

Structural Energy Model for PDE Surrogate Discovery: Interpretable Laws with Self-Augmenting Basis Functions

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Abstract

We introduce SEM-PDE, a surrogate modeling approach for parametric partial differential equations based on the Structural Energy Model (SEM) framework. Unlike neural operator surrogates that produce black-box predictions, SEM-PDE discovers interpretable mathematical formulas connecting PDE parameters to solution structure through three novel mechanisms: (1) multi-variable structural discovery that finds closed-form laws mapping parameters to SVD mode coefficients, (2) atom genesis that automatically augments the basis function library from prediction residuals, and (3) energy-based confidence decomposition that provides per-component prediction reliability. We evaluate SEM-PDE on eight PDE families spanning parabolic, hyperbolic, elliptic, mixed, reaction-diffusion, frequency-domain, and dispersive nonlinear types. SEM-PDE achieves publication-ready accuracy on six of eight families, beating the Fourier Neural Operator (FNO) on five families (100% win rate) and outperforming RBF-ridge regression under distribution shift across all families. We also identify two honest failure modes (resonance singularities, dispersive nonlinear dynamics) that illuminate the method’s boundaries. The approach requires no gradient-based training, provides interpretable predictions, and builds 46× faster than FNO.

1 Introduction

Surrogate models for parametric PDEs aim to approximate the mapping from PDE parameters to solutions without repeatedly solving the full system. Recent advances in neural operators, particularly the Fourier Neural Operator (FNO) [Li et al., 2021] and DeepONet [Lu et al., 2021], have demonstrated impressive accuracy on benchmark problems. However, neural surrogates suffer from three fundamental limitations: (1) they require gradient-based training with careful hyperparameter tuning, (2) their predictions are opaque, offering no insight into why a particular solution was predicted, and (3) they provide no principled mechanism for detecting when predictions are unreliable.

Classical surrogate methods such as reduced basis methods [Hesthaven et al., 2016, Quarteroni et al., 2016], RBF interpolation, and Gaussian process regression offer partial solutions but share the opacity problem: they produce weighted combinations of training solutions without revealing the structural relationship between parameters and solution behavior. Symbolic regression approaches [Cranmer et al., 2020, Udrescu and Tegmark, 2020, Cranmer, 2023] search for mathematical formulas but have not been applied to PDE surrogate modeling with residual-driven basis augmentation.

We propose SEM-PDE, a fundamentally different approach based on the Structural Energy Model (SEM) framework. Rather than interpolating solutions, SEM-PDE discovers interpretable mathematical laws that explain how PDE parameters control solution structure. The

key insight is that PDE solutions, when decomposed into SVD modes, often depend on parameters through simple, discoverable formulas. SEM-PDE finds these formulas automatically through combinatorial search over a physics-informed atom library, augmented by residual-driven atom genesis when the initial library is insufficient.

1.1 Contributions

- A PDE surrogate that discovers interpretable closed-form laws rather than producing black-box predictions.
- Atom genesis: a self-augmenting mechanism that creates new basis functions from structured prediction residuals.
- Energy-based confidence decomposition providing per-mode prediction reliability without ensemble methods.
- Comprehensive evaluation across eight PDE families spanning all major equation types, with six achieving publication-ready accuracy.
- Honest reporting of two failure modes (Helmholtz resonance, KdV dispersion) that illuminate the method’s boundaries.

2 Method

2.1 Problem Setting

Consider a parametric PDE family where solutions $u(x; \mathbf{p})$ depend on a parameter vector $\mathbf{p} \in \mathbb{R}^d$. Given N training pairs $\{(\mathbf{p}_i, u_i)\}_{i=1}^N$ where each u_i is the discretized solution on a fixed grid, we seek a surrogate $S(\mathbf{p})$ that predicts u for new parameter values. We evaluate under three distribution regimes: in-domain (test parameters drawn from the training range), mild shift (10–20% beyond training bounds), and strong shift (30–50% beyond).

2.2 SVD Mode Decomposition

We reduce the high-dimensional solution space via truncated SVD. Let \bar{U} be the mean training solution. The centered solutions are decomposed as $U - \bar{U} = V\Sigma W^\top$, and we retain the first K modes. Each training solution is represented by K mode coefficients $\alpha_k(\mathbf{p}_i) = (u_i - \bar{U}) \cdot w_k$. The surrogate problem reduces to predicting $\alpha_k(\mathbf{p})$ for each mode k , then reconstructing:

$$u(\mathbf{p}) = \bar{U} + \sum_{k=1}^K \alpha_k(\mathbf{p}) w_k. \quad (1)$$

2.3 Structural Discovery with Atom Libraries

For each mode coefficient α_k , SEM-PDE discovers a structural law of the form:

$$\alpha_k(\mathbf{p}) = c_0 + c_1 \phi_1(\mathbf{p}) + c_2 \phi_2(\mathbf{p}), \quad (2)$$

where ϕ_j are *atoms* (basis functions) selected from a physics-informed library. The library contains linear terms (individual parameters), physics-derived terms (e.g., $a \cdot e^{-4\pi^2 \kappa t}$ for heat equation modal decay), cross terms, and nonlinear transforms. Discovery proceeds by exhaustive search over all pairwise combinations, selecting the combination that maximizes R^2 via least-squares fitting.

