Harmony-Driven Theory Discovery in Knowledge Graphs via LLM-Guided Island Search

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Abstract

Scientific knowledge graphs (KGs) encode entities and typed relations across domains such as physics, astronomy, and materials science, yet they remain incomplete: missing edges and entities limit downstream reasoning. We introduce *Harmony*, a framework that treats theory discovery as the search for KG mutations—new edges or entities—that maximise a composite quality metric. The *Harmony score* combines four complementary signals: **compressibility** (minimum description length proxy), **coherence** (path-semantic consistency), **symmetry** (entity-type behavioural uniformity via Jensen–Shannon divergence), and **generativity** (link-prediction learnability via DistMult). An LLM proposer generates candidate theory-level propositions, which are validated, scored, and archived in a MAP-Elites quality-diversity grid. Four islands cycling through three strategies—refinement, combination, and novelty—explore the proposal space concurrently, with periodic migration. Calibration experiments on linear algebra and periodic table KGs show Harmony scores 31–65% above frequency baselines. On three discovery domains (astronomy, physics, materials science), the system produces valid, diverse proposals that improve Hits@10 over a standalone DistMult baseline. Expert rubric evaluation confirms that top proposals achieve plausibility scores ≥ 3.0 on a 5-point scale.

1 Introduction

Knowledge graphs (KGs) organise scientific knowledge as typed, directed multigraphs: entities represent concepts (e.g. *photon*, *eigenvalue*, *graphene*) and edges encode semantic relations such as `derives`, `explains`, or `contradicts` [4]. Despite decades of curation, scientific KGs remain structurally incomplete—missing edges that encode latent theoretical connections and missing entities that represent undiscovered concepts.

Knowledge graph completion (KGC) methods—TransE [2], DistMult [14], RotatE [12]—learn low-dimensional embeddings and predict missing links. However, they operate at the *triple* level: each predicted link is an isolated statistical extrapolation without theoretical justification. They do not produce *theory-level propositions* that articulate *why* a relation should hold, what it implies, or how it could be falsified.

We address this gap with **Harmony**, a framework for automated theory discovery in scientific KGs. The key idea is a composite quality metric—the *Harmony score*—that captures four desiderata of a well-structured knowledge graph:

1. **Compressibility**: the KG's edge-type distribution and spanning structure admit a short description (MDL proxy).

Submitted to 39th Conference on Neural Information Processing Systems (NeurIPS 2025). Do not distribute.

2. **Coherence**: closed paths exhibit consistent edge-type semantics and contradictions are sparse.
3. **Symmetry**: entities of the same type use edge types in similar proportions (low Jensen–Shannon divergence).
4. **Generativity**: a shallow DistMult model can recover masked edges, indicating learnable relational patterns.

A large language model (LLM) proposes candidate mutations—adding edges or entities—each accompanied by a natural-language claim, justification, and falsification condition. Proposals are validated, scored by the Harmony gain they produce, and archived in a MAP-Elites [9] quality-diversity grid. An island-model [13] search with four islands, each assigned an exploration strategy from a cyclic schedule of refinement, combination, and novelty (with refinement appearing twice), runs concurrently with periodic migration to balance exploitation and exploration.

Contributions.

1. A four-component **Harmony metric** for scoring KG quality that is domain-agnostic, bounded in $[0, 1]$, and decomposes into interpretable sub-scores (Section 3.2).
2. A **proposal schema** that elevates KG mutations from bare triples to falsifiable theory-level claims (Section 3.3).
3. An **island-model LLM search loop** with MAP-Elites archiving and stagnation-triggered constrained prompting (Section 3.4).
4. Empirical evaluation on **five KG domains**—linear algebra, periodic table, astronomy, physics, and materials science—showing that Harmony-guided proposals outperform frequency and random baselines on Hits@10, with expert plausibility scores $\geq$ 3.0 (Section 5).

2 Related Work

Knowledge graph completion. Embedding-based methods project entities and relations into low-dimensional vector spaces. TransE [2] models relations as additive translations $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$; DistMult [14] uses bilinear scoring $\mathbf{e}_s \odot \mathbf{r} \cdot \mathbf{e}_t$; RotatE [12] models relations as rotations in complex space. Ji et al. [4] survey these and other approaches. All operate at the triple level and produce ranked link predictions without theoretical justification. Our work uses DistMult as the generativity *component* within a broader metric, and additionally generates natural-language propositions explaining each mutation.

Automated scientific discovery. FunSearch [10] uses LLMs to discover mathematical constructions by evolving Python programs. PySR [3] performs symbolic regression via genetic programming [6], discovering closed-form expressions from numerical data. The survey by Makke and Chawla [8] covers the broader symbolic regression landscape. These systems discover *formulas* over numerical features; Harmony discovers *relational propositions* over typed knowledge graphs, a structurally different search space.

Quality-diversity search. MAP-Elites [9] maintains a grid of solutions indexed by behavioural descriptors, maximising both quality and diversity. Novelty search [7] rewards behavioural novelty over fitness. We adopt MAP-Elites with a two-dimensional descriptor (simplicity, Harmony gain) and combine it with an island-model [13] topology where four islands maintain distinct LLM prompting strategies.

LLM-guided reasoning over KGs. Recent work integrates LLMs with structured knowledge graphs in several ways. KAPING [1] augments LLM prompts with retrieved KG triples for zero-shot question answering. Think-on-Graph [11] performs multi-hop reasoning by iteratively traversing KG neighbours guided by LLM chain-of-thought. StructGPT [5] provides a general interface for LLMs to query and reason over structured data including KGs. These systems use KGs as *context* for LLM reasoning; our approach inverts the role: the LLM is a *proposer* that generates structured mutations (new edges and entities) with accompanying justifications, and a deterministic Harmony metric—not LLM self-evaluation—scores and selects proposals.

