

Shared Spatial Memory Through Predictive Coding

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ABSTRACT

Sharing and reconstructing a consistent spatial memory is a critical challenge in multi-agent systems, where partial observability and limited bandwidth often lead to catastrophic failures in coordination. We introduce a multi-agent predictive coding framework that formulate coordination as the minimization of mutual uncertainty among agents. Instantiated as an information bottleneck objective, it prompts agents to learn not only *who* and *what* to communicate but also *when*. At the foundation of this framework lies a grid-cell-like metric as internal spatial coding for self-localization, emerging spontaneously from self-supervised motion prediction. Building upon this internal spatial code, agents gradually develop a bandwidth-efficient communication mechanism and specialized neural populations that encode partners' locations—an artificial analogue of hippocampal *social place cells* (SPCs). These social representations are further enacted by a hierarchical reinforcement learning policy that actively explores to reduce joint uncertainty. On the Memory-Maze benchmark, our approach shows exceptional resilience to bandwidth constraints: success degrades gracefully from 73.5% to 64.4% as bandwidth shrinks from 128 to 4 bits/step, whereas a full-broadcast baseline collapses from 67.6% to 28.6%. Our findings establish a theoretically principled and biologically plausible basis for how complex social representations emerge from a unified predictive drive, leading to social collective intelligence.

Introduction

Collective intelligence is a cornerstone of biological success, enabling groups of organisms to perform complex tasks that far exceed the capabilities of any single individual [1, 4, 7, 29, 41]. From ant colonies forging optimal foraging trails to wolf packs executing intricate hunting strategies, the ability to form and act upon a shared understanding of the world is paramount [3, 14, 36]. This capacity is particularly salient in spatial navigation, where sociable animals such as bats in a cave complex or rats in a maze coordinate their movements by aligning internal representations of their environment [17, 33, 38]. Such alignment is often achieved through a sparse exchange of high-level cues, such as sonar chirps, ultrasonic squeaks, or visual signals, suggesting the existence of a shared cognitive map: a dynamic, distributed neural representation of the environment that includes the positions of resources, hazards, and, crucially, conspecifics [5, 13, 26, 45, 46].

The neural algorithms underlying these shared representations are thought to be a specialized extension of the mechanisms supporting individual cognition. In mammals, the hippocampal-entorhinal system provides the substrate for an individual's cognitive map, with place cells encoding specific locations and grid cells, providing a metric scaffold for space [15, 16, 18, 37]. The discovery of “social place cells”—neurons that fire when a partner is at a particular location—offers compelling evidence for a dedicated neural substrate that integrates the self with peers into this spatial framework [24, 40, 47]. These findings mean that the brain possesses sophisticated machinery not only for building a model of its own world but also for representing the world of others, a prerequisite for any meaningful social coordination. However, there is a critical distinction between representing others within a single brain and coordinating across brains. Within the centralized architecture of the hippocampal-entorhinal system, different neural populations can access and integrate social information through dense internal connectivity—communication is not a limiting factor. The computational challenge emerges at a different scale: when multiple individuals must align their internal spatial models through external communication that is severely bandwidth-constrained. This raises a fundamental question: What computational principles enable agents to develop socially-aware representations from individual experience and to coordinate these representations across a distributed system despite limited communication?

Similarly, in artificial multi-agent systems, replicating this biological prowess faces a same persistent challenge: the “communication bottleneck” [8, 10, 19, 30]. While multi-agent systems hold immense promise for applications in exploration, search, and rescue, their collective performance often degrades catastrophically as communication bandwidth becomes a bottleneck [20, 34, 35]. From an information theoretic perspective, the core issue is the inefficient management of statistical redundancy. When several agents explore an environment concurrently, their sensory observations are highly correlated. Naive

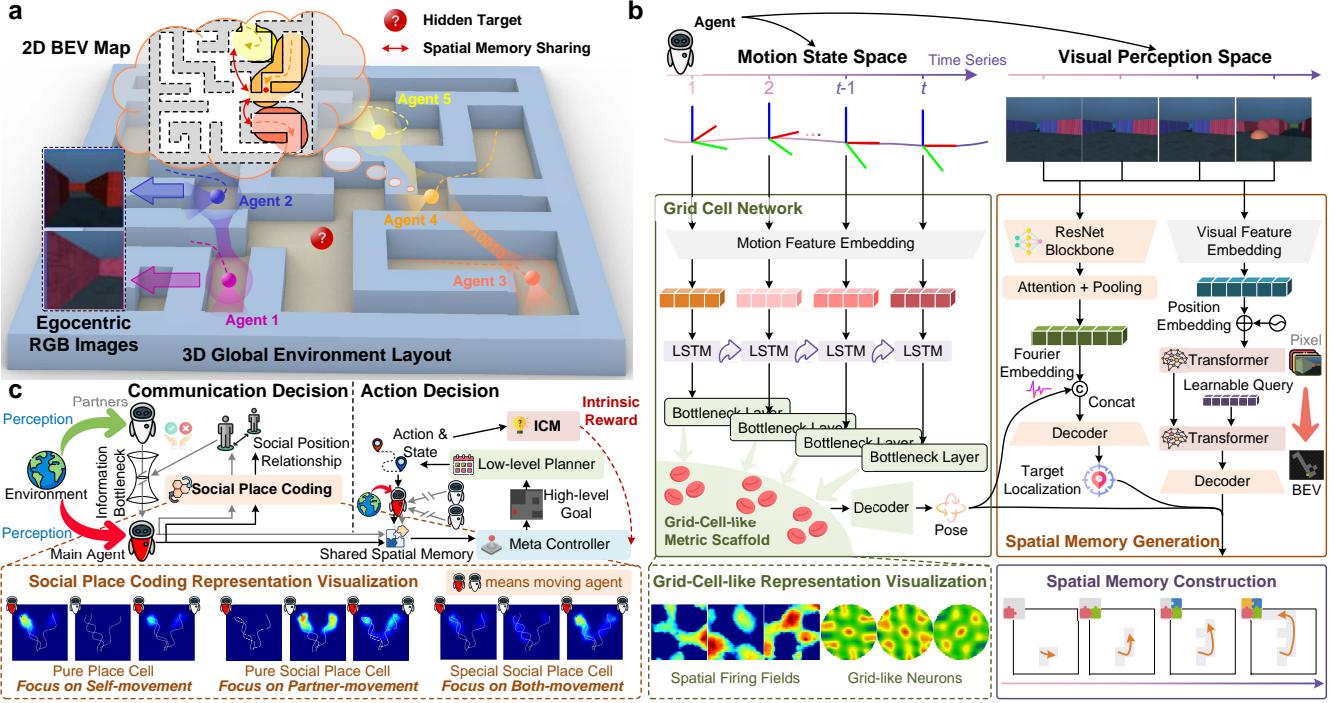


Figure 1. Overview of the predictive coding framework for sharing spatial memory. **a**, The multi-agent cooperative navigation task. Multiple agents, each with egocentric vision input, explore a 3D environment to find a hidden target. They coordinate by building and sharing a 2D bird's-eye-view (BEV) map via learned, emergent symbols. **b**, The single-agent spatial memory module. This module consists of two streams. The left stream, a Grid Cell Network, functions as an LSTM-based path integrator that processes the agent's motion state to estimate its pose. Its bottleneck layer spontaneously develops hexagonal activation patterns, mimicking biological grid cells. The right stream uses a Transformer-based network to generate a BEV map from visual inputs. The pose information from the path integrator is then used to accurately register the BEV map, constructing a coherent spatial memory of the maze layout. **c**, The agent's decision-making process via shared spatial memory. This process is divided into communication and action decisions. The communication decision is managed by an information bottleneck that adaptively adjusts data compression. Crucially, as this process must account for social peers, the network architecture gives rise to emergent social place cell-like activations. The action decision is handled by a hierarchical framework where a meta controller, trained with a multi-agent proximal policy optimization (MAPPO) algorithm and guided by an enhanced intrinsic curiosity module (ICM), directs a low-level planner to navigate toward regions that reduce the uncertainty of spatial memory.

communication strategies, such as broadcasting raw or compressed sensory data, inevitably lead to channel bandwidth starvation when transmitting vast amounts of redundant information that a partner could likely infer on its own [9, 11, 12, 43]. This leaves a critical gap in our understanding: **How can a decentralized system learn an efficient communication mechanism that is not only sparse, but also optimally informative, when transmitting only the essential information needed to resolve a partner's uncertainty?**

In this work, we demonstrate that shared spatial memory can emerge from a single computational principle: minimizing mutual predictive uncertainty between agents. We develop a multi-agent predictive coding framework that implements this principle through three integrated levels: **Level 1 (Individual Perception)**—spontaneous formation of grid-cell-like spatial metrics for self-localization; **Level 2 (Social Communication)**—bandwidth-efficient communication mechanisms and emergent social place cell representations; and **Level 3 (Strategic Exploration)**—hierarchical policies that reduce collective uncertainty through coordinated exploration.

To instantiate this principle, we ground our approach in the synthesis of predictive coding and information theory, constructing a robust shared spatial memory system that operates under extreme communication constraints. Our approach, summarized in **Fig. 1a-c**, addresses a cooperative navigation scenario where multiple agents leverage egocentric vision to explore an environment and interact via emergent symbols (**Fig. 1a**). The framework is designed to first enable each agent to individually build a predictive, allocentric bird's-eye-view (BEV) map from its own observations (**Fig. 1b**). Critically, it then provides a mechanism for agents to exchange these predictive insights through an information bottleneck, a process that minimizes their partners' future uncertainty and construct an efficient, socially grounded shared representation (**Fig. 1c**). Our framework

is realized through two tightly integrated mechanisms. First, each agent individually learns to perceive its environment by building a predictive model that generates a BEV map from egocentric vision input (**Fig. 1b**). We show that this complex visuospatial inference task is critically scaffolded by an internal path integrator that spontaneously self-organizes to produce a stable, grid-cell-like representation, providing a consistent metric for space without any explicit supervision (**Fig. 2**). This finding reinforces the idea that a robust internal model of self-motion is a foundational prerequisite for coherent world-building. Second, building upon this perceptual foundation, agents collaboratively develop a communication mechanism (**Fig. 1c**). Rather than exchanging raw observations, agents learn to transmit compressed, discrete symbols that are optimally tailored to reduce their partners' future uncertainty. This communication mechanism emerges from a variational information bottleneck (VIB) objective, which provides a principled trade-off between minimizing communication cost (rate) and maximizing predictive utility for a partner (distortion) [12, 22]. The fundamental observation is that agents can learn how to efficiently communicate with each other due to more interactions and hence sharing more prior information, which is similar to the fundamental principle of emergent communications[31, 32]. The communication mechanism is embedded within a hierarchical reinforcement learning framework (termed HRL-ICM), where an ICM-aided MAPPO algorithm makes strategic navigation decisions to efficiently reduce uncertainty [28, 42].

The proposed HRL-ICM framework achieves a level of performance and robustness that substantially exceeds current baselines such as *No Communication*, *Periodic Broadcast*, and *Full Broadcast*. As validated in the challenging Memory-Maze benchmark [27], our framework exhibits remarkable resilience to communication constraints. While the success rate of the *Full Broadcast* baseline collapses from 67.6% to 28.6% (a 58% relative decline) when the bandwidth is reduced from 128 to 4 bits/step, our method degrades slightly from 73.5% to 64.4% (only a 12% relative decline), maintaining superior performance even under extreme bandwidth constraints and underscoring the efficiency of the learned predictive communication mechanism (**Fig. 5g**). Most remarkably, we discover that the objective of predicting a partner's state drives the emergence of a functionally specialized neural substrate for social cognition. Within the network's social decoding module, neurons spontaneously segregate into distinct populations, including units that selectively encode the location of specific teammates—a striking artificial analogue of social place cells observed in the mammalian hippocampus (**Fig. 4**) [21]. Causal analyses confirm that these emergent representations are not epiphenomenal but functionally critical for effective coordination (**Fig. 6b** and **Supplementary Video 3**).

By unifying principles from predictive coding and information bottleneck theory [6, 38], our work provides a theoretically grounded and biologically explainable basis for shared spatial memory. The main contributions of this work are threefold. ① We develop a novel multi-agent framework that enables an efficient, semantically rich communication mechanism to emerge from first principles. ② We provide a plausible computational model for the function and emergence of social place cells, suggesting they arise as a necessary component of a social predictive coding system. ③ We validate this framework in a challenging benchmark, demonstrating state-of-the-art performance, scalability, and bandwidth insensitivity. This work paves the way for a new generation of collaborative agent systems that can coordinate with the efficiency and flexibility of their biological counterparts, grounded in a deeper understanding of the computational principles that may underlie collective intelligence itself.

Results

Grid-cell-like metric scaffold emerges spontaneously from self-supervised motion prediction

A fundamental prerequisite for our predictive coding framework is an agent's ability to form a stable internal model of its own state and surroundings. As outlined in **Fig. 1b**, this is achieved by solving two coupled prediction problems: predicting the visual appearance of the world (BEV mapping) and predicting the agent's own trajectory through it (path integration). This section presents results for this first component of our unified framework—the individual predictive model—demonstrating that solving the self-supervised task of continuous self-motion prediction naturally reinstates a spatial coding scheme, the reminiscent of biological grid cells, which in turn provides an essential metric scaffold for robust visual perception.

The core of the path integration module is an LSTM network, tasked with predicting its future pose based only on its past velocity commands. Under this predictive constraint, the network's hidden units spontaneously form periodic spatial firing patterns similar to the grid-cell representations previously reported in both biological and artificial agents [2, 37]. Many individual units developed highly structured spatial firing fields arranged in a triangular lattice (**Fig. 2a**). To quantitatively confirm this observation, we computed the spatial autocorrelogram for each unit's activation map. This analysis revealed a clear hexagonal symmetry in the firing patterns of key neurons (**Fig. 2b**), the defining physiological signature of grid cells. The mathematical formulation for calculating these rate maps, autocorrelograms, and the final gridness score is detailed in **Supplementary Method S1.1.3**.

This grid-like representation is not only a byproduct but also a computational regime that the network converges to when optimizing for stable self-motion prediction. To demonstrate this, we track the co-evolution of this neural code and the module's predictive performance throughout training. As the network learned, the gridness score of the most prominent units—a measure of hexagonal symmetry—steadily increased, while the path integration error, which quantifies the error in the predicted

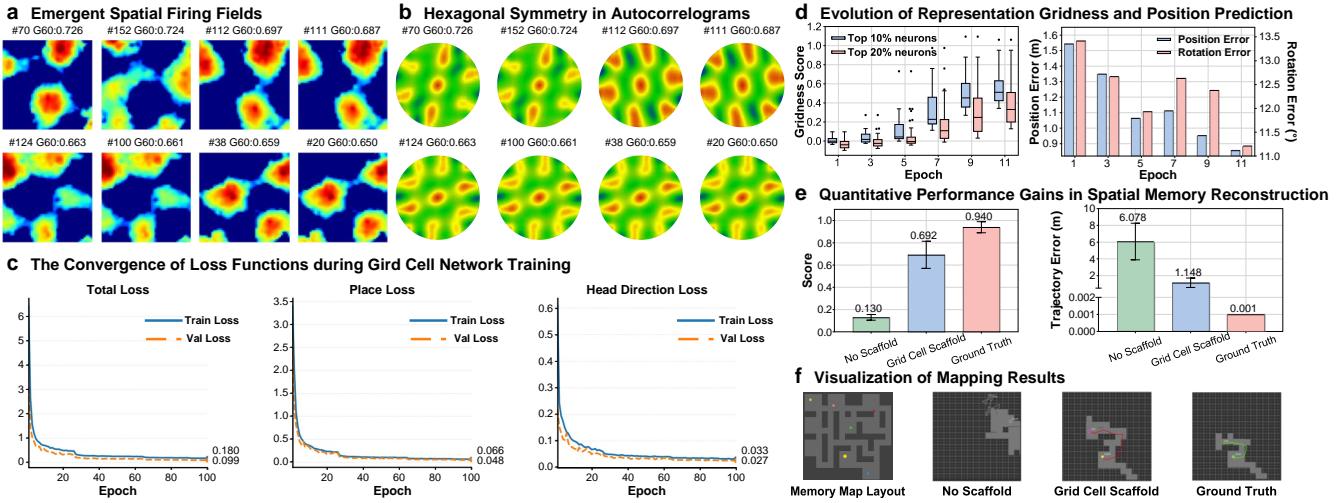


Figure 2. Grid-cell-like representations enhance robust global BEV mapping. **a**, 2D spatial firing rate maps of learned grid-like representations. **b**, Spatial autocorrelograms of representative grid-like neurons reveal hexagonal symmetry. **c**, The convergence of loss functions during grid cell network training. **d**, As training proceeds, top neuron gridness increases while path integration error decreases. **e**, Ablation study shows the full model achieves lower trajectory error and higher prediction confidence than the variant without the grid scaffold. **f**, Comparison of BEV map reconstructed by different configurations.

trajectory, concurrently and dramatically decreased (Fig. 2d and **Supplementary Fig. S4**). This tight correlation, along with the steady convergence of the training losses (Fig. 2c), demonstrates that the formation of a stable, periodic neural code is the very mechanism through which the network masters the task of motion prediction. The network learns to represent space metrically, enabling it to accurately integrate its movements over long distances and maintain a coherent belief about its location.

The primary function of this grid-like scaffold is to stabilize the agent's visual prediction process. By conditioning the BEV generation model on the latent state provided by the path integrator, the agent can correctly register and align transient visual inputs into a coherent allocentric frame. To isolate and quantify its functional role, we performed an ablation study, comparing the full predictive model against a variant where the grid-cell scaffold was disabled. The scaffold's contribution is clear: the full model achieved significantly lower trajectory error and higher prediction confidence (Fig. 2e). This improvement in self-localization directly translates into superior visual prediction. BEV maps from the scaffolded model are more complete and geometrically accurate, while the no-scaffold baseline products fragmented and distorted maps (Fig. 2f). **Supplementary Fig. S6** visualizes this full pipeline, showing how egocentric views are converted to BEV predictions and integrated into a persistent spatial memory. **Supplementary Fig. S7** illustrates the progressive and cumulative construction of the shared spatial memory, visualizing how the map is built up at sequential time intervals. Further examples of neural activations consistently show a transformation from disorganized firing to highly regular, grid-like fields (**Supplementary Fig. S4**). The dynamic evolution of this process is visualized in **Supplementary Video 5**, which shows the transformation from random initialization to highly structured grid-cell-like representations across training epochs. Therefore, these findings show that the emergence of grid-cell-like coding in our predictive model serves a necessary functional role for constructing a stable spatial memory, providing a computational foundation for coherent world modeling.

Structured communication mechanism emerges from the social predictive objective

Having established that individual agents can build robust predictive models of their environment, we next investigate how the framework extends this principle to the social domain. Agents learn to cooperate by developing a communication mechanism guided by a singular objective: transmit only the information that maximally reduces a partner's future uncertainty. This pressure compels the agents to collaboratively discover a communication system that is not only sparse but also intelligent and semantically structured.

A key property of the emergent protocol is its context-aware transmission strategy. Agents learn to communicate not periodically, but strategically at particular moments and locations where a partner's internal model is most likely to be inaccurate. We visualize the spatial distribution of communication events and find that agents concentrate their transmissions at points of high predictive uncertainty (Fig. 3a). For example, in mazes with a central hub, communication peaks in this area, where an agent's next move is most ambiguous. In such locations, information from others is crucial to avoid redundant exploration. Conversely, in mazes with long, deceptive dead ends, agents learn to communicate most frequently from deep within these

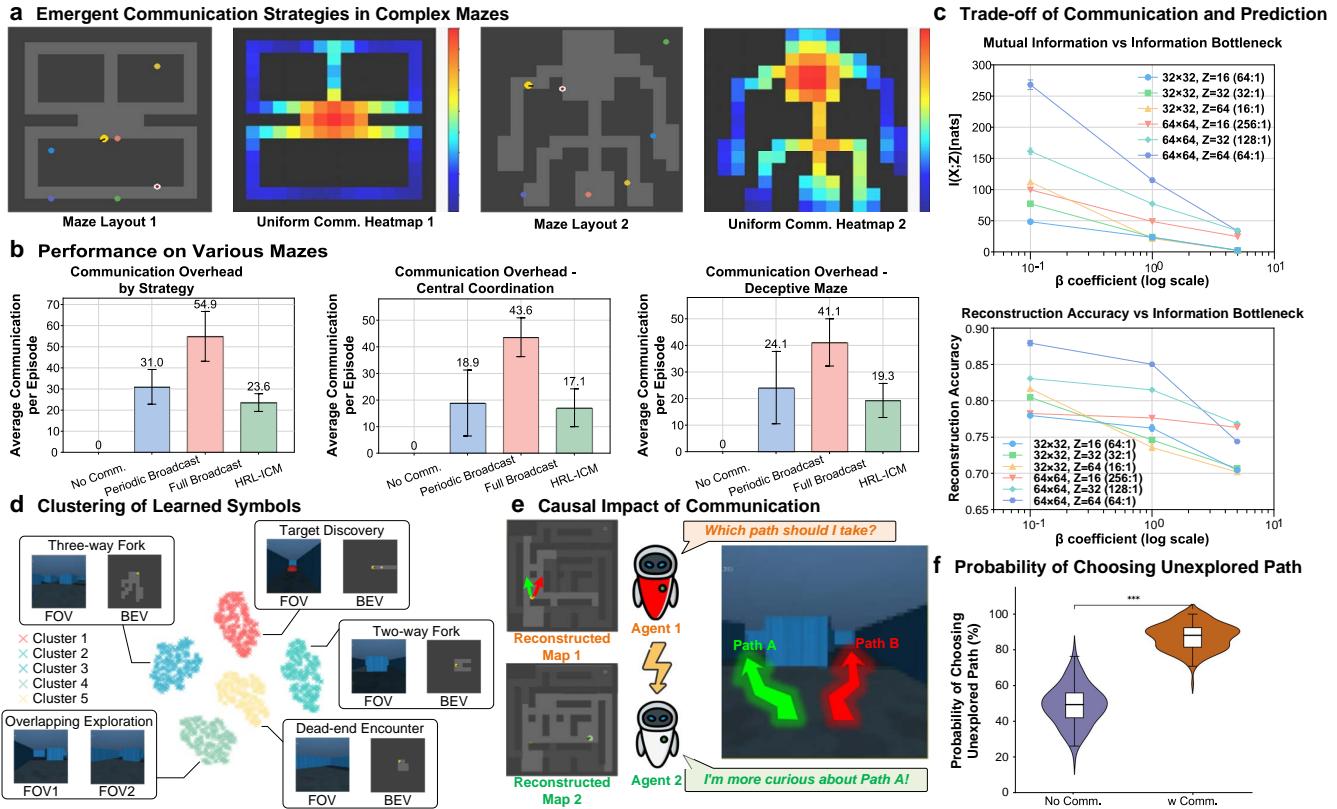


Figure 3. An efficient, structured, and intelligent communication mechanism emerges from a predictive objective. a. Intelligent communication strategies emerge, with message frequency (heatmaps) concentrated at critical decision points like coordination hubs or dead ends, demonstrating strategic triggering. **b.** The emergent protocol is highly bandwidth-efficient, consistently requiring the lowest communication overhead across diverse maze types when compared to full and periodic broadcast baselines. **c.** The protocol is theoretically controllable via the information bottleneck’s β coefficient, which enables a principled trade-off between message compression (compression ratio) and predictive utility (reconstruction accuracy). **d.** An emergent symbolic vocabulary is grounded in strategic contexts. A t-SNE visualization reveals distinct symbol clusters corresponding to high-level navigational situations, such as encountering a “Three-way Fork” or discovering the “Target”. **e.** Communication causally influences decision-making. In a controlled scenario where one agent faces a choice between an unexplored path (A) and a known one (B), communication from its partner allows it to identify Path A as the more informative route. **f.** The behavioral impact is statistically significant. A violin plot quantifying choices at two-way forks shows that communication leads to a significantly higher probability of selecting the unexplored, informative path compared to the no-communication baseline ($***p < 0.001$), confirming the protocol’s causal role in improving efficiency.

traps. This behavior is a direct solution to the social prediction problem: a message from a dead end serves as a powerful “prediction error” signal to teammates, effectively correcting their erroneous implicit prediction that the path might be fruitful. This strategic triggering, consistently observed across diverse maze topologies (Supplementary Fig. S7), demonstrates that agents learn an implicit model of their partners’ beliefs, sharing information precisely when it can best resolve uncertainty and prevent predictive mistakes.