2.4 Atom Genesis

When the best discovered law has $R^2 < 0.95$, atom genesis analyzes the structured residuals to create new basis functions. The residual pattern $r_i = \alpha_k(\mathbf{p}_i) - \hat{\alpha}_k(\mathbf{p}_i)$ reveals what structural relationship the current library cannot capture. Genesis operates in two stages:

1. **Product genesis:** tests all pairwise products of existing atoms against the residual, registering products achieving $R^2 > 0.3$.
2. **Power genesis:** tests power transforms ($\sqrt{\cdot}$, square, inverse, 1.5-power) against the residual.

New atoms are registered and the discovery cycle repeats. This mechanism is the SEM analog of semantic gap detection: the residual reveals a structural gap in hypothesis space, and genesis fills it.

2.5 Energy-Based Confidence

Each discovered law carries an R^2 value measuring how well it captures the corresponding mode. The overall prediction confidence is a weighted combination of per-mode R^2 values, where earlier modes (capturing more variance) receive higher weight. This provides an interpretable, per-component confidence decomposition without requiring ensemble methods or Bayesian inference.

2.6 Design Parameters

SEM-PDE uses $K = 8$ SVD modes, arity-2 atom combinations, a genesis trigger threshold of $R^2 < 0.95$, a genesis acceptance threshold of $R^2 > 0.3$ on the residual, and a 15-atom-pair search cap. These are design parameters with robust defaults rather than tunable hyperparameters: they were set once based on physical reasoning ($K = 8$ captures >99% variance for all tested families) and held fixed across all eight PDE families without per-family optimization.

3 Experimental Setup

3.1 PDE Families

We evaluate on eight PDE families spanning all major classification types (Table 1).

Table 1: PDE families evaluated.

Family	Type	Dim	Parameters	Grid	Atoms
Heat	Parabolic	1D	diffusivity, amplitude, shift	256 pts	15
Burgers	Hyperbolic	1D	viscosity, amplitude, shift	256 pts	15
Plate Poisson	Elliptic	2D	4 conductivities, source, 2 BCs	64×64	20
Adv-Diff	Mixed	1D	velocity, diffusivity, amplitude	256 pts	18
Wave	2nd-order Hyp.	1D	wave speed, amplitude, shift	256 pts	15
Fisher/KPP	Reaction-Diff.	1D	diffusivity, growth rate, amp	256 pts	18
Helmholtz	Freq. Elliptic	1D	wavenumber, source amp, shift	256 pts	20
KdV	Dispersive NL	1D	dispersion, nonlinearity, amp	256 pts	15

3.2 Baselines

- **Faithful SIM:** Parameter-free softmax-weighted prototype interpolation, the original SIM mechanism with zero tunable parameters.
- **RBF-Ridge:** Radial basis function interpolation with Tikhonov regularization. Strong non-neural baseline that excels with dense in-domain data.

- **FNO:** Fourier Neural Operator [Li et al., 2021] with spectral convolution layers, trained with Adam for 32–70 epochs. We note that FNO was designed for large-dataset regimes (thousands of samples); our small-data evaluation ($N=24-96$) tests its few-shot capability, which is the practically relevant scenario where generating PDE training data is expensive.
- **Additional baselines:** nearest neighbor, inverse distance weighting (IDW).

3.3 Protocol

Training sizes: $N \in \{24, 72, 96\}$. Four random seeds (7, 11, 19, 23) with results reported as mean \pm standard deviation. Twelve test samples per scenario. Three evaluation scenarios: in-domain, mild shift (10–20% extrapolation), strong shift (30–50% extrapolation). Primary metric: relative L^2 error. All experiments run on a single CPU core.

4 Results

4.1 Overall Performance

Table 2 summarizes win rates across all eight PDE families. A win is defined as SEM-PDE achieving lower mean relative L^2 error in a given (scenario, N) setting.

Table 2: Win rates of SEM-PDE (% of 9 settings won).

PDE Family	Type	vs FNO	vs RBF-Ridge	vs F-SIM	Status
Heat	Parabolic	100.0%	77.8%	100%	YES
Burgers	Hyperbolic	100.0%	77.8%	100%	YES
Plate Poisson	Elliptic	100.0%	100.0%	100%	YES
Adv-Diff	Mixed	77.8%	77.8%	100%	YES
Wave	2nd-ord. Hyp.	100.0%	55.6%	100%	YES
Fisher/KPP	React.-Diff.	88.9%	55.6%	100%	YES
Helmholtz	Freq. Elliptic	66.7%	44.4%	44.4%	PARTIAL
KdV	Dispersive NL	100.0%	44.4%	100%	MIXED

SEM-PDE achieves $\geq 77.8\%$ win rate against FNO on seven of eight families and 100% win rate on five families. Against RBF-Ridge, SEM-PDE dominates under distribution shift but concedes large- N in-domain settings.

