
Lie equivariance	$\hat{L}_j = K_j\mathbf{z}\cdot\nabla \pm K_j$	ℓ_{EQV}	B
Canonical eqvariance	$\hat{L}_j^{\mathbf{x}} = K_j\mathbf{x}\cdot\nabla_{\mathbf{x}} - K_j^t\mathbf{p}\cdot\nabla_{\mathbf{p}} + K_j^t$ $\hat{L}_j^{\mathbf{p}} = K_j\mathbf{x}\cdot\nabla_{\mathbf{x}} - K_j^t\mathbf{p}\cdot\nabla_{\mathbf{p}} - K_j$	ℓ_{CAN}	C
Hamiltonicity	$\hat{L}_{ij} = -\mathbf{m}_i^t\partial_j + \mathbf{m}_j^t\partial_i$	ℓ_{H}	A,B,C,D
Modularity	$\hat{L}_{ij} = \mathbf{A}_{ij}\hat{\mathbf{z}}_i^t\partial_j$	ℓ_{M}	D

Conservation laws

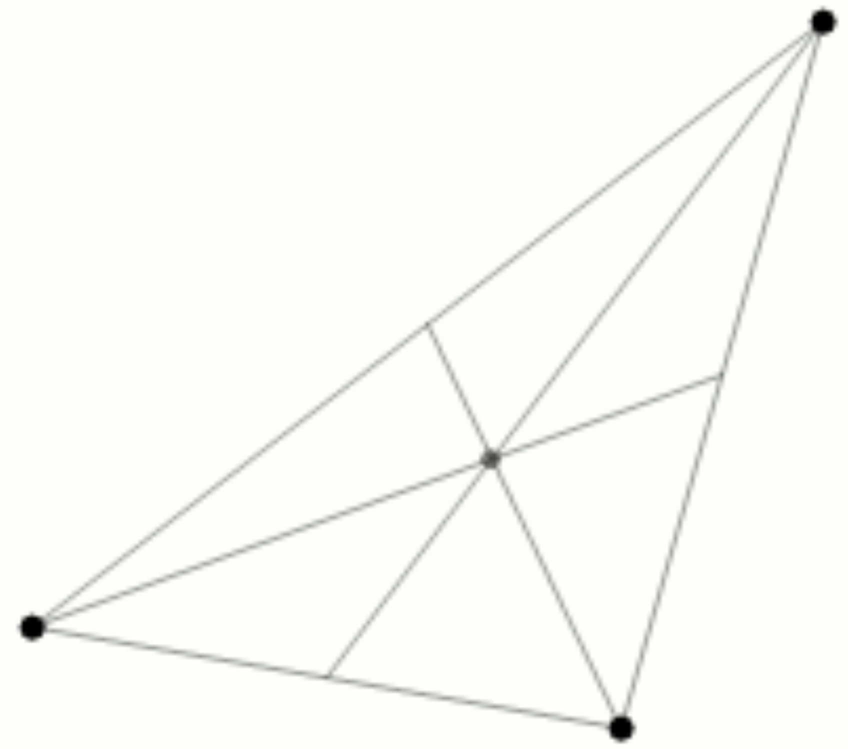


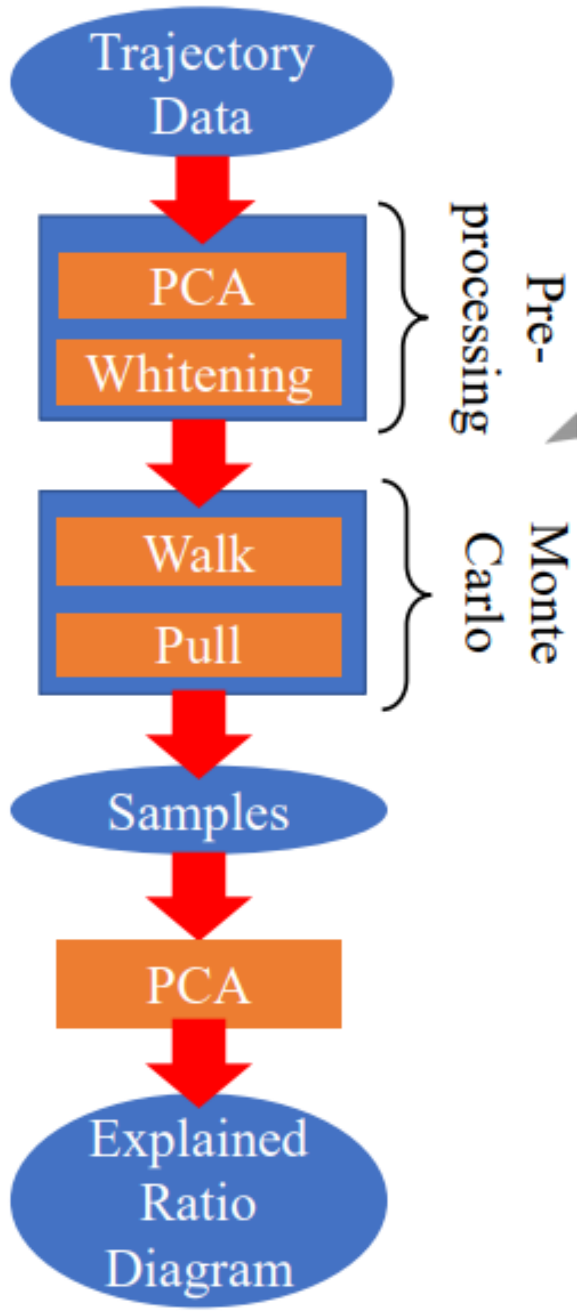
AI Poincare

Henri Poincaré (1854-1912)

6 conserved quantities out of 12 dof !

$$\ddot{\mathbf{r}}_1 = -Gm_2 \frac{\mathbf{r}_1 - \mathbf{r}_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3} - Gm_3 \frac{\mathbf{r}_1 - \mathbf{r}_3}{|\mathbf{r}_1 - \mathbf{r}_3|^3},$$
$$\ddot{\mathbf{r}}_2 = -Gm_3 \frac{\mathbf{r}_2 - \mathbf{r}_3}{|\mathbf{r}_2 - \mathbf{r}_3|^3} - Gm_1 \frac{\mathbf{r}_2 - \mathbf{r}_1}{|\mathbf{r}_2 - \mathbf{r}_1|^3},$$
$$\ddot{\mathbf{r}}_3 = -Gm_1 \frac{\mathbf{r}_3 - \mathbf{r}_1}{|\mathbf{r}_3 - \mathbf{r}_1|^3} - Gm_2 \frac{\mathbf{r}_3 - \mathbf{r}_2}{|\mathbf{r}_3 - \mathbf{r}_2|^3}.$$

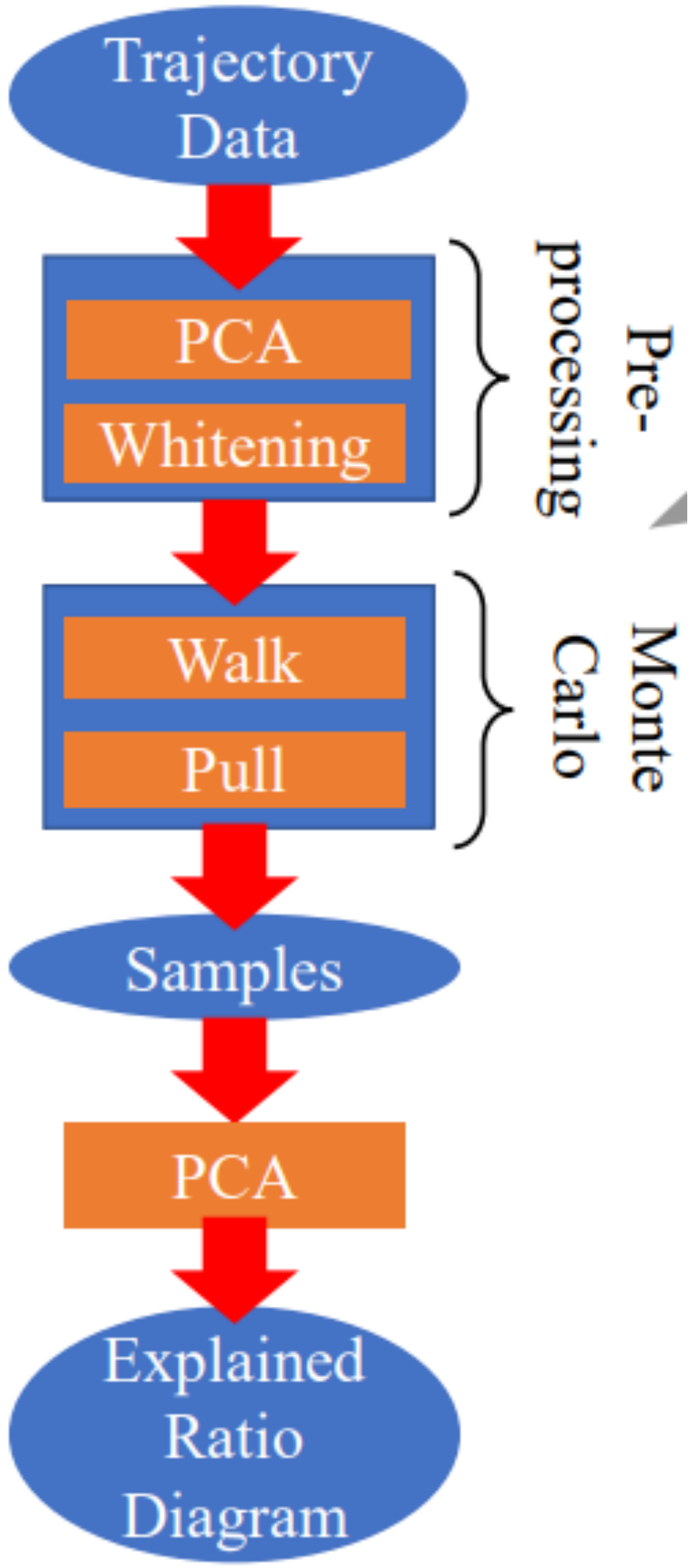




Henri Poincaré (1854-1912)