This strategy of transmitting only the most surprising, uncertainty-reducing information naturally gives rise to a highly bandwidth-efficient protocol. By eliminating the transmission of predictable, redundant information, the system minimizes its communication overhead. We quantify this by comparing the average number of messages per episode against standard baselines. Across thousands of randomly generated layouts, our framework consistently operates with a fraction of the bandwidth required by periodic or full-broadcast approaches (Fig. 3b), confirming that the social predictive objective is a powerful first principle for learning efficient communication.

Furthermore, the protocol is fundamentally structured and controllable, adhering to the principles of information bottleneck theory that underpin our social predictive model. The information bottleneck’s β coefficient allows for a principled tuning of the trade-off between compression (rate) and predictive utility (distortion). As we increase β , placing a stronger penalty

on information rate, the agents are forced to develop a more compressed, abstract symbolic representation (**Fig. 3c**). This comes at the expected cost of reduced predictive utility, confirming that the framework provides theoretical control over the communication channel's properties, allowing it to be adaptable to varying bandwidth constraints.

The uncertainty-driven compression scheme culminates in a meaningful symbolic vocabulary. A t-SNE visualization of the message latent space reveals that symbols are not used randomly but form distinct clusters corresponding to high-level strategic contexts (**Fig. 3d**). For instance, specific symbol families emerge for situations such as navigating a “Three-way Fork”, encountering a “Dead-end”, or discovering the “Target”. These are all contexts that demand clear communication to resolve ambiguity. To test for a causal link between these symbols and agent behavior, we conduct a controlled experiment (**Fig. 3e**). An agent at a fork could resolve its uncertainty about which path to choose only after receiving a message from its partner. We quantify these choices across thousands of trials and find that communication significantly and reliably guides agents to select the more informative, unexplored path over a known one (**Fig. 3f**). This provides compelling evidence that the social predictive objective forges a functional and intelligent communication system. The agents do not merely signal raw data; they learn to transmit compressed, symbolic representations of prediction errors to collaboratively refine their shared world model.

Predicting partner states forges an emergent social place code

A central challenge in collective intelligence is the capability to form and maintain representations of others. An agent must move beyond a purely egocentric worldview and model the states, locations, and potential actions of its partners. We hypothesize that the predictive objective of forecasting a teammate’s future sensory state would provide a sufficiently rich learning signal to induce a functionally specialized neural substrate for social spatial cognition. To test this, we design a social processing module that integrates the agent’s own state (S_1) with information about its partner’s state (S_2), and uses the resulting joint representation to predict future outcomes for both agents (**Fig. 4a**). Analysis of the learned internal representations revealed clear functional specialization with properties consistent with vector- and grid-like spatial coding in artificial agents [24, 40, 47].

Single-unit analyses indicate a spontaneous segregation into distinct, interpretable cell types (**Fig. 4b**). One substantial population behaved like classical place cells (network units encoding self-position, exhibiting sharp and stable firing fields tuned exclusively to the agent’s own location). These units are largely invariant to the partner’s motion or position, thereby providing a stable allocentric representation of self. In contrast, a second major population fired as a function of the partner’s location: these artificial social place cells (SPCs; units encoding partner position, distinct from the self-position-encoding place cells) showed strong spatial tuning to the partner’s location within the observer’s reference frame (**Fig. 4b**, Neurons 29 and 36), providing a substrate for tracking others. We also observe a population of mixed-selectivity units that conjunctively encode self- and partner-locations (**Fig. 4b**, Neuron 8). Representative galleries across four conditions (self-moving, partner-moving, both-moving, both-static) indicate that this specialization is expressed across units and task contingencies (**Supplementary Figs. S8-S10** and **Video 2**).

Beyond single-neuron effects, the specialized units form a population code for higher-order relational variables, most notably inter-agent distance. We identify subpopulations selectively tuned to near, mid-range, and far separations (**Fig. 4c**). Their graded tuning curves spanned the full range of separations encountered during exploration, yielding a tiling-like coverage of relational distance space and supporting a continuous representation of proximity to the partner (**Fig. 4c**, bottom right). This organization is consistent with the view that predictive objectives shape compact, task-relevant embeddings of spatial relations [24, 47].

We then quantitatively dissociate these populations using mutual information (MI) between firing rate and spatial variables. Place cells carry high MI about self-position but negligible MI about partner-position, whereas SPCs show the inverse profile (**Fig. 4d**, top). A scatter of Self MI versus Partner MI reveals clearly separable clusters under our metrics, corresponding to self-tuned, partner-tuned, and mixed-selectivity units (**Fig. 4d**, bottom). These results indicate that specialization is not confined to a small number of idiosyncratic units but reflects a broader division of labor induced by the social predictive objective.

To assess causal involvement, we perform *in-silico* lesions. Targeted lesioning of distance-tuned SPCs produced a marked, selective impairment in inter-agent distance prediction relative to pre-lesion performance and to size-matched random lesions (**Fig. 4e**). A broader lesion of the peer-processing module degrades general position prediction. Meanwhile, these patterns indicate that SPCs are causally important for computing relational social geometry in our setting, whereas self-tuned units primarily support self-localization. Control ablations that preserve overall parameter count but disrupt SPC-selective pathways yielded similar deficits in distance estimation (**Fig. 4e**).

We next link representation to learning dynamics and task performance. The fully trained network’s ability to predict a partner’s future trajectory depends on the integrity of SPCs: lesioning these units reduces predictive accuracy toward untrained levels (**Fig. 4f**, left). During training, validation loss decreases as the fraction of specialized units increases, with self-tuned and partner-tuned populations emerging in parallel (**Fig. 4f**, right). This co-evolution suggests that a functionally segregated social place code is not incidental but emerges as a principal mechanism by which the model solves partner-state prediction and coordination in our framework.

Finally, we clarify scope and relation to prior work. The present results do not claim a novel physiological class. Rather,

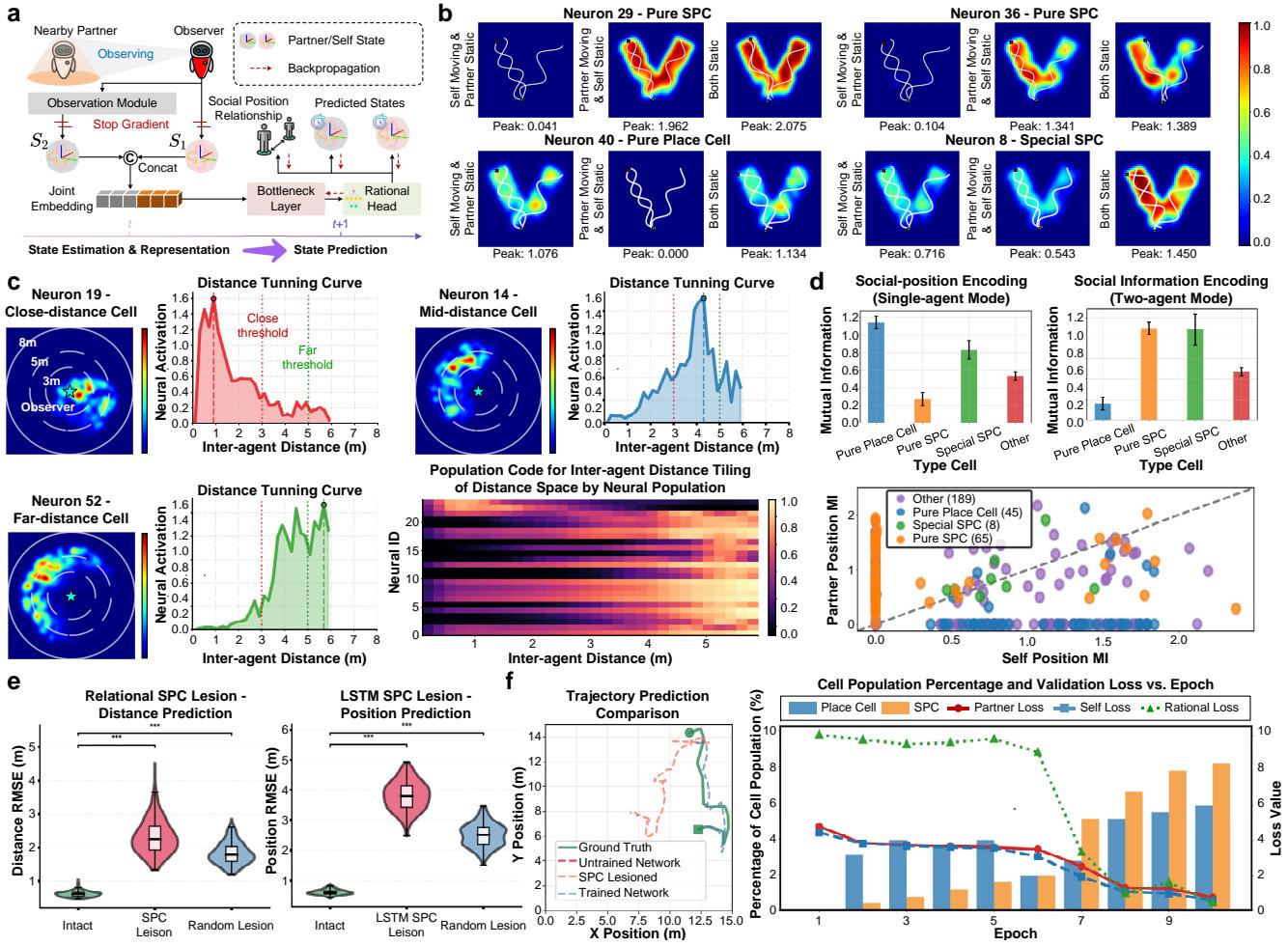


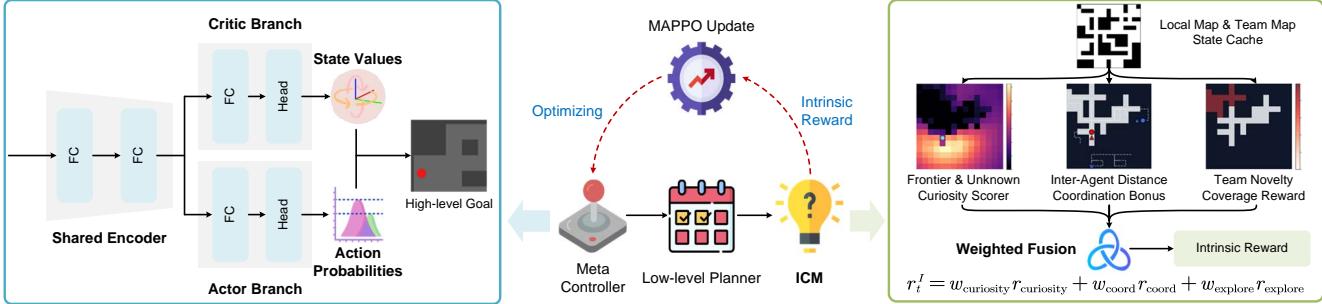
Figure 4. Predictive learning forges a functionally specialized social place code. **a**, Model architecture. Observer (S_1) and partner (S_2) states are processed through a bottleneck layer and relational head. The network is trained by back-propagating predictive error from self, partner, and social outputs. **b**, Functionally distinct neuron types. Heatmaps show spatial firing fields for representative “Pure SPCs” (tuned to partner location), “Pure Place Cells” (tuned to self location), and “Special SPCs” (mixed selectivity). **c**, Population code for inter-agent distance. Top panels show 2D maps and 1D tuning curves for neurons selective for close-, mid-, and far-distances. Bottom right, a heatmap of all distance-tuned neurons reveals a “tiling” of the distance space. **d**, Quantitative functional dissociation. Top, bar plots show high mutual information (MI) with self-position for Place Cells and with partner-position for SPCs. Bottom, a scatter plot of self MI vs. partner MI reveals specialized cell clusters. **e**, Causal necessity of SPCs demonstrated via in-silico lesioning. Targeted lesioning of distance-selective SPCs (“SPC Lesion”, left) specifically impairs distance prediction, while lesioning the entire peer LSTM module (right) impairs general position prediction, compared to controls. **f**, Co-evolution of performance and specialization. Left, trajectory predictions are accurate for the trained network but poor for untrained or SPC-lesioned networks. Right, validation loss decreases over training epochs as the proportion of specialized Place Cells and SPCs increases.

they show that under a social predictive objective, artificial networks reproduce a division of labor analogous to self- and partner-centered spatial coding, and this division carries demonstrable functional and causal relevance for constructing and exploiting a shared spatial memory. In combination with prior evidence that predictive pressures can organize grid- and distance-related codes in artificial agents [24, 40, 47], these findings support the view that minimizing mutual predictive uncertainty induces specialized representations for self and partner that jointly enable robust coordination under bandwidth and observability constraints.

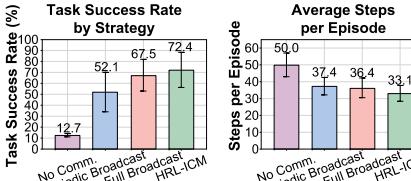
Integrated framework achieves superior cooperative navigation performance

The preceding sections demonstrate how a unified predictive objective forges specialized components for perception, communication, and social representation. Here, we evaluate the performance of the fully integrated system to validate its collective

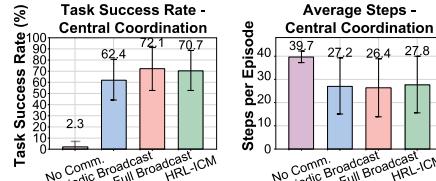
a Framework of HRL-ICM



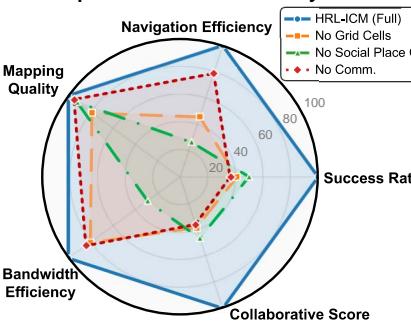
b Random Mazes



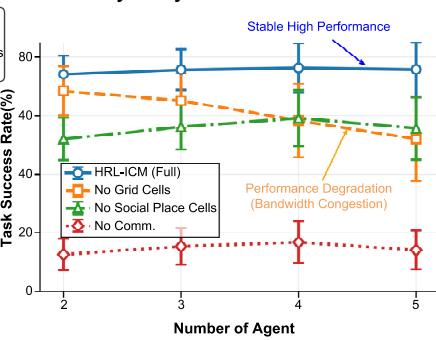
c Central Coordination Maze



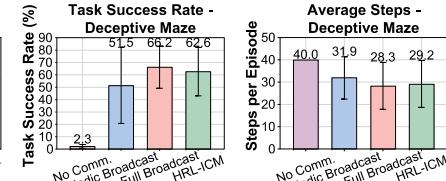
e Component Contribution Analysis



f Scalability Analysis



d Deceptive Maze



g Bandwidth Robustness Heatmap

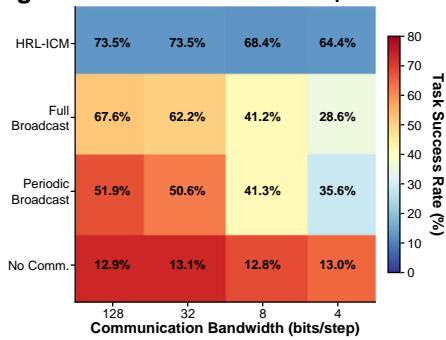


Figure 5. HRL-ICM framework achieves superior and robust cooperative performance. **a**, Architecture of the hierarchical reinforcement learning with intrinsic curiosity module (HRL-ICM). The ICM embodies the Level 3 predictive objective: it generates an intrinsic reward based on the agent’s inability to predict the consequences of its actions. This “prediction error” signal guides the high-level Meta Controller to select goals that maximally reduce uncertainty, which are then executed by a Low-level Planner. **b**, Superior success rates and efficiency across 10,000 random mazes. **c**, High performance maintained in a central coordination maze. **d**, Robustness demonstrated in a deceptive maze with numerous dead ends. **e**, Ablation analysis confirms that each predictive component (grid-cells, social cells, communication) is critical for performance, with communication being indispensable. **f**, The framework scales effectively as agent count increases, outperforming baseline strategies that suffer from performance degradation. **g**, Exceptional bandwidth robustness is shown as our method’s success rate degrades slightly when bandwidth shrinks, while the “Full Broadcast” baseline’s performance collapses.

effectiveness in solving complex, communication-constrained tasks. We assess the complete hierarchical reinforcement learning with intrinsic curiosity module (HRL-ICM) against strong baselines in the Memory-Maze benchmark (Fig. 5a). This framework implements the third level of our predictive coding hierarchy. It uses a policy guided by predictive uncertainty, where an intrinsic reward generated from prediction error directs agents to explore regions that maximally reduce their world model’s uncertainty.

We first assess the framework’s effectiveness across a wide range of navigation problems. In a large-scale test over 10,000 procedurally generated random mazes, HRL-ICM achieves the highest task success rate (72.4%) while simultaneously requiring the fewest steps on average to locate the goal (Fig. 5b). This strong average-case performance is mirrored in environments designed to probe specific aspects of collective intelligence. In a central coordination maze that demands efficient division of labor, our method again achieves the highest success rate of 72.0% (Fig. 5c). Furthermore, in a deceptive maze with numerous long dead-ends, the HRL-ICM agents maintain a high success rate of 66.0% (Fig. 5d). Besides, Supplementary Video 1 directly visualizes the performance comparison in memory maze. This resilience highlights the functional value of the emergent communication mechanism, which enables agents to share high-value negative information, a critical capability for efficient exploration.

To quantify the contribution of each core component to this performance, we conduct a systematic ablation study (Fig.

5e). The complete framework (HRL-ICM Full) outperforms all ablated variants across every metric, including success rate, navigation efficiency, and mapping quality. The removal of any single component resulted in a significant and interpretable performance degradation. Disabling the communication channel led to a collapse in collaborative score and success rate, confirming that cooperation is indispensable. Excising the social place cell module specifically degrades the agents' collaborative score and efficiency, providing further causal evidence that the emergent social representations are functionally critical for effective coordination. Similarly, removing the grid-cell scaffold compromises mapping quality and navigation efficiency, underscoring the foundational importance of a stable internal metric. This analysis demonstrates that the framework's success is attributable to the synergistic integration of its predictive components. The system's robustness is further evaluated against communication noise and environmental complexity (**Supplementary Fig. S11** and **Video 4**).

A critical test for any multi-agent system is scalability. We evaluate how the framework performs as the number of agents increased from two to five (**Fig. 5f**). Our HRL-ICM framework demonstrates high scalability, maintaining a stable success rate across varying numbers of agents. In contrast, baseline strategies that rely on naive broadcasting (Full and Periodic) suffers a clear performance decline as more agents are added. Their inability to manage the exponential growth in information flow leads to channel congestion and degraded coordination. Our framework's learned, predictive communication mechanism mitigates this issue by ensuring that only the most vital, non-redundant information is transmitted.

Finally, we test the framework's robustness under its core design constraint: limited communication bandwidth (**Fig. 5g**). The performance heatmap reveals the system's high resilience to bandwidth restrictions. As the available bandwidth is reduced from 128 bits/step to an extremely constrained 4 bits/step, HRL-ICM's success rate degrades only moderately from 73.5% to 64.4%. This contrasts sharply with the Full Broadcast baseline, whose performance collapsed under the same conditions, plummeting from 67.6% to 28.6%. This result provides compelling evidence for the efficacy of our approach. By learning to communicate only the essential prediction errors of their partners, the agents can sustain a high degree of coordinated action in austere communication environments where conventional methods fail. This demonstrates a robust solution to the challenge of communication-limited coordination.

Framework analysis: Convergence, causality, and generalization

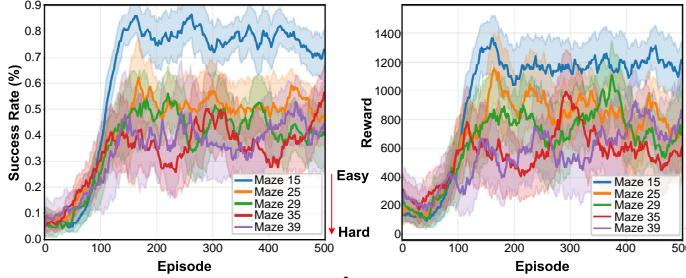
Having demonstrated the functional benefits of the integrated system, we next analyze its learning dynamics, the causal nature of its emergent communication, and its ability to generalize. A powerful internal model is only useful if it arises from a stable learning process, translates into effective behavior, and scales to challenges beyond its training distribution.

A prerequisite for any complex autonomous system is convergence to a stable, high-performance policy. We demonstrate this property by tracking the training dynamics of our framework across mazes of varying difficulty (**Fig. 6a**). In all tested environments, from 15×15 to 39×39 configurations, both the task success rate and the average reward per episode exhibit a steady and robust increase, ultimately converging to stable plateaus. This validates our end-to-end training approach. It also shows that the global objective of minimizing predictive uncertainty provides a consistent and effective learning signal for both visuomotor control and inter-agent communication. The learning process is not brittle but reliably guides agents toward a competent collaborative strategy.

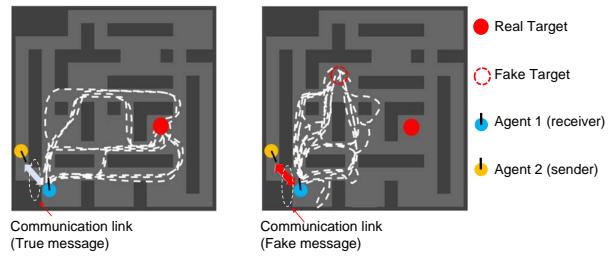
While the emergent communication mechanism is efficient, a critical question remains: *Do the learned symbols possess a grounded, causal meaning shared between agents?* To disambiguate this, we designed a causal intervention experiment (**Fig. 6b**). In a control scenario, a sender agent correctly identifies a target and transmits a corresponding message to a receiver, which then successfully navigates to the correct location. We then perform a counterfactual intervention by intercepting the true message and replacing it with a “fake message”, a symbol previously associates with a distractor's location. The effect is immediate and unambiguous. Upon receiving the fake message, the receiver predictably changes its trajectory and navigates directly to the fake target. This specific change in behavior in response to a manipulated signal provides powerful evidence that the learned symbols are not mere correlations but function as causal drivers of the receiver's actions. This confirms that the agents develop a shared, grounded understanding of the emergent symbols, forming the basis for language-driven coordination. Moreover, the causal intervention experiment is visualized in **Supplementary Video 3**, which demonstrates the receiver agent's trajectory being predictably altered by the manipulated message.

The ultimate test of the framework lies in its ability to generalize its learned strategies to environments more complex than those seen during training. We evaluate this by comparing the HRL-ICM framework against baselines across four scales of maze complexity, from 25×25 to 39×39 (**Fig. 6c**). The results demonstrate both superior performance and scalability. Across all maze sizes, our framework achieves a significantly higher task success rate (**Fig. 6d**) and requires fewer steps for completion (**Fig. 6e**) than all baselines. Critically, as environmental complexity increased, the performance of the baseline strategies degrades sharply. In contrast, our framework exhibits a much more graceful decline in performance. This superior scalability is a direct consequence of the framework's core principles. Instead of relying on brute-force information sharing, agents in our framework leverage their learned internal models, such as the grid-cell-like metric scaffold and social place cell code, to form a robust shared memory. They use the emergent communication mechanism to transmit only the most critical,

a Training Dynamics and Convergence Analysis



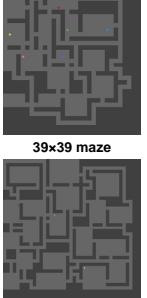
b Causal Intervention for Grounded Language Understanding



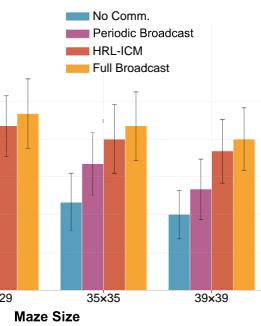
c 25x25 maze



d 29x29 maze



e 35x35 maze



f 39x39 maze

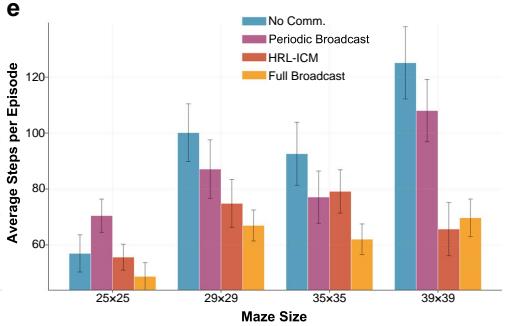


Figure 6. Comprehensive performance analysis of the HRL-ICM framework, demonstrating stable learning, causal language understanding, and robust generalization. **a**, Training dynamics and convergence across mazes of varying difficulty. The plots show steady improvement and convergence for both average reward and task success rate, indicating stable end-to-end learning. **b**, Causal intervention analysis reveals grounded language understanding. A receiver’s trajectory is predictably altered by a manipulated “fake” message (right) versus a true message (left), confirming the emergent symbols causally drive behavior. **c**, Example maze layouts of increasing complexity (from 25×25 to 39×39) used to test generalization. **d**, Task success rate across different maze sizes. HRL-ICM consistently outperforms baselines, showing superior performance. **e**, Average steps to completion. HRL-ICM demonstrates higher efficiency (fewer steps) than baselines, with its advantage growing in more complex environments.

uncertainty-reducing information. This is an inherently efficient strategy that is less susceptible to the combinatorial explosion of the state space. These findings validate that our theoretically-grounded approach resolves the trade-off between communication bandwidth and coordination effectiveness, yielding a generalizable and scalable solution for multi-agent intelligence.

