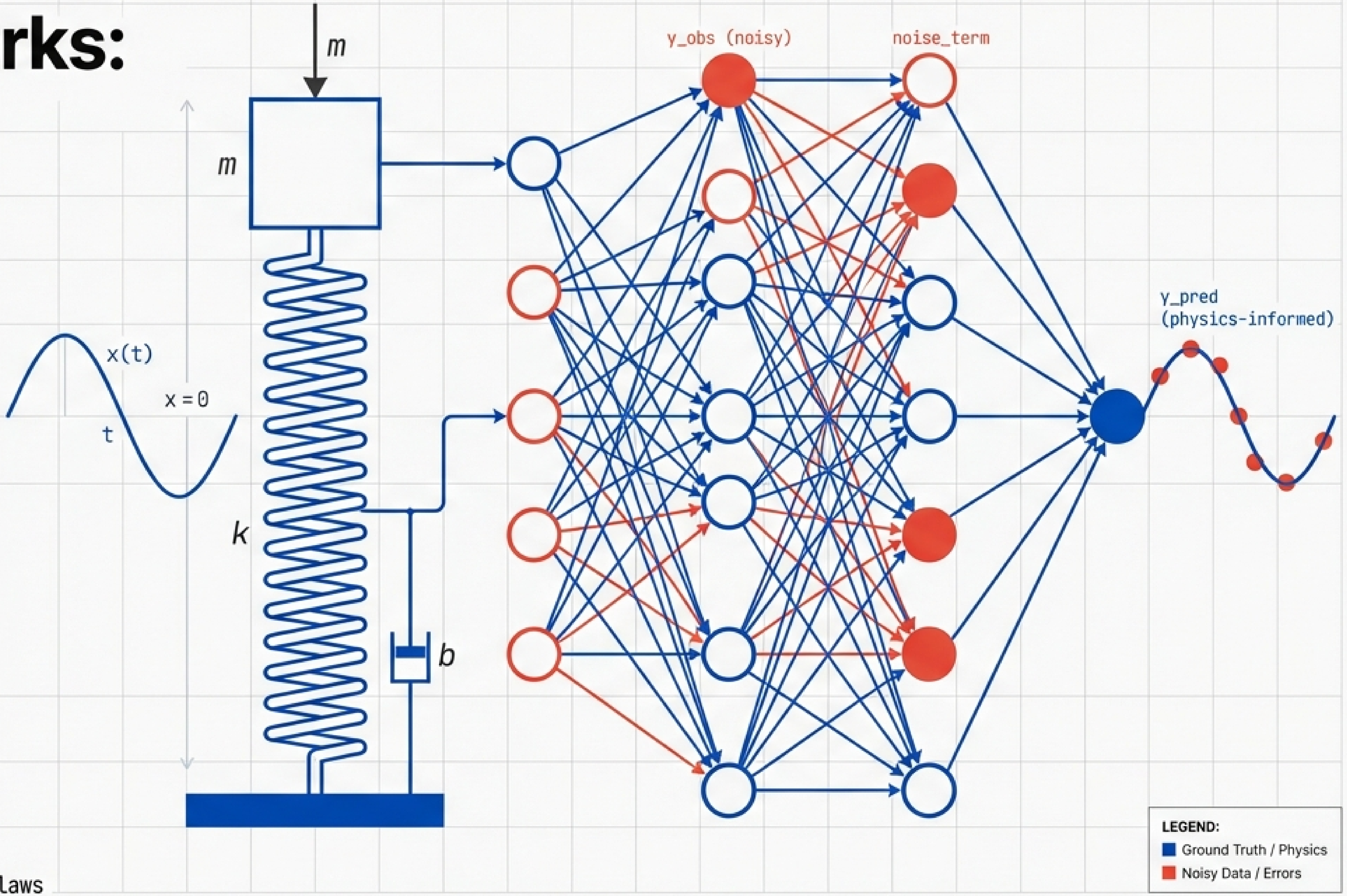
Physics-Informed Neural Networks: Discovery through JAX

Solving Inverse Problems for the Damped Harmonic Oscillator



Bridging the gap between noisy observational data and exact physical laws

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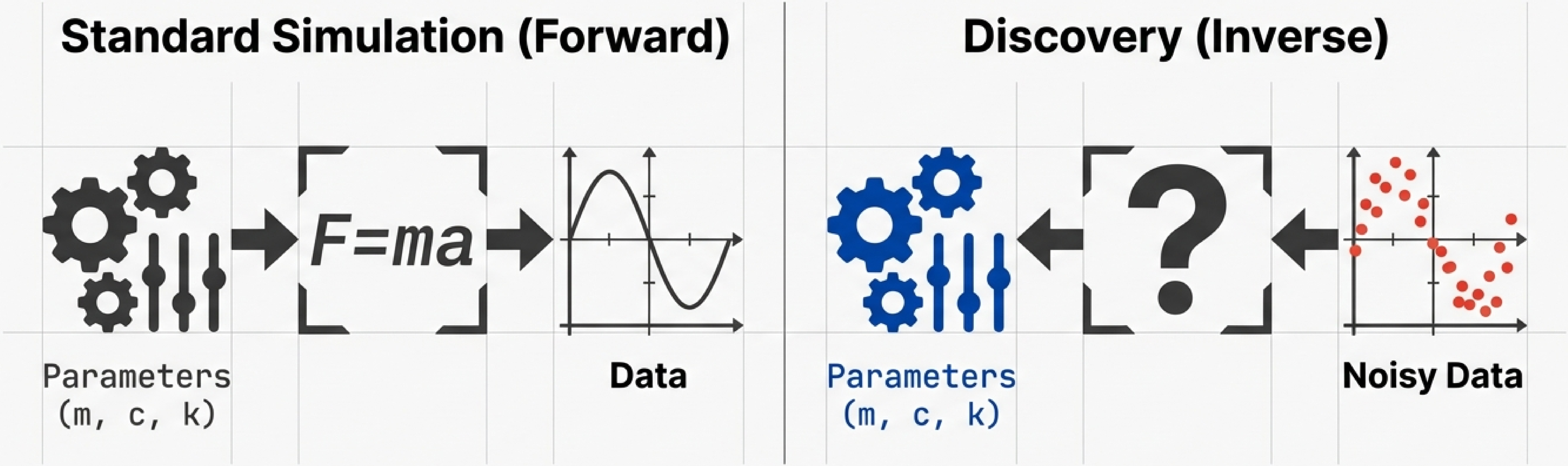
The Challenge: Solving the Inverse Problem



In traditional modeling, we input parameters to simulate motion. **In this experiment**, we **do the reverse: the AI observes the motion** and must **deduce the mass, stiffness**, and **damping coefficients** on its own.