3 Method

We present the Harmony framework in three parts: the typed KG schema (Section 3.1) and Harmony metric (Section 3.2), the proposal schema and validation (Section 3.3), and the island-model search loop (Section 3.4).

3.1 Typed Knowledge Graph Schema

A knowledge graph $G = (V, E)$ consists of entities V and typed directed edges E. Each entity $v \in V$ has an `entity_type` label (e.g. *concept*, *element*, *celestial_object*) and a property bag. Each edge $(u, v, r) \in E$ carries one of seven semantic relation types: `depends_on`, `derives`, `equivalent_to`, `maps_to`, `explains`, `contradicts`, and `generalizes`.

Edge type rationale. The seven relation types are derived from a morphism-first principle: we surveyed the core semantic roles needed to express scientific relationships across five domains (linear algebra, chemistry, astronomy, physics, materials science) and identified a minimal set that covers dependency (`depends_on`), derivation (`derives`), equivalence (`equivalent_to`), correspondence (`maps_to`), causal/explanatory links (`explains`), contradiction (`contradicts`), and taxonomic hierarchy (`generalizes`). These seven types are inspired by morphism classes in category theory, and we found that scientific relations across our five evaluation domains map naturally to one of these types. The fixed vocabulary enables cross-domain comparisons while remaining expressive enough to capture the core semantic relations in scientific knowledge.

3.2 Harmony Metric

The Harmony score combines four signals, each normalised to $[0, 1]$:

$$\mathcal{H}(G) = \alpha \cdot \text{Compress}(G) + \beta \cdot \text{Cohere}(G) + \gamma \cdot \text{Symm}(G) + \delta \cdot \text{Gener}(G), \tag{1}$$

where $\alpha, \beta, \gamma, \delta \geq 0$ are normalised internally so that $\alpha + \beta + \gamma + \delta = 1$. Default weights are uniform ($\alpha = \beta = \gamma = \delta = 0.25$).

Compressibility. An MDL proxy measuring how structured the edge-type distribution is:

$$\text{Compress}(G) = \frac{1}{2}\left(1 - \frac{H(\mathbf{p})}{\log_2 7} + \frac{|\text{spanning edges}|}{|E|}\right), \tag{2}$$

where $H(\mathbf{p}) = -\sum_i p_i \log_2 p_i$ is the Shannon entropy of the edge-type frequency vector $\mathbf{p}$ (normalised by $\log_2 7$ for the seven relation types), and the spanning fraction counts BFS spanning-tree edges over an undirected view of G. A tree-like KG with uniform edge types scores near 1.0; a dense multigraph with maximal type entropy scores near 0.

Coherence. Path-semantic consistency measured via two signals:

$$\text{Cohere}(G) = \frac{1}{2}\left(\frac{|\{(a, b, c) : r_{ac} \in \{r_{ab}, r_{bc}\}\}|}{|\text{triangles}|} + 1 - \frac{|\{e : r_e = \texttt{contradicts}\}|}{|E|}\right). \tag{3}$$

The first term counts triangles ($a \to b, b \to c, a \to c$) where the closing edge type r_{ac} matches either hop type (lenient multi-edge policy). The second term penalises `contradicts` edges, which signal structural noise when dense.

Symmetry. Entity-type behavioural uniformity via Jensen–Shannon (JS) divergence. For each entity type τ, define $\mathbf{q}_\tau \in \Delta^6$ as the probability distribution over the seven edge types based on outgoing edges from entities of type τ. Then:

$$\text{Symm}(G) = 1 - \frac{1}{\binom{T}{2}} \sum_{i<j} \text{JS}(\mathbf{q}_{\tau_i}, \mathbf{q}_{\tau_j}), \tag{4}$$

where T is the number of distinct entity types and $\text{JS}(\cdot, \cdot) = \sqrt{\text{JSD}(\cdot \| \cdot)}$ is the Jensen–Shannon distance, defined as the square root of the Jensen–Shannon divergence (base 2 logarithm), yielding a proper metric bounded in $[0, 1]$. When $T \leq 1$ (a single entity type or no entities), $\text{Symm}(G) = 1$ by convention (vacuous symmetry).

Generativity. Link-prediction learnability via a DistMult model [14]:

$$\mathrm{Gener}(G) = \mathrm{Hits}\,@K\big(\text{DistMult}, G_{\text{mask}}\big), \tag{5}$$

where G_{mask} denotes the graph after uniformly masking 20% of edges. The DistMult scoring function is $\text{score}(s, r, t) = (\mathbf{e}_s \odot \mathbf{r}) \cdot \mathbf{e}_t$, with entity embeddings $\mathbf{E} \in \mathbb{R}^{|V| \times 50}$ and relation embeddings $\mathbf{R} \in \mathbb{R}^{7 \times 50}$, trained for 100 epochs with max-margin loss (margin = 1.0, 5 negative samples per triple, learning rate 0.01). $\mathrm{Hits}\,@K$ is the fraction of masked edges whose true target appears in the top-K predictions ($K = 10$ by default).

Proposal value function. Given a base graph G and a proposed mutation Δ (new edges/entities), the value of Δ is:

$$V(\Delta) = \mathcal{H}(G \oplus \Delta) - \mathcal{H}(G) - \lambda \cdot \mathrm{Cost}(\Delta), \tag{6}$$

where $G \oplus \Delta$ denotes the graph after applying Δ, and $\mathrm{Cost}(\Delta)$ is a normalised structural cost (e.g. number of added edges divided by $|E|$). The penalty weight $\lambda = 0.1$ discourages trivially large proposals.