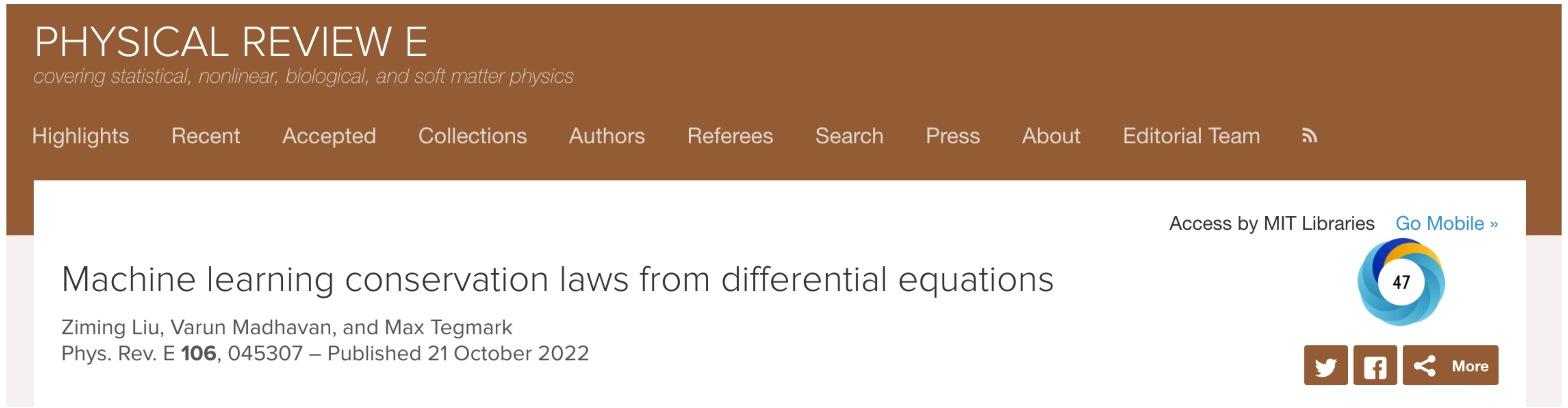
You're cheating!
You don't know what they are!!!
You only know how many!!!

Hold on…
I'm transforming…



Conservation laws

AI Poincare 2.0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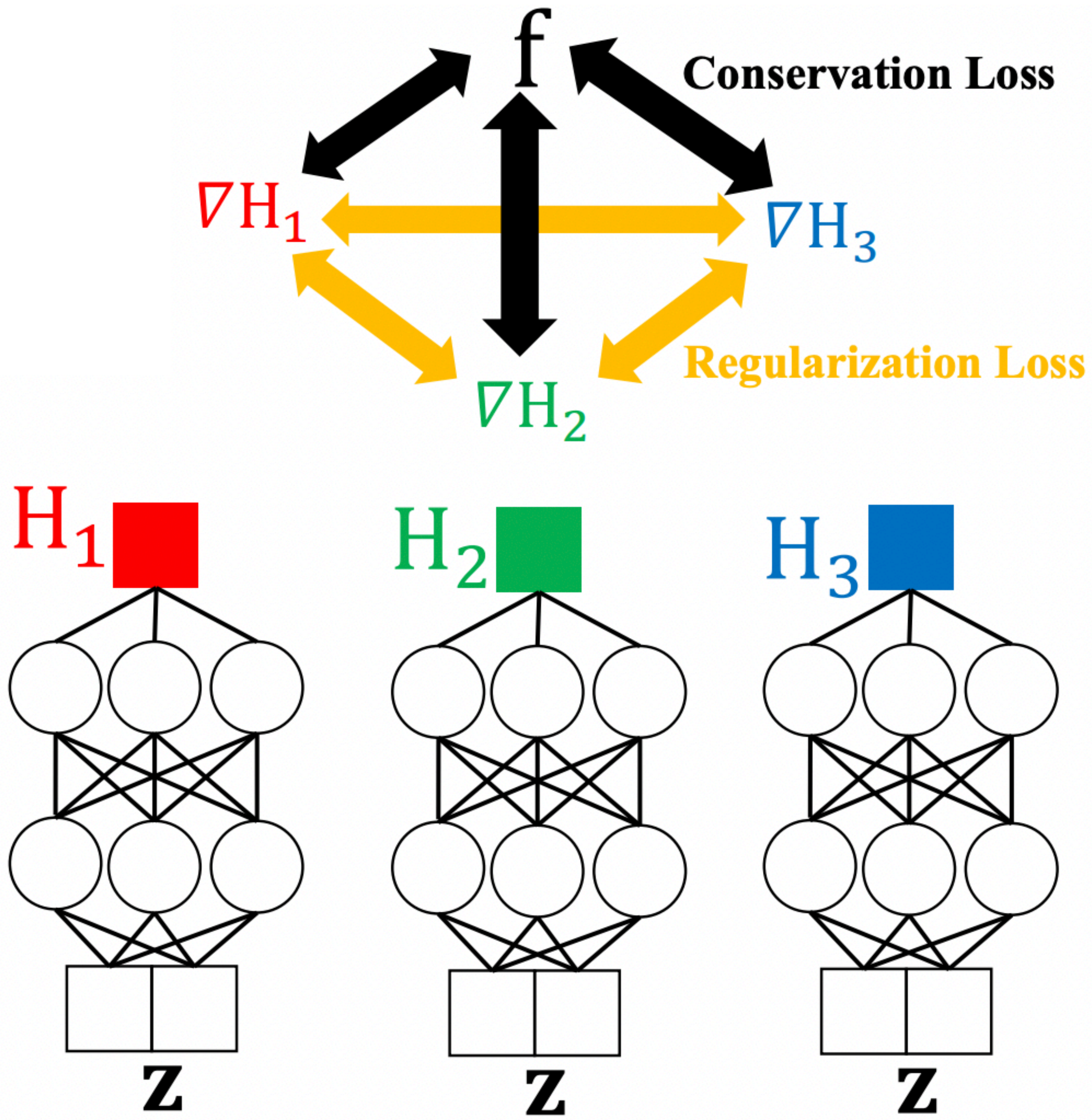
Machine learning conservation laws from differential equations

Ziming Liu, Varun Madhavan, and Max Tegmark
Phys. Rev. E **106**, 045307 – Published 21 October 2022

Henri Poincaré (1854-1912)

Go on…

How about now?



Conservation laws

arXiv > math > arXiv:1811.00961

Mathematics > Dynamical Systems

[Submitted on 2 Nov 2018]

Discovering conservation laws from data for control

Eurika Kaiser, J. Nathan Kutz, Steven L. Brunton

arXiv > cs > arXiv:2003.04630

Computer Science > Machine Learning

[Submitted on 10 Mar 2020 (v1), last revised 30 Jul 2020 (this version, v2)]

Lagrangian Neural Networks

Miles Cranmer, Sam Greydanus, Stephan Hoyer, Peter Battaglia, David Spergel, Shirley Ho