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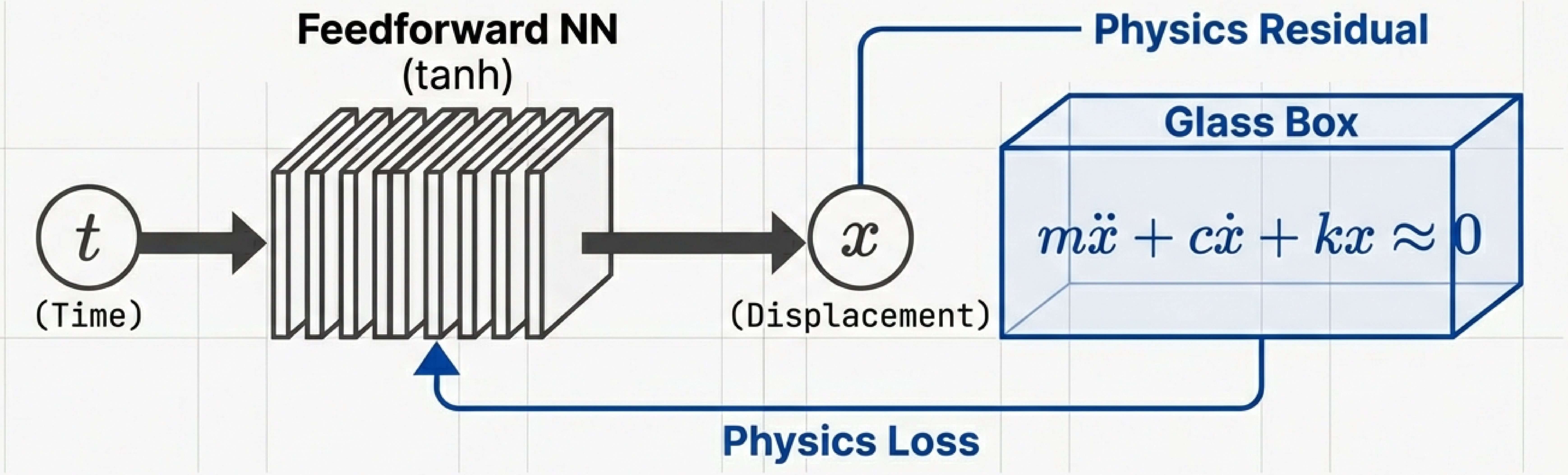
The "Glass Box" Architecture



Data Loss

Does the curve fit the dots?

Physics Loss

Does the curve obey the law?

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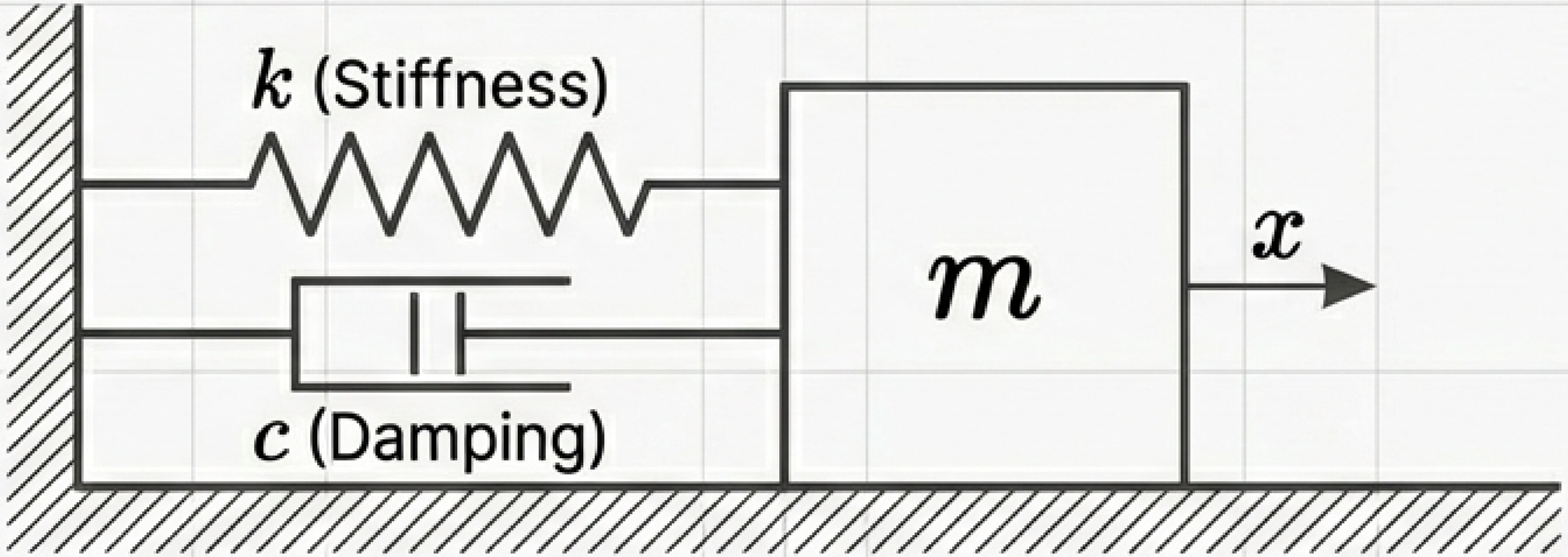
The Subject: The Damped Harmonic Oscillator

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0$$



m: Mass (Inertia)

c: Damping Coefficient (Friction/Drag)

k: Spring Stiffness (Restoring Force)

A fundamental system describing everything from mechanical vibrations to electrical circuits. We simulate an underdamped case ($\zeta < 1$) where oscillation decays over time.