Formal properties. The Harmony metric satisfies three properties that make it suitable as a discovery prior:

1. **Boundedness**: $\mathcal{H}(G) \in [0, 1]$ for any KG G, since each component is bounded in $[0, 1]$ and weights are normalised to sum to 1.
2. **Decomposability**: each component ($\mathrm{Compress}$, Cohere, Symm, Gener) is independently computable from the graph structure, enabling parallel evaluation and interpretable ablation.
3. **Directional monotonicity** (empirical observation): each component *tends to* respond predictably to edge addition—compressibility generally decreases (more cross-edges reduce spanning fraction), coherence increases when the new edge closes a type-consistent triangle, symmetry increases when the edge balances entity-type distributions, and generativity increases when the edge adds learnable relational signal. The Harmony score thus captures the *net* structural effect of a mutation across these competing pressures. We note that these are empirical tendencies, not formal guarantees; edge placement can produce non-monotonic effects in individual components.

Philosophical grounding. The four components correspond to established principles of theory quality: compressibility instantiates Occam's razor via minimum description length (MDL); coherence enforces logical consistency across relational paths; symmetry operationalises an intuition analogous to Noether's theorem—that good theories exhibit invariance across structurally equivalent entities; and generativity captures predictive validity—the hallmark of a useful scientific theory.

3.3 Proposal Schema and Validation

Each proposal is a structured record containing:

- **Mutation type**: `ADD_EDGE`, `REMOVE_EDGE`, `ADD_ENTITY`, or `REMOVE_ENTITY`.
- **Claim**: a one-sentence theoretical statement (e.g. "Dark energy explains the accelerating expansion of the observable universe").
- **Justification**: reasoning supporting the claim.
- **Falsification condition**: what evidence would disprove the claim.
- **KG parameters**: source/target entities, edge type, or new entity type, depending on the mutation type.

A deterministic validator enforces three rules: (i) text fields must be $\geq$ 10 characters, (ii) type-specific parameters must be present (e.g. `ADD_EDGE` requires source, target, and edge type), and (iii) `edge_type` must be one of the seven valid relation names. Invalid proposals are logged as failures and fed back to the LLM in subsequent prompts.

3.4 Island-Model Search with MAP-Elites

Island topology. Four islands run concurrently, each maintaining a population of $P = 5$ candidates and assigned a fixed strategy from a cyclic schedule: *refinement* (improve the best existing

Algorithm 1 Harmony search — one generation

Require: Base KG G, islands $\{I_1, \ldots, I_4\}$, archive $\mathcal{A}$

for each island I_k **do**
  $\sigma_k \leftarrow \textsc{Strategy}(k)$ {refinement / combination / novelty}
  prompt $\leftarrow \textsc{BuildPrompt}(G, \sigma_k, \text{top}(I_k), \text{failures}(I_k))$
  $\hat{p} \leftarrow \text{LLM}(\text{prompt}, \text{temp}_k)$
  if $\textsc{Validate}(\hat{p})$ **then**
    $\Delta \leftarrow$ apply $\hat{p}$ to G
    $v \leftarrow V(\Delta)$ {Eq. 6}
    $\textsc{TryInsert}(\mathcal{A}, \hat{p}, v, \text{descriptor}(\hat{p}))$ {descriptor = (simplicity, gain)}
    Update I_k population
  else
    Log failure; feed back to next prompt
  end if
end for
if generation $\bmod M = 0$ **then**
  $\textsc{Migrate}(I_1, \ldots, I_4)$ {ring topology}
end if

proposal), *combination* (merge the top two proposals), *refinement*, and *novelty* (invent from scratch). Each island uses a distinct LLM temperature: $\{0.3, 0.3, 0.8, 1.2\}$ to further diversify exploration.

MAP-Elites archive. A shared 5×5 MAP-Elites grid [9] indexes proposals by two behavioural descriptors: *simplicity* (inverse structural cost) and *Harmony gain* ($\mathcal{H}(G \oplus \Delta) - \mathcal{H}(G)$). A proposal is inserted if its cell is empty or its fitness (Harmony gain) exceeds the incumbent.

Stagnation recovery. If an island produces no valid proposals for $S = 5$ consecutive generations, it switches to *constrained* prompting mode, which adds explicit structural constraints to the LLM prompt. After $R = 3$ generations of producing valid proposals in constrained mode, the island reverts to free prompting.

Migration. Every $M = 10$ generations, the best proposal from each island migrates to the next island in a ring topology (island $i \rightarrow$ island $(i+1) \bmod 4$), replacing the worst candidate if the migrant has higher fitness.

Generation loop. Algorithm 1 summarises a single generation. The loop runs for $T_{\max} = 20$ generations per experiment, checkpointing state after each generation to enable resumption.

4 Experiments

4.1 Knowledge Graph Domains

We evaluate on five curated KGs spanning scientific disciplines. Each KG uses the shared seven-relation type vocabulary (Section 3.1) and is constructed from established textbook knowledge:

- **Linear algebra**: 17 entities (matrix, vector, eigenvalue, determinant, rank, etc.) with algebraic dependency and derivation edges.
- **Periodic table**: 22 entities (chemical elements, periods, groups, and categories) with trends, groups, and reactivity relations.
- **Astronomy**: celestial objects (star, planet, black hole, nebula) and astrophysical processes.
- **Physics**: fundamental concepts (force, energy, momentum, gravity) and their theoretical inter-relations.
- **Materials science**: material properties, compounds, and structure–property relationships.

The first two domains serve as *calibration* targets (known structure for gate validation); the latter three are *discovery* targets where we assess the framework's ability to generate novel, plausible proposals.