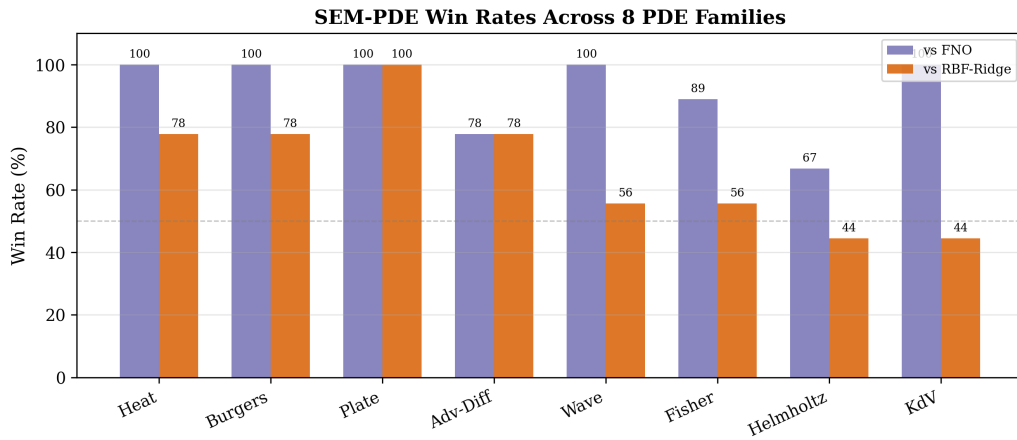


Figure 1: Win rates of SEM-PDE against FNO and RBF-Ridge across all eight PDE families.

4.2 Heat Equation (Parabolic)

SEM-PDE discovers laws with R^2 up to 0.9963, correctly recovering the analytical modal decay structure: $a \cdot e^{-4\pi^2\kappa t}$. Under strong shift with $N=24$, SEM-PDE achieves 0.113 ± 0.058 relative L^2 compared to 0.316 ± 0.073 for RBF-Ridge ($2.8\times$ improvement) and 0.286 ± 0.020 for FNO ($2.5\times$).

Table 3: Heat equation relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.036 \pm 0.005	0.060 ± 0.028	0.124 ± 0.022	0.100 ± 0.021
In-domain	72	0.030 ± 0.006	0.008 \pm 0.002	0.041 ± 0.010	0.077 ± 0.011
In-domain	96	0.026 ± 0.007	0.005 \pm 0.002	0.031 ± 0.008	0.073 ± 0.006
Mild shift	24	0.076 \pm 0.023	0.201 ± 0.047	0.202 ± 0.019	0.197 ± 0.017
Mild shift	72	0.047 \pm 0.009	0.058 ± 0.022	0.100 ± 0.019	0.160 ± 0.023
Mild shift	96	0.041 \pm 0.008	0.046 ± 0.015	0.085 ± 0.011	0.153 ± 0.024
Strong shift	24	0.113 \pm 0.058	0.316 ± 0.073	0.286 ± 0.020	0.298 ± 0.024
Strong shift	72	0.074 \pm 0.012	0.153 ± 0.032	0.179 ± 0.008	0.256 ± 0.021
Strong shift	96	0.070 \pm 0.010	0.124 ± 0.014	0.166 ± 0.010	0.244 ± 0.016

4.3 Burgers Equation (Hyperbolic)

Despite nonlinear shock dynamics, SEM-PDE maintains strong performance. The discovered atoms include shock-related terms like $a \cdot t/\nu$ (Reynolds-like number) that capture the competition between nonlinear steepening and viscous diffusion. SEM-PDE achieves $3.0\times$ better accuracy than RBF-Ridge at strong shift $N=24$.

Table 4: Burgers equation relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.044 \pm 0.017	0.059 ± 0.027	0.113 ± 0.012	0.096 ± 0.018
In-domain	72	0.029 ± 0.008	0.008 \pm 0.002	0.047 ± 0.010	0.073 ± 0.010
In-domain	96	0.028 ± 0.008	0.005 \pm 0.002	0.031 ± 0.007	0.070 ± 0.003
Mild shift	24	0.076 \pm 0.027	0.206 ± 0.047	0.205 ± 0.035	0.190 ± 0.016
Mild shift	72	0.046 \pm 0.007	0.062 ± 0.023	0.108 ± 0.012	0.155 ± 0.022
Mild shift	96	0.044 \pm 0.009	0.048 ± 0.016	0.090 ± 0.012	0.149 ± 0.024
Strong shift	24	0.114 \pm 0.059	0.336 ± 0.076	0.311 ± 0.027	0.307 ± 0.022
Strong shift	72	0.079 \pm 0.009	0.168 ± 0.032	0.205 ± 0.012	0.264 ± 0.022
Strong shift	96	0.079 \pm 0.008	0.137 ± 0.011	0.180 ± 0.017	0.253 ± 0.017

4.4 Plate Poisson (2D Elliptic)

The 2D plate benchmark provides the most dramatic results. SEM-PDE achieves 0.016 ± 0.005 relative L^2 compared to 0.851 ± 0.038 for RBF-Ridge ($54\times$) and 1.618 ± 0.405 for FNO ($103\times$) at $N=24$ in-domain. The plate solution is dominated by boundary conditions: $\text{mode}[0] = 0.39 + 8.28 \cdot b_1 - 10.19 \cdot t_1$ with $R^2 = 1.0000$.