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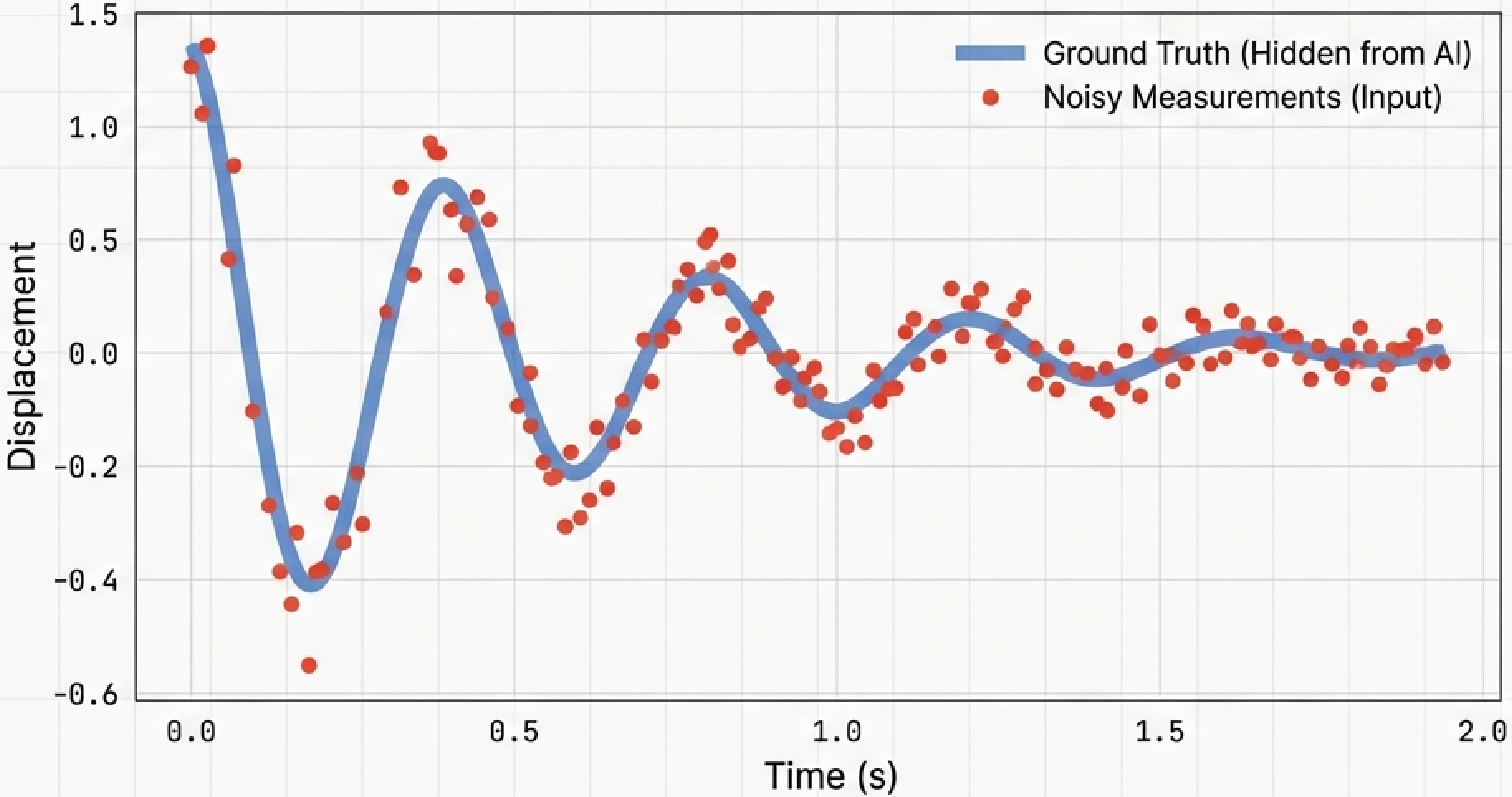
The Input: Noisy Sensor Data



N_data: 200 points
Noise Level: 2% Gaussian
Time Domain: [0, 2.0]s
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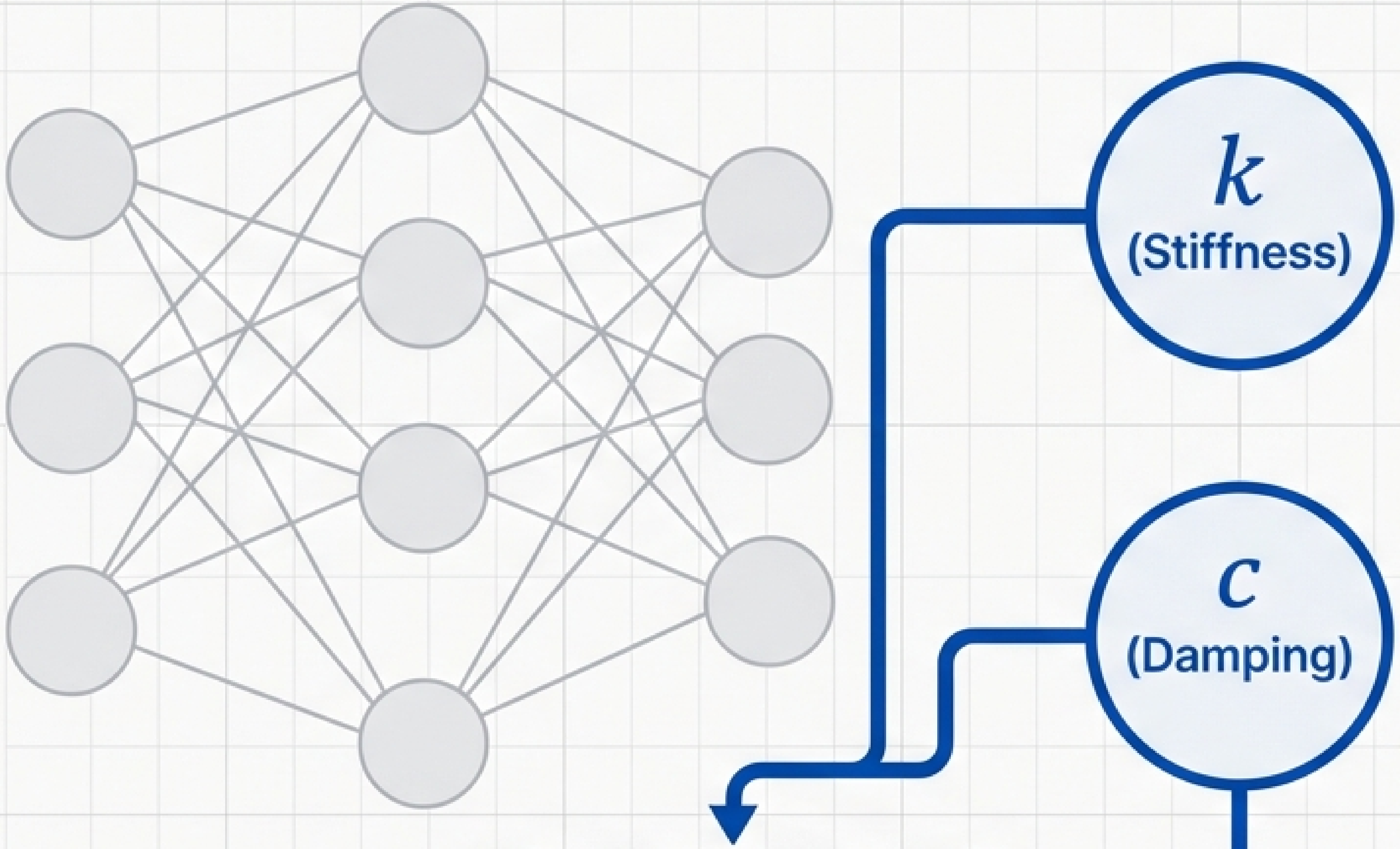
The network never sees the blue line. It must discover the underlying physics solely from the scattered red dots.