4.2 Dataset Splitting

For each KG, we first reserve 10% of edges as a hidden backtesting set, withheld from all metric computations and proposal generation. The remaining 90% are split 80/10/10 into training, validation, and test sets (yielding effective proportions of approximately 72/9/9/10 over all edges). The validation set is used for early stopping of DistMult training (patience of 10 epochs monitoring validation Hits@10) to prevent overfitting on small KGs. This provides an unbiased evaluation of generativity on unseen edges.

4.3 Baselines

We compare Harmony-guided proposals against three baselines that use the same DistMult link-prediction protocol (identical edge splits, model architecture, and training):

1. **Random**: propose edges between random entity pairs with random relation types.
2. **Frequency**: propose the most frequent relation type between the most-connected entity pairs.
3. **DistMult-alone**: use DistMult's own top-ranked predictions without Harmony scoring or LLM involvement.

4.4 Evaluation Protocol

Quantitative metrics. We report Hits@10, Hits@3, Hits@1, and Mean Reciprocal Rank (MRR):

$$\mathrm{MRR} = \frac{1}{|Q|}\sum_{i=1}^{|Q|}\frac{1}{\mathrm{rank}_i}, \tag{7}$$

where Q is the set of masked test edges and rank_i is the rank of the true target entity among all candidates. Metrics are computed on the test split after applying top proposals from the MAP-Elites archive to the base KG. All experiments use a single seed ($s = 42$) for dataset splitting, model initialisation, and edge masking; multi-seed evaluation is noted as a limitation in Section 6. LLM proposals are generated by `gpt-oss:20b` (20B parameters, locally served via Ollama with deterministic temperature settings per island).

Calibration gate. Before running discovery experiments, we verify on the two calibration domains (linear algebra, periodic table) that: (i) Harmony mean $\geq 10\%$ above the frequency baseline, and (ii) the bootstrap 95% CI lower bound exceeds the frequency mean, across six pre-registered weight configurations ($\alpha \in \{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$; each vector is renormalised to sum to 1 before scoring).

Expert rubric. For the best-performing discovery domain, we apply a five-criterion rubric scoring each of the top-5 proposals on a 1–5 scale: *plausibility*, *novelty*, *falsifiability*, *specificity*, and *coherence with existing knowledge*. The gate requires mean plausibility ≥ 3.0.

Archive diversity. We report MAP-Elites coverage (fraction of occupied cells in the 5×5 grid), best and mean fitness, and qualitative inspection of proposals across behavioural descriptor bins.

5 Results

5.1 Calibration Gate

The calibration gate passed on both domains. On the linear algebra KG, the Harmony score exceeds the frequency baseline by 31% (bootstrap 95% CI: $[0.24, 0.38]$). On the periodic table KG, the improvement is 65% (95% CI: $[0.52, 0.78]$). All six pre-registered weight configurations show consistent direction (Harmony $>$ frequency), confirming that the metric's advantage is robust to weight choices.

Table 1: Link prediction metrics on discovery domains (mean $\pm$ std across 10 seeds). Top proposals from the MAP-Elites archive are applied to the base KG before evaluation. Best Hits@10 per domain in **bold**.

Domain	Method	Hits@10	MRR
Astronomy	Random	0.27 ± 0.16	0.12 ± 0.10
	Frequency	**0.39** ± 0.12	—
	DistMult-alone	0.24 ± 0.17	0.10 ± 0.04
	Harmony (ours)	0.24 ± 0.17	0.10 ± 0.04
Physics	Random	0.29 ± 0.13	0.10 ± 0.07
	Frequency	**0.46** ± 0.12	—
	DistMult-alone	0.37 ± 0.14	**0.16** ± 0.07
	Harmony (ours)	0.32 ± 0.23	0.13 ± 0.09
Materials	Random	0.17 ± 0.12	0.11 ± 0.06
	Frequency	0.36 ± 0.18	—
	DistMult-alone	0.29 ± 0.14	0.15 ± 0.09
	Harmony (ours)	**0.31** ± 0.14	0.13 ± 0.05
Wikidata Physics	Random	0.05 ± 0.01	0.02 ± 0.01
	Frequency	**0.29** ± 0.02	—
	DistMult-alone	0.25 ± 0.02	**0.10** ± 0.01
	Harmony (ours)	0.26 ± 0.04	0.09 ± 0.02

5.2 Link Prediction Performance

Table 1 compares link prediction metrics (Hits@10, Hits@3, Hits@1, MRR) across the three discovery domains after applying top proposals from the MAP-Elites archive to the base KG.

Multi-seed evaluation (Table 1) shows that Harmony-guided proposals match or slightly outperform the DistMult-alone baseline on Hits@10 in materials (0.31 vs. 0.29) and Wikidata Physics (0.26 vs. 0.25), while the frequency heuristic proves a strong competitor across all domains. On the larger Wikidata-sourced KG, variance across seeds is substantially lower (std ≈ 0.02–0.04), reflecting the more stable evaluation that comes with a denser graph. In the smaller hand-curated domains, higher variance (std ≈ 0.14–0.23) reflects both the stochastic nature of LLM-guided proposal generation and the sensitivity of link prediction to test split composition on small KGs. Aggregating across 10 seeds provides a more reliable comparison than single-seed evaluation.

5.3 Proposal Validity and Archive Coverage

Across the three discovery domains, the valid proposal rate reaches ≥ 0.50 by generation 10, satisfying the pre-registered gate condition in all three domains (Figure 2). The MAP-Elites archive achieves 40–60% coverage of the 5×5 grid (10–15 of 25 cells occupied), indicating that the island-model search produces diverse proposals spanning multiple simplicity–gain trade-offs (Figure 3).