arXiv > cs > arXiv:1906.01563

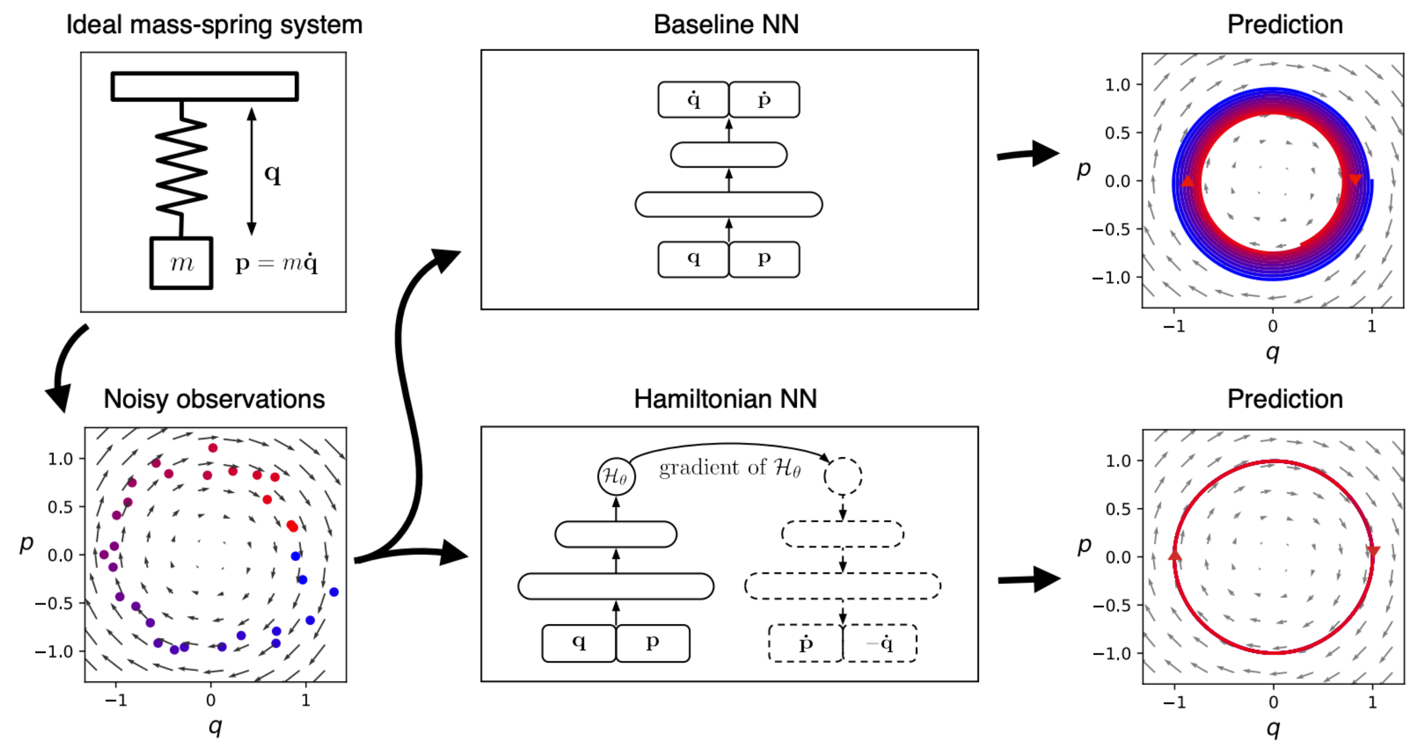
Computer Science > Neural and Evolutionary Computing

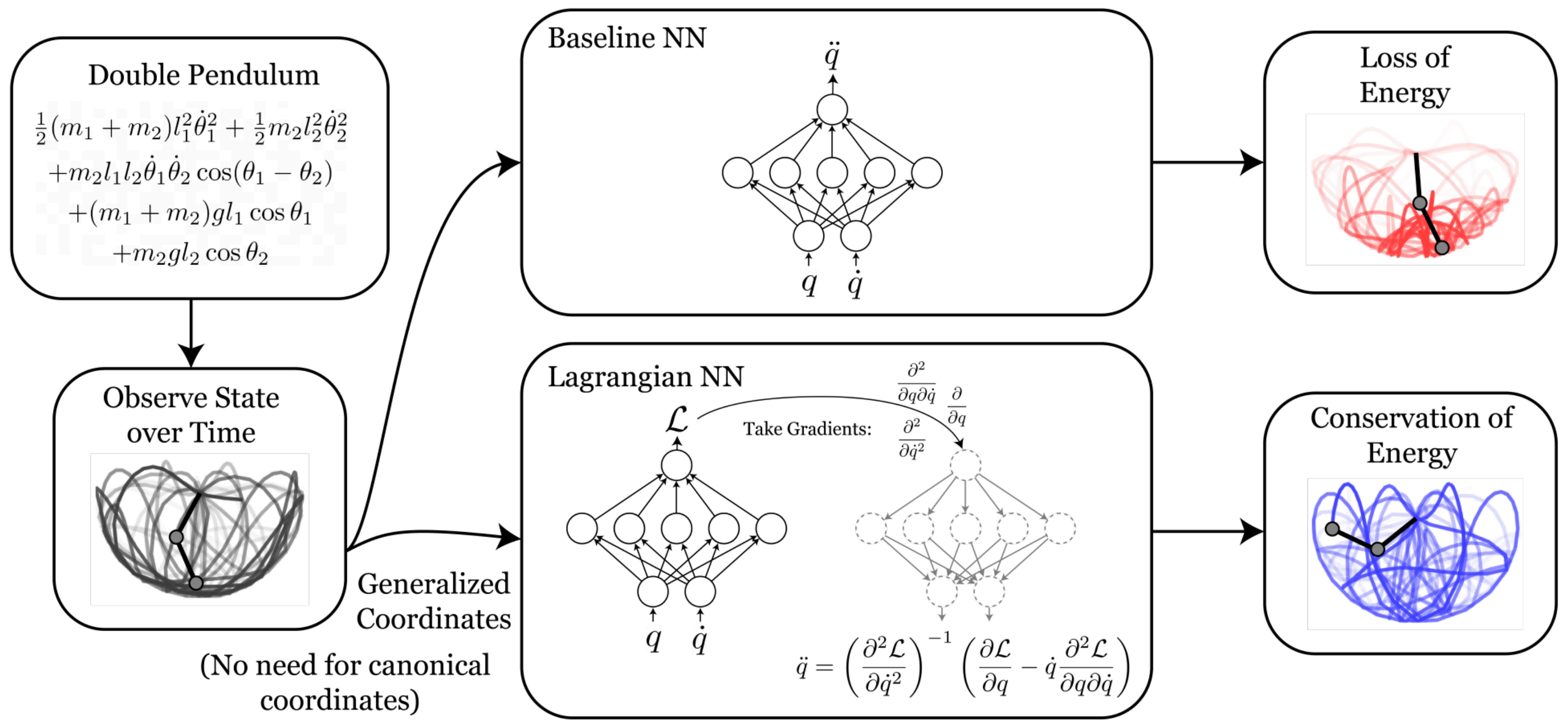
[Submitted on 4 Jun 2019 (v1), last revised 5 Sep 2019 (this version, v3)]

Hamiltonian Neural Networks

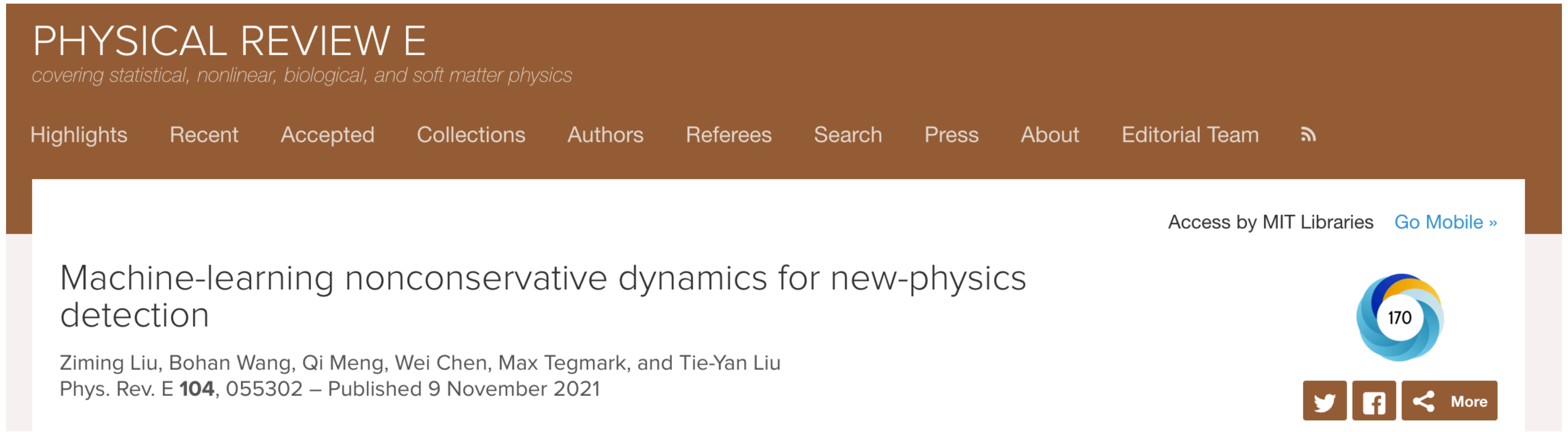
Sam Greydanus, Misko Dzamba, Jason Yosinski

SINDY-like





Non-conservation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Machine-learning nonconservative dynamics for new-physics detection

Ziming Liu, Bohan Wang, Qi Meng, Wei Chen, Max Tegmark, and Tie-Yan Liu
Phys. Rev. E **104**, 055302 – Published 9 November 2021