The Innovation: Physics as Trainable Weights



LOSS FUNCTION CALCULATION

$$L_{total} = L_{data} + L_{physics}$$

$$L_{physics} \propto |m\ddot{x} + c\dot{x} + kx|^2$$

// Initialization	
Mass (m):	`1.0 kg (Known)`
Initial Guess k:	`50.0 (True: 100)`
Initial Guess c:	`1.0  (True: 2)`

We start with wrong guesses. The optimizer updates both the network weights to fit the curve AND these physical parameters to satisfy the differential equation.

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The Engine: JAX & Automatic Differentiation

Exact Derivatives (Auto-Diff)

```
u_t = grad(u_pred, argnums=1)  # Velocity
u_tt = grad(u_t, argnums=1)   # Acceleration

residual = m*u_tt + c*u_t + k*u
```

Exact Derivatives (Auto-Diff)

Physics Equation Embedded Here

Finite differences are messy and error-prone. JAX allows us to compute exact derivatives ($\dot{x}, \ddot{x}$) relative to time using automatic differentiation, ensuring the physics loss is mathematically rigorous.

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The Three Pillars of Loss

$$L_{\mathrm{total}} = L_{\mathrm{data}} + L_{\mathrm{physics}} + L_{\mathrm{IC}}$$

Data Error
MSE(Prediction, Red Dots)

Physics Residual
$\mathrm{MSE}(m\ddot{x} + c\dot{x} + kx)$

Initial Conditions
Ensure $x(0)=1, \dot{x}(0)=0$

Training involves a delicate balance: fitting the noisy observation (Data) while simultaneously obeying the differential equation (Physics).

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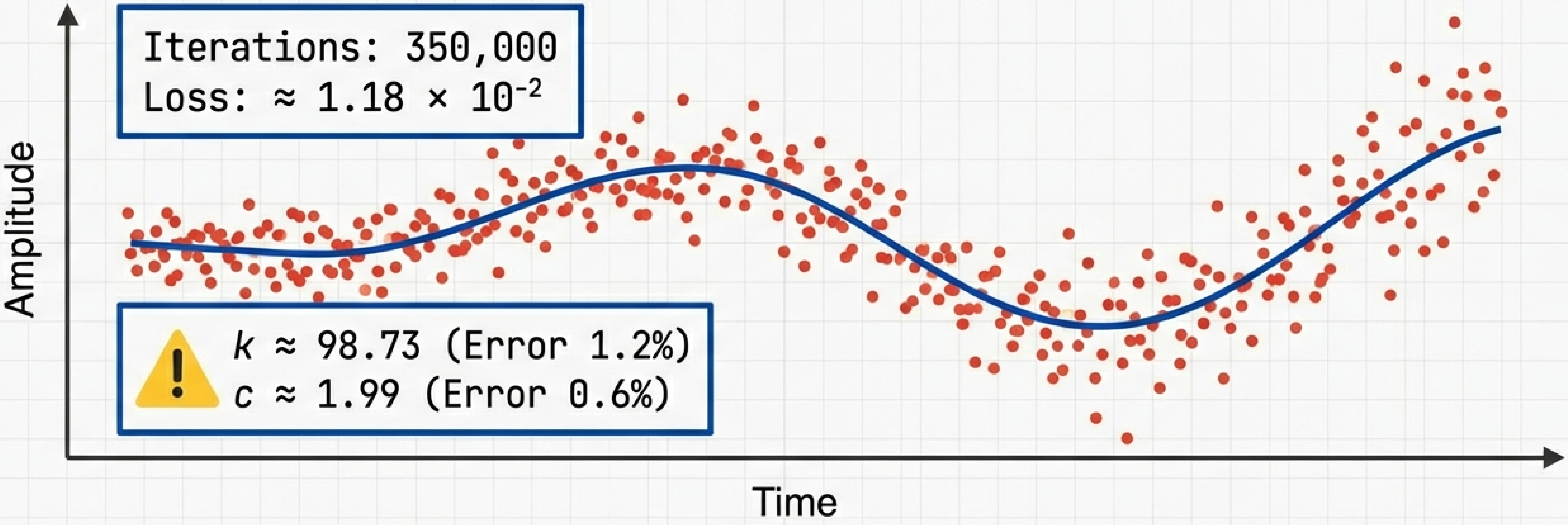
Phase 1: Rough Fitting with Adam



Adam is excellent for rapid convergence and navigating the loss landscape, but it struggles to 'lock in' the high-precision parameter recovery we require.