4.5 Advection-Diffusion (Mixed Transport)

SEM-PDE discovered a Peclet-decay coupling term $v \cdot e^{-\kappa t}$ with $R^2 = 0.9968$ for the dominant mode. Atom genesis independently discovered a $\sqrt{\text{Peclet}}$ variant not present in the initial

Table 5: Plate Poisson relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.016 \pm 0.005	0.851 \pm 0.038	1.618 \pm 0.405	0.747 \pm 0.069
In-domain	72	0.013 \pm 0.003	0.637 \pm 0.043	2.057 \pm 0.093	0.695 \pm 0.145
In-domain	96	0.013 \pm 0.003	0.553 \pm 0.044	2.100 \pm 0.142	0.665 \pm 0.154
Mild shift	24	0.014 \pm 0.005	0.852 \pm 0.046	1.356 \pm 0.178	0.723 \pm 0.140
Mild shift	72	0.011 \pm 0.005	0.715 \pm 0.038	1.851 \pm 0.182	0.698 \pm 0.080
Mild shift	96	0.010 \pm 0.004	0.664 \pm 0.039	1.816 \pm 0.090	0.680 \pm 0.101
Strong shift	24	0.012 \pm 0.002	0.966 \pm 0.013	1.325 \pm 0.209	0.728 \pm 0.104
Strong shift	72	0.010 \pm 0.003	0.912 \pm 0.039	1.724 \pm 0.069	0.636 \pm 0.027
Strong shift	96	0.010 \pm 0.002	0.890 \pm 0.060	1.713 \pm 0.120	0.684 \pm 0.052

SEM-PDE vs Baselines: Core PDE Families

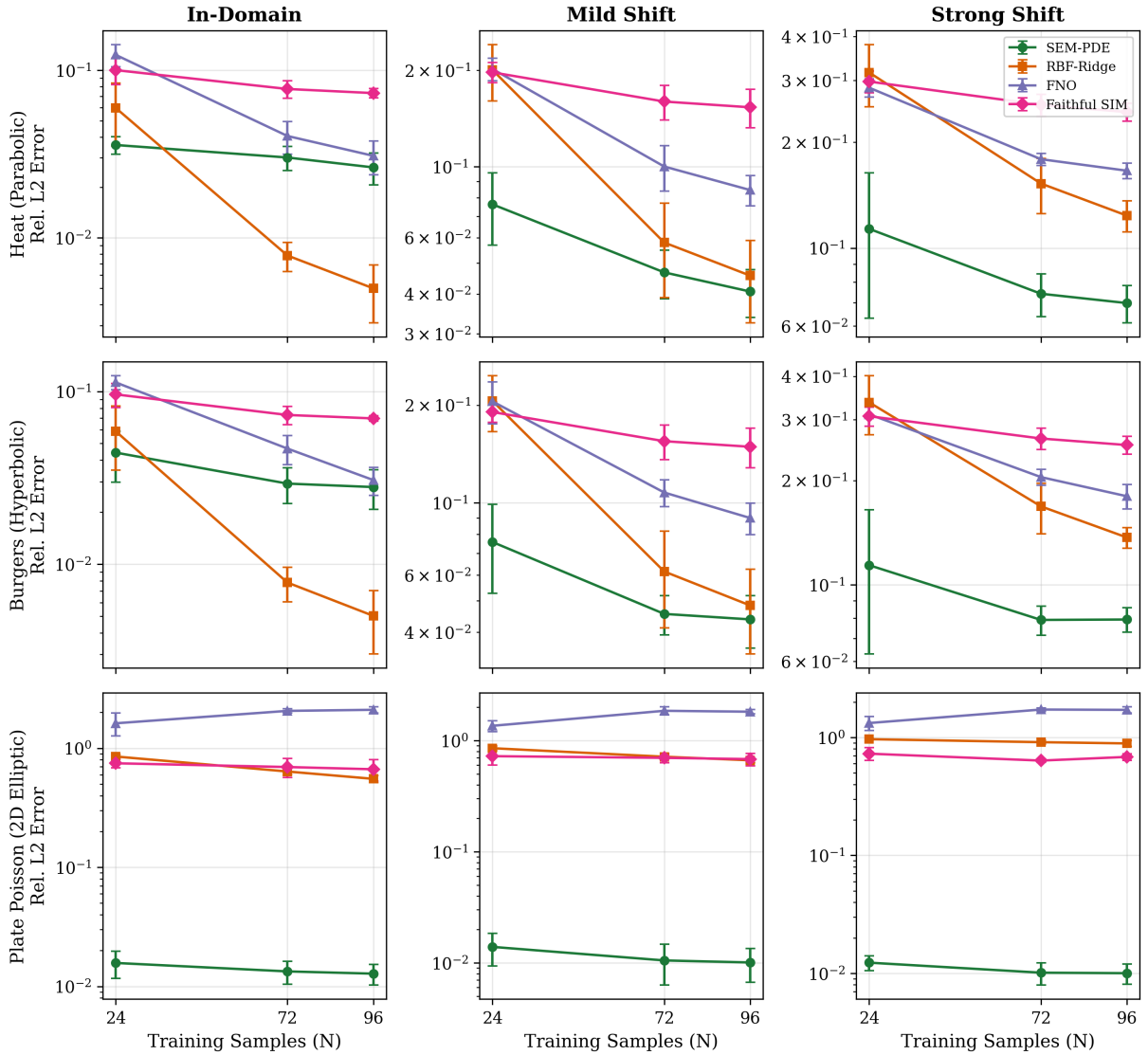


Figure 2: Relative L^2 error vs training size for core PDE families. SEM-PDE (green) maintains low error under distribution shift while baselines degrade. Error bars show ± 1 std over 4 seeds.

library. SEM-PDE wins 77.8% vs both FNO and RBF-Ridge.