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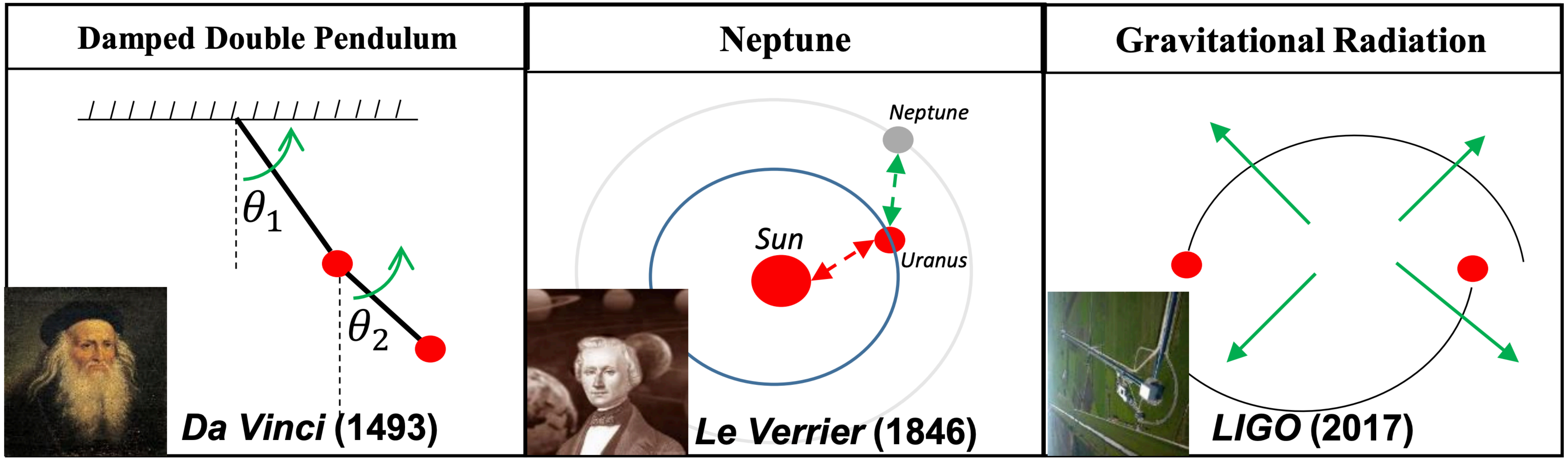
More



Dimensionless number: conservation in scale

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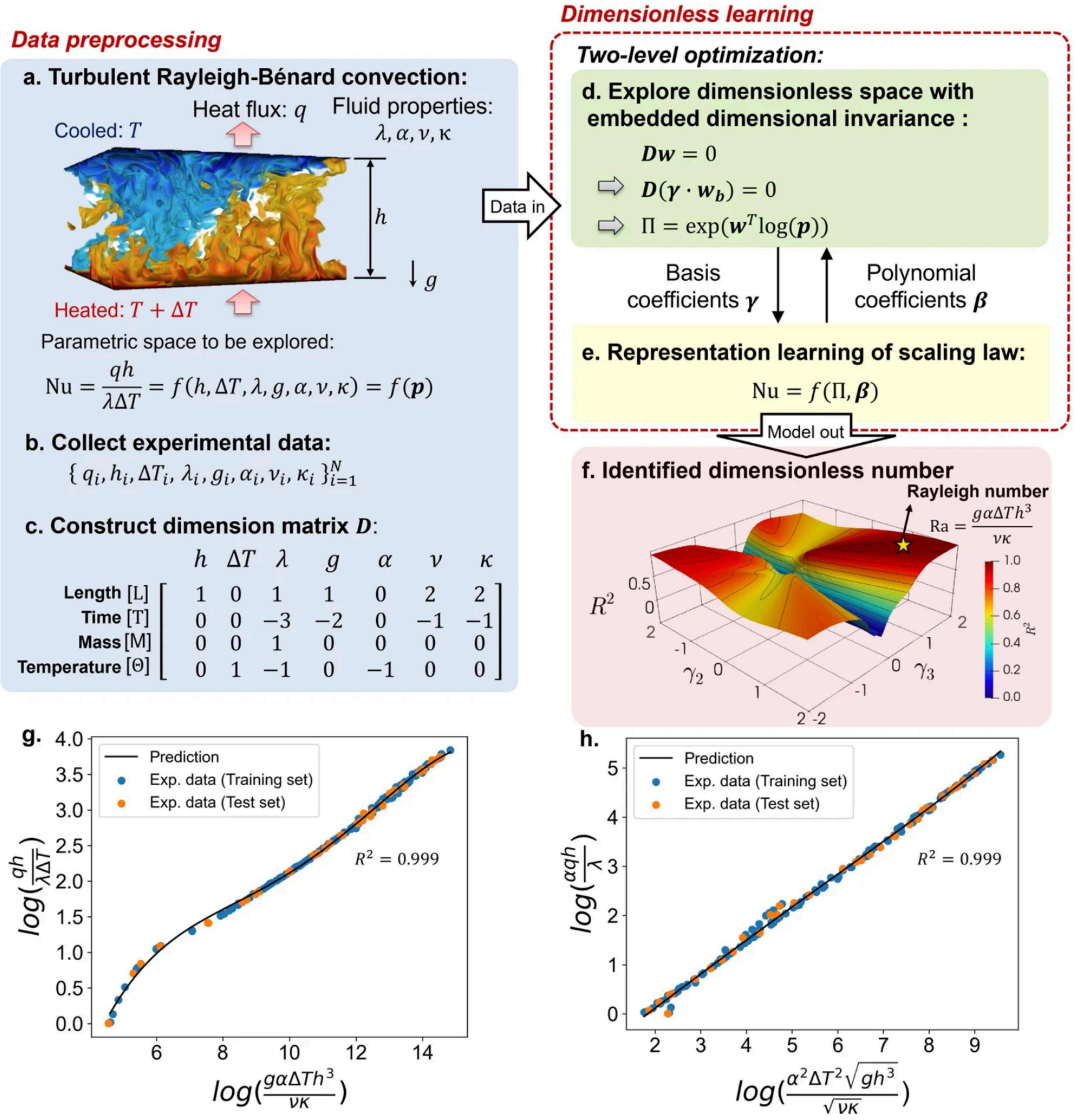
Nature Communications 13, Article number: 7562 (2022) | Cite this article



Neural New-Physics Detector (NNPhD)

Machine-Learning *Non-Conservation* for *New-Physics* Detection

Ziming Liu, Bohan Wang, Qi Meng, Wei Chen, Max Tegmark and Tie-Yan Liu
Joint work by MIT/IAIFI and Microsoft

Physical Review E 104,055302

NNPhD: Neural New Physics Detector

$$f = f_c + f_n$$

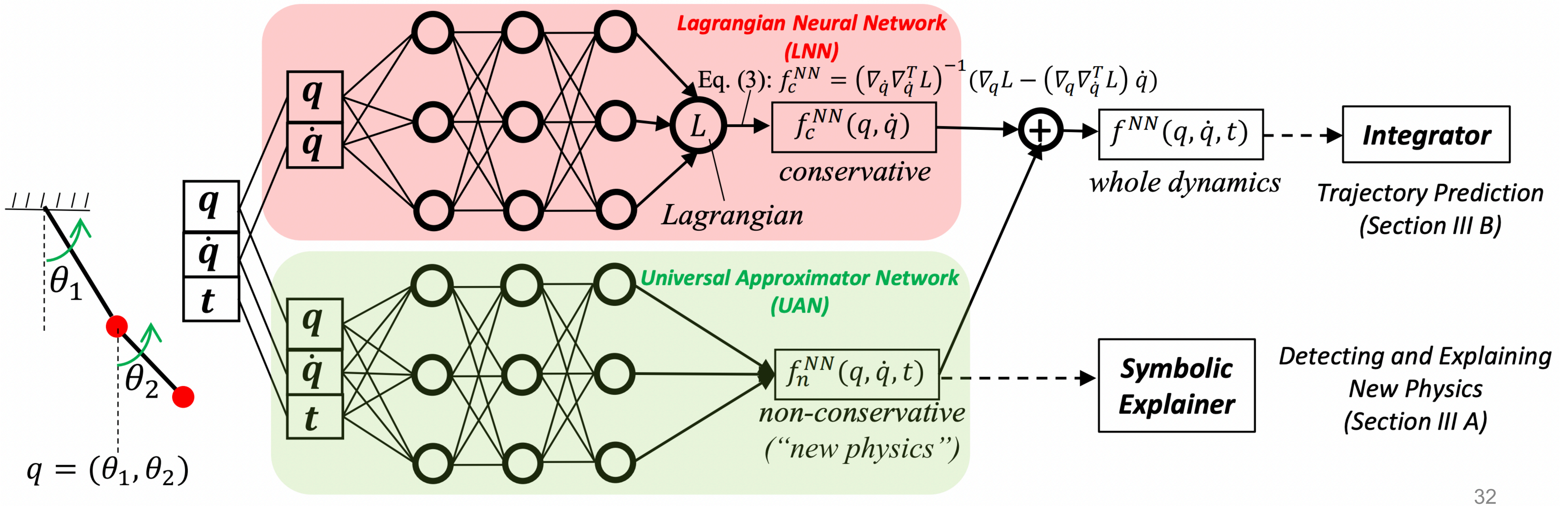
Conservative, LNN — Non-Conservative, MLP