Discussion

We propose that a single computational objective—the minimization of mutual predictive uncertainty—can serve as a first principle for the emergence of collective intelligence. We demonstrate that this unified predictive drive gives rise to a three-tiered hierarchy of phenomena: a stable, grid-cell-like spatial metric at the individual level; an efficient communication protocol at the inter-actional level; and a specialized neural substrate for social cognition, analogous to hippocampal social place cells, at the representational level. Our findings suggest that complex neural architectures supporting social navigation may not be distinct adaptations but are the computational consequence of this predictive learning framework. This frames social intelligence as an extension of individual cognition.

Our work is grounded in established principles of individual cognition. We first confirm that a stable personal spatial representation, scaffolded by an emergent, grid-cell-like metric critical for robust navigation [2], is a necessary foundational component (Fig. 2). While architectures such as the Tolman–Eichenbaum Machine provide a unifying account of how an *individual* agent learns and generalizes spatial and relational knowledge [37], our work addresses the subsequent challenge: how multiple agents, each possessing such internal models, achieve collective intelligence. We propose that the drive to minimize mutual uncertainty provides a computational bridge from individual cognition to shared understanding.

From this foundation, we address emergent communication. Unlike frameworks exploring asymmetric, teacher–student knowledge transfer [39], our setting resolves symmetric, peer-to-peer coordination. Framing communication through the information bottleneck principle, we show that agents can autonomously learn a protocol that balances communication cost and predictive utility (Fig. 3c), surpassing standard multi-agent reinforcement learning baselines, such as PPO and Dreamer, considered here [25]. A key consequence of this social predictive objective is the spontaneous formation of a functionally

specialized neural substrate for social cognition. Inspired by the discovery of hippocampal social place cells in bats [26], we provide a computational account consistent with their emergence under a social predictive objective. Whereas biological studies observe these neurons, our framework posits that the imperative to predict a partner’s future state encourages the development of functionally specialized units tuned to the location of others. Our *in-silico* lesion experiments (Fig. 4e, f) indicate that these emergent “social place cells” are causally important for social prediction, offering a functional interpretation for the “shared neural subspaces” reported in interacting systems [44].

The same principle mirrors the “next-token prediction” objective that underpins large language models (LLMs): while LLMs build a world model by predicting sequences of text, our agents build a shared spatial model by predicting sequences of each other’s sensory states. This parallel suggests that predictive learning is a general mechanism for constructing both individual and shared world models. The connection between understanding and effective compression, highlighted in recent work on lossless data compression [23], provides a theoretical link to the communication efficiency observed in our system. For multi-robot systems, this work offers a paradigm for designing communication-efficient swarms that learn to coordinate from first principles [25].

While our framework establishes these principles, it opens several avenues. The current model utilizes a discrete communication channel; future work could explore the emergence of more continuous or compositional communication structures [39]. Deploying our model-based learning approach on physical multi-robot systems to bridge the simulation-to-reality gap is a key next step [25]. More broadly, the phenomena of shared memory and social representation may arise not from intricate, pre-programmed rules, but from a single computational objective: the drive to predict the world of another.

Methods

Memory-Maze benchmark

All experiments are conducted within the Memory-Maze benchmark, a simulation environment specifically designed to rigorously evaluate agents’ long-term spatial memory and cooperative capabilities under partial observability [27]. The framework procedurally generates three-dimensional mazes with randomized layouts for each episode, which prevents task-specific overfitting and ensures that learned policies generalize across a wide distribution of environments. To systematically assess the scalability and robustness of our proposed model, we utilize a range of maze complexities, configuring the environment with progressively larger layouts, specifically 15×15 , 25×25 , 29×29 , 35×35 , and 39×39 grids. This setup allows for a thorough investigation of model performance as the state space and the demand on spatial memory and communication grow significantly.

Each agent in the multi-agent system operates based on egocentric sensory inputs and is subject to realistic physical and communication constraints. An agent’s perception is primarily driven by a forward-facing RGB camera providing a 75-degree field of view (FOV), which serves as its visual input. In addition to vision, each agent has access to its own proprioceptive information, namely its linear and angular velocities. The action space is discrete, consisting of move-forward, turn-left, turn-right, stay, enabling navigation through the maze corridors. A critical component of our experimental design is the constraint on inter-agent communication. Agents can only exchange information when they are within a pre-defined communication range, and the channel is subject to a configurable bandwidth bottleneck (e.g., 4 to 128 bits/step). This limitation mirrors real-world robotic applications and creates a strong selective pressure for the emergence of an efficient and targeted communication protocol, which is a central focus of our work. The collective objective for the team of N agents (where N is typically 2-4 in our experiments) is to collaboratively explore the unknown maze to locate a single, hidden target.

Unified framework for predictive coding

Throughout this paper, we use neuroscience-inspired terminology to describe artificial network components that exhibit functional properties analogous to biological neurons. Specifically, “place cells” refer to network units encoding spatial position with Gaussian receptive fields, “head-direction cells” encode heading orientation with von Mises tuning, and “grid cells” exhibit periodic hexagonal firing patterns. “Social place cells” (SPCs) are distinct units that encode partner locations rather than self-locations. These terms facilitate comparison with biological findings while denoting artificial neural network parameters that represent position and orientation information. Detailed mathematical definitions are provided in Supplementary Methods.

The cornerstone of our framework is the principle that intelligent agents build and share world models by continuously minimizing prediction error. We formalize the challenge of coordinated navigation as a multi-level prediction problem, where each agent’s objective is to build a generative model that predicts its own sensory inputs, the states of its partners, and the global state of the environment. This unified predictive objective is realized through three synergistic mechanisms: ① an individual predictive model for robust perception and self-localization, ② a social predictive coding model for emergent communication, and ③ a hierarchical policy guided by predictive uncertainty for strategic exploration.

Level 1: Individual predictive model for perception and self-localization

An agent must first form a coherent internal model of its own state and surroundings to serve as a foundation for any higher-level reasoning or social interaction. This is achieved not through a single monolithic network, but by the synergistic interplay of two specialized yet deeply integrated sub-systems that solve simultaneous, coupled prediction tasks. Meanwhile, these components function analogously to a visual simultaneous localization and mapping (SLAM) system, where the agent concurrently builds a map of its environment (perception) while predicting its location within it (localization). This dual predictive process is essential because each task regularizes the other: a stable location estimate prevents the map from becoming distorted, while a coherent map provides the landmarks necessary for accurate localization. This reciprocal relationship enables the construction of a reliable individual world model, which is the prerequisite for forming a shared spatial memory.

Visual predictive coding for BEV mapping. As shown in **Fig. 1b**, the primary perceptual task is framed as a visual prediction problem that addresses the challenge of inferring a stable world representation from a fleeting, ambiguous sensory stream. Specifically, the agent must learn a generative model of the physical world’s local geometry and appearance. It does so by learning to translate a high-dimensional, egocentric image, $O_{\text{Ego},t} \in \mathbb{R}^{3 \times H_{\text{in}} \times W_{\text{in}}}$ at time t , into a structured, allocentric BEV map, $\hat{O}_{\text{BEV},t} \in \mathbb{R}^{4 \times H_{\text{out}} \times W_{\text{out}}}$. This is a fundamentally ill-posed inverse problem, and the network is trained end-to-end to minimize the prediction error between its generated map and the ground truth. This error is quantified by a composite loss function, \mathcal{L}_{BEV} , which holistically evaluates the quality of the prediction across multiple modalities. Each component of this loss can be interpreted as imposing a different physical prior on the generative model, guiding it towards physically plausible solutions:

$$\mathcal{L}_{\text{BEV}} = w_{\text{occ}} \mathcal{L}_{\text{occ}} + w_{\text{rgb}} \mathcal{L}_{\text{rgb}} + w_{\text{smooth}} \mathcal{L}_{\text{smooth}}, \quad (1)$$

where w_{occ} , w_{rgb} , and w_{smooth} are weighting hyper-parameters. The occupancy loss, \mathcal{L}_{occ} , is a binary cross-entropy term on the predicted alpha channel ($\hat{\alpha}$) that forces the network to accurately predict the binary state of the world (i.e., navigable or occupied). The appearance loss, \mathcal{L}_{rgb} , a masked mean-squared error term, compels the model to predict the correct target color within navigable regions. Finally, the smoothness loss, $\mathcal{L}_{\text{smooth}}$, regularizes the predictive model by penalizing sharp spatial gradients, incorporating a prior that physical environments are generally continuous. To solve this complex, cross-view prediction task, we employ a sophisticated Transformer-based encoder-decoder architecture. The detailed layer-by-layer specification of this architecture is provided in **Supplementary Tables S4** and **S5**, which leverages a Transformer’s self-attention mechanism to overcome perspective distortion inherent in ground-level views. The encoder, E_{BEV} , uses a ResNet-18 backbone to extract spatial features. A key architectural innovation lies in treating the image’s vertical scanlines as a sequence. This allows the Transformer’s self-attention mechanism to disambiguate visual features by considering the global context along the vertical axis of the image, which is crucial for the predictive model to accurately infer depth and overcome perspective distortion. The decoder, D_{BEV} , then projects the resulting latent code into the final BEV map. The mathematical formulation and weighting of each loss component are detailed in **Supplementary Method S1.2**, which define the precise objective for learning photometrically and geometrically plausible BEV maps.

Predictive path integration for self-localization. As shown on the left side of **Fig. 1b**, the module’s objective is to minimize the prediction error $\mathcal{L}_{\text{path}}$, a heavily regularized, weighted sum of the Kullback-Leibler (KL) divergence between the predicted and target cell activations related to the agent’s pose:

$$\mathcal{L}_{\text{path}} = \mathcal{L}_{\text{KL}} + w_{\text{init}} \mathcal{L}_{\text{init}} + w_{\text{cont}} \mathcal{L}_{\text{cont}}. \quad (2)$$

The design of this loss function is critical for maintaining a stable predictive process over long trajectories. The primary term, \mathcal{L}_{KL} , applies a significantly higher weight to the prediction error in the initial trajectory frames, forcing the model to establish an accurate pose estimate early to prevent error accumulation. This is supplemented by an initial consistency term, $\mathcal{L}_{\text{init}}$, and a continuity regularizer, $\mathcal{L}_{\text{cont}}$. This structured learning pressure compels the LSTM’s hidden units to discover the most efficient neural code for representing Euclidean space under translational motion. Remarkably, the optimal representation that emerges spontaneously to best solve this temporal self-prediction task is a grid-cell-like code, exhibiting the hexagonal symmetry found in the mammalian entorhinal cortex. This provides strong evidence that such complex, biologically-plausible neural structures can arise not from explicit design, but as a fundamental and convergent solution to the problem of continuous self-prediction in a spatial environment. This emergent metric scaffold provides the essential, stable foundation upon which the local visual predictions can be reliably integrated, forming a coherent and robust individual spatial memory. Theoretically, this learning process allows the LSTM to function as an amortized Bayesian filter, effectively performing probabilistic state estimation, as detailed in **Supplementary Method S1.1**. The architecture and training details are listed in **Supplementary Tables S1** and **S2**.

Theoretical justification for predictive path integration. Here we provide a theoretical justification for how the self-prediction objective compels neural networks to spontaneously develop structured, grid-like spatial representations. The key insight is that the geometry of path integration—specifically, the requirement to maintain a consistent spatial metric under continuous

motion—fundamentally constrains the form of efficient neural codes. We demonstrate that hexagonal grid patterns emerge not from architectural engineering, but as the unique solution to satisfying geometric consistency under representational efficiency constraints.

Probabilistic formulation. We formalize path integration as a problem of sequential state inference. The agent’s pose at time t is characterized by the state vector $s_t = (\mathbf{r}_t, \theta_t) \in \mathbb{R}^2 \times \mathbb{S}^1$, where $\mathbf{r}_t = (r_{x,t}, r_{y,t})^\top$ denotes the position and θ_t denotes the heading angle. The agent’s kinematics follow the dynamics:

$$\begin{aligned}\theta_{t+1} &= \theta_t + \omega_t \Delta t \pmod{2\pi}, \\ \mathbf{r}_{t+1} &= \mathbf{r}_t + R(\theta_t) \mathbf{v}_t \Delta t,\end{aligned}$$

where $u_t = (\mathbf{v}_t, \omega_t)$ is the control input comprising egocentric translational and angular velocities, and $R(\theta_t)$ is the rotation matrix (**Supplementary Definition 2**) that transforms egocentric motor commands to allocentric position updates.

The path integrator network receives no direct supervision on the latent pose s_t during trajectory execution. Instead, its sole learning signal derives from predicting the activity of virtual place and head-direction cells (artificial network units that encode spatial position and heading orientation, respectively, using biologically-inspired activation patterns; see **Supplementary Method S1.1** for detailed definitions) at the final timestep. These spatial cells exhibit tuning curves with log-potentials $\phi_\ell(s)$: place cells use Gaussian receptive fields $\phi_i(\mathbf{r}) = -\|\mathbf{r} - \mu_i\|^2/(2\sigma_i^2)$ while head-direction cells employ von Mises tuning $\phi_j(\theta) = \kappa_j \cos(\theta - \mu_j)$. The probability of observing cell ℓ active in pose s_t follows a softmax distribution over these potentials:

$$p(y_t = \ell \mid s_t) = \frac{\exp\{\phi_\ell(s_t)\}}{\sum_{m=1}^C \exp\{\phi_m(s_t)\}},$$

where C denotes the total number of cells and y_t is the random variable for the active cell identity. The LSTM path integrator is trained to map a sequence of control inputs $\{u_t\}_{t=1}^T$ and an initial observation y_0 to a predictive distribution $\hat{p}(\cdot \mid y_0, \{u_t\})$ over cell activations at the final time T . The training objective minimizes the expected Kullback–Leibler (KL) divergence between the true activation distribution and the network’s prediction:

$$\mathcal{L}(\Theta) = \mathbb{E}_{y_0, \{u_t\}} [\text{KL}(p(\cdot \mid s_T) \parallel \hat{p}(\cdot \mid y_0, \{u_t\}))], \quad (3)$$

where y_0 denotes the initial spatial cell observation encoding starting pose s_0 , u_t represents the sequence of motor commands, s_T is the true final pose after path integration, $p(\cdot \mid s_T)$ is the target sensory distribution at the final pose, $\hat{p}(\cdot \mid y_0, u_t)$ is the LSTM’s predicted distribution, and Θ denotes the network parameters. Minimizing this prediction error over diverse trajectories compels the network to internalize the geometric structure of spatial navigation.

Architectural design for temporal integration. The recurrent structure of an LSTM is particularly well-suited for path integration because its gated cell state mechanism enables stable accumulation of incremental motion signals over extended time horizons. The LSTM’s cell state \mathbf{c}_t serves as a continuous memory substrate that is updated at each timestep by integrating velocity inputs through its gating architecture:

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t,$$

where \mathbf{f}_t and \mathbf{i}_t are the forget and input gates, and $\tilde{\mathbf{c}}_t$ is the candidate update. Critically, we impose a representational bottleneck by projecting the LSTM hidden state through a low-dimensional layer before prediction (**Supplementary Table S1**). This architectural choice is essential: the bottleneck forces the network to discover a compressed, information-efficient encoding of pose that can support accurate long-term prediction. It is this efficiency pressure, combined with the predictive objective, that catalyzes the emergence of structured spatial codes.

Emergence of hexagonal representations from geometric constraints. Finally, we justify why hexagonal activity patterns spontaneously emerge as the optimal solution. The path integration task fundamentally requires representing accumulated two-dimensional displacements in a compressed latent space with limited dimensionality. As established in Supplementary Information through **Supplementary Proposition 1** and **Theorem 1**, any representation that faithfully performs path integration must satisfy translation equivariance: a physical displacement $\Delta \mathbf{r}$ must correspond to a consistent linear transformation in the latent space, independent of starting location. This geometric constraint, combined with the information efficiency requirement under the bottleneck architecture, necessitates a periodic encoding. **Supplementary Theorem 2** proves that the minimal isotropic representation in two dimensions requires exactly three frequency directions uniformly distributed at 120° angular separation, uniquely determined by first-order isotropy (zero mean) and second-order isotropy (identity-proportional metric). As demonstrated in **Supplementary Corollary 3**, these three directions generate effective six-fold symmetry due to cosine function parity: their superposition creates an interference pattern whose peak activations form a hexagonal lattice with 60° rotational symmetry. Consequently, minimizing prediction error under equivariance and efficiency constraints causes LSTM hidden units to self-organize into grid-cell-like hexagonal patterns, providing the consistent spatial metric needed for path integration and forming the computational foundation for downstream prediction and planning.

Level 2: Social predictive coding for emergent communication

Having established a robust individual predictive model, the next challenge is to synchronize these models across agents. Central to this is a neural substrate designed to form a unified representation of the multi-agent system, which serves as the foundation for communication. We employ a dual-stream LSTM network that concurrently processes egocentric motion inputs (linear and angular velocities) from both the self-agent and its partner. The network is trained under a multi-faceted predictive objective: it must simultaneously predict its own future location, its partner’s future location, and, critically, the future Euclidean distance between them via a dedicated relational regression head. This compound predictive pressure compels the network’s shared latent representation to functionally specialize. This process gives rise to distinct neural populations, including units selectively tuned to the partner’s location—an artificial analogue of social place cells (SPCs; distinct from the self-position-encoding place cells described above, these units specifically encode partner locations within the observer’s reference frame), as detailed in our results (Fig. 4). This emergent social representation provides the rich, unified state, $S_{i,t}$, that informs the communication protocol. Furthermore, the explicit distance prediction serves as a critical gating mechanism for determining **who and when** communication is feasible, as detailed in **Supplementary Method S1.4.1** (Social place cell module architecture in Table S11).

This architecture sets the stage for extending the predictive coding principle to the multi-agent domain, where we reformulate communication not as mere data transfer, but as a mechanism for collaborative prediction. The question shifts from “What information should I send?” to “What piece of my knowledge will maximally reduce my partner’s future uncertainty?” This is the essence of social predictive coding: agents learn to transmit only information that is novel and decision-relevant from the receiver’s perspective. To formalize this, we employ the information bottleneck (IB) principle. The goal is to learn a stochastic encoder, $p(m_{i,t} | S_{i,t})$, that maps the sender agent i ’s state $S_{i,t}$ to a compressed message $m_{i,t}$. The optimal encoding must balance two competing objectives: maximizing the message’s predictive utility for the receiver while minimizing communication cost. Following the rate-distortion framework, we formulate this as minimizing a loss function that trades off distortion (predictive loss) against rate (compression cost):

$$\mathcal{L}_{\text{IB}} = \underbrace{-I(m_{i,t}; O_{j,t+1} | S_{j,t})}_{\text{Distortion}} + \beta \underbrace{I(S_{i,t}; m_{i,t})}_{\text{Rate}}, \quad (4)$$

where $I(\cdot; \cdot)$ denotes mutual information, which is a measure of the mutual dependence between the two variables. $O_{j,t+1}$ is the future observation of the receiving agent j , $S_{j,t}$ is the receiver’s current state (serving as side information), and $\beta > 0$ is a hyper-parameter balancing the trade-off. The **Distortion** term quantifies the negative of the information the message provides about the receiver’s future conditioned on what the receiver already knows—minimizing distortion thus maximizes predictive utility. The **Rate** term quantifies the information the message retains about the sender’s state—minimizing rate enforces compression. The parameter β controls this trade-off: larger β prioritizes compression, while smaller β prioritizes predictive accuracy.

Directly optimizing Eq. (4) is intractable because computing mutual information requires integrating over high-dimensional and unknown data distributions. We therefore derive a tractable surrogate objective by constructing variational bounds for both the rate and distortion terms. We introduce a parametric encoder $q_\varphi(z | S_{i,t})$ that maps the sender’s state to a latent variable z (representing the message $m = g(z)$, where $g(\cdot)$ is message decoder), and a parametric decoder $p_\vartheta(O_{j,t+1} | z, S_{j,t})$ that predicts the receiver’s future observation.

First, we derive a tractable upper bound for the communication rate, $I(S_{i,t}; m_{i,t})$. By introducing a fixed prior distribution $p(z)$ over the latent message space, the rate can be bounded by the Kullback-Leibler (KL) divergence between the approximate posterior and the prior:

$$I(S_{i,t}; m_{i,t}) \leq \mathbb{E}_{p(S_{i,t})} \left[D_{\text{KL}}(q_\varphi(z | S_{i,t}) \| p(z)) \right]. \quad (5)$$

Minimizing this KL divergence thus serves to minimize an upper bound on the true communication rate, effectively enforcing compression.

Second, we derive a tractable upper bound for the distortion term, $-I(m_{i,t}; O_{j,t+1} | S_{j,t})$. Using the entropy decomposition, the conditional mutual information can be written as $I(m_{i,t}; O_{j,t+1} | S_{j,t}) = H(O_{j,t+1} | S_{j,t}) - H(O_{j,t+1} | m_{i,t}, S_{j,t})$. Since the baseline entropy $H(O_{j,t+1} | S_{j,t})$ is independent of model parameters, minimizing distortion $-I(m_{i,t}; O_{j,t+1} | S_{j,t})$ is equivalent to minimizing the conditional entropy $H(O_{j,t+1} | m_{i,t}, S_{j,t})$. We upper-bound this entropy using a parametric decoder $p_\vartheta(O_{j,t+1} | z, S_{j,t})$, yielding:

$$-I(m_{i,t}; O_{j,t+1} | S_{j,t}) \leq -H(O_{j,t+1} | S_{j,t}) + \mathbb{E}_{p(S_{i,t}, S_{j,t}, O_{j,t+1})} \left[\mathbb{E}_{q_\varphi(z | S_{i,t})} \left[-\log p_\vartheta(O_{j,t+1} | z, S_{j,t}) \right] \right]. \quad (6)$$

Since $H(O_{j,t+1} | S_{j,t})$ is constant, minimizing this bound is equivalent to minimizing the expected negative log-likelihood (reconstruction error). Combining these bounds yields the variational information bottleneck (VIB) objective, which is a

tractable surrogate for the intractable IB loss. By substituting the upper bound for rate and the upper bound for distortion (omitting the constant $H(O_{j,t+1} | S_{j,t})$), we obtain:

$$\mathcal{L}_{\text{VIB}}(\varphi, \vartheta) = \underbrace{\mathbb{E}_{p(S_{i,t}, S_{j,t}, O_{j,t+1})} \left[\mathbb{E}_{q_\varphi(z|S_{i,t})} \left[-\log p_\vartheta(O_{j,t+1} | z, S_{j,t}) \right] \right]}_{\text{Distortion (Reconstruction Loss)}} + \beta \underbrace{\mathbb{E}_{p(S_{i,t})} \left[D_{\text{KL}}(q_\varphi(z | S_{i,t}) \| p(z)) \right]}_{\text{Rate (KL Regularizer)}} \quad (7)$$

where expectations are taken over the joint data distribution. The first term minimizes the reconstruction error, maximizing the message's predictive utility. The second term minimizes the KL divergence from the prior, enforcing compression. We operationalize this using a convolutional variational autoencoder (VAE) architecture, where the entire system is trained end-to-end to minimize \mathcal{L}_{VIB} . The encoder implements a hierarchical downsampling structure that maps a 64×64 spatial memory map to a compressed latent message z , while the decoder symmetrically reconstructs the partner's predicted occupancy map from this compressed representation (detailed architecture specifications in **Supplementary Tables S8** and **S9**).