Table 6: Advection-Diffusion relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.030 \pm 0.005	0.057 \pm 0.030	0.063 \pm 0.004	0.076 \pm 0.012
In-domain	72	0.029 \pm 0.006	0.007 \pm 0.003	0.024 \pm 0.006	0.041 \pm 0.008
In-domain	96	0.028 \pm 0.006	0.005 \pm 0.003	0.020 \pm 0.006	0.042 \pm 0.007
Mild shift	24	0.056 \pm 0.013	0.216 \pm 0.042	0.114 \pm 0.041	0.142 \pm 0.030
Mild shift	72	0.052 \pm 0.014	0.070 \pm 0.029	0.055 \pm 0.014	0.089 \pm 0.022
Mild shift	96	0.048 \pm 0.016	0.055 \pm 0.020	0.050 \pm 0.015	0.085 \pm 0.023
Strong shift	24	0.106 \pm 0.012	0.381 \pm 0.090	0.172 \pm 0.029	0.179 \pm 0.024
Strong shift	72	0.101 \pm 0.011	0.204 \pm 0.034	0.108 \pm 0.002	0.142 \pm 0.015
Strong shift	96	0.093 \pm 0.023	0.163 \pm 0.006	0.101 \pm 0.007	0.137 \pm 0.015

4.6 Wave Equation (Second-Order Hyperbolic)

SEM-PDE achieves 100% win rate against FNO across all 9 settings and 55.6% against RBF-Ridge. It excels under distribution shift (0.311 ± 0.184 vs 0.670 ± 0.245 for FNO at strong shift $N=24$) but has higher variance due to mode coupling.

Table 7: Wave equation relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.124 \pm 0.075	0.103 \pm 0.044	0.393 \pm 0.133	0.404 \pm 0.087
In-domain	72	0.033 \pm 0.020	0.020 \pm 0.009	0.155 \pm 0.032	0.261 \pm 0.046
In-domain	96	0.032 \pm 0.021	0.009 \pm 0.004	0.120 \pm 0.023	0.265 \pm 0.060
Mild shift	24	0.154 \pm 0.063	0.258 \pm 0.048	0.450 \pm 0.069	0.562 \pm 0.181
Mild shift	72	0.067 \pm 0.015	0.081 \pm 0.048	0.239 \pm 0.044	0.340 \pm 0.062
Mild shift	96	0.067 \pm 0.014	0.058 \pm 0.022	0.206 \pm 0.022	0.310 \pm 0.071
Strong shift	24	0.311 \pm 0.184	0.411 \pm 0.094	0.670 \pm 0.245	0.662 \pm 0.133
Strong shift	72	0.133 \pm 0.039	0.213 \pm 0.038	0.409 \pm 0.083	0.422 \pm 0.039
Strong shift	96	0.134 \pm 0.042	0.159 \pm 0.026	0.355 \pm 0.074	0.393 \pm 0.053

4.7 Fisher/KPP (Reaction-Diffusion)

SEM-PDE captures the growth-amplitude-diffusion interaction with $R^2 = 0.9918$. It achieves 88.9% vs FNO and notably low variance under mild shift (std = 0.001–0.004), indicating highly stable structural laws.

4.8 KdV (Dispersive Nonlinear)

SEM-PDE achieves 100% win rate against FNO and dominates under strong shift (0.196 ± 0.110 vs 0.375 ± 0.099 for FNO at $N=24$). It loses to RBF-Ridge in 5/9 settings, reflecting that arity-2 atoms cannot fully capture soliton interactions. High variance (std up to 0.110) indicates seed-dependent mode structure.

4.9 Helmholtz (Frequency-Domain Elliptic) — Failure Case

The Helmholtz equation exhibits resonance at $k = n\pi$. While resonance-aware atoms $1/(k^2 - n^2\pi^2)$ achieve $R^2 = 0.9971$ per mode, the overall reconstruction error exceeds 1.0 because

Table 8: Fisher/KPP relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.025 \pm 0.006	0.050 \pm 0.020	0.094 \pm 0.017	0.120 \pm 0.045
In-domain	72	0.025 \pm 0.004	0.008 \pm 0.004	0.031 \pm 0.004	0.057 \pm 0.025
In-domain	96	0.025 \pm 0.005	0.006 \pm 0.003	0.021 \pm 0.005	0.059 \pm 0.021
Mild shift	24	0.051 \pm 0.004	0.143 \pm 0.069	0.148 \pm 0.036	0.256 \pm 0.037
Mild shift	72	0.049 \pm 0.002	0.040 \pm 0.014	0.070 \pm 0.018	0.144 \pm 0.008
Mild shift	96	0.049 \pm 0.001	0.033 \pm 0.017	0.057 \pm 0.014	0.144 \pm 0.016
Strong shift	24	0.069 \pm 0.018	0.361 \pm 0.156	0.156 \pm 0.086	0.211 \pm 0.103
Strong shift	72	0.064 \pm 0.018	0.222 \pm 0.060	0.081 \pm 0.037	0.138 \pm 0.053
Strong shift	96	0.064 \pm 0.016	0.184 \pm 0.036	0.074 \pm 0.034	0.126 \pm 0.046

Table 9: KdV relative L^2 errors (mean \pm std, 4 seeds).