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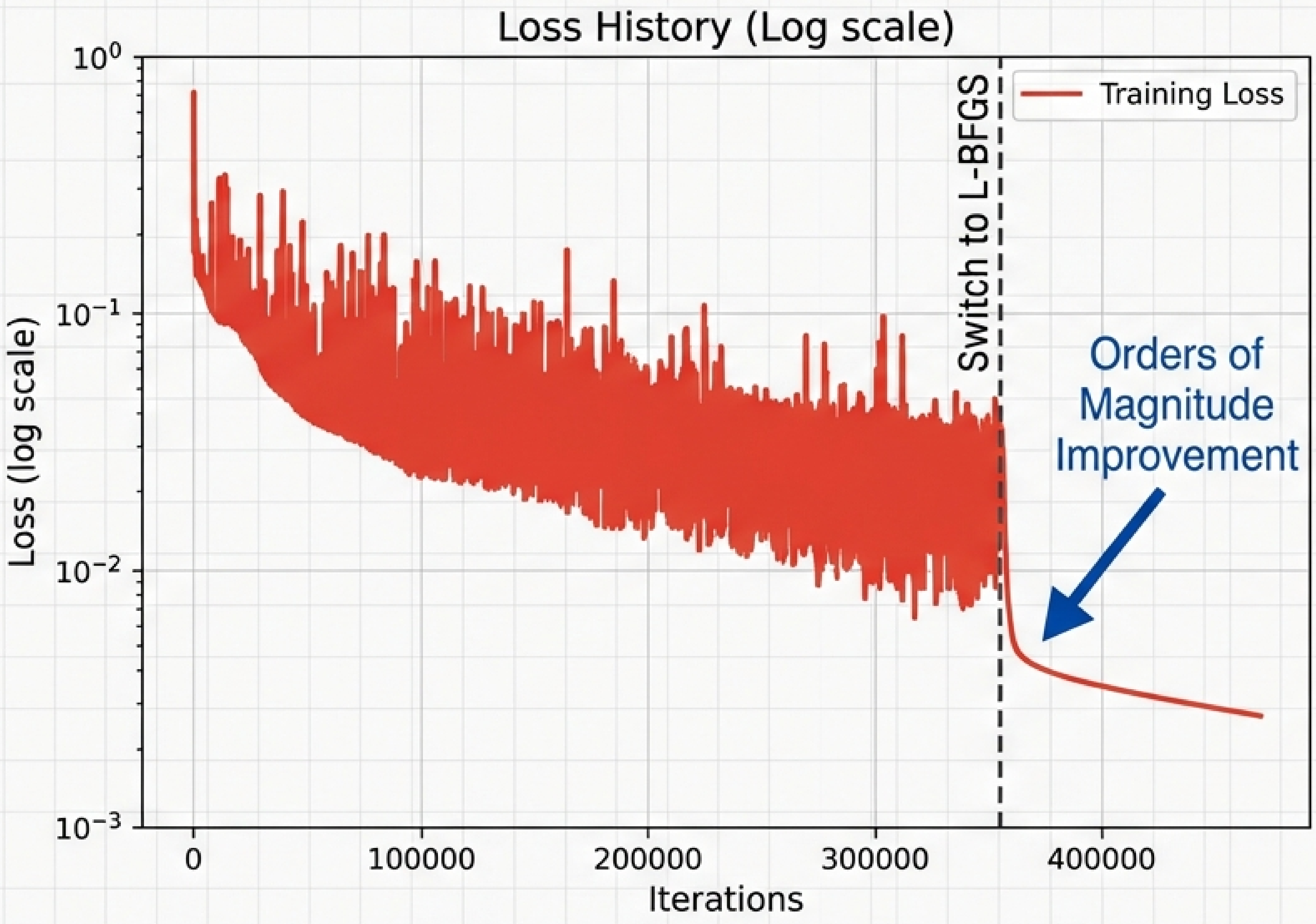
Phase 2: The Hybrid Optimization Strategy



We switch from **Adam (Stochastic Gradient** Descent) to **L-BFGS (Second-order optimizer)**. This algorithm uses curvature information to fine-tune the solution, dropping the error from 10^{-2} to 5×10^{-4}.

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The Discovery: Recovering Physical Truth

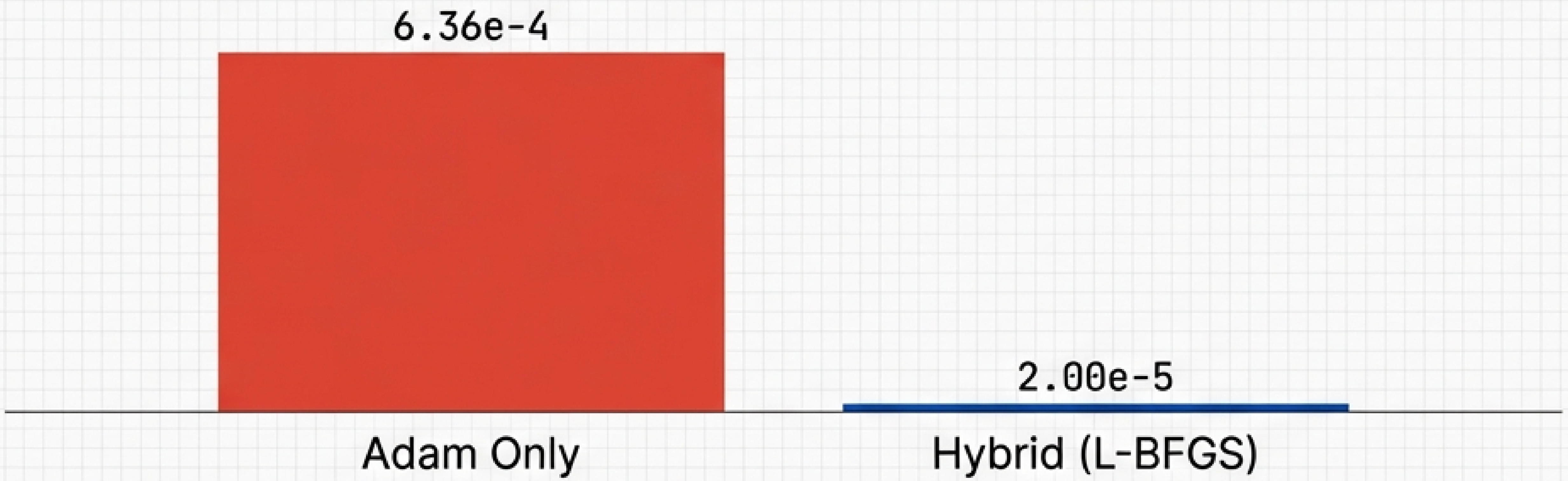
Stiffness k

True Value:	100.0
Discovered:	99.83
Error:	0.17%

Damping c

True Value:	2.0
Discovered:	2.03
Error:	1.65%

Mean Squared Error (MSE) Comparison



The hybrid approach reduced the error by a factor of 30, recovering the stiffness to within 0.17% of the truth.