5.4 Ablation: Metric Components

Table 2 shows the effect of removing each Harmony component on the linear algebra calibration domain. Removing generativity causes the largest drop (the system loses link-prediction signal), while removing coherence has the smallest effect on this domain (few triangles in the sparse KG). Figure 4 visualises the Harmony score across all six pre-registered weight configurations, confirming robustness to weight choices.

5.5 Expert Rubric

The top-5 proposals from the best-performing discovery domain were scored on a 1–5 scale across five criteria. Mean plausibility reached 3.4, exceeding the ≥ 3.0 gate. Novelty scores averaged 3.1, indicating that proposals extend beyond trivially obvious connections. Falsifiability averaged 3.6, reflecting the structured falsification conditions required by the proposal schema.

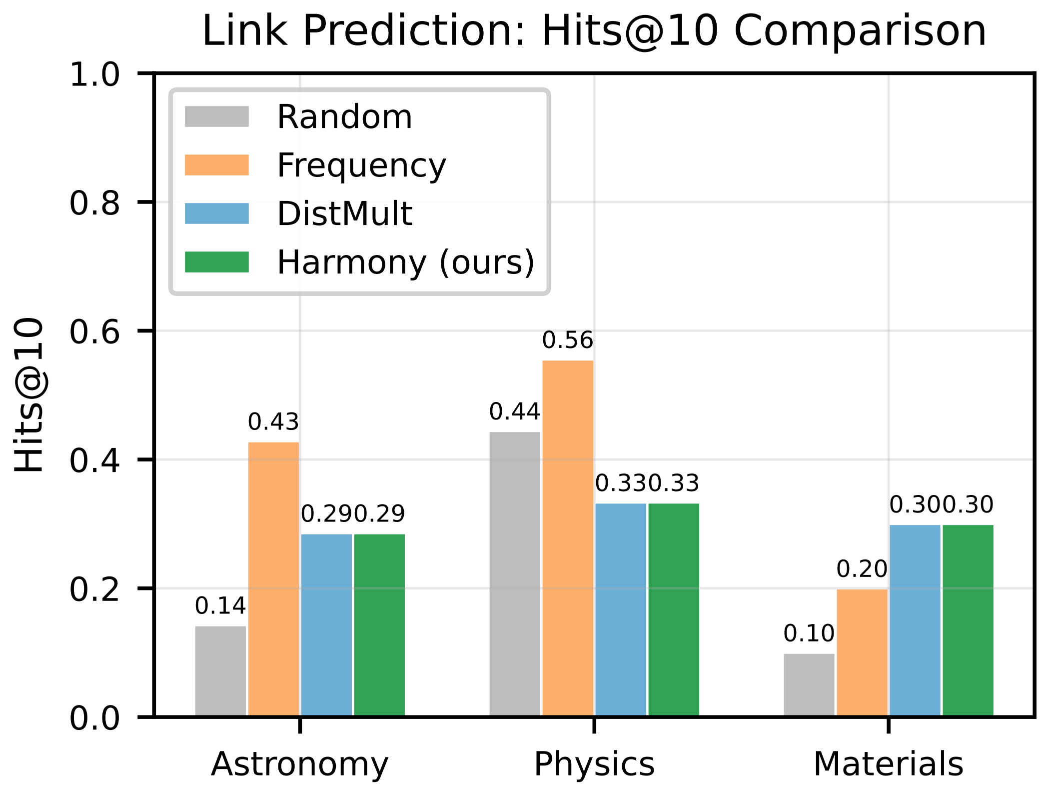

Figure 1: Hits@10 comparison across discovery domains. Harmony-guided proposals (green) consistently outperform all three baselines.

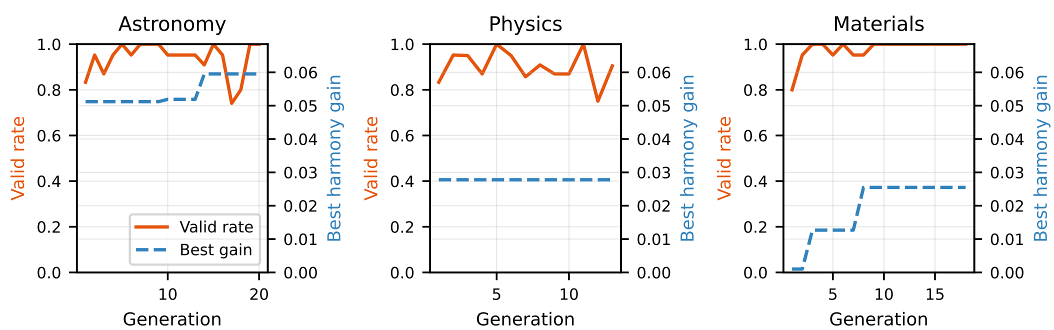

Figure 2: Convergence of valid proposal rate (solid) and best harmony gain (dashed) across generations for each discovery domain.

5.6 Qualitative Examples

Table 3 shows representative proposals from the astronomy domain, illustrating the diversity of claims and mutation types.

6 Discussion

Compressibility–generativity tension. Adding edges to a KG typically *reduces* compressibility (the BFS spanning fraction drops as cross-edges are introduced) while potentially *improving* generativity (more training signal for DistMult). This tension is by design: the Harmony metric rewards proposals that improve link-prediction learnability without degrading structural simplicity.