Each term in this loss directly implements a component of the social predictive coding framework. The first term (reconstruction loss) corresponds to distortion, minimizing prediction error and thereby maximizing the message's utility for the receiver. The second term (KL divergence) corresponds to rate, enforcing compression and driving the emergence of efficient symbolic protocols. The hyperparameter β enables systematic exploration of the rate-distortion trade-off, revealing how bandwidth constraints shape emergent communication structure (training configuration in **Supplementary Table S10**). The full derivation of the variational bounds is provided in **Supplementary Method S1.6**.

Level 3: Predictive uncertainty as a guide for strategic exploration

The predictive coding framework culminates at the level of strategic decision-making. Having established models to predict its environment (Level 1) and its partners' states (Level 2), the agent must now decide how to act in order to improve these predictive models over time. This transforms the agent from a passive observer into an active learner, a concept known as active inference. The optimal exploration strategy, from a predictive coding perspective, is to seek out experiences that maximally reduce the uncertainty of the agent's internal generative model. In a large, partially-observable environment, this requires a principled approach to balance exploration and exploitation, a challenge we address with a hierarchical reinforcement learning (HRL) framework explicitly guided by predictive uncertainty.

This framework decomposes the complex navigation problem into two levels. The low-level controller is a deterministic planner (A* search) that executes concrete navigational sub-goals based on the agent's current understanding of the shared world map. This offloads the complexities of pathfinding, allowing the high-level policy (meta-controller) to focus exclusively on the strategic question: “*Where should I go next to learn the most?*” The meta-controller is implemented as an actor-critic network and trained using multi-agent proximal policy optimization (MAPPO), a robust algorithm for cooperative settings. To fulfil this, each agent first partitions its occupancy grid into a 4×4 regional summary, generating a 48-dimensional feature vector that includes the exploration ratio, walkability, and agent occupancy for each region. These features are fed into a shared actor-critic network with two fully connected layers (256 units, ReLU activation) to extract a common embedding. This embedding then branches into an actor head, which outputs a masked categorical distribution over the 16 regions for goal selection, and a critic head, which predicts scalar state values (**Supplementary Table S12**). The crucial insight is that the reward signal driving this high-level policy is not based on sparse, external rewards (like finding the target), but is instead generated intrinsically from the agent's own state of uncertainty.

This is realized through an enhanced intrinsic curiosity module (ICM), which functions as the direct implementation of the active inference principle. Rather than relying on a learned forward dynamics model, our ICM directly estimates epistemic uncertainty by analyzing the geometry of the known-unknown boundary in the agent's local map, augmented with social spatial information from the SPC module (Level 2). The composite intrinsic reward signal, r_t^{int} , is a weighted sum of three components, each reflecting a different facet of uncertainty reduction:

$$r_t^{\text{int}} = w_{\text{curiosity}} r_{\text{curiosity}} + w_{\text{coord}} r_{\text{coord}} + w_{\text{explore}} r_{\text{explore}}. \quad (8)$$

Specifically, these components are implemented as follows: (1) The curiosity reward, $r_{\text{curiosity}}$, is a frontier-based score that directly rewards the selection of high-level goals in regions bordering unknown territory, where the shared predictive map is most uncertain. (2) The coordination reward, r_{coord} , promotes spatial division of labor by leveraging the inter-agent distance estimates $\hat{d}_{ij,t}$ provided by the SPC module. This component discourages redundant exploration by rewarding goal selections that maintain appropriate separation from teammates, directly operationalizing the principle that distributed exploration maximizes information gain. Critically, this establishes a computational dependency: the SPC module's learned distance-tuned neurons (**Fig. 4c**) provide the essential geometric information that enables the ICM to generate coordination signals. (3) The exploration reward, r_{explore} , grants credit for discovering map cells that are unknown to the entire team, targeting states that

are, by definition, maximally unpredictable. More details about ICM reward formulations and communication protocols are provided in **Supplementary Method S1.4**.

By training the MAPPO policy to maximize this rich, uncertainty-driven intrinsic reward, the HRL-ICM framework learns a sophisticated, coordinated exploration strategy from first principles. It does not rely on hand-crafted heuristics for exploration but instead learns to perform a form of Bayesian experimental design, constantly choosing actions to gather the most informative data. The entire system is trained end-to-end with the SPC module providing continuous geometric awareness of partner states, the ICM translating this into strategic exploration incentives, and the meta-controller selecting goals based on these incentives (hyperparameters and training configuration in **Supplementary Table S13**). Thus, from the lowest level of perception to the highest level of strategic planning, the entire architecture is unified under the overarching goal of building and refining a predictive model of the world by actively seeking out and resolving uncertainty.

Data Availability

The datasets used in this study are based on procedurally generated environments within the Memory-Maze benchmark, which has been made publicly available at <https://github.com/jurgisp/memory-maze>. All environment configurations, agent spawn locations, and goal placements used in our experiments are provided in the supplementary repository. Additional raw data (e.g., agent trajectories, BEV reconstructions, and communication transcripts) are available from the corresponding author upon reasonable request.

Code Availability

The full source code for the predictive coding framework, including training scripts, network architectures, and experiment configurations, will be released at <https://github.com/fangzr/SSM-PC> upon publication. To facilitate reproducibility, the repository also includes pretrained models, instructions for reproducing the Memory-Maze benchmark results, and detailed documentation. A permanent versioned archive will be deposited in Zenodo prior to final acceptance.

Author Contributions

Z.F., Y.G. and J.W. conceived the predictive coding framework. Z.F., Y.G. Y.Z. and H.A. performed all experiments and data analysis. Y.G and H.A. contributed to the conception of the HRL-ICM framework and data collection. J.W. and Y.F. supervised the entire project. Y.W., and Y.F. wrote and reviewed the manuscript. All authors discussed the results and provided critical feedback on the manuscript. J.W. and Y.F. provided funding.

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Supplementary Information

Shared Spatial Memory Through Predictive Coding

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S1 Supplementary Methods

S1.1 Grid cell network: Biological-inspired spatial representation

A fundamental cognitive capability for navigation is the ability to maintain a dynamic estimate of self-location and orientation from idiothetic cues—a process known as path integration. In mammals, this function is robustly implemented by the hippocampal-entorhinal system, which provides a canonical example of a stable internal metric for space. Inspired by this biological solution [2], we developed a computational model (termed grid cell network) designed to test the hypothesis that the characteristic neural codes for space, such as grid cells, can emerge from a general predictive learning objective, without being explicitly engineered into the system’s architecture. Grid cell network, a recurrent neural network, is tasked not only with path integration, but also with a more fundamental objective: to predict its own future sensory state given a sequence of self-motion cues. We demonstrate that to solve this continuous self-prediction problem efficiently [3], the network is compelled to develop a highly structured internal representational scheme. This scheme, we show, is a convergent solution that recapitulates key properties of biological spatial representations, most notably the spontaneous formation of hexagonally symmetric grid-like firing patterns.

S1.1.1 Network architecture

The core of our grid cell network is a recurrent neural network (RNN) formulated as a predictive state-space model. Its objective is to learn the transition dynamics of an agent’s pose by continuously predicting its future location and orientation. The sequential and cumulative nature of path integration presents a significant challenge involving long-term temporal dependencies and the integration of noisy velocity signals. To address this, we selected a long short-term memory (LSTM) network as the central recurrent component [6]. The LSTM’s gating mechanisms are exceptionally well-suited to learning to retain or discard information over extended time horizons, providing a robust substrate for integrating velocity commands while mitigating the vanishing gradient problems that would plague a simpler RNN architecture in this task. The network’s full architecture is specified in **Fig. S1** and **Table S1**.

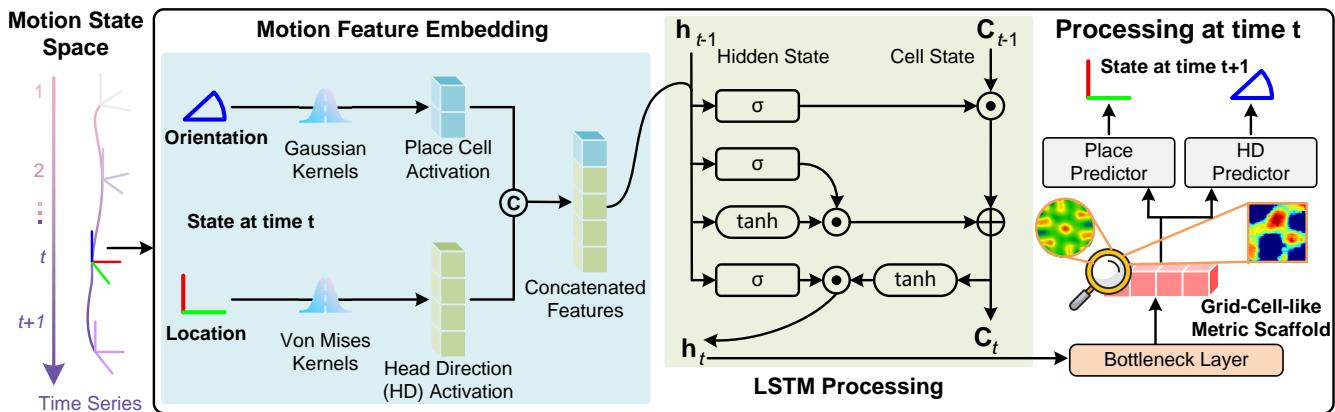


Figure S1. Architecture of grid cell network.

The computational flow is designed to test a key principle of biological navigation: the anchoring of a dynamic, self-motion-based estimate of position to stable, absolute sensory cues. The process begins by with encoding the agent’s initial pose (s_0) into a high-dimensional, distributed representation using ensembles of virtual place and head direction (HD) cells [3]. This initial representation, grounded in an absolute reference frame, is projected through learnable linear layers to initialize the LSTM’s hidden state (h_0) and cell state (c_0). This initialization strategy is not a mere technical convenience; it is a critical design choice that simulates the neural mechanism of “remapping” or “resetting” observed when an animal enters a new environment. By grounding the integrator’s initial state in a veridical sensory observation, we prevent the unbounded accumulation of drift that is the primary failure mode of pure idiothetic integration.

From this anchored starting point, the LSTM iteratively updates its internal state by processing the sequence of velocity inputs. At each timestep, the LSTM’s hidden state—its internal representation of the agent’s current pose—is passed through a linear bottleneck layer before prediction. This bottleneck is a central element of our experimental design. By constraining the dimensionality of the representation passed to the predictors, we impose a powerful efficiency constraint on the network. This forces the network to discover a compressed, abstract, and maximally informative latent code for pose. The central scientific question this architecture addresses is: What is the geometry of this emergent representation? Is it an unstructured code, or does it converge to a structured, periodic representation, such as the hexagonal lattice of grid cells, which is hypothesized to be an information-theoretically optimal code for 2D space? Finally, two linear predictor heads decode this latent representation back

Table S1. Details of grid cell network. B and Seq mean the batch size and sequence length, respectively.

Component	Input Size	Output Size	Parameters
Velocity Processing			
Velocity Input	$B \times Seq \times 3$	$B \times Seq \times 3$	-
Initial State Computation			
Place Cell Activation	$B \times 2$	$B \times 256$	Gaussian Kernels
Head Direction Activation	$B \times 1$	$B \times 32$	Von Mises Kernels
Concatenated Features	$B \times 288$	$B \times 288$	-
LSTM Processing			
Initial Hidden State (h_0)	$B \times 288$	$1 \times B \times 128$	Linear(288, 128)
Initial Cell State (c_0)	$B \times 288$	$1 \times B \times 128$	Linear(288, 128)
LSTM Layer	$B \times Seq \times 3$	$B \times Seq \times 128$	1 layer, 128 units
Bottleneck and Prediction			
Bottleneck Layer	$B \times Seq \times 128$	$B \times Seq \times 256$	Linear + Dropout(0.5)
Place Predictor	$B \times Seq \times 256$	$B \times Seq \times 256$	Linear(256, 256)
HD Predictor	$B \times Seq \times 256$	$B \times Seq \times 32$	Linear(256, 32)

into the “sensory” space of place and head direction cell activations. The entire network is trained end-to-end by minimizing the discrepancy between these predictions and the ground-truth sensory states, thereby closing the predictive loop and forcing the internal dynamics of the model to learn the dynamics of the external world.

S1.1.2 Place and head direction cell ensembles as a sensory ground truth

To provide the network with a stable, biologically-plausible sensory ground truth for its predictive task, we constructed virtual ensembles of place cells and head direction cells. These cell types are not merely convenient choices; they are well-established models for neural representations of location and orientation, respectively. Their tuning profiles provide a smooth, distributed, and overcomplete basis for representing the agent’s state, a feature that confers robustness to noise and local errors.

Place cell ensemble. Location is encoded by an ensemble of place cells with Gaussian receptive fields distributed uniformly across the environment. This creates a population code where each location elicits a unique pattern of activation. The activation of each cell i is a normalized Gaussian function of the agent’s position \mathbf{x} :

$$a_i(\mathbf{x}) = \frac{\exp\left(-\frac{\|\mathbf{x} - \mu_i\|^2}{2\sigma_i^2}\right)}{\sum_{j=1}^N \exp\left(-\frac{\|\mathbf{x} - \mu_j\|^2}{2\sigma_j^2}\right)}, \quad (S1)$$

where μ_i is the preferred location of cell i . This normalization ensures the population vector of activations forms a probabilistic distribution over the state space.

Head direction cell ensemble. Orientation is encoded by an ensemble of head direction cells whose firing is tuned to the agent’s heading angle. We model these using von Mises distributions, the circular analogue of the Gaussian distribution, which accurately captures the tuning curves of biological head direction cells. The activation of each cell j is given by:

$$b_j(\theta) = \frac{\exp(\kappa_j \cos(\theta - \phi_j))}{\sum_{k=1}^M \exp(\kappa_k \cos(\theta - \phi_k))}, \quad (S2)$$

where θ is the heading angle, ϕ_j is the cell’s preferred direction, and κ_j controls the tuning width, allowing for a diversity of specificities within the population.

S1.1.3 Objective function for predictive spatial learning

To drive the emergence of structured representations, we design a specialized, multi-component loss function that guides the learning process. This objective function is not arbitrary but is carefully structured to enforce key constraints on the predictive

task, which can be defined as:

$$\mathcal{L}_{\text{total}} = \sum_{t=0}^{T-1} w_t \left(\mathcal{L}_{\text{place}}^{(t)} + \mathcal{L}_{\text{HD}}^{(t)} \right) + w_{\text{init}} \mathcal{L}_{\text{init}} + w_{\text{cont}} \mathcal{L}_{\text{cont}}. \quad (\text{S3})$$

Probabilistic loss and temporal weighting. We frame the prediction task in probabilistic terms by using the Kullback-Leibler (KL) divergence between the network’s predicted distribution of cell activations and the ground-truth distribution. This treats learning as a process of minimizing the informational “surprise” between the model’s belief and reality, a more principled approach than simple regression for dealing with distributed neural codes.

$$\mathcal{L}_{\text{place}}^{(t)} = \text{KL} \left(\text{softmax}(\hat{\mathbf{p}}_t) \parallel \mathbf{p}_t^{\text{target}} \right), \quad (\text{S4})$$

$$\mathcal{L}_{\text{HD}}^{(t)} = \text{KL} \left(\text{softmax}(\hat{\mathbf{h}}_t) \parallel \mathbf{h}_t^{\text{target}} \right). \quad (\text{S5})$$

Furthermore, path integration errors are cumulative; small initial errors can propagate and corrupt the entire trajectory estimate. To counteract this, we implement a temporally-weighted loss scheme. The weights w_t place a strong emphasis on accuracy in the initial phase of a trajectory, effectively creating a curriculum that forces the network to first master the fundamental single-step dynamics.

$$w_t = \begin{cases} 2 \cdot w_{\text{init}} & \text{if } t = 0 \\ w_{\text{init}} \cdot \rho^{t-1} & \text{if } 1 \leq t < 5 \quad \text{with } w_{\text{init}} = 5.0, \rho = 0.8. \\ 1.0 & \text{if } t \geq 5 \end{cases} \quad (\text{S6})$$

Regularization for spatial and temporal coherence. Two additional regularization terms enforce plausible constraints on the spatial representation. The initial consistency loss, $\mathcal{L}_{\text{init}}$, explicitly penalizes any mismatch between the network’s initial prediction and the initial sensory ground truth. This reinforces the “anchoring” mechanism described previously.

$$\mathcal{L}_{\text{init}} = 2.0 \cdot \text{KL} \left(\text{softmax}(\hat{\mathbf{p}}_0) \parallel \mathbf{p}_0^{\text{target}} \right). \quad (\text{S7})$$

The continuity loss, $\mathcal{L}_{\text{cont}}$, encourages smoothness in the network’s predictions over consecutive timesteps. This is a biologically plausible prior, as an agent’s belief about its location should not change drastically. This term regularizes the learned dynamics, preventing jittery state estimates and promoting the learning of a continuous manifold representation.

$$\mathcal{L}_{\text{cont}} = \frac{1}{5} \sum_{t=1}^5 (1 - 0.15(t-1)) \cdot \text{KL} \left(\text{softmax}(\hat{\mathbf{p}}_t) \parallel \text{softmax}(\hat{\mathbf{p}}_{t-1}) \right). \quad (\text{S8})$$

More details about grid cell network training are listed in [Table S2](#).

S1.1.4 Quantitative analysis of emergent spatial representations

To objectively determine whether the network’s learned representations exhibit the characteristic firing patterns of grid cells, we employ a standardized quantitative analysis pipeline adapted directly from the field of neurophysiology. This procedure allows us to rigorously identify the presence of hexagonal periodicity in the activity of individual units within the network’s bottleneck layer, providing the crucial empirical link between our computational model and the biological phenomenon it seeks to explain.

Rate map. For any given unit, we first compute an occupancy-normalised firing rate map, which represents its average activation as a function of the agent’s 2D position. For a unit with activation sequence $\{a_t\}_{t=1}^T$ along a trajectory $\{(x_t, y_t)\}_{t=1}^T$, the arena is discretised into bins (i, j) . The rate map $R(i, j)$ is calculated by dividing the total activation within a bin, $\mathcal{S}(i, j)$, by the time spent in that bin, $\mathcal{O}(i, j)$:

$$R(i, j) = \begin{cases} \mathcal{S}(i, j) / \mathcal{O}(i, j), & \mathcal{O}(i, j) > 0, \\ \text{NaN}, & \text{otherwise.} \end{cases} \quad (\text{S9})$$

This map is typically smoothed with a Gaussian kernel to mitigate sampling noise. Let the mask of visited bins be $\mathcal{V} = \{(i, j) : \mathcal{O}(i, j) > 0\}$.

Table S2. Training configuration of grid cell network.

Parameter Category	Parameter	Value
Loss Weights	Initial Frame Weight (w_{init})	5.0
	Decay Factor (ρ)	0.8
	Initial Consistency Weight (w_{init})	2.0
	Continuity Weight (w_{cont})	0.1
	Sequence Length	100 time steps
	Temporal Focus Window	First 5 time steps
Network Parameters	LSTM Hidden Size	128
	Bottleneck Size	256
	Dropout Rate	0.5
	Input Velocity Dimension	3 (2D + angular)
Training Setup	Batch Size	64
	Learning Rate	1×10^{-3}
	Environment Size	15×15 m

Spatial autocorrelogram (SAC). To reveal periodic structure in the rate map, we compute its 2D spatial autocorrelation. The autocorrelogram, $\text{SAC}(\mathbf{d})$, measures the Pearson correlation between the rate map R and a spatially shifted version of itself for every possible offset $\mathbf{d} = (d_x, d_y)$.

$$\text{SAC}(\mathbf{d}) = \frac{\sum_{(i,j) \in \mathcal{V}_d} (R(i,j) - \mu_d) (R(i+d_x, j+d_y) - \mu_{d'})}{\sqrt{\sum_{(i,j) \in \mathcal{V}_d} (R(i,j) - \mu_d)^2} \sqrt{\sum_{(i,j) \in \mathcal{V}_d} (R(i+d_x, j+d_y) - \mu_{d'})^2}}, \quad (\text{S10})$$

where \mathcal{V}_d is the set of overlapping valid bins for a given shift, and $\mu, \mu', \sigma, \sigma'$ are the respective sample means and standard deviations. A hexagonally periodic firing pattern manifests as a central peak at $\mathbf{d} = \mathbf{0}$ surrounded by a ring of six additional peaks, forming a hexagonal lattice in the correlogram.

Gridness score calculation. To quantify the degree of hexagonal symmetry, we compute a “gridness score”. This involves isolating the ring of peaks in the SAC surrounding the central peak using an annular mask, $\mathcal{A}(r_{\min}, r_{\max})$. We then measure the rotational symmetry of the pattern within this annulus by calculating the Pearson correlation, C_θ , between the annulus and a version of itself rotated by an angle θ .

$$C_\theta(r_{\min}, r_{\max}) = \frac{\sum_{\mathbf{d} \in \mathcal{A}(r_{\min}, r_{\max})} (S(\mathbf{d}) - \bar{s}) (S_\theta(\mathbf{d}) - \bar{s})}{\sum_{\mathbf{d} \in \mathcal{A}(r_{\min}, r_{\max})} (S(\mathbf{d}) - \bar{s})^2}, \quad (\text{S11})$$

where S is the SAC image and \bar{s} its mean value over the annulus. $S_\theta(\mathbf{d}) = S(\mathbf{R}_\theta \mathbf{d})$, where the matrix \mathbf{R}_θ is a rotation matrix: $\mathbf{R}_\theta = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$. The final gridness score contrasts the correlations at angles consistent with a hexagonal lattice ($60^\circ, 120^\circ$) with those at inconsistent angles ($30^\circ, 90^\circ, 150^\circ$).

$$G_{60}(r_{\min}, r_{\max}) = \frac{C_{60} + C_{120}}{2} - \frac{C_{30} + C_{90} + C_{150}}{3}, \quad (\text{S12})$$

where C_θ omits (r_{\min}, r_{\max}) , defined by Eq. (S11). A high positive score indicates strong hexagonal symmetry. For robustness, this score is maximized over a range of possible annulus radii (r_{\min}, r_{\max}) for each unit. An analogous score, G_{90} , can be computed to test for four-fold (square) symmetry.

$$G_{90}(r_{\min}, r_{\max}) = C_{90} - \frac{1}{2} (C_{45} + C_{135}). \quad (\text{S13})$$

This rigorous, standardized methodology allows for a direct, quantitative comparison between the representations learned by our model and those observed in electrophysiological recordings.

Table S3. Details of ResNet-based target detection network.