Loss Function

$$L = L_e + \lambda L_b$$

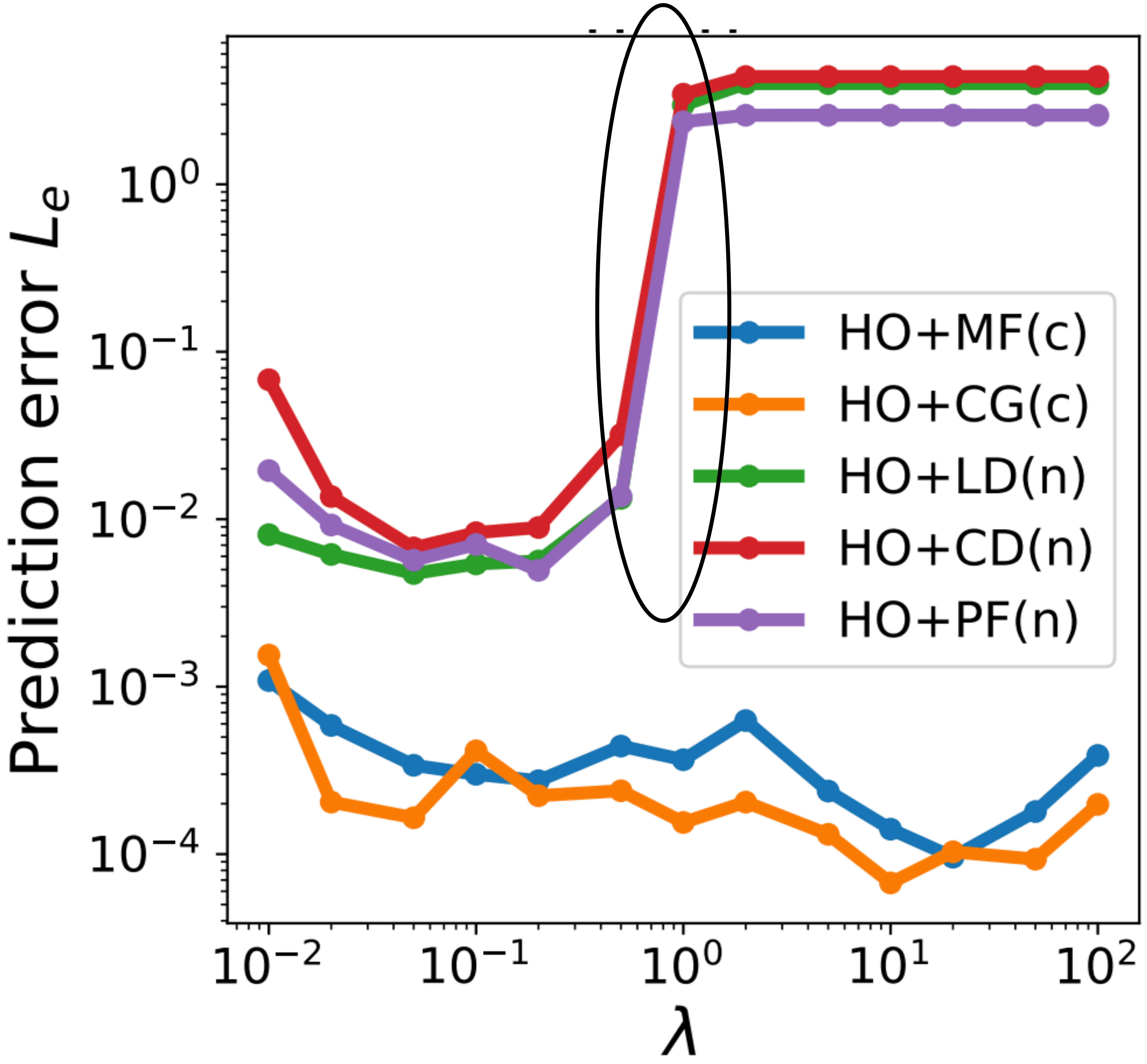
$$L_e = || f - (f_c + f_n) ||$$

$$L_b = || f_n ||$$

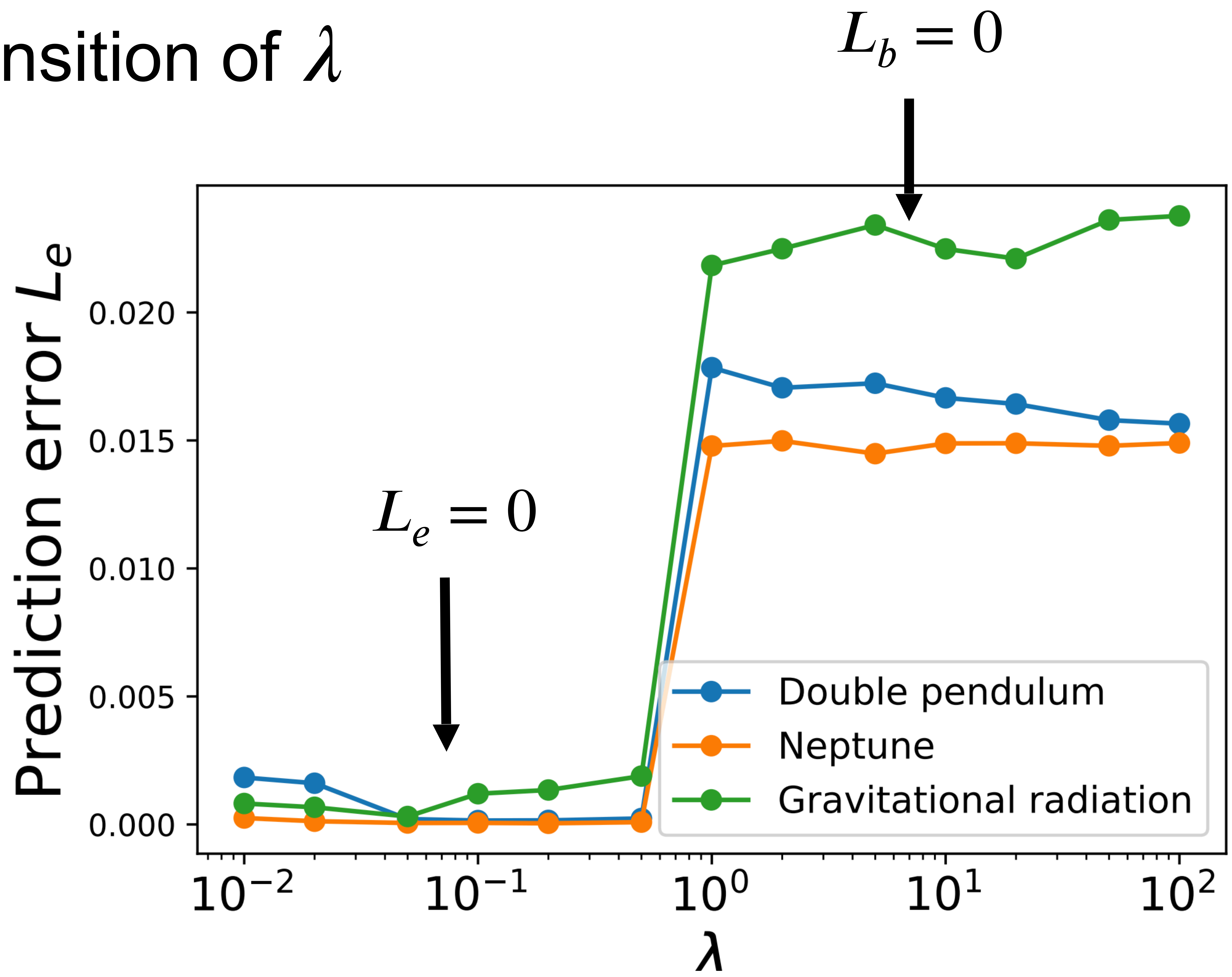


Phase Transition of λ

Phase transitions:
Indication of new physics (non-conservation) !