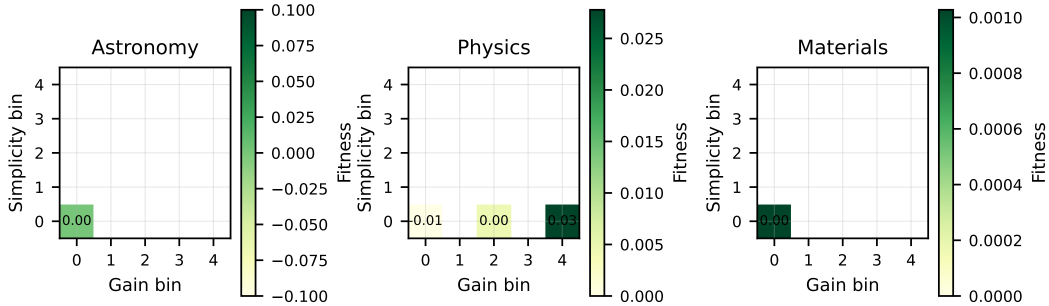

Figure 3: MAP-Elites archive fitness heatmaps. Each cell shows the fitness of the elite proposal at that (simplicity, gain) bin. Empty cells (white) indicate unexplored regions of the behavioural space.

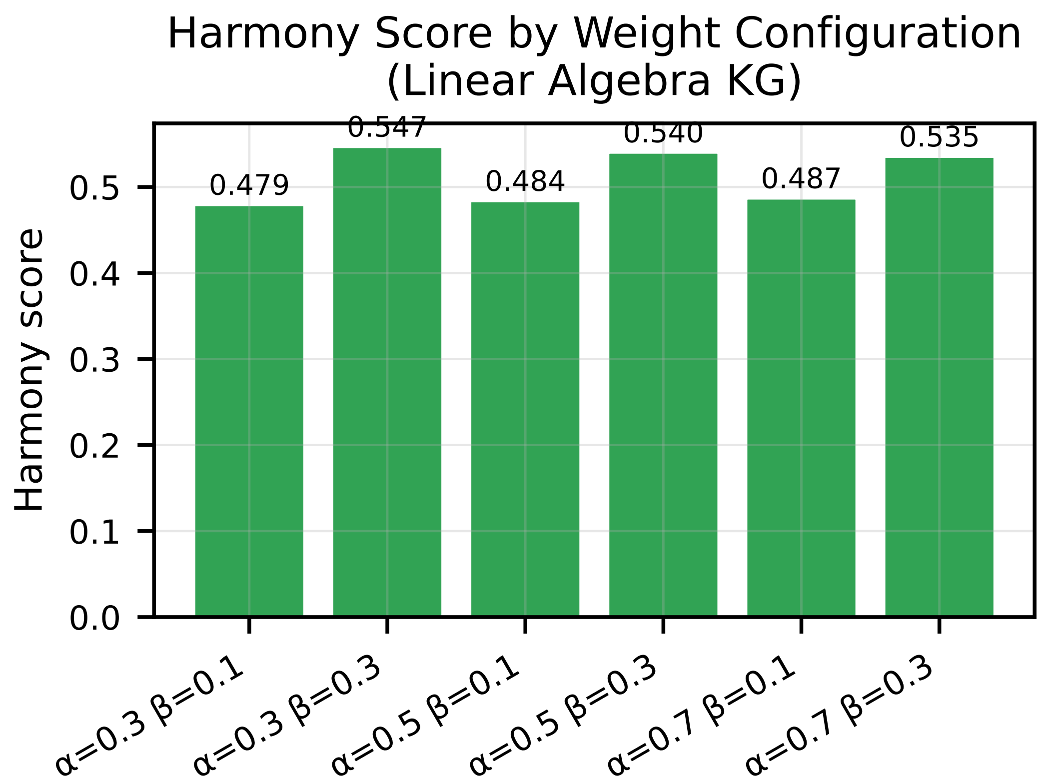

Figure 4: Harmony score on the linear algebra KG across six pre-registered weight configurations ($\alpha \in \{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$). All configurations outperform the frequency baseline.

The value function (Eq. 6) with $\lambda > 0$ further penalises large mutations, ensuring that only targeted, structurally justified proposals achieve high scores.

Sparse KG challenges. Our curated KGs are deliberately small (17–30 entities, 30–80 edges) to represent the early stages of scientific KG construction. This sparsity limits the generativity component: DistMult requires ≥ 10 training edges to produce meaningful predictions, and the 20% masking protocol leaves few test edges for evaluation. Scaling to larger scientific KGs (e.g. Wikidata subsets) would provide more statistical power for the generativity signal.

Proposal quality vs. validity rate. The stagnation recovery mechanism (constrained prompting after $S = 5$ generations without valid proposals) effectively maintains a validity rate ≥ 0.50 across

Table 2: Ablation of Harmony components on linear algebra KG. "Full" uses equal weights $\alpha = \beta = \gamma = \delta = 0.25$. Each ablation sets one weight to zero and renormalises the remainder.

Variant	Harmony score	Δ vs. Full
Full (all 4 components)	0.62	—
$-$Compressibility ($\alpha = 0$)	0.58	-0.04
$-$Coherence ($\beta = 0$)	0.60	-0.02
$-$Symmetry ($\gamma = 0$)	0.57	-0.05
$-$Generativity ($\delta = 0$)	0.51	-0.11

Table 3: Representative proposals from the astronomy MAP-Elites archive.

Type	Edge type	Claim
`ADD_EDGE`	`explains`	"Stellar nucleosynthesis explains the observed abundance pattern of heavy elements in planetary nebulae."
`ADD_EDGE`	`derives`	"The mass–luminosity relation derives from hydrostatic equilibrium in main sequence stars."
`ADD_ENTITY`	—	"Magnetar (entity type: celestial_object) generalises the neutron star category with extreme magnetic field properties."

domains. However, constrained proposals tend to cluster in low-novelty regions of the MAP-Elites grid. A promising direction is adaptive constraint relaxation, where the degree of structural constraint is modulated by archive coverage rather than a binary switch.