Layer	Input Size	Output Size	Parameters	Activation
Spatial Feature Extractor				
Input Image	$3 \times 64 \times 64$	$3 \times 64 \times 64$	-	-
ResNet18 Conv1	$3 \times 64 \times 64$	$64 \times 32 \times 32$	$k = 7, s = 2, p = 3$	ReLU
BatchNorm + MaxPool	$64 \times 32 \times 32$	$64 \times 16 \times 16$	$k = 3, s = 2, p = 1$	-
ResNet18 Layer1	$64 \times 16 \times 16$	$64 \times 16 \times 16$	2 residual blocks	ReLU
ResNet18 Layer2	$64 \times 16 \times 16$	$128 \times 8 \times 8$	2 residual blocks	ReLU
ResNet18 Layer3	$128 \times 8 \times 8$	$256 \times 8 \times 8$	2 residual blocks	ReLU
Conv2d Compression	$256 \times 8 \times 8$	$128 \times 8 \times 8$	$k = 1$	ReLU
BatchNorm2d	$128 \times 8 \times 8$	$128 \times 8 \times 8$	-	-
Conv2d Refinement	$128 \times 8 \times 8$	$64 \times 8 \times 8$	$k = 3, p = 1$	ReLU
BatchNorm2d	$64 \times 8 \times 8$	$64 \times 8 \times 8$	-	-
Position Predictor ($N_{\text{obj}} = 6$)				
Shared Attention Conv	$64 \times 8 \times 8$	$32 \times 8 \times 8$	$k = 1$	ReLU
BatchNorm2d	$32 \times 8 \times 8$	$32 \times 8 \times 8$	-	-
Attention Logits	$32 \times 8 \times 8$	$6 \times 8 \times 8$	$k = 1$	-
Spatial Softmax	$6 \times 8 \times 8$	$6 \times 8 \times 8$	Per-object norm	-
Weighted Pooling	$(64 \times 8 \times 8) \times 6$	6×64	Attention-weighted	-
Concat w/ Orientation	6×64	6×66	Angle: $[\cos \theta, \sin \theta]$	-
Position MLP-1	6×66	6×64	Linear + LayerNorm	ReLU
Dropout	6×64	6×64	$p = 0.2$	-
Position Output	6×64	6×2	Linear(64, 2)	-
Visibility Predictor				
Global Avg Pool	$64 \times 8 \times 8$	64	Spatial reduction	-
Concat w/ Orientation	64	66	Angle: $[\cos \theta, \sin \theta]$	-
Visibility MLP-1	66	64	Linear + LayerNorm	ReLU
Dropout	64	64	$p = 0.2$	-
Visibility Output	64	6	Linear(64, 6)	Sigmoid
Output Composition				
Masked Positions	$(6 \times 2) \times (6 \times 1)$	6×2	Element-wise product	-

S1.2 Spatial memory generation module

The generation of a stable, allocentric spatial memory from a stream of egocentric visual inputs is a cornerstone of an agent’s individual world model. This process addresses a fundamentally ill-posed inverse problem: inferring a structured, top-down world representation from ambiguous, high-dimensional localized sensory data. Our architecture is designed as a hierarchical processing pipeline consisting of three primary stages: (1) object-centric feature extraction from the raw first-person view, (2) cross-view encoding of visual features into a latent representation, and (3) decoding into a structured bird’s-eye-view (BEV) spatial map [10, 11]. This pipeline leverages the complementary strengths of convolutional and transformer-based networks, and is trained end-to-end under a composite predictive objective that imposes a set of physical priors on the generative model, guiding it toward geometrically and photometrically plausible solutions. We describe each processing stage in detail below.

S1.2.1 Target localization network

Accurate detection and localization of task-relevant objects within the egocentric visual field is a prerequisite for effective spatial memory construction. This module addresses a fundamental challenge in embodied perception: extracting sparse, object-centric representations from dense, pixel-level observations under significant geometric ambiguity. The target localization network must simultaneously solve three interrelated inference problems—identifying which objects are visible, estimating their relative positions in the agent’s reference frame, and filtering out visual distractors—all from a single monocular image acquired from a dynamically moving viewpoint.

Our design is grounded in a biologically-inspired hierarchical processing principle observed in the ventral visual stream

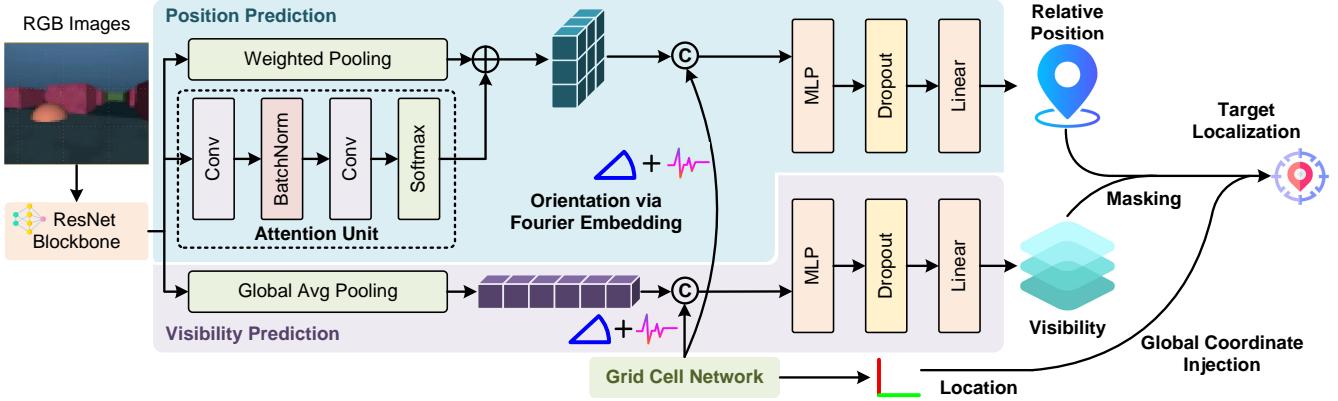


Figure S2. Architecture of target localization network.

of the primate brain, where object recognition emerges through a cascade of increasingly abstract feature representations. Early visual cortex extracts local edge orientations and textures, intermediate areas construct viewpoint-invariant part-based representations, and higher areas in the inferotemporal cortex achieve categorical object identity. Analogously, our architecture employs a convolutional backbone to progressively abstract the raw visual input into a hierarchy of increasingly semantic features, culminating in explicit position and visibility estimates for each potential target object. This hierarchical abstraction is critical for achieving robustness to variations in lighting, viewing angle, and partial occlusions that plague end-to-end direct regression approaches.

The network architecture, specified in **Fig. S2** and **Table S3**, is composed of three functionally distinct stages. The *Spatial Feature Extractor* leverages a truncated ResNet-18 backbone, retaining only the initial convolutional stem and the first three residual blocks (up to layer3). This design choice reflects a deliberate trade-off: deeper layers of ResNet are optimized for semantic categorization tasks, whereas our task requires preserving fine-grained spatial structure for accurate localization. The truncated backbone outputs a 256-channel feature map at 1/8 spatial resolution, which is subsequently refined by a compact spatial processing module consisting of two 1×1 and 3×3 convolutional layers that compress the representation to 64 channels while enhancing locality-sensitive features through grouped convolutions and batch normalization.

The *Position Predictor* implements a spatial attention mechanism to extract object-specific representations from the shared feature map. Rather than employing independent processing streams for each object—which would scale poorly and ignore inter-object spatial relationships—we utilize a shared convolutional attention generator that produces a multi-channel attention map, with each channel corresponding to one potential target. This design enforces a structural prior that object locations are spatially disentangled and can be decoded through weighted spatial pooling. For each object $k \in \{1, \dots, N_{\text{obj}}\}$, the attention map $\mathbf{A}_k \in \mathbb{R}^{H \times W}$ is normalized via spatial softmax, yielding a probability distribution over image locations. The attended feature vector $\mathbf{f}_k = \sum_{i,j} \mathbf{A}_k(i, j) \cdot \mathbf{F}(i, j)$ is then concatenated with a 2-dimensional encoding of the agent’s head orientation (represented as $[\cos \theta, \sin \theta]$) and passed through a compact MLP to produce the object’s relative position (x_k, y_k) in the agent’s local coordinate frame. The inclusion of orientation information is critical, as the same visual observation corresponds to different relative positions depending on the agent’s heading direction.

The *Visibility Predictor* operates on global context, aggregating the spatial feature map via spatial average pooling to produce a holistic scene descriptor. This global representation is fused with the orientation encoding and processed by a lightweight MLP with layer normalization and dropout (rate 0.2) to predict a per-object visibility score. The sigmoid activation enforces a probabilistic interpretation, allowing the network to express graded uncertainty about object presence. During inference, the predicted positions are masked by the visibility scores, effectively gating the position estimates to suppress hallucinated detections for occluded or out-of-view objects. This architectural separation of position estimation (which operates on spatially-localized features) and visibility prediction (which requires holistic scene understanding) reflects the computational principle of divide-and-conquer, enabling each sub-module to specialize on complementary aspects of the detection task.

The network is trained using a multi-task loss function that jointly optimizes position accuracy and visibility classification. For position estimation, we employ a masked mean squared error (MSE) loss that is computed only for ground-truth visible objects, preventing the network from being penalized for arbitrary predictions on occluded targets. For visibility prediction, we use binary cross-entropy (BCE) loss. The composite objective is formulated as:

$$\mathcal{L}_{\text{detector}} = \frac{1}{N_{\text{obj}}} \sum_{k=1}^{N_{\text{obj}}} \left[v_k^{\text{gt}} \cdot \|\mathbf{p}_k - \mathbf{p}_k^{\text{gt}}\|_2^2 + \lambda_{\text{vis}} \cdot \text{BCE}(\hat{v}_k, v_k^{\text{gt}}) \right], \quad (\text{S14})$$

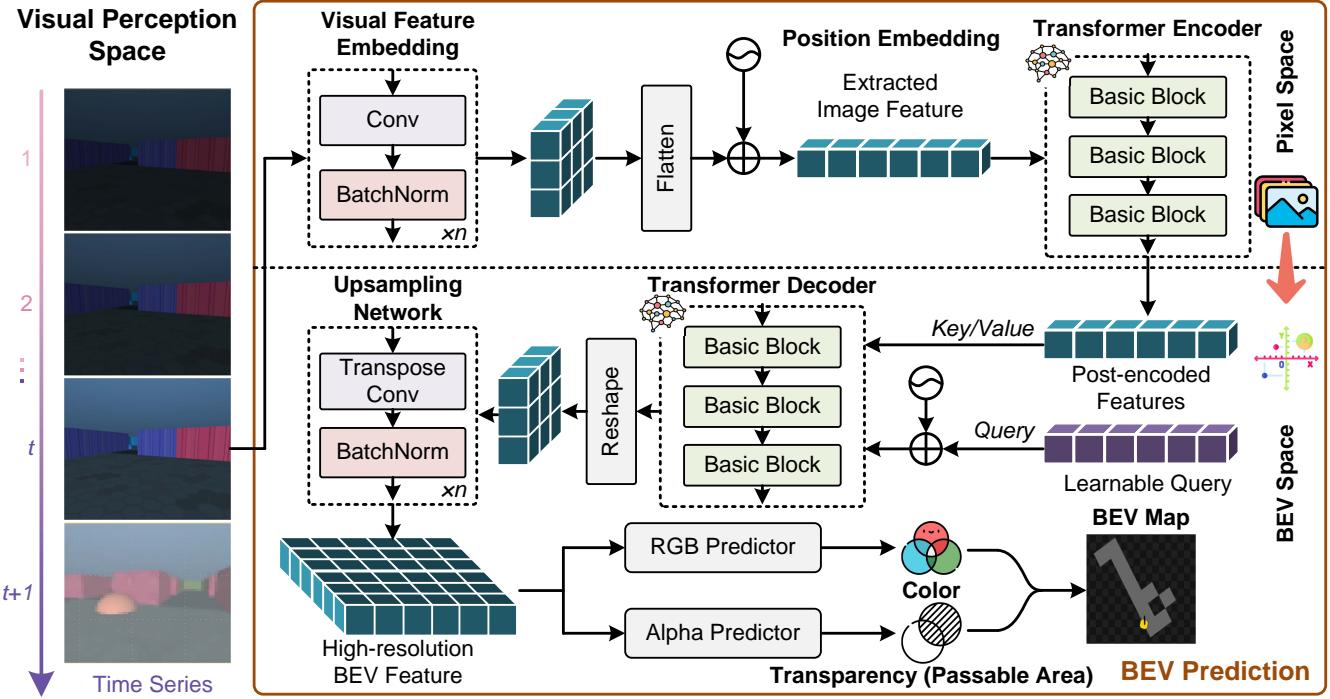


Figure S3. Architecture of BEV prediction network.

where $v_k^{\text{gt}} \in \{0, 1\}$ is the ground-truth visibility label, $\mathbf{p}_k \in \mathbb{R}^2$ is the predicted position, \mathbf{p}_k^{gt} is the ground-truth position, \hat{v}_k is the predicted visibility score, and $\lambda_{\text{vis}} = 1.0$ balances the two objectives. This formulation ensures that the position predictor receives meaningful gradients only for visible objects, while the visibility predictor learns a robust binary classifier across all object states. The use of a pre-trained ResNet-18 backbone (trained on ImageNet) provides strong initialization for low-level feature extraction, significantly accelerating convergence and improving sample efficiency in the target detection task. The entire module is trained with the Adam optimizer using a learning rate of 1×10^{-4} and weight decay of 1×10^{-5} for regularization.

S1.2.2 BEV prediction network

Encoder. The encoder’s primary function is to transform a raw, first-person-view image into a compact and contextually-rich latent representation suitable for cross-view translation. This transformation must overcome severe geometric distortions inherent in ground-level perspectives, where depth cues are ambiguous and distant objects appear compressed. To address this challenge, our encoder employs a two-stage processing pipeline that combines hierarchical convolutional feature extraction with global contextual reasoning via transformer-based attention.

The first stage employs a standard convolutional neural network (CNN) backbone to extract a hierarchy of spatial features from an input image. This initial processing stage, detailed in **Fig. S3** and **Table S4**, consists of four progressive downsampling blocks, each halving the spatial resolution while doubling the channel capacity. This pyramid structure effectively captures low-level visual world patterns such as edges, textures, and local shapes in early layers, while deeper layers encode increasingly abstract semantic features such as object boundaries and surface orientations. Each convolutional layer is followed by batch normalization to stabilize training dynamics and ReLU activation to introduce non-linearity.

The critical architectural innovation lies in the subsequent processing stage, where we treat the vertical scanlines of the resulting $256 \times 4 \times 4$ feature map as a sequence. This reformulation enables the application of a Transformer encoder, whose self-attention mechanism can integrate information across the entire vertical axis of the image. This global context is essential for accurately inferring depth relationships and disambiguating occluded regions—tasks at which purely convolutional architectures often struggle due to their limited receptive fields. The transformer processes 4 vertical scanlines, each represented as a sequence of 4 spatial tokens with 256-dimensional feature vectors. Sinusoidal positional encodings are added to preserve spatial ordering, and 3 transformer layers with 8 attention heads refine the representation by modeling long-range dependencies. This encoder design enables the network to effectively bridge the perspective gap between egocentric observation and allocentric representation.

Decoder. The decoder is tasked with projecting the abstract latent code generated by the encoder into a structured, allocentric bird’s-eye-view (BEV) map. This inverse mapping must reconstruct fine-grained spatial details from a heavily compressed

Table S4. Encoder architecture of BEV prediction. B means the batch size.

Layer	Input Size	Output Size	Parameters	Activation
Visual Feature Embedding				
Conv2d-1	$3 \times 64 \times 64$	$32 \times 32 \times 32$	$k = 3, s = 2, p = 1$	ReLU
BatchNorm2d-1	$32 \times 32 \times 32$	$32 \times 32 \times 32$	-	-
Conv2d-2	$32 \times 32 \times 32$	$64 \times 16 \times 16$	$k = 3, s = 2, p = 1$	ReLU
BatchNorm2d-2	$64 \times 16 \times 16$	$64 \times 16 \times 16$	-	-
Conv2d-3	$64 \times 16 \times 16$	$128 \times 8 \times 8$	$k = 3, s = 2, p = 1$	ReLU
BatchNorm2d-3	$128 \times 8 \times 8$	$128 \times 8 \times 8$	-	-
Conv2d-4	$128 \times 8 \times 8$	$256 \times 4 \times 4$	$k = 3, s = 2, p = 1$	ReLU
BatchNorm2d-4	$256 \times 4 \times 4$	$256 \times 4 \times 4$	-	-
Transformer Processing				
Reshape	$256 \times 4 \times 4$	$4 \times (B \times 4) \times 256$	-	-
Position Embedding	$4 \times (B \times 4) \times 256$	$4 \times (B \times 4) \times 256$	$d_{\text{model}} = 256$	-
Transformer Encoder	$4 \times (B \times 4) \times 256$	$4 \times (B \times 4) \times 256$	3 layers, 8 heads	-

representation, requiring both spatial upsampling and semantic refinement. Our decoder architecture, specified in [Fig. S3](#) and [Table S5](#), implements this transformation through a two-stage process combining transformer-based cross-attention with hierarchical convolutional upsampling.

The first stage employs a Transformer decoder to establish spatial correspondences between the encoded visual features and the target BEV grid. We initialize a set of learnable query vectors arranged in an 8×8 spatial grid, with each query corresponding to a specific location in the coarse-resolution BEV map. These queries are augmented with sinusoidal positional encodings to inject spatial awareness. The transformer decoder then refines these queries through 3 layers of cross-attention, where each query attends to the encoder’s output memory to extract relevant visual evidence for its corresponding spatial location. This attention mechanism effectively implements a learned, content-dependent resampling operation that warps the egocentric visual features into the allocentric frame. The output is a 256-channel feature map at 8×8 resolution, representing a semantically-rich but spatially-coarse BEV representation.

The second stage progressively upsamples this coarse representation to the final 250×250 resolution through a cascade of five transposed convolutional layers. Each upsampling block doubles the spatial resolution while halving the channel depth, gradually translating abstract semantic features into concrete pixel-level predictions. Batch normalization and ReLU activations are applied after each layer to maintain stable gradients and non-linear expressiveness. The final 4-channel output is partitioned into RGB appearance channels and a single alpha channel representing occupancy probability. Both outputs are resized to 250×250 via bilinear interpolation and passed through sigmoid activations to enforce valid probability ranges. This hierarchical decoder design ensures that the network can reconstruct both the geometric layout (via the alpha channel) and the visual appearance (via RGB channels) of the environment from a unified latent representation.

Transformer component. The capacity and performance of the transformer-based components are critical to the model’s ability to reason about long-range spatial dependencies. The specific hyperparameters, detailed in [Table S6](#), were chosen to balance representational power with computational efficiency. A model dimension (d_{model}) of 256 provides a sufficiently high-dimensional space for embedding complex visual features. The use of 8 attention heads allows the model to simultaneously focus on different aspects of the visual input—for instance, attending to distant landmarks with one head while focusing on nearby wall textures with another. The 3-layer depth for both the encoder and decoder was empirically determined to be deep enough to learn complex cross-view transformations without incurring excessive computational cost or overfitting. These parameters collectively equip the module with the necessary capacity to learn the non-trivial mapping from a narrow, first-person perspective to a comprehensive, top-down allocentric map.

Loss function details. To guide the learning process toward physically plausible world models, the module is optimized by minimizing a composite loss function, \mathcal{L}_{BEV} , which holistically evaluates the quality of the BEV prediction. This objective function is a weighted sum of three distinct terms, each imposing a different physical prior on the model’s predictions. The primary term, the occupancy loss (\mathcal{L}_{occ}), uses binary cross-entropy to enforce geometric consistency, compelling the network to make a clear distinction between navigable space and solid obstacles. The appearance loss (\mathcal{L}_{rgb}) employs a masked mean-squared error to ensure photorealistic accuracy, forcing the model to predict the correct surface textures but only within regions identified as navigable. Finally, a smoothness loss ($\mathcal{L}_{\text{smooth}}$) acts as a regularizer, penalizing sharp, unnatural gradients in

Table S5. Decoder architecture of BEV prediction. B means the batch size.

Layer	Input Size	Output Size	Parameters	Activation
Transformer Decoder				
Query Init	-	$64 \times (B \times 4) \times 256$	8×8 spatial	-
PositionalEncoding	$64 \times (B \times 4) \times 256$	$64 \times (B \times 4) \times 256$	$d_{\text{model}} = 256$	-
TransformerDecoder	Memory + Query	$(B \times 4) \times 256 \times 8 \times 8$	3 layers, 8 heads	-
Linear Projection	$(B \times 4) \times 256$	256×256	-	-
Upsampling Network				
ConvTranspose2d-1	$256 \times 8 \times 8$	$128 \times 16 \times 16$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-1	$128 \times 16 \times 16$	$128 \times 16 \times 16$	-	-
ConvTranspose2d-2	$128 \times 16 \times 16$	$64 \times 32 \times 32$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-2	$64 \times 32 \times 32$	$64 \times 32 \times 32$	-	-
ConvTranspose2d-3	$64 \times 32 \times 32$	$32 \times 64 \times 64$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-3	$32 \times 64 \times 64$	$32 \times 64 \times 64$	-	-
ConvTranspose2d-4	$32 \times 64 \times 64$	$16 \times 128 \times 128$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-4	$16 \times 128 \times 128$	$16 \times 128 \times 128$	-	-
ConvTranspose2d-5	$16 \times 128 \times 128$	$8 \times 256 \times 256$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-5	$8 \times 256 \times 256$	$8 \times 256 \times 256$	-	-
Conv2d-Final	$8 \times 256 \times 256$	$4 \times 256 \times 256$	$k = 3, p = 1$	-
Output Processing				
RGB Channels	$3 \times 256 \times 256$	$3 \times 250 \times 250$	Bilinear Resize	Sigmoid
Alpha Channel	$1 \times 256 \times 256$	$1 \times 250 \times 250$	Bilinear Resize	Sigmoid

the predicted occupancy map and incorporating the prior that physical environments are generally continuous. The mathematical formulation and weighting of each component are detailed in **Table S7**.

S1.3 Emergent communication mechanism architecture

To operationalize the principle of Social Predictive Coding, we design a communication architecture that directly implements the variational information bottleneck (VIB) framework [1, 16]. The central hypothesis is that an efficient communication mechanism need not be manually designed but can emerge share when agents are optimized to transmit only the information that is maximally reductive of their partner’s future uncertainty. Consequently, the network architecture is not merely a tool for data compression, but a principled mechanism for learning a compact, structured, and task-relevant symbolic language from the ground up. This process is built upon a neural substrate capable of generating a rich, unified social representation, which serves as the input to the communication module. We first detail this substrate, followed by the communication architecture itself.

S1.3.1 Social representation substrate: Emergence of social place cells

Before an agent can decide what information to transmit, it must first form a comprehensive internal representation of the whole multi-agent system system [4]. This state, denoted as $S_{i,t}$ in our method, serves as the foundation for the entire communication mechanism. To this end, we design a specialized neural architecture, the **Social Place Coding**, to learn this rich social representation, as shown in the main text (**Fig. 4a**).

The network’s backbone is a dual-stream path integration module built upon a single recurrent LSTM core. This LSTM concurrently processes egocentric motion inputs (linear and angular velocities) from both the self-agent and its partner. A key design choice is the use of an asymmetric input representation: the self-agent’s velocity vector is concatenated with a learned **ego_token**, while the partner’s velocity is concatenated with a zero vector. This allows the shared LSTM to distinguish between self and other motion streams while processing them with the same set of weights, encouraging the development of a unified representational space.

The hidden states from both processing streams are then fused via element-wise addition to form a **joint_representation**. This unified state is then passed through a bottleneck layer. This shared latent representation is compelled to functionally specialize under a multi-faceted predictive objective. The network is trained not only to predict its own future location (place and head-direction cell activations) and its partner’s future location, but also, critically, the future Euclidean distance between them via a dedicated **relational_head** (the relative positioning). This compound predictive pressure ensures that the

Table S6. Details of transformer component in BEV prediction.

Component	Parameter	Value
Transformer Encoder	Model Dimension (d_{model})	256
	Number of Heads	8
	Feed-forward Dimension	2048
	Number of Layers	3
	Dropout Rate	0.1
Transformer Decoder	Model Dimension (d_{model})	256
	Number of Heads	8
	Feed-forward Dimension	2048
	Number of Layers	3
	Dropout Rate	0.1
Positional Encoding	Max Sequence Length	5000
	Encoding Type	Sinusoidal

Table S7. Details of loss function in BEV prediction.

Loss Component	Mathematical Form	Weight
Alpha Loss	$\mathcal{L}_{\text{occ}} = -\sum_{i,j} [y_{ij} \log(\hat{y}_{ij}) + (1 - y_{ij}) \log(1 - \hat{y}_{ij})]$	$w_{\alpha} = 1.0$
RGB Loss	$\mathcal{L}_{\text{rgb}} = \frac{1}{ M } \sum_{(i,j) \in M} \ \mathbf{c}_{ij} - \hat{\mathbf{c}}_{ij}\ _2^2$	$w_{\text{rgb}} = 0.5$
Smoothness Loss	$\mathcal{L}_{\text{smooth}} = \frac{1}{2} (\mathbb{E}[\ \nabla_x \alpha\] + \mathbb{E}[\ \nabla_y \alpha\])$	$w_{\text{smooth}} = 0.1$

joint_representation encodes not just individual trajectories but also the dynamic spatial relationship between the agents. It is this relational predictive task that catalyzes the emergence of specialized neural populations, including social place cells (SPCs) that are selectively tuned to the partner’s location. This emergent social representation provides the rich, disentangled state $S_{i,t}$ that is subsequently fed into the VIB communication encoder, forming a crucial bridge between social cognition and emergent communication.