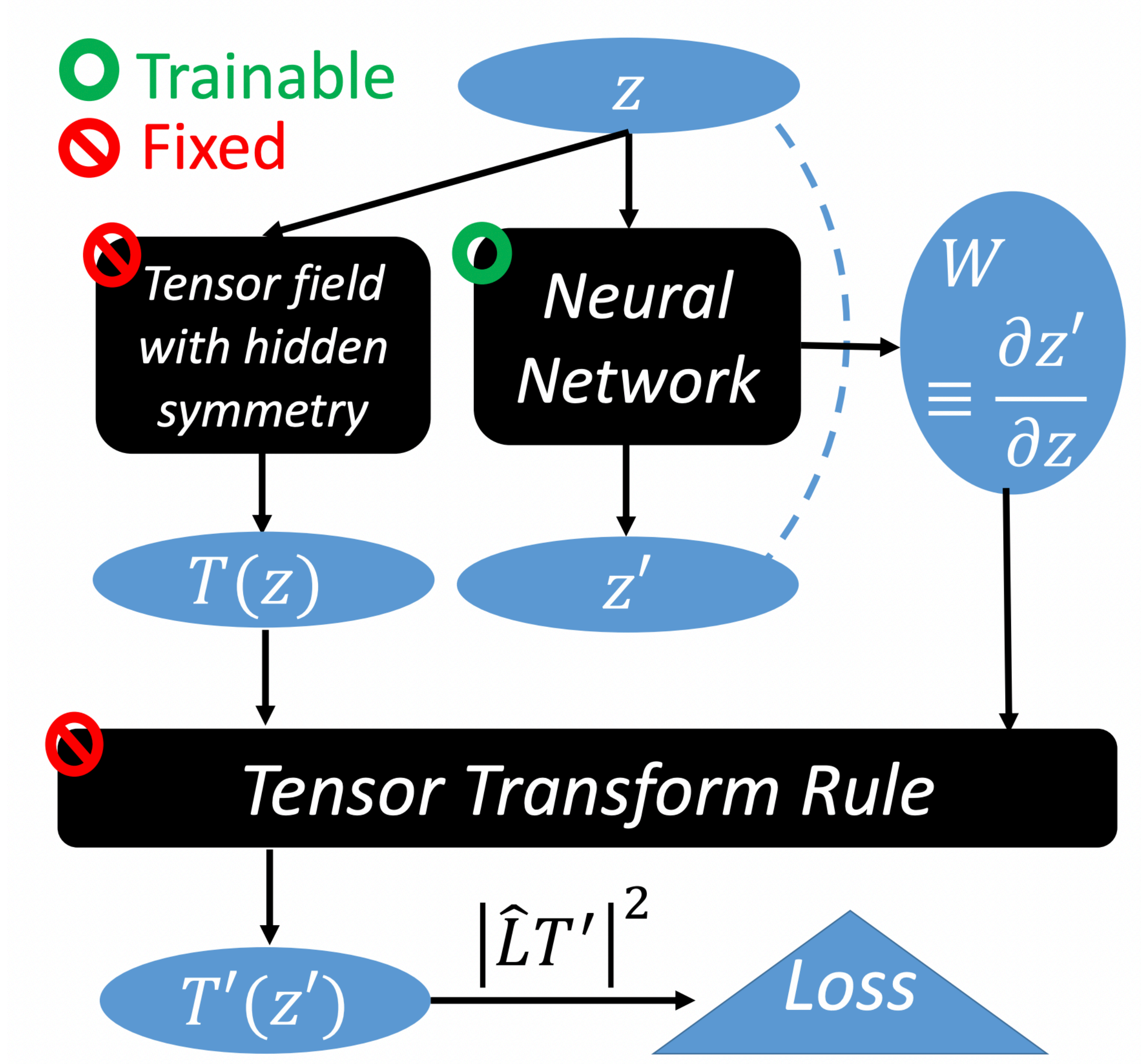


Phase Transition of λ



Theory: Check out the Theorem 1 of our paper!

Machine-Learning Hidden Symmetries



"Machine-learning hidden symmetries", Ziming Liu and Max Tegmark.

Phys. Rev. Lett. 128, 180201

What happens inside black holes?

$$\mathbf{g}=\begin{pmatrix} 1-\frac{2M}{r} & 0 & 0 & 0 \\ 0 & -1-\frac{2Mx^2}{(r-2M)r^2} & -\frac{2Mxy}{(r-2M)r^2} & -\frac{2Mxz}{(r-2M)r^2} \\ 0 & -\frac{2Mxy}{(r-2M)r^2} & -1-\frac{2My^2}{(r-2M)r^2} & -\frac{2Myz}{(r-2M)r^2} \\ 0 & -\frac{2Mxz}{(r-2M)r^2} & -\frac{2Myz}{(r-2M)r^2} & -1-\frac{2Mz^2}{(r-2M)r^2} \end{pmatrix}$$

$$\begin{pmatrix} t' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} t+2M\left[2u+\ln\frac{u-1}{u+1}\right] \\ x \\ y \\ z \end{pmatrix}$$

$$u \equiv \sqrt{(r/2M)}$$

$$\mathbf{g}=\begin{pmatrix} 1-\frac{2M}{r} & -\sqrt{\frac{2M}{r}}\frac{x}{r} & -\sqrt{\frac{2M}{r}}\frac{y}{r} & -\sqrt{\frac{2M}{r}}\frac{z}{r} \\ -\sqrt{\frac{2M}{r}}\frac{x}{r} & -1 & 0 & 0 \\ -\sqrt{\frac{2M}{r}}\frac{y}{r} & 0 & -1 & 0 \\ -\sqrt{\frac{2M}{r}}\frac{z}{r} & 0 & 0 & -1 \end{pmatrix}$$

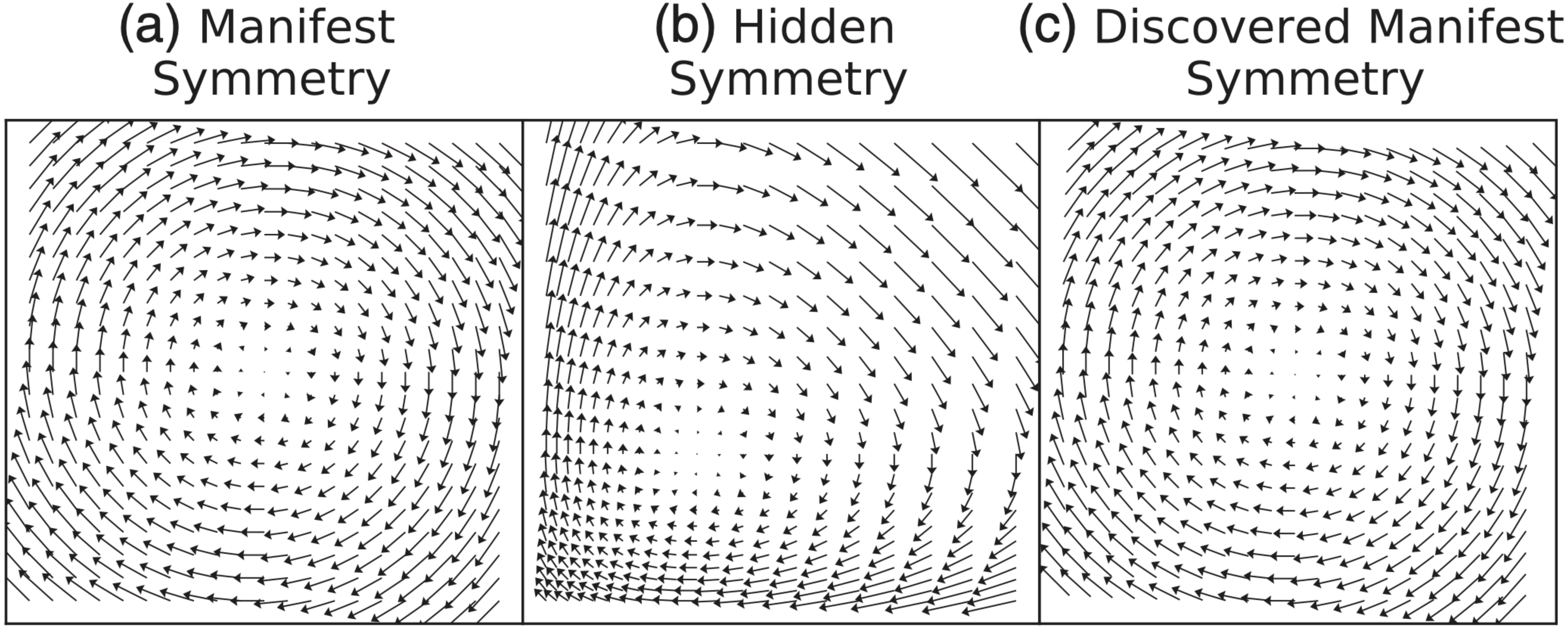
You die!

Schwarzschild 1915

Not right away!