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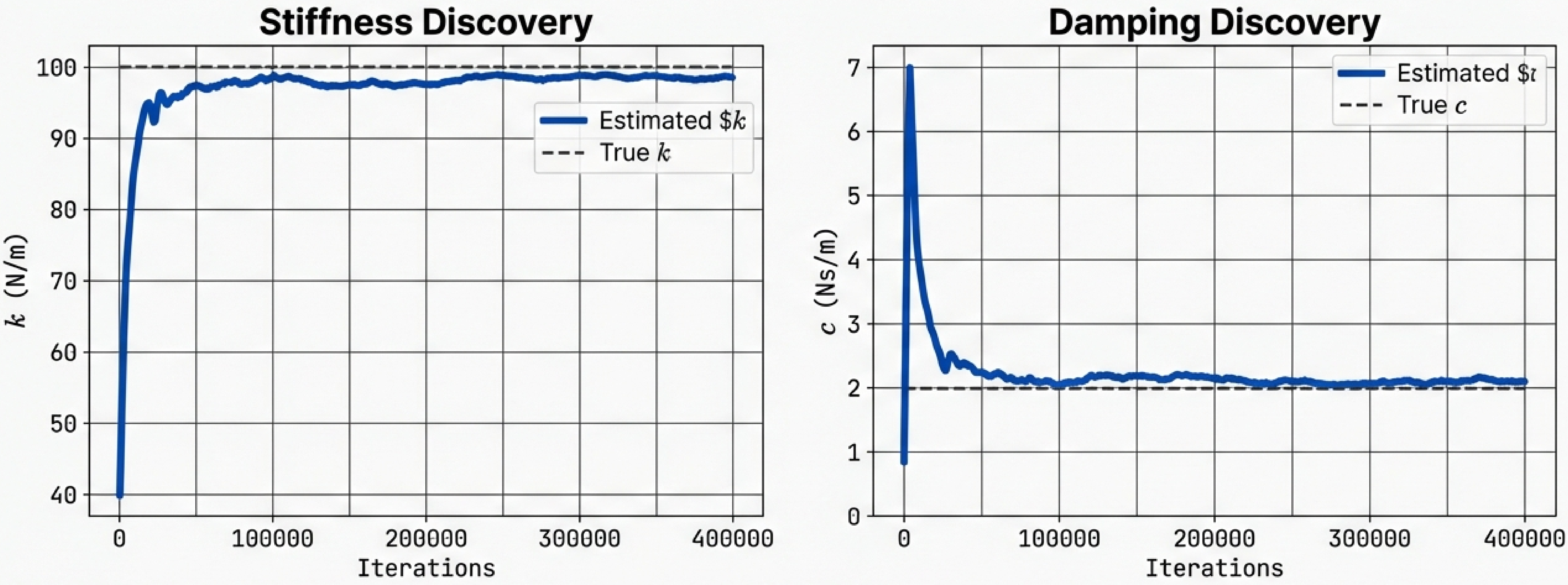
Visualizing the Search for k and c



The 'dashboard' of discovery. We can watch the AI converge on the physical constants as training progresses.

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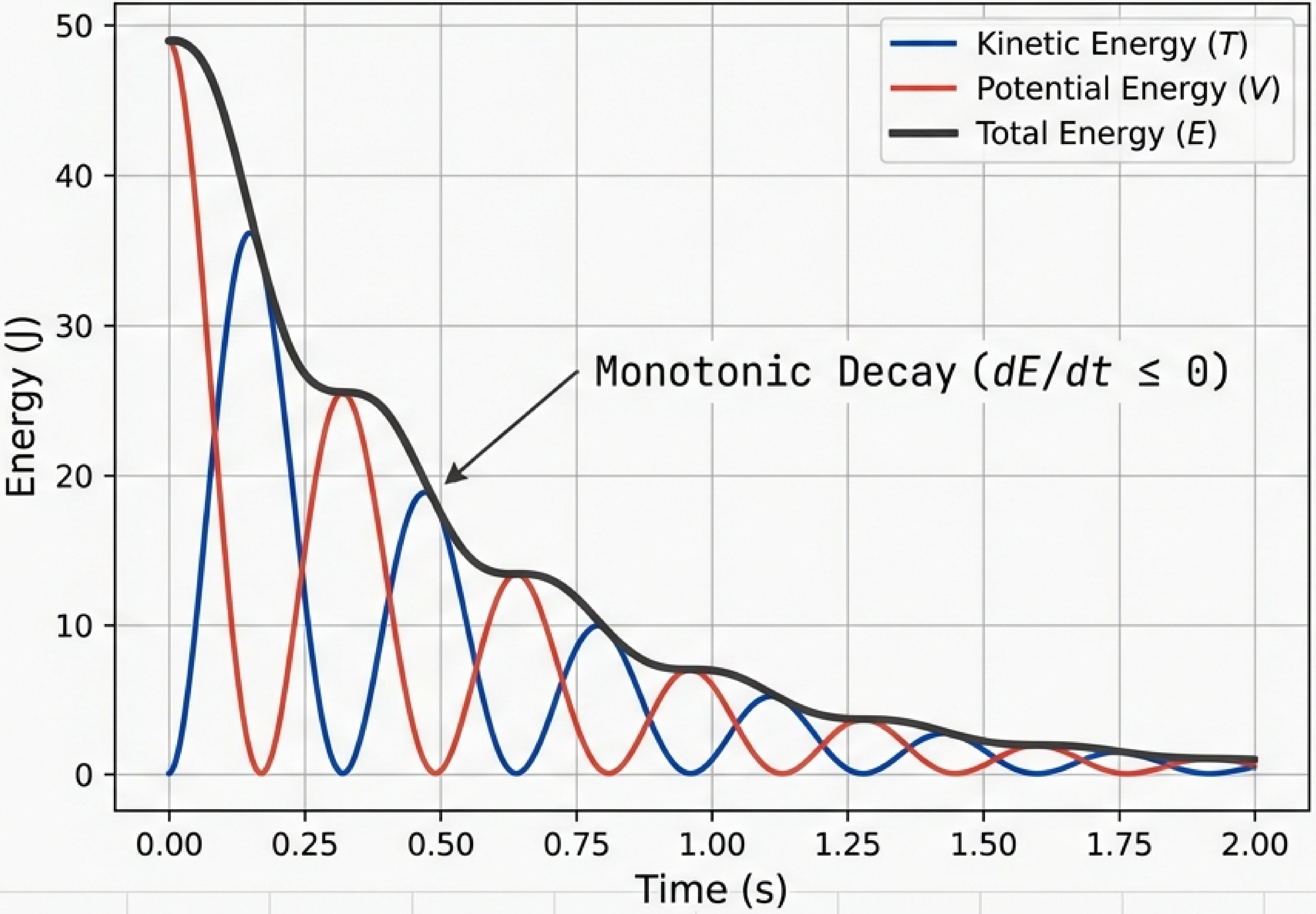
Verification I: Energy Dissipation



$$E = T + V = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2$$

Even though the AI wasn't explicitly told about 'Energy," the solution perfectly conserves the thermodynamics of dissipation.