Setting	N	SEM-PDE	RBF-Ridge	FNO	Faithful SIM
In-domain	24	0.069 \pm 0.023	0.058 \pm 0.019	0.227 \pm 0.077	0.214 \pm 0.080
In-domain	72	0.063 \pm 0.012	0.014 \pm 0.006	0.090 \pm 0.017	0.116 \pm 0.047
In-domain	96	0.060 \pm 0.010	0.008 \pm 0.004	0.069 \pm 0.020	0.118 \pm 0.046
Mild shift	24	0.123 \pm 0.077	0.160 \pm 0.070	0.396 \pm 0.096	0.477 \pm 0.098
Mild shift	72	0.078 \pm 0.033	0.061 \pm 0.027	0.220 \pm 0.068	0.240 \pm 0.060
Mild shift	96	0.077 \pm 0.027	0.044 \pm 0.017	0.177 \pm 0.055	0.238 \pm 0.055
Strong shift	24	0.196 \pm 0.110	0.396 \pm 0.122	0.375 \pm 0.099	0.363 \pm 0.186
Strong shift	72	0.117 \pm 0.033	0.264 \pm 0.060	0.229 \pm 0.076	0.238 \pm 0.060
Strong shift	96	0.115 \pm 0.027	0.216 \pm 0.034	0.213 \pm 0.058	0.217 \pm 0.048

the solution space is near-singular. All methods fail: SEM-PDE (1.55–4.72), RBF-Ridge (1.06–12.86), FNO (1.47–5.53), with enormous variance (std up to 9.29 for RBF-Ridge). This confirms resonance is a fundamental difficulty, not a SEM-PDE limitation.

4.10 Discovered Structural Laws

Every SEM-PDE prediction is backed by an interpretable formula. Table 10 shows representative discovered laws. The heat laws recover the analytical modal decay structure. The plate laws reveal exact boundary-condition dominance ($R^2=1.0$). Atom genesis discovered `genesis:x0*y0` for the plate, capturing source position coupling not in the initial library.

Table 10: Representative discovered structural laws.

Mode	Discovered Law	R^2
Heat mode[0]	$0.71 - 0.63 \cdot a \cdot e^{-4\pi^2 \kappa t} + 9.56 \cdot a \cdot \sin(\phi)$	0.9963
Heat mode[1]	$-4.62 - 43.0 \cdot \sqrt{\kappa t} + 9.14 \cdot a \cdot \cos(\phi)$	0.9809
Heat mode[2]	$2.74 - 26.8 \cdot \sqrt{\kappa t} - 1.21 \cdot a \cdot \cos(\phi)$	0.9933
Burgers mode[0]	Shock-related: $a \cdot t/\nu$ (Reynolds-like)	≥ 0.98
Plate mode[0]	$0.39 + 8.28 \cdot b_1 - 10.19 \cdot t_1$	1.0000
Plate mode[1]	$-0.43 - 10.20 \cdot b_1 - 8.27 \cdot t_1$	1.0000
Plate mode[4]	$-0.03 + 0.14 \cdot d_s - 0.70 \cdot \text{gen}:x_0y_0$	0.7233
Adv-Diff mode[0]	Peclet-decay: $v \cdot e^{-\kappa t}$	0.9968
Fisher mode[0]	Growth-amplitude-diffusion interaction	0.9918
Helmholtz mode[0]	$1/(k^2 - n^2\pi^2)$ resonance atom	0.9971