S1.3.2 Encoder architecture: Implementing the VIB compression term

The encoder’s role is to transform the sender’s high-dimensional state, an occupancy map $S_{i,t}$ of size 64×64 , into a compressed latent message z . This directly corresponds to learning the stochastic mapping $q_{\varphi}(z | S_{i,t})$ in our VIB formulation. Our choice of a deep convolutional structure is critical for this task. Unlike fully-connected networks that would discard spatial topology, convolutional layers impose a strong and relevant inductive bias—namely, locality and translation equivariance. This ensures that the learned features capture the geometric nature of the agent’s environment.

The architecture, detailed in **Table S8**, employs a symmetric downsampling hierarchy. Each block halves the spatial resolution while doubling the channel capacity, creating a pyramid of progressively more abstract and semantically rich feature maps. This hierarchical processing allows the network to capture not just fine-grained local details (e.g., narrow corridors) in its initial layers, but also the global layout and topological structure of the environment in its deeper layers. This multi-scale feature extraction is essential for generating a message that is both comprehensive and compact.

The information bottleneck itself is realized at the VAE’s latent space. The flattened 4096-dimensional feature vector is projected onto the parameters of a diagonal Gaussian distribution, μ and $\log \sigma^2$. The stochastic message z is then sampled using the reparameterization trick ($z = \mu + \epsilon\sigma, \epsilon \sim \mathcal{N}(0, I)$), which permits gradient flow during backpropagation. This stochastic encoding is the key to rate-limiting the communication channel. The KL-divergence term in the loss function, \mathcal{L}_{KL} , penalizes the encoded distribution $q_{\varphi}(z | S_{i,t})$ for deviating from the uninformative prior $p(z)$. This pressure constrains the mutual information $I(S_{i,t}; z)$, forcing the encoder to discard non-essential information and retain only the most salient features of the input map.

S1.3.3 Decoder architecture: Implementing the VIB predictive utility term

The decoder’s function is to quantify the predictive utility of the message z . It operationalizes the predictive model $p_{\theta}(O_{j,t+1} | z, S_{j,t})$ from our VIB framework, where its primary goal is to reconstruct the receiving agent’s future state from the compressed message. The architecture, detailed in **Table S9**, symmetrically mirrors the encoder. It first projects the latent code z back to a high-dimensional feature space (4096 dimensions) and reshapes it into a spatial tensor ($256 \times 4 \times 4$).

Table S8. Communication encoder architecture. This network implements the compression stage of the VIB, mapping a spatial map to a stochastic latent variable z .

Layer	Input Size	Output Size	Parameters	Activation
Spatial Memory Input				
Input Map	$1 \times 64 \times 64$	$1 \times 64 \times 64$	-	-
Convolutional Downsampling				
Conv2d-1	$1 \times 64 \times 64$	$32 \times 32 \times 32$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-1	$32 \times 32 \times 32$	$32 \times 32 \times 32$	-	-
Conv2d-2	$32 \times 32 \times 32$	$64 \times 16 \times 16$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-2	$64 \times 16 \times 16$	$64 \times 16 \times 16$	-	-
Conv2d-3	$64 \times 16 \times 16$	$128 \times 8 \times 8$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-3	$128 \times 8 \times 8$	$128 \times 8 \times 8$	-	-
Conv2d-4	$128 \times 8 \times 8$	$256 \times 4 \times 4$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-4	$256 \times 4 \times 4$	$256 \times 4 \times 4$	-	-
VAE Latent Space Projection				
Flatten	$256 \times 4 \times 4$	4096	-	-
Mean Projection (μ)	4096	z_{dim}	Linear(4096, z_{dim})	-
LogVar Projection ($\log \sigma^2$)	4096	z_{dim}	Linear(4096, z_{dim})	-
Reparameterization	z_{dim}	z_{dim}	$z = \mu + \epsilon \cdot \sigma$	-

A sequence of transposed convolutional layers then hierarchically upsamples this representation, progressively doubling the spatial resolution while halving the channel depth. This process effectively inverts the abstraction performed by the encoder, translating the compact, semantic message back into a concrete spatial map. The final layer applies a sigmoid activation function to produce pixel-wise occupancy probabilities, yielding a reconstructed map \hat{y} that represents the agent’s prediction of its partner’s view. The quality of this reconstruction serves as the measure of the message’s utility.

S1.3.4 VIB objective: Driving the emergence of efficient communication

The encoder and decoder are trained jointly by minimizing the VIB objective function, which is functionally equivalent to the VAE’s evidence lower bound (ELBO). This loss function elegantly captures the fundamental rate-distortion trade-off at the heart of our theory:

$$\mathcal{L}_{\text{VIB}} = \underbrace{\mathcal{L}_{\text{reconstruction}}}_{\text{Predictive Utility}} + \underbrace{\beta \cdot \mathcal{L}_{\text{KL}}}_{\text{Communication Cost}}. \quad (\text{S15})$$

Reconstruction loss: Maximizing predictive utility. The reconstruction loss, a pixel-wise binary cross-entropy, drives the decoder to produce accurate predictions, thereby rewarding messages that contain high predictive utility:

$$\mathcal{L}_{\text{reconstruction}} = - \sum_{i,j} [y_{ij} \log(\hat{y}_{ij}) + (1 - y_{ij}) \log(1 - \hat{y}_{ij})]. \quad (\text{S16})$$

This term directly instantiates the distortion component of the VIB framework, ensuring that compressed messages z retain sufficient information to enable accurate reconstruction of the receiver’s spatial map.

KL divergence loss: Enforcing communication efficiency. Simultaneously, the KL-divergence loss regularizes the encoder, penalizing deviation from the simple Gaussian prior and thus minimizing the information capacity of the communication channel. This term operationalizes the rate constraint in the VIB formulation. Specifically, the KL term measures the information-theoretic divergence between the learned variational posterior $q_\varphi(z | S_{i,t})$ produced by the encoder and the standard Gaussian prior $p(z) = \mathcal{N}(\mathbf{0}, \mathbf{I})$. By definition, the Kullback-Leibler divergence is:

$$\mathcal{L}_{\text{KL}} = D_{\text{KL}}(q_\varphi(z | S_{i,t}) \| p(z)) = \mathbb{E}_{q_\varphi(z | S_{i,t})} [\log q_\varphi(z | S_{i,t}) - \log p(z)]. \quad (\text{S17})$$

This expectation quantifies the average “surprise” or information cost of encoding the agent’s state $S_{i,t}$ relative to the uninformative prior. Minimizing this divergence ensures that the latent code z remains statistically indistinguishable from the prior unless the information is essential for prediction.

Table S9. Communication decoder architecture. This network instantiates the predictive component of the VIB, reconstructing a spatial map from the latent message z .

Layer	Input Size	Output Size	Parameters	Activation
Latent Space Processing				
Latent Input	z_{dim}	z_{dim}	-	-
Projection	z_{dim}	4096	Linear(z_{dim} , 4096)	ReLU
Reshape	4096	$256 \times 4 \times 4$	-	-
Transposed Convolutional Upsampling				
ConvTranspose2d-1	$256 \times 4 \times 4$	$128 \times 8 \times 8$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-1	$128 \times 8 \times 8$	$128 \times 8 \times 8$	-	-
ConvTranspose2d-2	$128 \times 8 \times 8$	$64 \times 16 \times 16$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-2	$64 \times 16 \times 16$	$64 \times 16 \times 16$	-	-
ConvTranspose2d-3	$64 \times 16 \times 16$	$32 \times 32 \times 32$	$k = 4, s = 2, p = 1$	ReLU
BatchNorm2d-3	$32 \times 32 \times 32$	$32 \times 32 \times 32$	-	-
ConvTranspose2d-4	$32 \times 32 \times 32$	$1 \times 64 \times 64$	$k = 4, s = 2, p = 1$	Sigmoid
Spatial Map Output				
Reconstructed Map	$1 \times 64 \times 64$	$1 \times 64 \times 64$	Continuous $[0, 1]$	-

Table S10. Training configuration and performance metrics of communication mechanism.

Parameter Category	Parameter	Value
Architecture	Input Map Size	64×64 pixels
	Latent Dimensions (z_{dim})	128 (Optimal)
	Compression Ratio	32:1
	Reconstruction Error	< 4.1%
Training	Optimizer	Adam
	Batch Size	32
	Learning Rate	1×10^{-3}
	Training Epochs	50
VIB Objective	Reconstruction Weight	1.0
	KL Divergence Weight (β)	1.0

Closed-form solution under Gaussian assumptions. Our encoder architecture parametrizes the variational posterior as a diagonal Gaussian distribution:

$$q_{\varphi}(z|S_{i,t}) = \mathcal{N}(\boldsymbol{\mu}(S_{i,t}), \text{diag}(\boldsymbol{\sigma}^2(S_{i,t}))), \quad (\text{S18})$$

where $\boldsymbol{\mu} = [\mu_1, \dots, \mu_{z_{\text{dim}}}]^{\top}$ and $\boldsymbol{\sigma}^2 = [\sigma_1^2, \dots, \sigma_{z_{\text{dim}}}^2]^{\top}$ are outputs of the encoder's mean and log-variance projection layers, respectively. The diagonal covariance structure reflects the architectural assumption that latent dimensions are conditionally independent given the input state. Under this Gaussian parametrization with a standard normal prior $p(z) = \mathcal{N}(\mathbf{0}, \mathbf{I})$, the KL divergence factorizes across dimensions:

$$D_{\text{KL}}(q_{\varphi}(z|S_{i,t})\|p(z)) = \sum_{k=1}^{z_{\text{dim}}} D_{\text{KL}}(\mathcal{N}(\mu_k, \sigma_k^2)\|\mathcal{N}(0, 1)). \quad (\text{S19})$$

For any two univariate Gaussian distributions $\mathcal{N}(\mu_k, \sigma_k^2)$ and $\mathcal{N}(0, 1)$, the KL divergence has the well-known closed form:

$$D_{\text{KL}}(\mathcal{N}(\mu_k, \sigma_k^2)\|\mathcal{N}(0, 1)) = \frac{1}{2} (\sigma_k^2 + \mu_k^2 - 1 - \log \sigma_k^2). \quad (\text{S20})$$

This expression is derived by evaluating the expectation in Eq. (S17) under the Gaussian density functions and simplifying the resulting integral.

Summing over all latent dimensions, we obtain the final training objective:

$$\mathcal{L}_{\text{KL}} = \frac{1}{2} \sum_{k=1}^{z_{\text{dim}}} (\mu_k^2 + \sigma_k^2 - 1 - \log \sigma_k^2), \quad (\text{S21})$$

where (μ_k^2) penalizes the encoder for shifting the posterior distribution's mean away from zero. This term encourages the latent code to be centered, preventing the encoder from arbitrarily offsetting the representation space. The variance regularization $(\sigma_k^2 - 1)$ penalizes deviation of the posterior variance from unity. When $\sigma_k^2 > 1$, the distribution is overly diffuse, indicating the encoder is uncertain; when $\sigma_k^2 < 1$, the distribution is overly concentrated, indicating overconfidence. This term encourages calibrated uncertainty. Besides, variance collapse prevention $(-\log \sigma_k^2)$ acts as a negative log-determinant term that becomes large (highly penalizing) as $\sigma_k^2 \rightarrow 0$. This prevents the posterior from collapsing to a delta function, which would eliminate stochasticity and reduce the model to deterministic encoding. The stochastic bottleneck is essential for learning representations robust to input variations.

The rate-distortion trade-off. The hyperparameter β serves as the Lagrange multiplier from the original information bottleneck formulation, allowing explicit control over this trade-off. A larger β intensifies the pressure to compress, forcing the system to discover a more abstract and efficient communication mechanism. It is this pressure that catalyzes the emergence of a specialized symbolic system. When the channel capacity is limited, the agents learn that the most valuable, uncertainty-reducing information often pertains to the locations and trajectories of other agents. The VIB objective thus guides the latent space to develop a disentangled structure where specific dimensions become selectively tuned to this critical social-spatial information. This process explains the spontaneous emergence of social place cell (SPC)-like representations within the communication code—not as a pre-programmed feature, but as the optimal solution to the problem of collaborative prediction under bandwidth constraints. As shown in our training configuration (Table S10), this architecture achieves a 32:1 compression ratio with under 5% reconstruction error, demonstrating the efficacy of this emergent communication.

S1.4 HRL-ICM framework

To operationalize the strategic exploration policy described in the main text, we implement a hierarchical reinforcement learning framework augmented with an intrinsic curiosity module (HRL-ICM). This architecture decomposes the navigation task into strategic goal selection (handled by a learned meta-controller) and tactical path execution (delegated to a deterministic A* planner). The framework is trained using multi-agent proximal policy optimization (MAPPO), a robust variant of the PPO algorithm adapted for cooperative multi-agent [19]. By separating strategic and tactical reasoning, the system can learn long-horizon exploration strategies without the burden of low-level motor control, enabling efficient credit assignment and scalable coordination across multiple agents.

Critically, the framework's ability to coordinate exploration across agents depends on accurate estimation of inter-agent spatial relationships. This is achieved through the social place cell (SPC) module described in the main text, which provides the essential relational geometry required for the ICM to compute coordination rewards and for the communication gating policy to make informed transmission decisions. We first describe the integration of this social spatial representation module before detailing the meta-controller and ICM components.

S1.4.1 Social place cell module for partner state estimation

The social place cell module serves as the perceptual foundation for multi-agent coordination by continuously estimating partner locations and computing inter-agent distances. This module extends the grid-cell-based path integration architecture described in **Method S1.1** to the social domain through a dual-stream processing design.

The architecture consists of two parallel LSTM encoders that concurrently process motion information from both the observing agent (self) and its partner. The self-stream receives the agent's proprioceptive velocity commands $\mathbf{v}_{\text{self},t} = (v_x, v_y, \omega)$ as direct sensory input. The partner-stream processes estimated partner velocities $\hat{\mathbf{v}}_{\text{partner},t}$, which are inferred from visual observations of the partner's motion across multiple frames. Specifically, when a partner is visible within the agent's field of view, its displacement and orientation change over a short temporal window (typically 3-5 frames) are used to estimate its instantaneous translational and angular velocities. This visual motion estimation provides a noisy but informative signal about the partner's navigation state.

Both streams are initialized at episode start using the respective agents' known starting poses, encoded through ensembles of virtual place cells and head-direction cells identical to those used in the individual path integration module (detailed in **Method S1.1**). The two LSTM hidden states, $\mathbf{h}_{\text{self},t}$ and $\mathbf{h}_{\text{partner},t}$, are then fused via element-wise summation to form a unified joint representation $\mathbf{h}_{\text{joint},t} = \mathbf{h}_{\text{self},t} + \mathbf{h}_{\text{partner},t}$. This shared representation is passed through a bottleneck layer (256 units, 50% dropout) that enforces a compressed, information-efficient encoding of the two-agent system state.

Table S11. Details of social place cell module.

Component	Input Dim	Output Dim	Description
Input Processing			
Self Velocity	3	3	(v_x, v_y, ω)
Partner Velocity (est.)	3	3	Visual motion estimation
Initial Pose Encoding	2+1	288	Place (256) + HD (32) cells
Dual-Stream LSTM			
Self LSTM	3	128	Hidden state \mathbf{h}_{self}
Partner LSTM	3	128	Hidden state $\mathbf{h}_{\text{partner}}$
Fusion (sum)	128×2	128	$\mathbf{h}_{\text{joint}}$
Bottleneck & Prediction Heads			
Bottleneck Layer	128	256	Dropout 0.5
Self Place Predictor	256	256	KL loss
Self HD Predictor	256	32	KL loss
Partner Place Predictor	256	256	KL loss
Partner HD Predictor	256	32	KL loss
Distance Regression	256	1	MSE loss

The network is trained under a multi-task predictive objective with three supervision signals, each computed at the final timestep T of a trajectory segment:

$$\mathcal{L}_{\text{SPC}} = \mathcal{L}_{\text{self}} + \mathcal{L}_{\text{partner}} + w_{\text{dist}} \mathcal{L}_{\text{distance}}, \quad (\text{S22})$$

where $\mathcal{L}_{\text{self}}$ and $\mathcal{L}_{\text{partner}}$ are KL divergences between predicted and target place/head-direction cell activations for the self and partner agents, respectively (identical in form to the individual path integration loss), and $\mathcal{L}_{\text{distance}}$ is a mean-squared error on the Euclidean distance between agents, $\|\mathbf{r}_{\text{self},T} - \mathbf{r}_{\text{partner},T}\|_2$. The distance prediction is implemented via a dedicated regression head (linear layer) that projects the bottleneck representation to a scalar distance estimate. We set $w_{\text{dist}} = 1.0$ to balance the three objectives.

This compound predictive objective compels the bottleneck representation to develop functionally specialized subpopulations. As demonstrated in the main text (Fig. 4), analysis of the learned representations reveals distinct neuron types: pure place cells tuned exclusively to self-position, social place cells (SPCs) selective for partner position, and mixed-selectivity units encoding conjunctions of self- and partner-locations. Critically, a subset of units forms a population code for inter-agent distance, exhibiting graded tuning curves that tile the distance space from close proximity to far separation. This distance-tuned population is causally necessary for accurate distance estimation, as confirmed by targeted *in-silico* lesion experiments (Fig. 4e).

For integration into the HRL-ICM framework, the SPC module operates continuously during exploration. At each timestep, the module outputs: (1) an updated estimate of the partner’s position $\hat{\mathbf{r}}_{\text{partner},t}$ (decoded from the partner place cell activations), and (2) a predicted inter-agent distance \hat{d}_t (from the relational regression head). These outputs are consumed by downstream components: the distance estimate \hat{d}_t directly informs the ICM’s coordination reward (detailed below), while the partner position estimate enables the communication gating policy to assess whether agents are within communication range. The SPC module thus closes the loop between perception and coordination, transforming visual observations of partners into structured spatial representations that guide strategic decision-making. The architecture specifications are provided in **Table S11**.

S1.4.2 Meta-controller architecture

The meta-controller is implemented as a shared actor-critic network that maps high-level spatial abstractions to goal selections. To construct a tractable state representation from the high-dimensional occupancy map, each agent first partitions its local $H \times W$ grid into a coarse $g \times g$ regional summary (typically $g = 4$, yielding 16 macro-regions). For each region $k \in \{1, \dots, g^2\}$, the agent computes three summary statistics: the *exploration ratio* (proportion of cells with known occupancy), the *walkability ratio* (proportion of known cells that are navigable), and a binary *agent presence indicator*. These features are concatenated into a $3g^2$ -dimensional state vector that serves as input to the policy network.

The network architecture follows a standard actor-critic design with shared feature extraction. Two fully-connected layers (each with 256 hidden units and ReLU activation) process the regional feature vector to produce a shared embedding. This embedding then branches into two specialized heads. The *actor head* projects the embedding through an additional hidden layer (256 units, ReLU) before outputting a g^2 -dimensional logit vector, which is normalized via softmax to yield a categorical

Table S12. Details of meta-controller actor-critic.

Component	Input Dim	Output Dim	Activation
Shared Feature Extraction			
FC-1	48	256	ReLU
FC-2	256	256	ReLU
Actor Branch			
Actor FC	256	256	ReLU
Action Logits	256	16	Softmax
Critic Branch			
Critic FC	256	256	ReLU
Value Output	256	1	Linear

distribution over candidate goal regions. The *critic head*, operating in parallel, projects the shared embedding through its own hidden layer to produce a scalar state-value estimate. All network weights are initialized using orthogonal initialization with a gain of 0.01, a choice that promotes stable early-stage training by preventing gradient explosion. The architecture is formally specified in **Table S12**.

S1.4.3 Intrinsic curiosity module

The intrinsic curiosity module (ICM) translates the abstract principle of uncertainty-driven exploration into a concrete, dense reward signal that guides the meta-controller’s learning [7, 15]. Rather than relying on a learned forward dynamics model, which can be sample-inefficient in high-dimensional discrete spaces, our ICM directly estimates epistemic uncertainty by analyzing the geometry of the known-unknown boundary in the agent’s local map, augmented with social spatial information from the SPC module. The module generates a composite intrinsic reward r_t^{int} as a weighted sum of three interpretable components:

$$r_t^{\text{int}} = w_{\text{curiosity}} r_{\text{curiosity}} + w_{\text{coord}} r_{\text{coord}} + w_{\text{explore}} r_{\text{explore}}, \quad (\text{S23})$$

where $(w_{\text{curiosity}}, w_{\text{coord}}, w_{\text{explore}}) = (1.0, 0.5, 0.3)$ are fixed hyperparameters that balance the contribution of each term. The *curiosity reward* $r_{\text{curiosity}}$ encourages agents to select goal regions that border unknown territory. It computes a spatial “curiosity map” by identifying frontier pixels—known navigable cells adjacent to unexplored areas—and weighting them by their proximity to the agent and the local density of unknown neighbors. The reward is then the normalized curiosity value of the selected goal region, effectively incentivizing movement toward the boundary of the agent’s knowledge.

The *coordination reward* r_{coord} promotes spatial division of labor by leveraging the inter-agent distance estimates provided by the SPC module. This component discourages redundant exploration by rewarding goal selections that maintain appropriate separation from teammates. For each agent i , the SPC module continuously estimates the distances $\{\hat{d}_{ij,t}\}_{j \neq i}$ to all partner agents. When agent i selects a goal region centered at \mathbf{g}_i , the coordination reward is computed as:

$$r_{\text{coord}}^i = \sum_{j \neq i} \min \left(\frac{\hat{d}_{ij,t}}{d_{\text{norm}}}, 1.0 \right) \cdot \mathbb{1}[\hat{d}_{ij,t} \geq d_{\text{min}}], \quad (\text{S24})$$

where $d_{\text{norm}} = 10.0$ grid cells is a normalization constant, $d_{\text{min}} = 3.0$ grid cells is a minimum desired separation threshold, and $\mathbb{1}[\cdot]$ is an indicator function that provides a bonus only when agents maintain at least the minimum distance. This design creates a repulsive force between agents proportional to their estimated separation, directly operationalizing the principle that distributed exploration maximizes information gain. Critically, this component relies entirely on the SPC module’s distance predictions $\hat{d}_{ij,t}$ —without accurate distance estimation, agents cannot effectively coordinate their exploration strategies. This establishes a direct computational dependency: the SPC module’s learned distance-tuned neurons (described in **Fig. 4c**) provide the essential geometric information that enables the ICM to generate coordination signals.

The *exploration reward* r_{explore} provides a direct bonus for discovering cells that were previously unknown to the entire team, quantified by counting newly revealed map cells in a local neighborhood around the agent and applying an exponential distance decay with decay constant $\alpha = 0.1$:

$$r_{\text{explore}} = \sum_{(x,y) \in \mathcal{N}(\mathbf{r}_i, r_{\text{local}})} \mathbb{1}[M_{x,y,t-1}^{\text{shared}} = 0 \wedge M_{x,y,t}^i > 0] \cdot \exp(-\alpha \|\mathbf{r}_i - (x,y)\|_2), \quad (\text{S25})$$

where $\mathcal{N}(\mathbf{r}_i, r_{\text{local}})$ is a local neighborhood of radius $r_{\text{local}} = 2$ grid cells around the agent's position \mathbf{r}_i , M^{shared} denotes the team's collective map, and M^i is agent i 's local map. This three-component design ensures that agents are simultaneously attracted to informative frontiers, repelled from teammates to avoid overlap (mediated by SPC distance estimates), and directly rewarded for expanding the collective map.

S1.4.4 Communication mechanism

Inter-agent communication is realized through a bandwidth-limited message-passing system that operates in parallel with the high-level decision loop, with communication feasibility determined by the SPC module's distance estimates. Each agent is endowed with a finite budget of *communication tokens* (typically 10 per episode), which depletes with each message transmission and regenerates slowly over time (refill rate $\rho_{\text{refill}} = 1/60$ per step). The decision to communicate involves two stages: first, the SPC module determines which partners are within communication range (defined as $\hat{d}_{ij,t} \leq d_{\text{comm}}$), establishing the set of feasible communication targets; second, a learned gating policy decides whether to actually transmit a message to these reachable partners.