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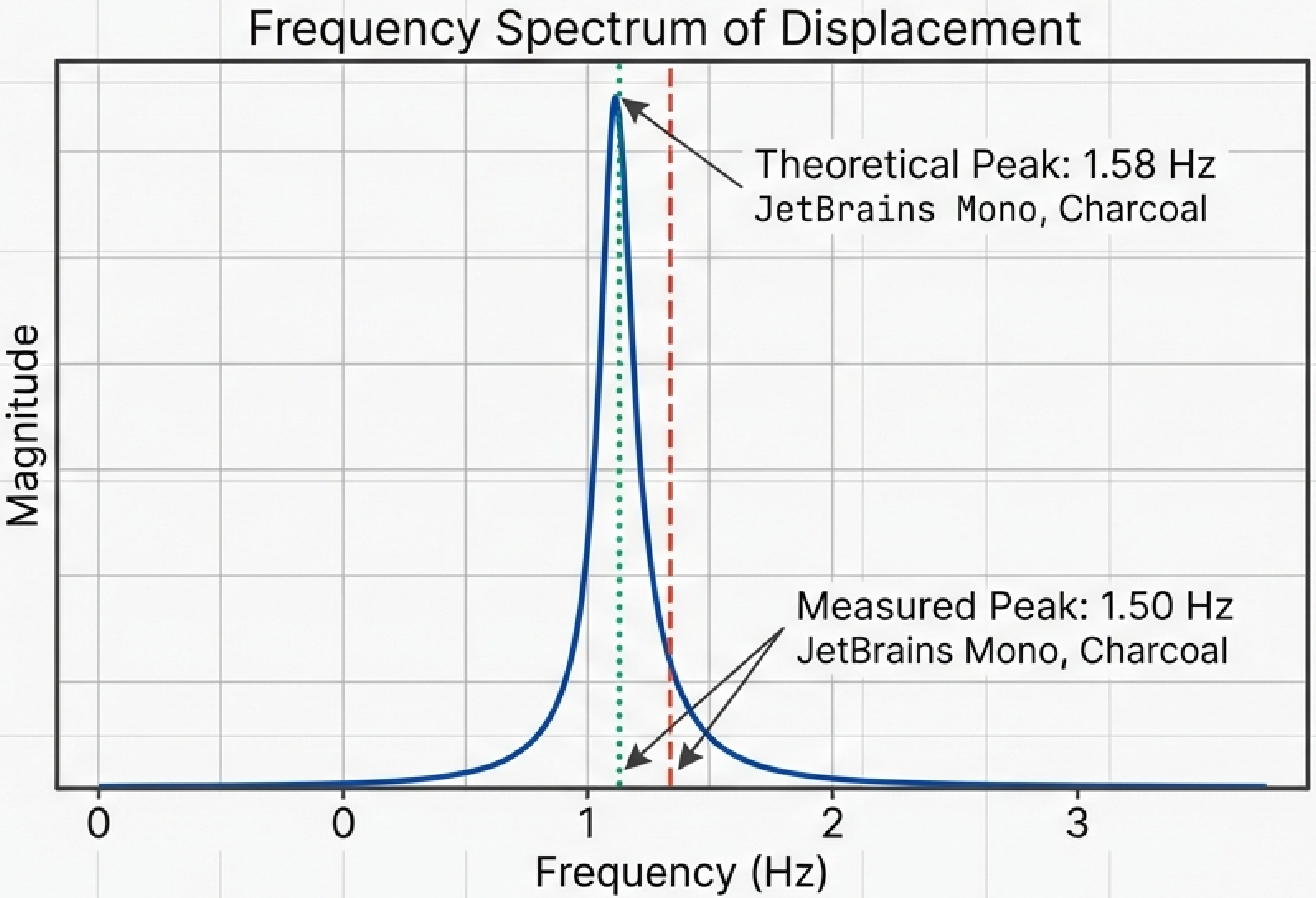
Verification II: Frequency Analysis



A Fast Fourier Transform (**FFT**) confirms the network captured the correct dominant frequency of the system, aligning closely with the damped natural frequency ω_d.

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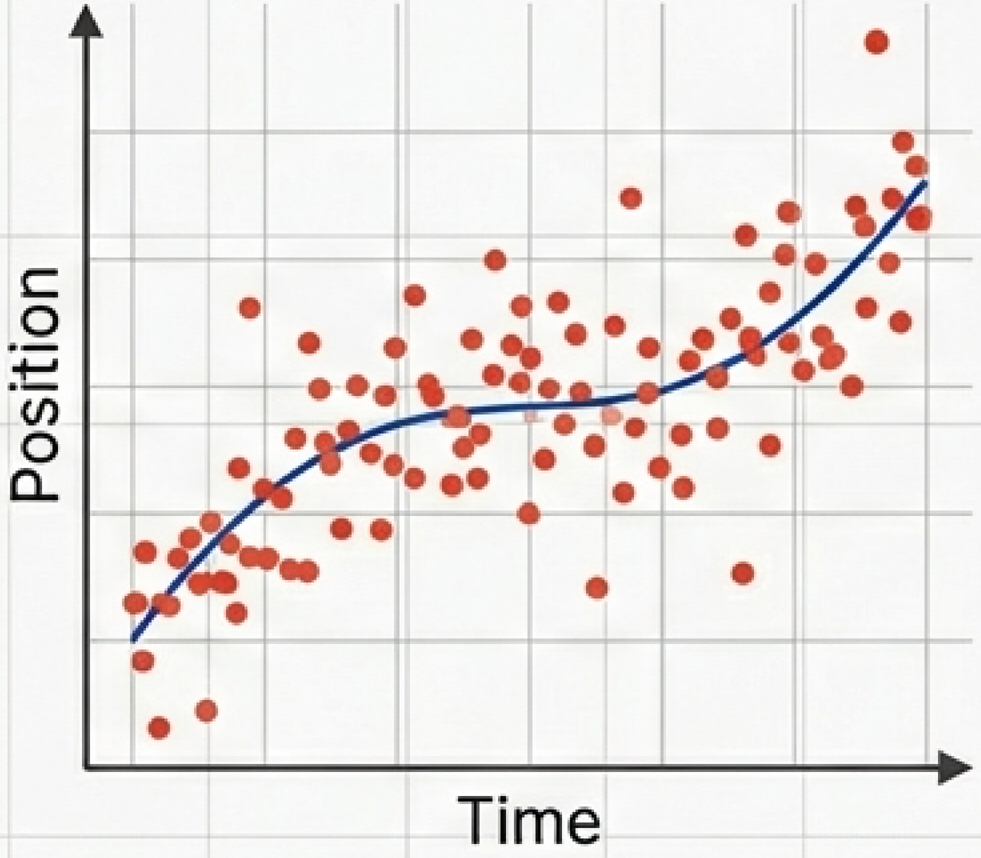
From Noise to Laws