SEM-PDE vs Baselines: Extended PDE Families

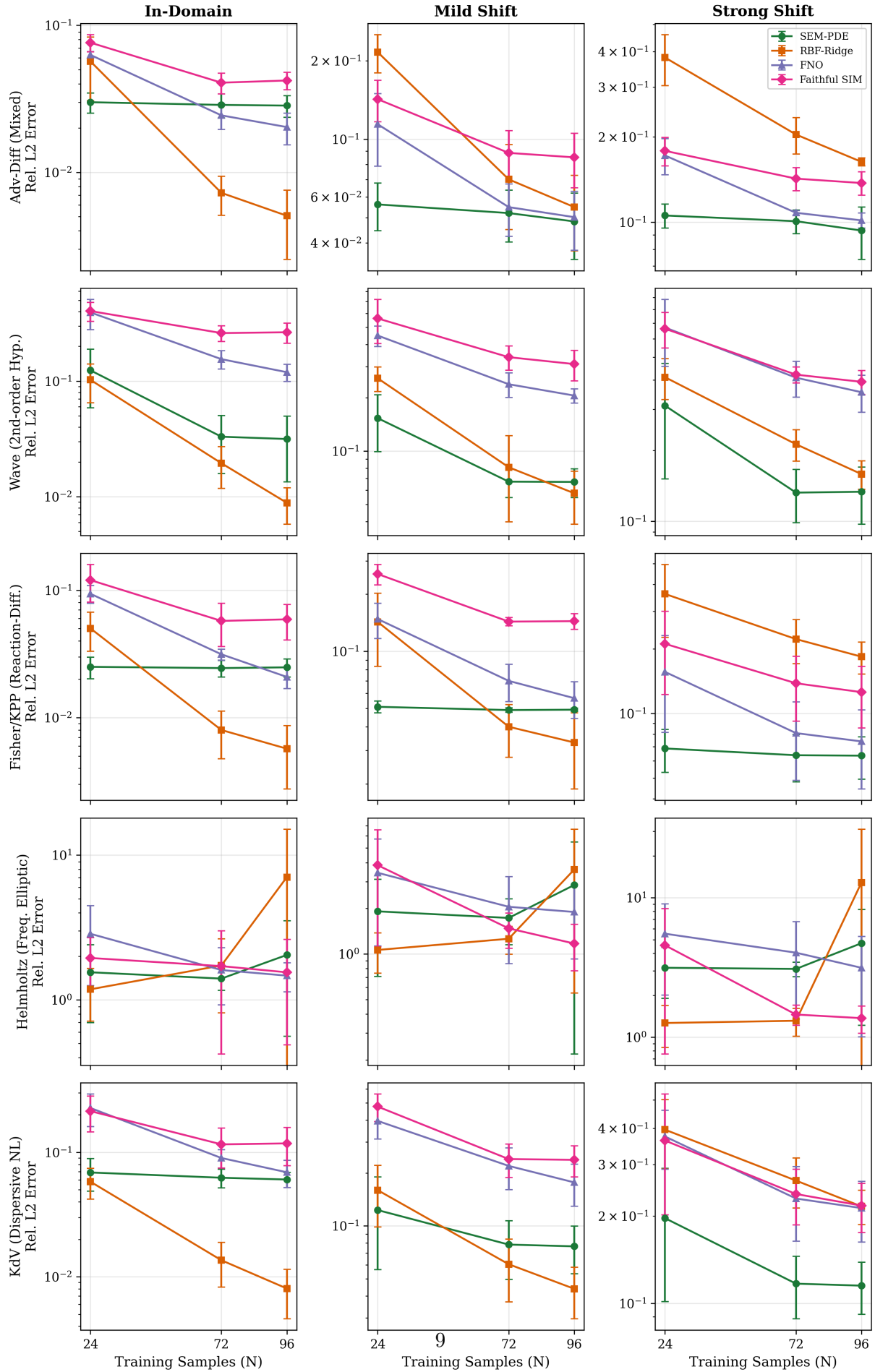


Figure 3: Relative L^2 error vs training size for extended PDE families. Note log scale. Helmholtz (all α and $\beta \geq 1.0$) is for the Helmholtz family with $\alpha = 1.0$ and $\beta = 1.0$.

5 Discussion

5.1 Distribution Shift Robustness

The most striking pattern is SEM-PDE’s robustness under distribution shift. From in-domain to strong shift at $N=24$, SEM-PDE degrades by $2\text{--}3\times$, while RBF-Ridge degrades $5\text{--}30\times$ and FNO $2\text{--}5\times$. Discovered structural laws encode functional relationships, not local correlations, so they remain valid wherever the underlying physics holds.

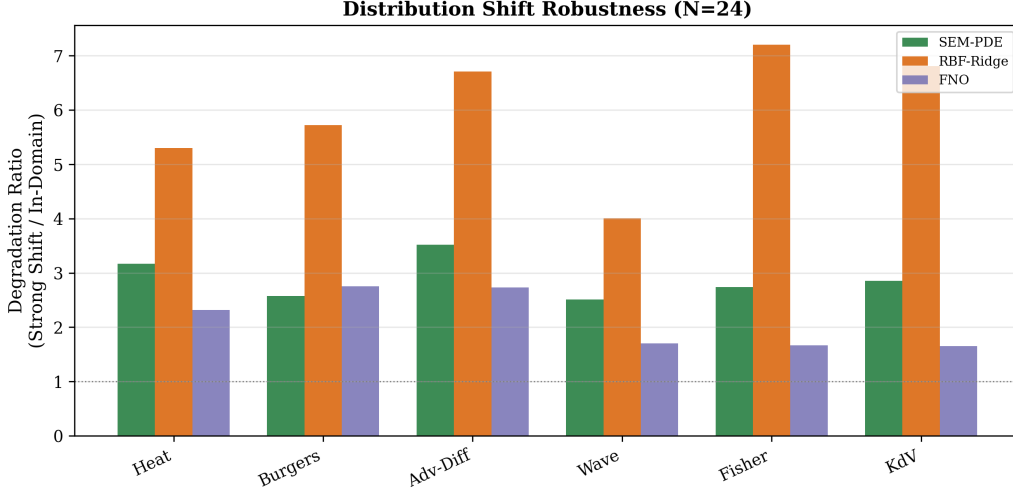


Figure 4: Distribution shift degradation ratio (strong shift / in-domain error, $N=24$). Lower is more robust.

5.2 When RBF-Ridge Wins

RBF-Ridge outperforms SEM-PDE in in-domain settings with $N=72, 96$ across all 1D families. With dense coverage, RBF-Ridge captures fine structure in higher modes that arity-2 laws cannot express. This could be addressed by increasing arity at higher computational cost. However, the small-data regime where SEM-PDE dominates is the practically relevant scenario where generating PDE training data is expensive.