The gating policy is modeled as a logistic classifier that takes as input a 9-dimensional feature vector encoding: (1) the agent's current exploration progress (mean exploration ratio across regions), (2) remaining token budget (normalized by initial budget), (3) local map confidence (average confidence in visible region), (4) spatial connectivity (number of adjacent navigable cells), (5-8) a one-hot encoding of location type (junction, corridor, dead-end, open-area), and (9) a bias term. Critically, this feature vector does *not* explicitly include partner distance—the distance constraint is enforced at the architectural level by the SPC module's range-gating, ensuring that communication is only physically possible when $\hat{d}_{ij,t} \leq d_{\text{comm}}$. The policy outputs a binary communication decision via a sigmoid activation: $p_{\text{comm}} = \sigma(\mathbf{w}^\top \mathbf{f}_t + b)$, where $\mathbf{w} \in \mathbb{R}^9$ are learned weights, \mathbf{f}_t is the feature vector, and b is a learned bias. When an agent elects to communicate and has available tokens, it broadcasts its local occupancy map and current position to all teammates within the SPC-determined communication range.

This design establishes a clear functional hierarchy: the SPC module's distance-tuned neurons provide the low-level geometric constraint that defines when communication is physically feasible (mimicking limited-range radio communication), while the learned gating policy operates within these constraints to decide when communication is strategically valuable. This separation ensures that the system respects realistic communication limitations while still learning an intelligent transmission strategy. The causal necessity of accurate distance estimation is evident: if the SPC module's distance predictions $\hat{d}_{ij,t}$ are inaccurate (as occurs after SPC lesioning, **Fig. 4e**), agents will incorrectly estimate which partners are reachable, leading to failed communication attempts or missed opportunities for coordination.

Upon receiving a message from a partner confirmed to be within range (via bidirectional SPC distance checks), the recipient performs an intelligent map fusion operation. Rather than naively overwriting its local map, the agent maintains auxiliary *confidence* and *timestamp* matrices that track the reliability and recency of each cell's occupancy estimate. When integrating received information, conflicting observations are resolved via a multi-criteria decision rule: more recent information is preferred over stale data, higher-confidence estimates override lower-confidence ones, and in cases of equal confidence, wall observations are given precedence over free-space observations as a safety heuristic. This confidence-weighted fusion mechanism ensures that the shared spatial memory remains coherent despite asynchronous and potentially noisy observations, while the token-based gating prevents communication saturation and encourages agents to transmit selectively at moments of high informational value.

S1.4.5 Training configuration and optimization

The entire HRL-ICM system is trained end-to-end using the MAPPO algorithm with the following configuration. The meta-controller makes a high-level goal selection every $K = 20$ environment steps, during which the low-level A* planner executes primitive movement actions (move-forward, turn-left, turn-right, stay) to navigate toward the chosen region. Extrinsic rewards include a large bonus (+500) for task success (locating the hidden goal), a small step penalty (−0.01) to encourage efficiency, and a collision penalty (−3). The total reward at each decision point is the sum of extrinsic and intrinsic components. Advantages for policy gradient updates are computed using Generalized Advantage Estimation (GAE) with discount factor $\gamma = 0.99$ and trace parameter $\lambda = 0.95$. The policy is optimized using the Adam optimizer with a learning rate of 3×10^{-4} , gradient clipping at norm 1.0, and an entropy regularization coefficient of $\eta = 0.01$ to maintain exploration. Training is conducted over multiple episodes on procedurally generated mazes of varying sizes (15 × 15 to 39 × 39), ensuring that the learned policy generalizes across diverse spatial layouts rather than overfitting to a fixed map. The key hyperparameters are summarized in **Table S13**.

The hierarchical training procedure ensures that all components are jointly optimized. The SPC module is pre-trained on trajectory prediction tasks to establish stable distance estimation before being integrated into the full HRL-ICM loop. During full system training, the SPC parameters are kept frozen for the first 10^4 environment steps to allow the meta-controller and ICM to stabilize, after which all components are fine-tuned end-to-end. This staged training strategy prevents the SPC module from adapting to spurious reward signals and ensures that its distance predictions remain grounded in the geometric structure of agent trajectories. The integration of these components creates a complete computational loop: the SPC module provides

Table S13. Training configuration of HRL-ICM.

Category	Parameter	Value
Meta-Controller	Regional Grid Size ($g \times g$)	4×4
	Hidden Dimension	256
	Input Feature Dimension	48
	Output Actions (Regions)	16
SPC Module	LSTM Hidden Size	128
	Bottleneck Dimension	256
	Distance Loss Weight (w_{dist})	1.0
	Distance Normalization (d_{norm})	10.0 cells
	Min. Coordination Distance (d_{min})	3.0 cells
ICM Weights	Curiosity Weight ($w_{\text{curiosity}}$)	1.0
	Coordination Weight (w_{coord})	0.5
	Exploration Weight (w_{explore})	0.3
	Exploration Radius (r_{local})	2 cells
	Distance Decay (α)	0.1
Communication	Token Budget	10
	Refill Rate (ρ_{refill})	1/60 per step
	Gating Feature Dimension	9
	Communication Range (d_{comm})	5.0 cells
MAPPO Training	Algorithm	MAPPO
	High-Level Decision Interval (K)	20 steps
	Learning Rate	3×10^{-4}
	Discount Factor (γ)	0.99
	GAE Parameter (λ)	0.95
	Entropy Coefficient (η)	0.01
	Gradient Clip Norm	1.0
Rewards	Task Success	+500
	Step Penalty	-0.01
	Collision Penalty	-3

geometric awareness of partner states, the ICM translates this into strategic exploration incentives, the meta-controller selects goals based on these incentives, and the communication mechanism leverages distance estimates to coordinate information sharing—all unified under the MAPPO training objective.

S1.5 Theoretical framework: Path integration and grid cell emergence

This section establishes a rigorous mathematical framework demonstrating how recurrent networks trained on predictive coding objectives naturally discover path integration dynamics and hexagonally-periodic spatial representations. We develop a principled theoretical argument showing that these solutions emerge from fundamental geometric constraints imposed by the task structure through three stages: (1) establishing preliminaries, (2) proving equivariance-driven path integration, and (3) deriving hexagonal symmetry from isotropy requirements.

S1.5.1 Preliminaries: Mathematical foundations

We formalize the mathematical structure underlying two-dimensional spatial navigation, establishing notation and dynamical equations that any successful path integration system typically incorporate.

State space and kinematics.

Definition 1 (Pose and state space). *An agent navigating in two-dimensional space is characterized by its pose $s_t = (\mathbf{r}_t, \theta_t) \in \mathbb{R}^2 \times \mathbb{S}^1$, where $\mathbf{r}_t = (r_{x,t}, r_{y,t})^\top \in \mathbb{R}^2$ denotes the position vector in Cartesian coordinates (allocentric reference frame) and $\theta_t \in [0, 2\pi]$ denotes the heading angle measured counterclockwise from the positive x -axis. Throughout this work, boldfaced lowercase letters denote column vectors while regular lowercase letters denote scalars.*

Definition 2 (Rotation Matrix). *The rotation matrix $R(\alpha) \in SO(2)$ rotates vectors in \mathbb{R}^2 counterclockwise by angle α [9]:*

$$R(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix}. \quad (\text{S26})$$

Lemma 1 (Rotation matrix properties). *The rotation matrices satisfy: (i) composition law $R(\alpha)R(\gamma) = R(\alpha + \gamma)$, (ii) identity $R(0) = I_2$, (iii) inverse $R(\alpha)^{-1} = R(-\alpha) = R(\alpha)^\top$, and (iv) orthogonality $R(\alpha)^\top R(\alpha) = I_2$, implying norm preservation $\|R(\alpha)\mathbf{v}\| = \|\mathbf{v}\|$ [9].*

Proof. Property (i) follows from trigonometric angle addition formulas:

$$\begin{aligned} R(\alpha)R(\gamma) &= \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \cos \gamma & -\sin \gamma \\ \sin \gamma & \cos \gamma \end{pmatrix} \\ &= \begin{pmatrix} \cos(\alpha + \gamma) & -\sin(\alpha + \gamma) \\ \sin(\alpha + \gamma) & \cos(\alpha + \gamma) \end{pmatrix} = R(\alpha + \gamma), \end{aligned} \quad (\text{S27})$$

where the second equality uses $\cos(\alpha + \gamma) = \cos \alpha \cos \gamma - \sin \alpha \sin \gamma$ and $\sin(\alpha + \gamma) = \sin \alpha \cos \gamma + \cos \alpha \sin \gamma$. Properties (ii)-(iv) follow by direct computation. \square

Motor commands naturally arise in the egocentric (body-centered) frame, while stable spatial memory requires allocentric representations. A vector \mathbf{v}^{ego} in egocentric coordinates transforms to allocentric coordinates via $\mathbf{v}^{\text{allo}} = R(\theta_t)\mathbf{v}^{\text{ego}}$, mediating the heading-dependent transformation central to path integration.

Definition 3 (Path integration dynamics). *At each discrete time step t with uniform interval $\Delta t > 0$, the agent receives motor command $u_t = (\mathbf{v}_t, \omega_t) \in \mathbb{R}^2 \times \mathbb{R}$ specifying egocentric translational velocity $\mathbf{v}_t = (v_{x,t}, v_{y,t})^\top$ and angular velocity ω_t . The pose evolves according to:*

$$\theta_{t+1} = \theta_t + \omega_t \Delta t \pmod{2\pi}, \quad (\text{S28})$$

$$\mathbf{r}_{t+1} = \mathbf{r}_t + \Delta \mathbf{r}_t, \quad \text{where} \quad \Delta \mathbf{r}_t = R(\theta_t)\mathbf{v}_t \Delta t [5]. \quad (\text{S29})$$

Given initial pose $s_0 = (\mathbf{r}_0, \theta_0)$ and command sequence $\{u_t\}_{t=0}^{T-1}$, the cumulative final pose is $\mathbf{r}_T = \mathbf{r}_0 + \sum_{t=0}^{T-1} R(\theta_t)\mathbf{v}_t \Delta t$ and $\theta_T = \theta_0 + \sum_{t=0}^{T-1} \omega_t \Delta t \pmod{2\pi}$.

Remark (Position encoding vs Full pose). *Although complete pose (\mathbf{r}, θ) requires three dimensions of information (two for position, one for heading), our subsequent analysis focuses exclusively on position encoding $\mathbf{r} \in \mathbb{R}^2$ since: (i) position integration $\sum R(\theta_t)\mathbf{v}_t \Delta t$ involves heading-dependent rotations and is computationally complex while heading integration $\sum \omega_t \Delta t$ is simple scalar accumulation, (ii) biological grid cells specifically encode position independent of heading while head direction cells separately encode orientation, and (iii) LSTM hidden states $\mathbf{h} \in \mathbb{R}^d$ can decompose into independent subspaces for position (requiring sophisticated encoding) and heading (requiring simple integration).*

Learning objective. The latent pose s_t is not directly observed. Instead, the system observes activity from C spatial cells with log-firing potential $\phi_i : \mathbb{R}^2 \times \mathbb{S}^1 \rightarrow \mathbb{R}$. Place cells use Gaussian receptive fields $\phi_i(\mathbf{r}) = -\|\mathbf{r} - \mu_i\|^2 / (2\sigma_i^2)$ while head-direction cells use von Mises tuning $\phi_j(\theta) = \kappa_j \cos(\theta - \mu_j)$. Observations follow softmax distribution $p(y = \ell \mid s) = \exp\{\phi_\ell(s)\} / \sum_{m=1}^C \exp\{\phi_m(s)\}$.

Definition 4 (Prediction objective). *An LSTM network with hidden state $h_t \in \mathbb{R}^d$ receives initial observation y_0 and command sequence $\{u_t\}_{t=1}^T$, producing predictive distribution $\hat{p}(\cdot \mid y_0, \{u_t\})$ over the final sensory pattern. The learning objective minimizes prediction error:*

$$\mathcal{L}(\Theta) = \mathbb{E}_{y_0, \{u_t\}} [\text{KL}(p(\cdot \mid s_T) \parallel \hat{p}(\cdot \mid y_0, \{u_t\}))], \quad (\text{S30})$$

where s_T is the true final pose from Eqs. (S28)–(S29), and the expectation is over diverse trajectories. Θ denotes the network parameters. This objective does not explicitly prescribe path integration or specific internal representations; rather, path integration emerges as the optimal strategy for minimizing prediction error over diverse navigation trajectories.

Roadmap. The emergence of hexagonal grid patterns proceeds through three steps: **Proposition 1** proves equivariance under rigid body transformations, **Theorem 1** derives cosine-sine phase encoding from stability constraints, and **Corollary 3** establishes hexagonal symmetry from isotropy requirements.

S1.5.2 Equivariance under rigid body transformations

Having established the dynamical foundations of path integration, we now demonstrate that these dynamics possess a critical geometric property: equivariance under rigid body transformations. This symmetry fundamentally constrains how neural networks can represent spatial information.

Definition 5 (Rigid body transformation). *A rigid body transformation $G_{\delta, \Phi}$ parameterized by translation $\delta \in \mathbb{R}^2$ and rotation angle $\phi \in [0, 2\pi)$ acts on pose $s = (\mathbf{r}, \theta)$ as $G_{\delta, \Phi}(\mathbf{r}, \theta) = (R(\phi)\mathbf{r} + \delta, \theta + \phi)$, rotating position by ϕ then translating by δ while simultaneously rotating heading. The set $\{G_{\delta, \Phi}\}$ forms the special Euclidean group $SE(2)$, the symmetry group of planar rigid motions.*

Proposition 1 (Equivariance of physical dynamics). *The path integration Eqs. (S28)–(S29) are equivariant with respect to rigid body transformations: if trajectory $\{s_t\}_{t=0}^T$ evolves from initial condition s_0 under motor commands $\{u_t\}_{t=0}^{T-1}$, then for any $G_{\delta, \Phi}$, the transformed trajectory $\{\tilde{s}_t\}_{t=0}^T$ defined by $\tilde{s}_t = G_{\delta, \Phi}(s_t)$ evolves from transformed initial condition $\tilde{s}_0 = G_{\delta, \Phi}(s_0)$ under the same command sequence.*

Proof. Since $t \in \{0, 1, 2, \dots, T\}$ is a discrete index enumerating time steps (with each step having duration $\Delta t > 0$), we proceed by mathematical induction on $P(t)$: $(\tilde{\mathbf{r}}_t, \tilde{\theta}_t) = (R(\phi)\mathbf{r}_t + \delta, \theta_t + \phi)$. Base case ($t = 0$): $P(0)$ holds by definition. Inductive step: assuming $P(k)$ holds, applying Eqs. (S28)–(S29) to transformed state \tilde{s}_k with motor command $u_k = (\mathbf{v}_k, \omega_k)$ yields for heading $\tilde{\theta}_{k+1} = \tilde{\theta}_k + \omega_k \Delta t = (\theta_k + \phi) + \omega_k \Delta t = \theta_{k+1} + \phi$, and for position:

$$\begin{aligned} \tilde{\mathbf{r}}_{k+1} &\stackrel{(S29)}{=} \tilde{\mathbf{r}}_k + R(\tilde{\theta}_k)\mathbf{v}_k \Delta t \stackrel{P(k)}{=} (R(\phi)\mathbf{r}_k + \delta) + R(\theta_k + \phi)\mathbf{v}_k \Delta t \\ &\stackrel{\text{Lem.1}(i)}{=} (R(\phi)\mathbf{r}_k + \delta) + R(\phi)R(\theta_k)\mathbf{v}_k \Delta t = R(\phi)(\mathbf{r}_k + R(\theta_k)\mathbf{v}_k \Delta t) + \delta \\ &\stackrel{(S29)}{=} R(\phi)\mathbf{r}_{k+1} + \delta, \end{aligned} \quad (S31)$$

where we used rotation composition $R(\theta_k + \phi) = R(\phi)R(\theta_k)$ and matrix distributivity. Thus $P(k+1)$ holds and by induction, $P(t)$ holds for all $t \geq 0$. \square

Corollary 1 (Equivariance constraint on learned representations). *Any network achieving zero prediction error on objective (S30) must learn an internal representation that respects the equivariance structure of the physical dynamics established in Proposition 1.*

Proof. Suppose the network achieves zero prediction error, meaning $\hat{p}(\cdot \mid y_0, \{u_t\}) = p(\cdot \mid s_T)$ almost surely where s_T results from the dynamics in Eqs. (S28)–(S29). Consider a transformed trajectory starting from $\tilde{s}_0 = G_{\delta, \Phi}(s_0)$ with corresponding initial observation \tilde{y}_0 . The network receives the same control sequence $\{u_t\}$ and must predict the spatial cell activations at the final transformed pose \tilde{s}_T . By Proposition 1, we know $\tilde{s}_T = G_{\delta, \Phi}(s_T)$. Since the place and head-direction cell activations are determined uniquely by pose, perfect prediction on both the original and transformed trajectories requires that the network's internal state evolution mirrors the geometric transformation: if the network maps $(y_0, \{u_t\})$ to some internal representation \mathbf{h}_T that encodes pose s_T , then it must map $(\tilde{y}_0, \{u_t\})$ to a representation $\tilde{\mathbf{h}}_T$ that encodes the transformed pose $\tilde{s}_T = G_{\delta, \Phi}(s_T)$. This equivariance constraint on the latent representation is a necessary consequence of achieving zero prediction error across all possible trajectories and their rigid transformations. \square

This geometric constraint, combined with stability requirements for recurrent integration, uniquely determines the structure of position-encoding neural codes as demonstrated next.

S1.5.3 Emergence of sinusoidal phase encoding

Having established that learned networks must exhibit equivariance, we now examine how LSTM hidden states encode position information. The key insight is that stable, composable position updates naturally lead to periodic representations. We posit that the LSTM hidden state $\mathbf{h} \in \mathbb{R}^d$ contains at least one two-dimensional subspace $\mathbf{y} = (y_1, y_2)^\top \in \mathbb{R}^2$ encoding position $\mathbf{r} \in \mathbb{R}^2$ through invertible linear mapping $\mathbf{r} = W\mathbf{y} + \mathbf{b}$ where $W \in \mathbb{R}^{2 \times 2}$ is invertible ($\det(W) \neq 0$) and $\mathbf{b} \in \mathbb{R}^2$ is bias[12]. The subspace updates via $\mathbf{y}_{t+1} = M(\Delta\mathbf{r}_t)\mathbf{y}_t$ where $M : \mathbb{R}^2 \rightarrow \mathbb{R}^{2 \times 2}$ is an update operator and $\Delta\mathbf{r}_t = \mathbf{r}_{t+1} - \mathbf{r}_t$ is position increment. This analyses one encoding frequency; multiple subspaces with different frequencies may coexist as shown later in Corollary 3.

Lemma 2 (Update operator constraints). *To support stable, composable path integration, we impose the following four constraints on the update operator M : (i) identity at zero $M(\mathbf{0}) = I_2$ ensuring no change under no displacement, (ii) continuity in $\Delta\mathbf{r}$ reflecting smooth neural dynamics, (iii) composable $M(\mathbf{a})M(\mathbf{b}) = M(\mathbf{a} + \mathbf{b})$ ensuring path-independence, and (iv) orthogonality $M(\Delta\mathbf{r})^\top M(\Delta\mathbf{r}) = I_2$ preserving norm for stability.*

Justification. Property (i): For path integration to be well-defined, zero displacement should not change the internal representation for any initial state \mathbf{y}_t , the requirement that $\mathbf{y}_{t+1} = M(\mathbf{0})\mathbf{y}_t = \mathbf{y}_t$ for all \mathbf{y}_t , which implies $M(\mathbf{0}) = I_2$. Property (ii): LSTM operations (matrix multiplications, additions, smooth activations) are continuous functions, naturally yielding continuity of M in $\Delta\mathbf{r}$. Property (iii): Consider two successive displacements $\mathbf{r}_t \xrightarrow{\mathbf{a}} \mathbf{r}_{t+1} = \mathbf{r}_t + \mathbf{a}$ yielding $\mathbf{y}_{t+1} = M(\mathbf{a})\mathbf{y}_t$ and $\mathbf{r}_{t+1} \xrightarrow{\mathbf{b}} \mathbf{r}_{t+2} = \mathbf{r}_{t+1} + \mathbf{b}$ yielding $\mathbf{y}_{t+2} = M(\mathbf{b})\mathbf{y}_{t+1} = M(\mathbf{b})M(\mathbf{a})\mathbf{y}_t$; path-independence requires this equals direct displacement result $\mathbf{y}_{t+2} = M(\mathbf{a} + \mathbf{b})\mathbf{y}_t$ for all \mathbf{y}_t , giving $M(\mathbf{a})M(\mathbf{b}) = M(\mathbf{a} + \mathbf{b})$. Property (iv): To avoid gradient explosion/vanishing during recurrent updates, we require norm preservation $\|\mathbf{y}_{t+1}\| = \|\mathbf{y}_t\|$ for all \mathbf{y}_t , giving $\|M(\Delta\mathbf{r}_t)\mathbf{y}_t\|^2 = \mathbf{y}_t^\top M^\top M \mathbf{y}_t = \|\mathbf{y}_t\|^2$ for all \mathbf{y}_t , implying $M^\top M = I_2$. \square

Theorem 1 (Rotation matrix structure with linear phase). *Any operator $M : \mathbb{R}^2 \rightarrow \mathbb{R}^{2 \times 2}$ satisfying the four properties in **Lemma 2** must have the form $M(\Delta\mathbf{r}) = R(\mathbf{q} \cdot \Delta\mathbf{r})$ for some frequency vector $\mathbf{q} = (q_x, q_y)^\top \in \mathbb{R}^2$, where $\mathbf{q} \cdot \Delta\mathbf{r} = q_x \Delta r_x + q_y \Delta r_y$ and $R(\cdot)$ is the rotation matrix from **Definition 2**.*

Proof. The proof proceeds by leveraging each constraint from **Lemma 2** systematically to determine the unique functional form of M . We divide the procedure of proof into the following 4 steps:

Step 1: M maps to the rotation group $SO(2)$. Property (iv) in **Lemma 2** establishes that $M(\Delta\mathbf{r})$ is orthogonal: $M(\Delta\mathbf{r})^\top M(\Delta\mathbf{r}) = I_2$. This means $M(\Delta\mathbf{r}) \in O(2)$, the orthogonal group. Additionally, Property (i) gives $M(\mathbf{0}) = I_2$ which has determinant +1. By Property (ii), M is continuous in $\Delta\mathbf{r}$, so $\det(M(\Delta\mathbf{r}))$ varies continuously with $\Delta\mathbf{r}$ while remaining in $\{-1, +1\}$ (the only possible determinants for orthogonal matrices). Since $\det(M(\mathbf{0})) = \det(I_2) = +1$ and determinant cannot jump discontinuously, we conclude $\det(M(\Delta\mathbf{r})) = +1$ for all $\Delta\mathbf{r}$. Therefore, $M(\Delta\mathbf{r}) \in SO(2)$, the special orthogonal group of rotation matrices.