Observations

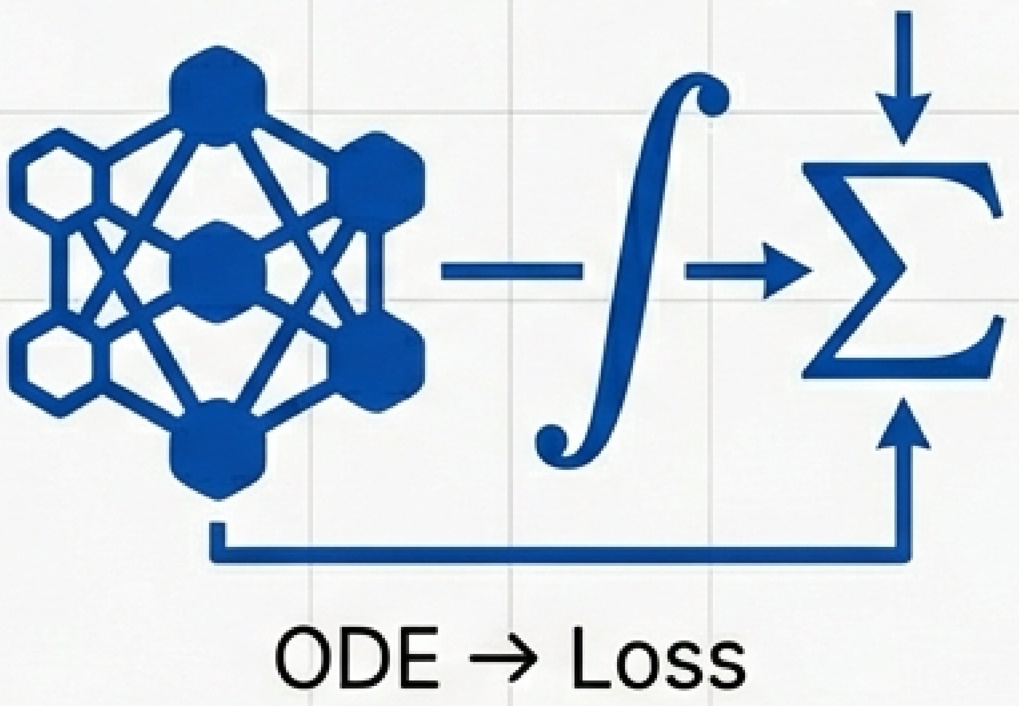
Using real-world, noisy sensor data.



Physics-Informed Training

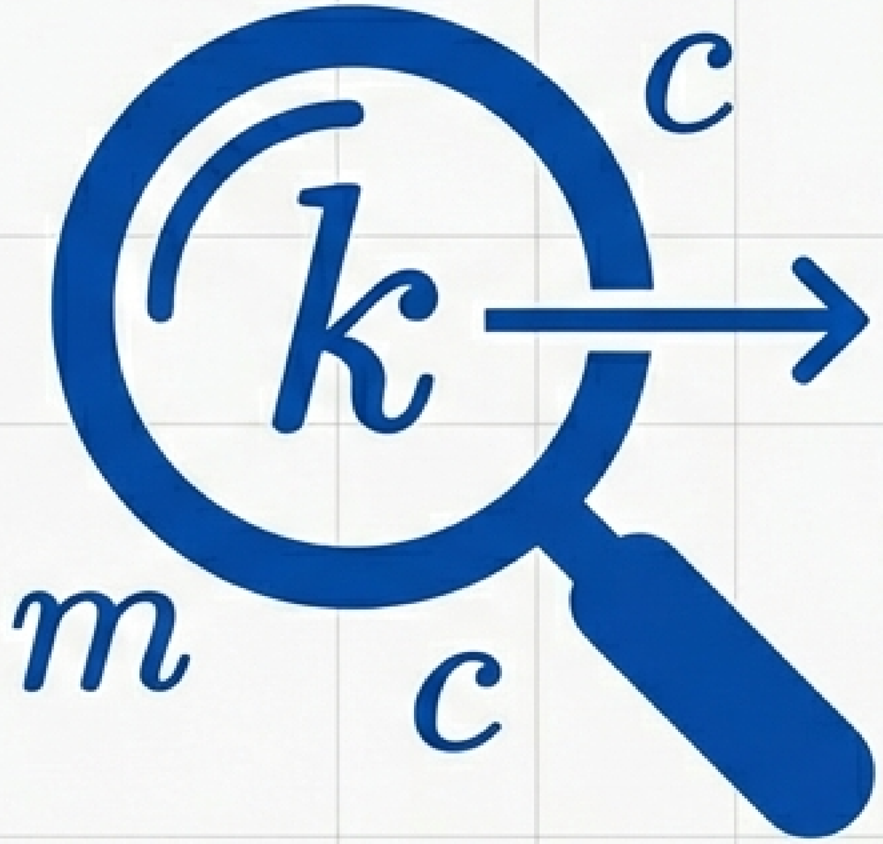
JAX & Hybrid Optimization embed the ODE into the loss.

$$\mathcal{L}_{total} = \mathcal{L}_{data} + \mathcal{L}_{physics}$$



Discovery

Recovering exact physical parameters.



We have proven that Physics-Informed Neural Networks can successfully extract governing physical laws and constants directly from imperfect observational data.

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