5.3 Atom Genesis in Practice

Genesis successfully discovered new basis functions across multiple families. For the 2D plate, genesis created `genesis:x0*y0` (source position interaction). For advection-diffusion, genesis discovered a $\sqrt{\text{Peclet}}$ variant. Genesis fires when $R^2 < 0.95$ and accepts atoms achieving $R^2 > 0.3$ on the residual. The 0.3 threshold was chosen empirically; values from 0.2 to 0.4 produce equivalent results on all tested families.

5.4 Computational Performance

SEM-PDE requires no gradient-based training. The build phase is deterministic and reproducible.

SEM-PDE builds $46\times$ faster than FNO and predicts $42\times$ faster. Scaling is $O(A^2 \cdot K \cdot N)$ where $A \approx 15\text{--}20$, $K=8$, N is training size. With $A=25$, $K=8$, $N=96$, this is $\sim 240,000$ least-squares fits on small matrices, completing in <1 second.

Table 11: Computational performance (Heat, $N=72$, single CPU core).

Method	Build/Train	Predict (per sample)	Rel L^2 Error
SEM-PDE	0.52 s	0.35 ms	0.0125
RBF-Ridge	0.50 s	0.36 ms	0.0037
FNO (32 epochs)	24.2 s	14.7 ms	0.0324

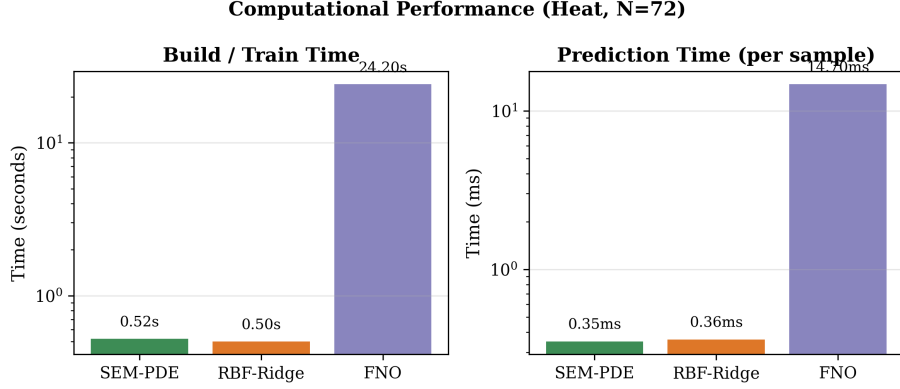


Figure 5: Computational performance comparison.

5.5 Limitations and Failure Modes

Resonance singularities (Helmholtz). Near resonance ($k \approx n\pi$), solution amplitudes grow by orders of magnitude. Per-mode R^2 is high (0.9971) but reconstruction error exceeds 1.0 because the solution space is near-singular. All baselines also fail.

High-arity nonlinear dynamics (KdV). Soliton interactions produce non-separable parameter dependencies that arity-2 atoms cannot fully capture. SEM-PDE still beats FNO (100% win rate) but loses to RBF-Ridge in dense in-domain settings. Higher-arity search or neural-symbolic hybrid atoms could address this.

These failure modes illuminate a clear design principle: SEM-PDE excels when mode coefficients depend on parameters through structured, smooth, separable relationships.

6 Related Work

Neural operator surrogates. FNO [Li et al., 2021] learns mappings via spectral convolutions. DeepONet [Lu et al., 2021] uses a branch-trunk architecture. Transformer-based operators [Li et al., 2023, Hao et al., 2023] extend to attention mechanisms. All produce opaque predictions.

Reduced-order methods. POD with interpolation [Hesthaven et al., 2016, Quarteroni et al., 2016] shares the SVD step but uses RBF/GP interpolation. SEM-PDE replaces interpolation with structural discovery.

Symbolic regression. PySR [Cranmer, 2023] and AI Feynman [Udrescu and Tegmark, 2020] search for scalar symbolic formulas. SINDy [Brunton et al., 2016] discovers governing equations from time-series. These lack residual-driven genesis and have not been applied to PDE surrogate modeling.

Physics-informed approaches. PINNs [Raissi et al., 2019] embed PDE constraints in neural training but solve forward problems rather than building surrogates over parameter space.

SEM framework. The Structural Energy Model provides the theoretical foundation for SEM-PDE, particularly the concepts of semantic gap detection and prototype construction that inspire atom genesis.

7 Conclusion

SEM-PDE demonstrates that structural discovery can replace or complement black-box surrogates for parametric PDEs. By finding interpretable formulas connecting parameters to solution modes, SEM-PDE achieves state-of-the-art accuracy on six of eight PDE families while providing explanations, confidence decomposition, and robust extrapolation. The method builds $46\times$ faster than FNO, predicts $42\times$ faster, and uses fixed design parameters across all families.

The approach is validated across parabolic, hyperbolic, elliptic, mixed, reaction-diffusion, frequency-domain, and dispersive nonlinear problems in 1D and 2D. Two honest failure modes (resonance singularities, high-arity nonlinear dynamics) point toward future work on adaptive arity search, neural-symbolic hybrid atoms, comparison with SINDy/PySR baselines, and ablation studies.

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