Gullstrand & Painlevé 1932

Toy example: 1D Harmonic oscillator

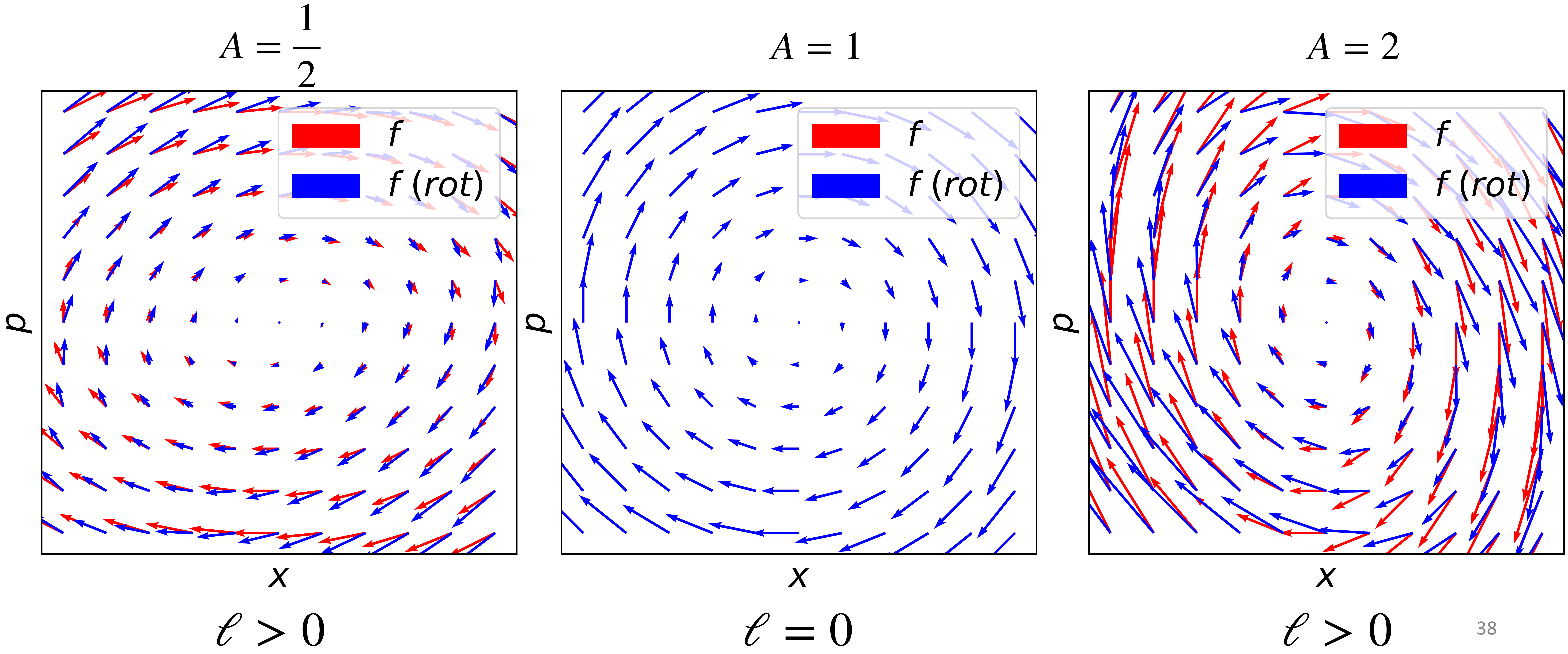


$$\frac{d}{dt}\begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} p \\ -x \end{pmatrix} \xrightarrow{\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} e^{x/2} - 1 \\ e^{p/2} - 1 \end{pmatrix}} \frac{d}{dt}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} (1+a)\ln(1+b) \\ -(1+b)\ln(1+a) \end{pmatrix}$$

Measure symmetry violation

$$\frac{d}{dt}\begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} p \\ -Ax \end{pmatrix}$$

$$\ell \sim |f(Rz) - Rf(z)|^2, \quad R = \text{rotation}$$



Measure symmetry violation

$$\ell \sim |f(gz) - gf(z)|^2, \quad g \in \mathbf{G}$$

Some Lie group

Symmetry

$$g = \exp(\sum_{i=1}^{d} \theta_i K_i), \quad K_i \text{ are geneartors}$$

$$\frac{d(f(gz) - gf(z))}{d\theta_i}\Big|_{\theta=0} = \text{math} \ldots = \nabla f(z) K_i z - K_i f(z)$$

Linear PDE (operator)

Theorem $f(z)$ is G − equivariant $\leftrightarrow \hat{L}_i f = 0, \; \hat{L}_i f \equiv \nabla f(z) K_i z - K_i f(z)$

$$\ell \sim |\hat{L}_i f|^2 = |\nabla f(z) K_i z - K_i f(z)|^2$$

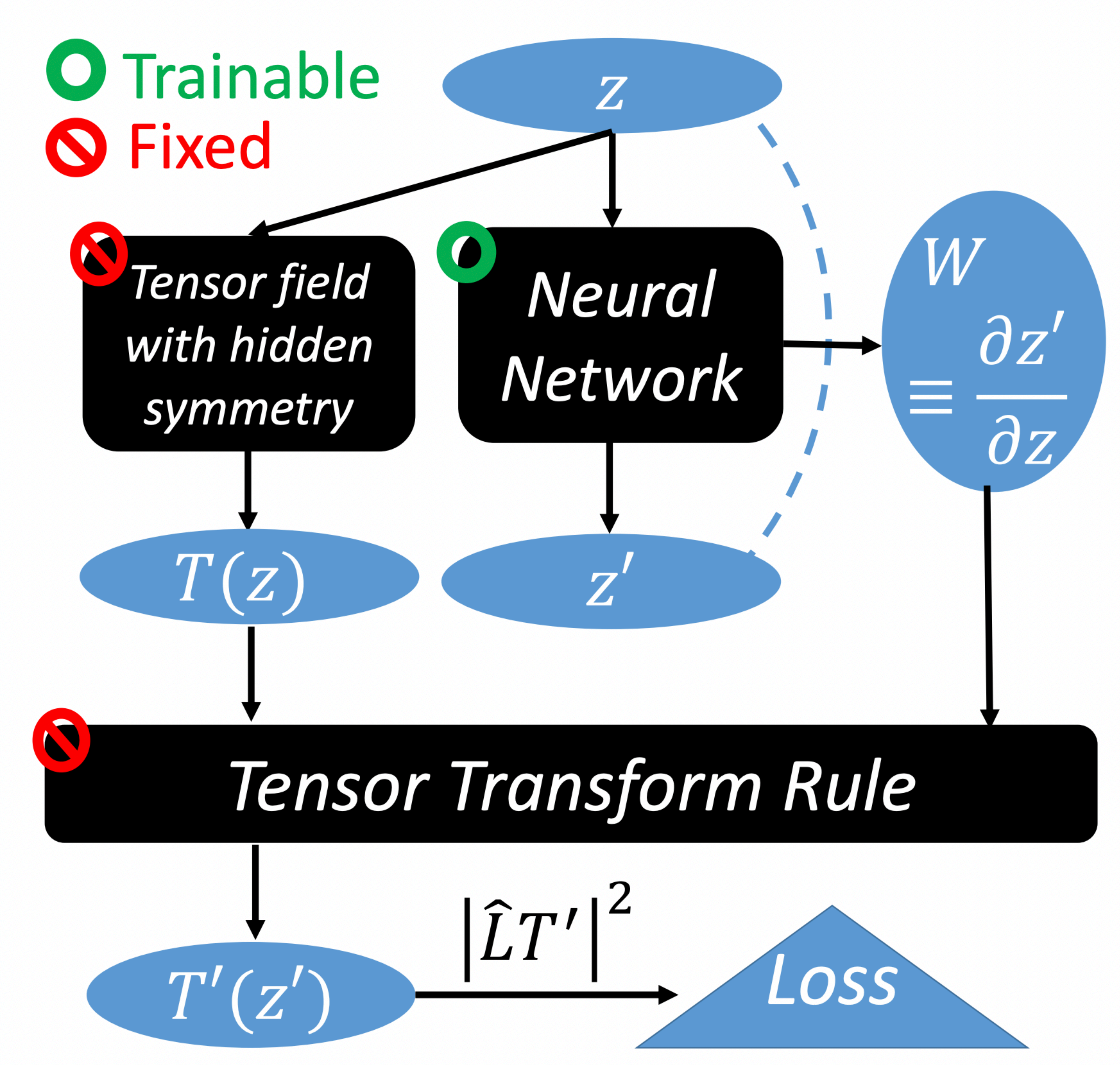
Loss function

Symmetries & PDEs

TABLE I: PDE and Losses for Generalized Symmetries

Generalized symmetry	Linear operator $\hat{L}$	Loss ℓ	Examples
Translation invariance	$\hat{L}_j = \partial_j$	ℓ_{TI}	A,E,F
Lie invariance	$\hat{L}_j = K_j \mathbf{z} \cdot \nabla$	ℓ_{INV}	E,F
Lie equivariance	$\hat{L}_j = K_j \mathbf{z} \cdot \nabla \pm K_j$	ℓ_{EQV}	B
Canonical eqvariance	$\hat{L}_j^{\mathbf{x}} = K_j \mathbf{x} \cdot \nabla_{\mathbf{x}} - K_j^t \mathbf{p} \cdot \nabla_{\mathbf{p}} + K_j^t$ $\hat{L}_j^{\mathbf{p}} = K_j \mathbf{x} \cdot \nabla_{\mathbf{x}} - K_j^t \mathbf{p} \cdot \nabla_{\mathbf{p}} - K_j$	ℓ_{CAN}	C
Hamiltonicity	$\hat{L}_{ij} = -\mathbf{m}_i^t \partial_j + \mathbf{m}_j^t \partial_i$	ℓ_{H}	A,B,C,D
Modularity	$\hat{L}_{ij} = \mathbf{A}_{ij} \hat{\mathbf{z}}_i^t \partial_j$	ℓ_{M}	D