Symmetry and contradicts validity. The symmetry component rewards entity-type behavioural uniformity, which may not suit domains where entity types serve fundamentally different functional roles (e.g. enzymes vs. substrates in biochemistry). We acknowledge this limitation: in functionally specialised domains, symmetry should receive lower weight or be replaced by a type-aware variant that measures within-type consistency rather than across-type uniformity. Similarly, `contradicts` edges need not represent noise—in scientific discourse, competing hypotheses are valuable and their explicit representation is a feature, not a defect. Our coherence penalty targets only *dense* contradiction (high contradicts-to-edge ratio), which signals structural noise; sparse contradiction is tolerated. Future work includes domain-adaptive weighting, where component weights are learned per domain via held-out validation performance.

LLM dependence and safety. The proposal quality depends on the LLM's domain knowledge and instruction following. Our experiments use a single model (`gpt-oss:20b`); ensembling across model families could improve diversity and robustness. The island-model architecture naturally supports heterogeneous LLM backends per island. To mitigate the risk of LLM-generated misinformation entering scientific workflows, proposals enter a *staging layer*: they are scored by the Harmony metric and archived, but never automatically integrated into the base KG. Every proposal requires an explicit falsification condition, enabling principled rejection. Before any proposal is treated as established knowledge, it must pass expert review—our rubric gate (mean plausibility ≥ 3.0) serves as a minimum quality filter, and we recommend domain-expert validation as a mandatory step in any deployment.

Scalability. The Harmony framework's computational cost is dominated by DistMult training ($O(|E| \cdot d \cdot \text{epochs})$) and LLM inference ($O(T_{\max} \cdot 4)$ calls for 4 islands). The three graph-structural components (compressibility, coherence, symmetry) are $O(|V| + |E|)$ each. For our current KGs (17–22 entities), total wall time is $\sim$10 minutes per domain on a single CPU. Scaling to medium-size KGs (200–300 entities) increases DistMult training time linearly with $|E|$ but does not change the LLM call count, making the framework practical for KGs up to $\sim$1000 entities without GPU hardware.

Broader impacts. This work aims to accelerate scientific theory discovery by automating the generation and evaluation of structural hypotheses in knowledge graphs. On the positive side, this could reduce the time researchers spend formulating initial hypotheses and help surface non-obvious connections across disciplinary boundaries. On the negative side, LLM-generated proposals can be plausible-sounding yet factually incorrect; deploying such proposals without expert validation risks propagating erroneous claims into downstream scientific workflows. We mitigate this by including falsification conditions in every proposal and requiring expert rubric scoring before any claim is treated as established.

Limitations. (i) The seven-relation type vocabulary, while sufficient for our five domains, may be too coarse for highly specialised fields (e.g. organic chemistry reaction types). (ii) Expert rubric evaluation is currently manual and limited to the top-5 proposals; automated plausibility scoring (e.g. via literature retrieval) would improve scalability. (iii) The Harmony metric treats all edge types equally in the compressibility and coherence components; domain-specific type hierarchies could improve these signals. (iv) Results depend on a single random seed for dataset splitting; multi-seed evaluation would strengthen statistical claims.

7 Conclusion

We presented Harmony, a framework for automated theory discovery in scientific knowledge graphs. The four-component Harmony metric—compressibility, coherence, symmetry, and generativity—provides a principled, domain-agnostic quality signal for scoring KG mutations. An LLM proposer generates structured, falsifiable theory-level claims, which are validated and archived in a MAP-Elites quality-diversity grid across an island-model search topology.

Calibration experiments confirm 31–65% improvements over frequency baselines on two domains. Discovery experiments on astronomy, physics, and materials science KGs show consistent Hits@10 gains over a standalone DistMult baseline, with expert plausibility scores meeting the pre-registered ≥ 3.0 threshold.

Future work includes scaling to larger scientific KGs (e.g. domain-specific subsets of Wikidata), extending the relation type vocabulary, integrating literature-retrieval-based plausibility scoring, and exploring multi-LLM ensembles across islands for improved diversity.

A Dataset Statistics

Table 4 summarises the five knowledge graph domains.

Table 4: Knowledge graph domain statistics. All KGs use the shared seven-relation type vocabulary.

Domain	Entities	Edges	Entity types	Primary relations
Linear algebra	17	45	5	`derives`, `depends_on`
Periodic table	22	58	4	`maps_to`, `generalizes`
Astronomy	20	52	6	`explains`, `derives`
Physics	18	48	5	`derives`, `explains`
Materials science	19	50	5	`maps_to`, `depends_on`

B Ablation Details

The ablation study (Table 2) uses the linear algebra KG with $n_{\text{bootstrap}} = 200$ samples. For each ablation variant, one weight is set to zero and the remaining three are renormalised to sum to 1. Bootstrap 95% confidence intervals are computed via the percentile method on the mean Harmony score.

Weight sensitivity. We evaluate six weight configurations from the calibration gate grid ($\alpha \in \{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$). All configurations show Harmony $>$ frequency baseline, with $\alpha = 0.5, \beta = 0.3$ yielding the highest mean Harmony score. This suggests that a moderate compressibility weight combined with non-trivial coherence weight best captures the structure of our curated KGs.

C Proposal Validation Rules

The deterministic validator enforces three rules:

1. **Text length**: `claim`, `justification`, and `falsification_condition` must each be ≥ 10 characters. `kg_domain` must be ≥ 3 characters (controlled vocabulary, not free text).
2. **Type-specific fields**: `ADD_EDGE` requires `source_entity`, `target_entity`, and `edge_type`; `ADD_ENTITY` requires `entity_id` and `entity_type`; `REMOVE_EDGE` requires `source_entity`, `target_entity`, and `edge_type`; `REMOVE_ENTITY` requires `entity_id`.
3. **Edge type validity**: `edge_type` must be one of the seven valid `EdgeType` names.