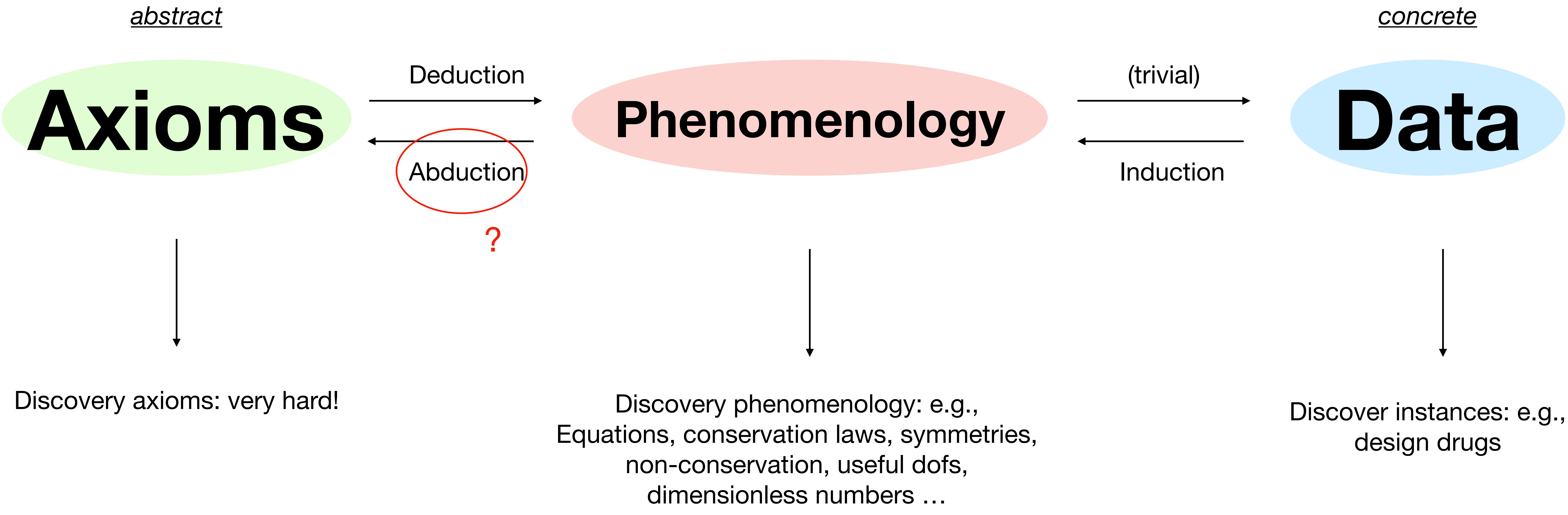
Searching for manifest coordinates



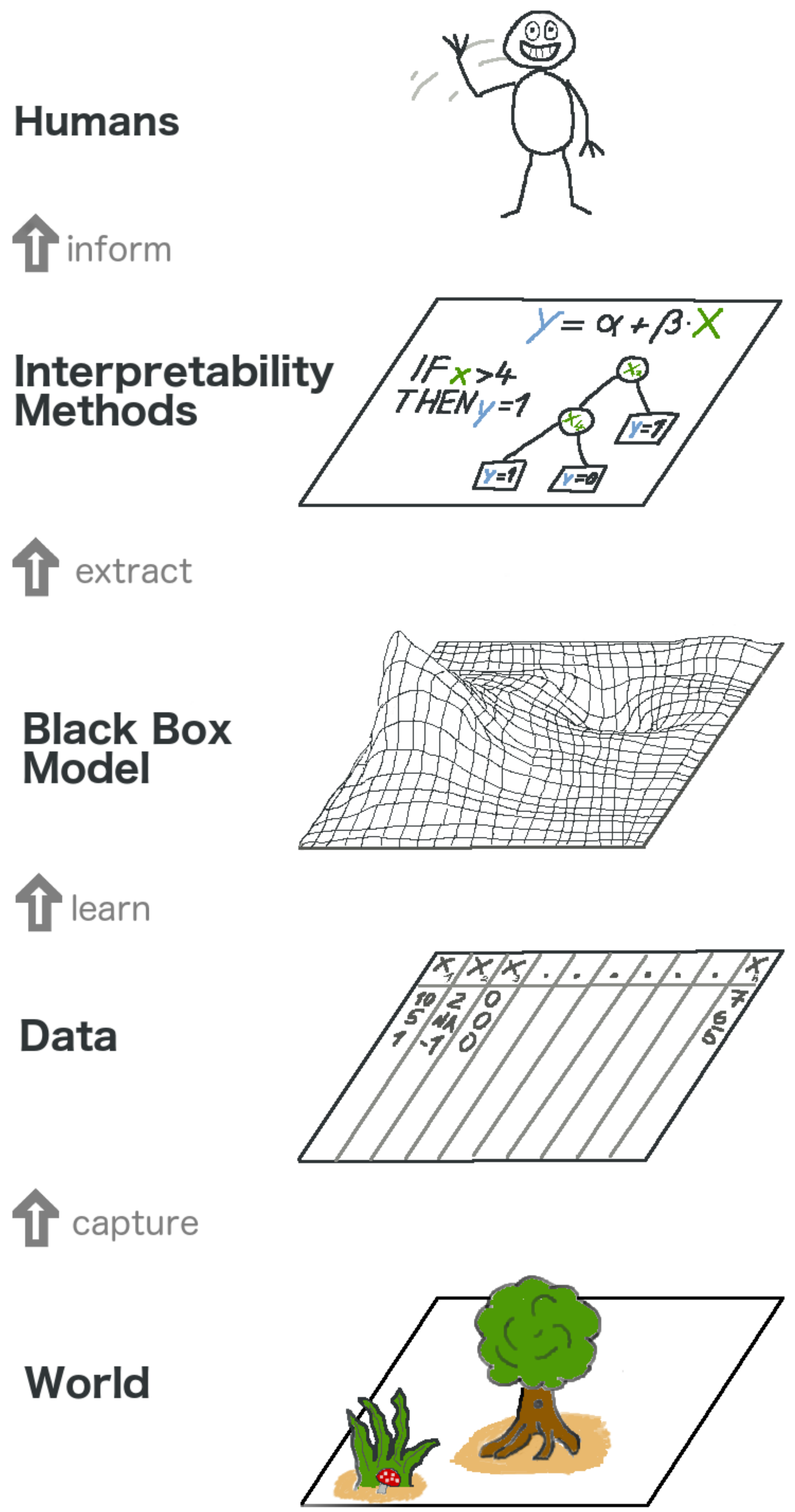
$$T'^{i'_1 \cdots i'_m}_{j'_1 \cdots j'_n} = \mathbf{W}^{i'_1}_{\ i_1} \cdots \mathbf{W}^{i'_m}_{\ i_m} (\mathbf{W}^{-1})^{j_1}_{\ j'_1} \cdots (\mathbf{W}^{-1})^{j_n}_{\ j'_n} T^{i_1 \cdots i_m}_{j_1 \cdots j_n}$$

Open questions

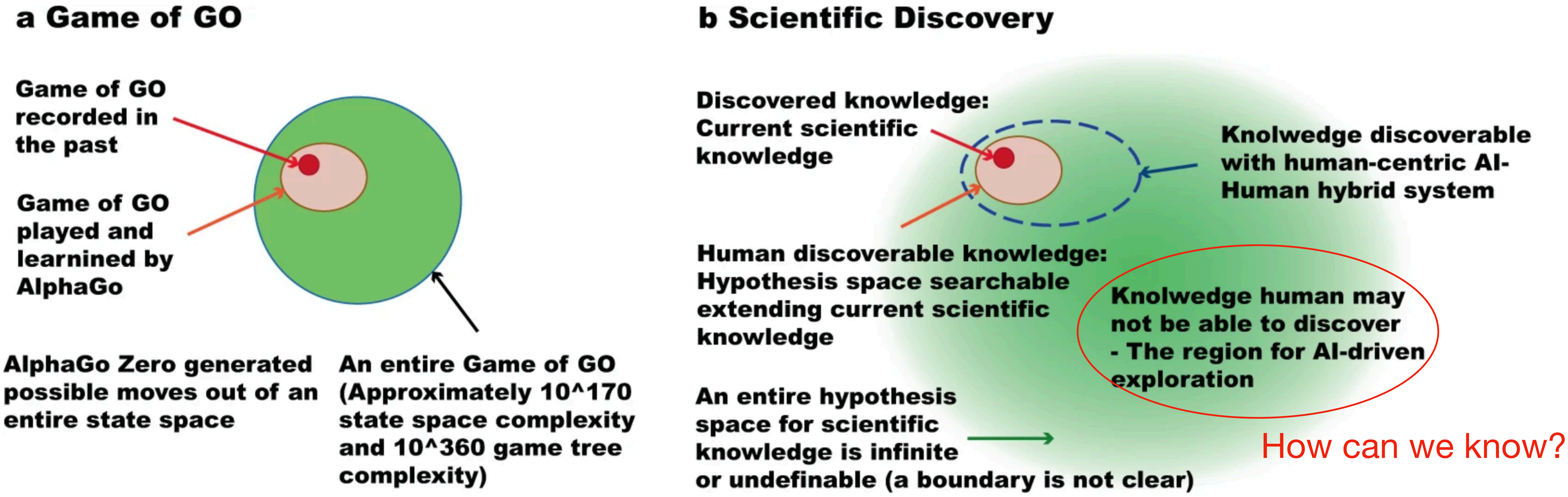
1. Abduction


abstract
concrete
Axioms
Deduction
Abduction
?
Phenomenology
(trivial)
Induction
Data
Discovery axioms: very hard!
Discovery phenomenology: e.g., Equations, conservation laws, symmetries, non-conservation, useful dofs, dimensionless numbers …
Discover instances: e.g., design drugs

2. Interpretability



3. Level of discovery



Search space structures for **a** perfect information games as represented by the Game of GO and **b** scientific discovery are illustrated with commonalities and differences. While the search space for the Game of GO is well-defined, the search space for scientific discovery is open-ended. A practical initial strategy is to augment search space based on current scientific knowledge with human-centric AI-Human Hybrid system. An extreme option is to set search space broadly into distant hypothesis spaces where AI Scientist may discover knowledge that was unlikely to be discovered by the human scientist.