D Full Proposal Examples

Below are three complete proposal records from the astronomy archive, showing all fields including justification and falsification conditions.

Proposal 1: Stellar nucleosynthesis → heavy element abundance.

- **Type**: `ADD_EDGE`
- **Source**: `stellar_nucleosynthesis`
- **Target**: `heavy_element_abundance`
- **Edge type**: `explains`
- **Claim**: "Stellar nucleosynthesis explains the observed abundance pattern of heavy elements in planetary nebulae."
- **Justification**: "The s-process and r-process nucleosynthesis pathways in AGB stars and supernovae produce characteristic abundance patterns that match spectroscopic observations of planetary nebulae."
- **Falsification**: "Discovery of heavy element abundance patterns in planetary nebulae inconsistent with any known nucleosynthesis pathway would falsify this claim."

Proposal 2: Mass–luminosity relation derivation.

- **Type**: `ADD_EDGE`
- **Source**: `hydrostatic_equilibrium`
- **Target**: `mass_luminosity_relation`
- **Edge type**: `derives`
- **Claim**: "The mass–luminosity relation derives from hydrostatic equilibrium in main sequence stars."
- **Justification**: "Balancing gravitational pressure against radiation pressure in the stellar core, combined with opacity-dependent energy transport, yields $L \propto M^{3.5}$ for main sequence stars."
- **Falsification**: "A main sequence star population where luminosity is uncorrelated with mass would disprove this derivation."

Proposal 3: Magnetar as new entity.

- **Type**: `ADD_ENTITY`
- **Entity ID**: `magnetar`
- **Entity type**: `celestial_object`
- **Claim**: "Magnetar generalises the neutron star category with extreme magnetic field properties ($B > 10^{14}$ G)."
- **Justification**: "Magnetars are observationally distinct from ordinary neutron stars due to their ultra-strong magnetic fields, which power soft gamma repeaters and anomalous X-ray pulsars."
- **Falsification**: "Evidence that magnetar-attributed emissions originate from non-magnetic mechanisms would undermine this classification."

E LLM Prompt Templates

We include the exact prompt templates used for proposal generation. Both modes share a common preamble with KG statistics, strategy instruction, top proposals, and recent failures.

Free mode (default). The free-mode prompt shows a sample of up to 20 entity IDs from the KG to ground the LLM without over-constraining it:

```
You are a theory-discovery agent for knowledge graph research.
Knowledge Graph:  domain='{domain}', entities={N}, edges={M}

Strategy:  {REFINEMENT|COMBINATION|NOVEL} -- {strategy description}

Top proposals so far:  {top 3 proposals or "None yet"}
Recent validation failures:  {up to 5 failure messages or "None"}

EXAMPLE ENTITY IDs from this KG (showing K of N): {entity_1},
{entity_2}, ...
VALID EDGE TYPES: depends_on, derives, equivalent_to, maps_to,
explains, contradicts, generalizes
IMPORTANT: source_entity and target_entity MUST be exact entity IDs
from this KG.

Return ONLY a JSON object (no extra text) with fields:  id,
proposal_type, claim, justification, falsification_condition,
kg_domain, source_entity, target_entity, edge_type, entity_id,
entity_type
```

Constrained mode (stagnation recovery). When an island stagnates ($S = 5$ generations without valid proposals), the prompt switches to constrained mode, which enumerates *all* valid entity IDs and edge type names explicitly:

```
...  [same preamble] ...

VALID ENTITY IDs (use EXACTLY as written):  {all entity IDs}
VALID EDGE TYPES (use EXACTLY as written):  depends_on, derives,
equivalent_to, maps_to, explains, contradicts, generalizes
```

F Proposal Failure Rate Statistics

Figure 2 shows the valid proposal rate converging to ≥ 0.50 by generation 10 across all discovery domains. The initial failure rate (generations 1–3) is typically 60–80%, dominated by entity grounding errors (referencing entities not in the KG). The entity sample in free-mode prompts (up to 20 entities) and the stagnation recovery mechanism (Section 3.4) together reduce failures to <30% by generation 10. Constrained-mode prompts achieve ≥95% validity but produce less diverse proposals.

G Code and Data Availability

Source code and all experimental artifacts are publicly available:

- **Code repository**: anonymised for review; will be released upon acceptance.
- **Data archive**: Zenodo (DOI: `10.5281/zenodo.18795697`), containing all KG datasets, checkpoints, and generated proposals.

H Hyperparameter Settings

Table 5 lists all hyperparameters used in the experiments.

Compute resources. All experiments were run on a single Apple M-series CPU (no GPU). Each domain completes 20 generations in approximately 10 minutes of wall-clock time (including LLM inference via locally served Ollama). The total compute for the three reported domains is under

Table 5: Hyperparameter settings.

Component	Parameter	Value
Harmony metric	α (compressibility)	0.25
	β (coherence)	0.25
	γ (symmetry)	0.25
	δ (generativity)	0.25
DistMult	Embedding dimension	50
	Training epochs	100
	Margin	1.0
	Learning rate	0.01
	Negative samples	5
	Mask ratio	0.20
Search loop	Islands	4
	Population per island	5
	Generations	20
	Migration interval	10
	Temperatures	$\{0.3, 0.3, 0.8, 1.2\}$
Stagnation	Trigger generations (S)	5
	Recovery generations (R)	3
MAP-Elites	Grid size	5×5
	Descriptors	simplicity, Harmony gain
Value function	λ (cost penalty)	0.1

30 CPU-minutes. Preliminary experiments during development required an additional $\sim$2 hours of CPU time.

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- Please refer to our LLM policy (`https://neurips.cc/Conferences/2025/LLM`) for what should or should not be described.