Step 2: Deriving the functional equation from composability. Property (iii) in **Lemma 2** states $M(\mathbf{a})M(\mathbf{b}) = M(\mathbf{a} + \mathbf{b})$ for all $\mathbf{a}, \mathbf{b} \in \mathbb{R}^2$. Applying this recursively with $\mathbf{a} = \mathbf{b} = \Delta\mathbf{r}$ yields:

$$M(2\Delta\mathbf{r}) = M(\Delta\mathbf{r} + \Delta\mathbf{r}) = M(\Delta\mathbf{r})M(\Delta\mathbf{r}) = M(\Delta\mathbf{r})^2. \quad (\text{S32})$$

Continuing inductively, $M(n\Delta\mathbf{r}) = M(\Delta\mathbf{r})^n$ for any positive integer $n \in \mathbb{N}$. For negative integers, using Property (i) we have $I_2 = M(\mathbf{0}) = M(\Delta\mathbf{r} + (-\Delta\mathbf{r})) = M(\Delta\mathbf{r})M(-\Delta\mathbf{r})$, so $M(-\Delta\mathbf{r}) = M(\Delta\mathbf{r})^{-1}$, extending the power rule to all integers $n \in \mathbb{Z}$. For rational exponents, consider $n, m \in \mathbb{N}$ with $m \neq 0$. Let $\mathbf{w} = \Delta\mathbf{r}/m$. Then, we have $M(\Delta\mathbf{r}) = M(m\mathbf{w}) = M(\mathbf{w})^m$. In $SO(2)$, every rotation $R(\theta)$ has m distinct m -th roots: $R(\theta/m + 2\pi k/m)$ for $k = 0, 1, \dots, m-1$. However, by continuity of M (Property (ii)) and $M(\mathbf{0}) = I_2$, for small $\|\Delta\mathbf{r}\|$, we must have $M(\Delta\mathbf{r})$ close to I_2 , which uniquely determines the principal root with $k = 0$. Extending by continuity for all $\Delta\mathbf{r}$, we obtain $M(\mathbf{w}) = M(\Delta\mathbf{r})^{1/m}$ as the unique continuous choice. Therefore:

$$M\left(\frac{n}{m}\Delta\mathbf{r}\right) = M(n\mathbf{w}) = M(\mathbf{w})^n = \left(M(\Delta\mathbf{r})^{1/m}\right)^n = M(\Delta\mathbf{r})^{n/m}. \quad (\text{S33})$$

Thus $M(\alpha\Delta\mathbf{r}) = M(\Delta\mathbf{r})^\alpha$ holds for all $\alpha \in \mathbb{Q}$ (Set of rational number). Invoking Property (ii), continuity of M in $\Delta\mathbf{r}$, combined with density of rationals in reals, extends this to all $\alpha \in \mathbb{R}$:

$$M(\alpha\Delta\mathbf{r}) = M(\Delta\mathbf{r})^\alpha \quad \text{for all } \alpha \in \mathbb{R}, \Delta\mathbf{r} \in \mathbb{R}^2. \quad (\text{S34})$$

Step 3: Characterizing rotation matrices via one-parameter subgroups. Since $M(\Delta\mathbf{r}) \in SO(2)$ (from Step 1), we can write $M(\Delta\mathbf{r}) = R(\theta(\Delta\mathbf{r}))$ for some angle function $\theta : \mathbb{R}^2 \rightarrow \mathbb{R}$. From Property (iii), the composability $M(\mathbf{a})M(\mathbf{b}) = M(\mathbf{a} + \mathbf{b})$ translates to:

$$R(\theta(\mathbf{a}))R(\theta(\mathbf{b})) \stackrel{\text{Lem.1(i)}}{=} R(\theta(\mathbf{a}) + \theta(\mathbf{b})) = R(\theta(\mathbf{a} + \mathbf{b})). \quad (\text{S35})$$

Since $R(\cdot)$ is injective modulo 2π , this gives $\theta(\mathbf{a} + \mathbf{b}) = \theta(\mathbf{a}) + \theta(\mathbf{b}) \pmod{2\pi}$. Property (ii) ensures θ is continuous. Property (i) provides $M(\mathbf{0}) = I_2 = R(0)$, thus $\theta(\mathbf{0}) = 0 \pmod{2\pi}$. Choosing the continuous branch with $\theta(\mathbf{0}) = 0$, we obtain the additive Cauchy functional equation:

$$\theta(\mathbf{a} + \mathbf{b}) = \theta(\mathbf{a}) + \theta(\mathbf{b}), \quad \theta(\mathbf{0}) = 0. \quad (\text{S36})$$

Step 4: Solving the Cauchy equation yields linear form. The continuous solution to the additive functional **Eq. (S36)** on \mathbb{R}^2 must be linear: $\theta(\Delta\mathbf{r}) = \mathbf{q} \cdot \Delta\mathbf{r}$ for some constant vector $\mathbf{q} = (q_x, q_y)^\top \in \mathbb{R}^2$. To see this, first restrict to one-dimensional subspaces. For any fixed unit vector $\mathbf{e} \in \mathbb{R}^2$ with $\|\mathbf{e}\| = 1$, define $f_{\mathbf{e}}(\xi) = \theta(\xi\mathbf{e})$ for $\xi \in \mathbb{R}$. Then **Eq. (S36)** gives:

$$f_{\mathbf{e}}(\xi + \eta) = \theta(\xi\mathbf{e} + \eta\mathbf{e}) = \theta(\xi\mathbf{e}) + \theta(\eta\mathbf{e}) = f_{\mathbf{e}}(\xi) + f_{\mathbf{e}}(\eta), \quad (\text{S37})$$

with $f_{\mathbf{e}}(0) = 0$. Since θ is continuous (Property (ii)), $f_{\mathbf{e}}$ is also continuous. The unique continuous solution to Cauchy's functional equation $f(\xi + \eta) = f(\xi) + f(\eta)$ on \mathbb{R} is $f_{\mathbf{e}}(\xi) = c_{\mathbf{e}}\xi$ for some constant $c_{\mathbf{e}} \in \mathbb{R}$. Thus $\theta(\xi \mathbf{e}) = c_{\mathbf{e}}\xi$.

For a general displacement $\Delta \mathbf{r} = \Delta r_x \mathbf{e}_x + \Delta r_y \mathbf{e}_y$ where $\mathbf{e}_x = (1, 0)^\top$ and $\mathbf{e}_y = (0, 1)^\top$ are the standard basis vectors, linearity of θ from **Eq. (S36)** yields:

$$\begin{aligned}\theta(\Delta \mathbf{r}) &= \theta(\Delta r_x \mathbf{e}_x + \Delta r_y \mathbf{e}_y) = \theta(\Delta r_x \mathbf{e}_x) + \theta(\Delta r_y \mathbf{e}_y) \\ &= c_{\mathbf{e}_x} \Delta r_x + c_{\mathbf{e}_y} \Delta r_y = \mathbf{q} \cdot \Delta \mathbf{r},\end{aligned}\quad (\text{S38})$$

where we defined $\mathbf{q} = (c_{\mathbf{e}_x}, c_{\mathbf{e}_y})^\top = (q_x, q_y)^\top$. This is the inner product between frequency vector \mathbf{q} and displacement $\Delta \mathbf{r}$.

Combining Steps 1–4, we have established that $M(\Delta \mathbf{r}) = R(\theta(\Delta \mathbf{r})) = R(\mathbf{q} \cdot \Delta \mathbf{r})$, where the rotation angle is a linear function of the displacement. Each of the four properties in **Lemma 2** was essential: Property (i) fixed the identity element and normalization, Property (ii) enabled application of continuous functional equation theory, Property (iii) imposed the group homomorphism structure yielding the additive Cauchy equation, and Property (iv) restricted the image to rotation matrices in $SO(2)$. The frequency vector \mathbf{q} emerges as the unique free parameter characterizing the rate of phase advance per unit displacement, thereby determining the spatial periodicity of the neural representation. \square

Corollary 2 (Cosine-Sine phase encoding). *Under rotation update $M(\Delta \mathbf{r}) = R(\mathbf{q} \cdot \Delta \mathbf{r})$, accumulated displacement $\mathbf{R} = \mathbf{r}_T - \mathbf{r}_0$ from initial $\mathbf{y}_0 = (1, 0)^\top$ yields $\mathbf{y}_T = (\cos(\mathbf{q} \cdot \mathbf{R}), \sin(\mathbf{q} \cdot \mathbf{R}))^\top$, revealing position encoding through sinusoidal functions in quadrature—the fundamental signature of grid cells.*

Proof. Iterating the update equation $\mathbf{y}_{t+1} = M(\Delta \mathbf{r}_t) \mathbf{y}_t$ from $t = 0$ to $T - 1$ yields $\mathbf{y}_T = \prod_{t=0}^{T-1} M(\Delta \mathbf{r}_t) \mathbf{y}_0$. Substituting $M(\Delta \mathbf{r}_t) = R(\mathbf{q} \cdot \Delta \mathbf{r}_t)$ from **Theorem 1** and using composition property from **Lemma 1(i)** gives $\mathbf{y}_T = R\left(\sum_{t=0}^{T-1} \mathbf{q} \cdot \Delta \mathbf{r}_t\right) \mathbf{y}_0 = R(\mathbf{q} \cdot \mathbf{R}) \mathbf{y}_0$ where $\mathbf{R} = \sum_{t=0}^{T-1} \Delta \mathbf{r}_t = \mathbf{r}_T - \mathbf{r}_0$ is the cumulative displacement. Taking $\mathbf{y}_0 = (1, 0)^\top$ as initial state and applying **Definition 2**, we have:

$$\mathbf{y}_T = R(\mathbf{q} \cdot \mathbf{R}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(\mathbf{q} \cdot \mathbf{R}) & -\sin(\mathbf{q} \cdot \mathbf{R}) \\ \sin(\mathbf{q} \cdot \mathbf{R}) & \cos(\mathbf{q} \cdot \mathbf{R}) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(\mathbf{q} \cdot \mathbf{R}) \\ \sin(\mathbf{q} \cdot \mathbf{R}) \end{pmatrix}. \quad (\text{S39})$$

Thus, path integration over arbitrary trajectories reduces to evaluating sinusoidal functions of the net displacement's projection onto frequency vector \mathbf{q} . The phase $\phi = \mathbf{q} \cdot \mathbf{R}$ linearly encodes position, while the quadrature pair $(\cos \phi, \sin \phi)$ provides full 2π -periodic coverage necessary for unambiguous spatial representation—the fundamental computational signature observed in biological grid cells. \square

S1.5.4 Hexagonal symmetry from directional isotropy

Having derived sinusoidal phase encoding for individual subspaces, we now address how multiple frequency components combine to produce hexagonal spatial patterns. The crucial insight is that robust spatial representation requires directional isotropy—uniform sensitivity across all navigation directions. For this purpose, LSTM hidden states employ multiple independent two-dimensional subspaces $\{\mathbf{y}^{(j)}\}_{j=1}^K$ each with frequency vector $\mathbf{q}_j \in \mathbb{R}^2$ of equal magnitude $\|\mathbf{q}_j\| = q > 0$ with unit direction $\mathbf{u}_j = \mathbf{q}_j/q$ with $\|\mathbf{u}_j\| = 1$. Multiple frequencies provide spatial resolution at various granularities, robustness against noise, and disambiguation through coarse-fine scale combinations.

Definition 6 (Directional isotropy). *A multi-frequency representation achieves directional isotropy (uniform sensitivity across all displacement directions) if: (i) first-order isotropy $\sum_{j=1}^K \mathbf{u}_j = \mathbf{0}$, ensuring no net directional bias, and (ii) second-order isotropy $\sum_{j=1}^K \mathbf{u}_j \mathbf{u}_j^\top = \lambda I_2$ for some $\lambda > 0$, ensuring equal representational capacity along all axes. The outer product $\mathbf{u}_j \mathbf{u}_j^\top \in \mathbb{R}^{2 \times 2}$ is a rank-one matrix encoding directional concentration.*

Lemma 3 (Minimal configuration size). *The minimum number of unit vectors satisfying both isotropy conditions is $K = 3$.*

Proof. For $K = 1$, first-order condition gives $\mathbf{u}_1 = \mathbf{0}$ contradicting $\|\mathbf{u}_1\| = 1$, thus $K = 1$ is impossible. For $K = 2$, first-order condition gives $\mathbf{u}_1 + \mathbf{u}_2 = \mathbf{0}$, implying $\mathbf{u}_2 = -\mathbf{u}_1$. Then $\sum_{j=1}^2 \mathbf{u}_j \mathbf{u}_j^\top = \mathbf{u}_1 \mathbf{u}_1^\top + (-\mathbf{u}_1)(-\mathbf{u}_1)^\top = 2\mathbf{u}_1 \mathbf{u}_1^\top$, which is a rank-1 matrix (all rows are multiples of \mathbf{u}_1^\top) while λI_2 has rank 2 for any $\lambda > 0$, yielding contradiction. Thus $K \geq 3$. \square

Theorem 2 (Minimal isotropic configuration). *For $K = 3$, the unique configuration (up to global rotation) satisfying both isotropy conditions comprises three unit vectors equally spaced by 120° angular separation.*

Proof. We construct the solution systematically from the isotropy conditions. Parametrize the three unit vectors as $\mathbf{u}_j = (\cos \alpha_j, \sin \alpha_j)^\top$ for $j = 1, 2, 3$ where $\alpha_j \in [0, 2\pi)$ denote the angles measured counterclockwise from the positive x -axis. Our goal is to determine the angular configuration $\{\alpha_1, \alpha_2, \alpha_3\}$ uniquely from the two isotropy conditions in **Definition 6**.

Without loss of generality, we fix $\alpha_1 = 0$ by rotational invariance, reducing the problem to finding α_2 and α_3 . The first-order isotropy condition $\sum_{j=1}^3 \mathbf{u}_j = \mathbf{0}$ decomposes into two scalar equations by examining the x and y components separately:

$$\cos 0 + \cos \alpha_2 + \cos \alpha_3 = 1 + \cos \alpha_2 + \cos \alpha_3 = 0, \quad (\text{S40})$$

$$\sin 0 + \sin \alpha_2 + \sin \alpha_3 = \sin \alpha_2 + \sin \alpha_3 = 0. \quad (\text{S41})$$

From **Eq. (S41)**, we obtain $\sin \alpha_3 = -\sin \alpha_2$. This constraint has two families of solutions: either $\alpha_3 = -\alpha_2 \pmod{2\pi}$, which gives $\alpha_3 = 2\pi - \alpha_2$ for $\alpha_2 \in (0, 2\pi)$, or $\alpha_3 = \pi + \alpha_2$. We examine each case separately.

For the First case $\alpha_3 = \pi + \alpha_2$, substituting into **Eq. (S40)**, we have:

$$1 + \cos \alpha_2 + \cos(\pi + \alpha_2) = 1 + \cos \alpha_2 - \cos \alpha_2 = 1 \neq 0, \quad (\text{S42})$$

producing a contradiction. Thus this case is impossible.

For the second case $\alpha_3 = 2\pi - \alpha_2$, substituting into **Eq. (S40)** yields:

$$1 + \cos \alpha_2 + \cos(2\pi - \alpha_2) = 1 + \cos \alpha_2 + \cos \alpha_2 = 1 + 2 \cos \alpha_2 = 0, \quad (\text{S43})$$

where we used $\cos(2\pi - \alpha_2) = \cos(-\alpha_2) = \cos \alpha_2$. Solving **Eq. (S43)**, we obtain $\cos \alpha_2 = -1/2$. Since $\alpha_2 \in (0, 2\pi)$ and $\alpha_2 \neq \pi$ (else $\alpha_3 = \pi$, violating distinctness), we have $\alpha_2 = 2\pi/3 = 120^\circ$ or $\alpha_2 = 4\pi/3 = 240^\circ$. If $\alpha_2 = 120^\circ$, we have $\alpha_3 = 2\pi - 120^\circ = 240^\circ$, giving the configuration $\{0^\circ, 120^\circ, 240^\circ\}$ with consecutive spacing of 120° . We conclude that the unique angular configuration is $\{\alpha_1, \alpha_2, \alpha_3\} = \{0^\circ, 120^\circ, 240^\circ\}$, corresponding to the explicit unit vectors:

$$\mathbf{u}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix}, \quad \mathbf{u}_3 = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix}. \quad (\text{S44})$$

To verify completeness, we confirm the second-order isotropy condition. Computing the outer products:

$$\mathbf{u}_1 \mathbf{u}_1^\top = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{u}_2 \mathbf{u}_2^\top = \begin{pmatrix} 1/4 & -\sqrt{3}/4 \\ -\sqrt{3}/4 & 3/4 \end{pmatrix}, \quad \mathbf{u}_3 \mathbf{u}_3^\top = \begin{pmatrix} 1/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & 3/4 \end{pmatrix}, \quad (\text{S45})$$

and summing them up, we obtain $\sum_{j=1}^3 \mathbf{u}_j \mathbf{u}_j^\top = \begin{pmatrix} 3/2 & 0 \\ 0 & 3/2 \end{pmatrix} = \frac{3}{2} I_2$, confirming second-order isotropy with $\lambda = 3/2$. The configuration is unique up to global rotation since fixing $\alpha_1 = 0$ removes the rotational degree of freedom, and the choice $\alpha_2 = 240^\circ$ simply corresponds to rotating the entire configuration by 120° . \square

Corollary 3 (Hexagonal periodicity from cosine symmetry). *The three-directional isotropic configuration induces hexagonal spatial periodicity with 60° rotational symmetry in neural firing patterns.*

Proof. From **Corollary 2**, the two-dimensional neural activity in subspace j is given by $\mathbf{y}^{(j)} = (\cos(\mathbf{q}_j \cdot \mathbf{r}), \sin(\mathbf{q}_j \cdot \mathbf{r}))^\top$.

Directional symmetry from cosine evenness: The cosine function possesses even symmetry: $\cos(-\mathbf{q}_j \cdot \mathbf{r}) = \cos(\mathbf{q}_j \cdot \mathbf{r})$. This means that frequency vector \mathbf{q}_j and its opposite $-\mathbf{q}_j$ produce identical spatial modulation in the cosine component. When considering the combined activity pattern formed by summing cosine terms from all subspaces, the three frequency directions $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ at angles $\{0^\circ, 120^\circ, 240^\circ\}$ generate stripe patterns whose interference is equivalent to that produced by six plane-wave components at angles $\{0^\circ, 60^\circ, 120^\circ, 180^\circ, 240^\circ, 300^\circ\}$ evenly spaced by 60° . This six-fold directional symmetry in the cosine-based firing pattern is the hallmark of hexagonal geometry[8].

Stripe pattern superposition: The combined neural activity aggregating contributions from all three subspaces takes the form:

$$A(\mathbf{r}) = \sum_{j=1}^3 \cos(\mathbf{q}_j \cdot \mathbf{r}). \quad (\text{S46})$$

Each individual term $\cos(\mathbf{q}_j \cdot \mathbf{r})$ represents a periodic stripe pattern in two-dimensional space: regions where $\mathbf{q}_j \cdot \mathbf{r} \approx 0 \pmod{2\pi}$ exhibit high activity (bright stripes, such as red area in **Fig. S4**), while regions where $\mathbf{q}_j \cdot \mathbf{r} \approx \pi \pmod{2\pi}$ exhibit low activity (dark stripes, such as green or blue area in **Fig. S4**). The stripes are parallel lines perpendicular to direction \mathbf{u}_j , repeating with spatial period $\lambda = 2\pi/q$ where $q = \|\mathbf{q}_j\|$. Thus, $A(\mathbf{r})$ represents the superposition of three stripe patterns oriented at $0^\circ, 120^\circ$, and 240° , each with identical spatial frequency.

Interference creates triangular grid: The superposition $A(\mathbf{r})$ achieves its global maximum value of 3 precisely at positions where all three stripe patterns simultaneously reach their individual peaks, satisfying $\mathbf{q}_j \cdot \mathbf{r} = 2\pi n_j$ for integers $n_j \in \mathbb{Z}$,

$j = 1, 2, 3$. Geometrically, this occurs at the intersection points of bright stripes from all three orientations. Consider three families of parallel lines in the plane, each family rotated 120° from the others. Elementary geometry establishes that such a configuration produces intersection points forming an equilateral triangular grid: each “cell” bounded by six line segments forms a regular hexagon, and the vertices of these hexagons constitute a triangular lattice. Specifically, any intersection point has six nearest-neighbor intersection points arranged symmetrically at 60° intervals around a circle, all at equal distance.

Hexagonal periodicity from triangular symmetry: The triangular lattice of peak firing locations possesses 60° rotational symmetry: rotating the entire pattern by 60° maps the lattice onto itself. Equivalently, we can describe this structure as a hexagonal lattice by noting that each lattice point is surrounded by six equidistant neighbors forming a regular hexagon. The spatial periodicity repeats with characteristic length scale (determined by q), and the firing pattern exhibits the hallmark signatures of biological grid cells: hexagonal arrangement of firing fields, 60° rotational symmetry, and periodic tiling of the navigable space. This demonstrates that the three-direction isotropic configuration from **Theorem 2** necessarily produces hexagonal spatial representations through wave interference, bridging the abstract frequency-space symmetry to the concrete real-space geometry observed in neural recordings. \square

Corollary 3 posits hexagonal symmetry as a necessary consequence of geometric isotropy, offers a distinct perspective from mechanisms centered on nonlinear optimization. For instance, recent work demonstrates that hexagonal patterns are actively selected as the optimal solution when a nonnegativity constraint on firing rates is imposed [13]. In that framework, nonnegativity acts as a nonlinear stabilization force that breaks the degeneracy of many possible linear solutions (i.e., plane waves on an annulus), thereby favoring the 120° triplet configuration. Our theory, in contrast, establishes this 120° configuration not merely as a selected optimum, but as the unique minimal ($K = 3$) solution that fundamentally satisfies the kinematic requirement for directional isotropy.

S1.6 Derivation of the variational bound for the predictive information bottleneck

This section establishes a rigorous mathematical framework for optimizing emergent communication protocols through variational inference. This framework is based on the well-known Information Bottleneck (IB) theory [1, 16], an elegant but intractable information theoretic solution, which is to optimize the inference quality under communication bandwidth constraints between two agents for fulfilling a specific mission. The resulting solution is the IB principle that balances the compression ratio for a certain level of inference quality and bandwidth consumption for such compressed information sharing. The core challenge lies in translating the IB principle into a computationally feasible training procedure. To use IB theory to solve our current problem at hand, its formulation naturally balances communication efficiency against predictive power by simultaneously minimizing the compression cost (rate) and maximizing the utility of transmitted messages for predicting the receiver’s future observations (distortion). However, direct optimization is fundamentally intractable, as it requires computing mutual information between high-dimensional neural representations governed by unknown probability distributions. We resolve this obstacle through variational inference, deriving tight upper for communication efficiency and lower bounds for prediction accuracy that transform the abstract IB objective into a fully differentiable loss function amenable to gradient-based optimization. This derivation proceeds as follows: we first establish notation and mathematical preliminaries, then derive tractable bounds for the rate term (**Method S1.6.1**), followed by bounds for the distortion term (**Method S1.6.2**), and finally synthesize these components into the unified variational information bottleneck (VIB) objective (**Method S1.6.3**).

Notation and problem formulation. Throughout this derivation, we adopt the following notation for clarity and consistency. The sender agent i at time t maintains internal state $S_i \equiv S_{i,t}$, encoding its current environmental context, sensory history, and predictive model. The receiver agent j possesses analogous state $S_j \equiv S_{j,t}$, representing its own perspective. Communication occurs through a latent message variable $z \equiv m_{i,t}$ generated stochastically by the sender’s encoder. The receiver’s future observation $O'_j \equiv O_{j,t+1}$ serves as the prediction target whose uncertainty we seek to minimize through communication. In multi-agent coordination tasks, effective communication requires transmitting information that maximally reduces the receiver’s uncertainty about its own future sensory experience, conditioned on what the receiver already knows from its current state.

The Information Bottleneck objective from the main text **Eq. (4)** formalizes this principle as a loss function that balances predictive accuracy against communication cost:

$$\mathcal{L}_{\text{IB}} = \underbrace{-I(z; O'_j | S_j)}_{\text{Distortion}} + \beta \underbrace{I(S_i; z)}_{\text{Rate}}, \quad (\text{S47})$$

where $I(\cdot; \cdot)$ denotes mutual information, and $\beta > 0$ is a hyperparameter controlling the rate-distortion trade-off. We minimize \mathcal{L}_{IB} with respect to the encoder distribution. The **Distortion** term $-I(z; O'_j | S_j)$ is the negative conditional mutual information—minimizing distortion maximizes the information the message provides about the receiver’s future observation O'_j beyond what the receiver can infer from its current state S_j alone. The **Rate** term $I(S_i; z)$ quantifies the communication cost—the amount of information the message retains about the sender’s state after communication, which is to minimize for

compression. The parameter β implements a soft bandwidth constraint: larger β penalizes communication cost more severely, promoting compressed, abstract representations.

Direct optimization of Eq. (S47) is intractable for three fundamental reasons. First, computing mutual information requires integrating over the joint distribution of high-dimensional continuous variables (neural network hidden states), which cannot be evaluated analytically or estimated efficiently from finite samples. Second, the conditional mutual information $I(z; O'_j | S_j)$ involves the true data distribution $p(O'_j | S_j, z)$ governing environment dynamics, which is unknown and potentially complex. Third, even if these distributions were known, the required high-dimensional integrals lack closed-form solutions and suffer from exponential computational complexity. We therefore seek variational surrogates—computable bounds that preserve the essential structure of the IB objective while enabling practical optimization through standard deep learning tools.

S1.6.1 Deriving a tractable upper bound for the communication rate

Considering the intractability of the IB objective in Eq. (S47), we now construct a tractable surrogate for the communication rate term $I(S_i; z)$, which quantifies the bandwidth of intended transmitted messages. We proceed through three steps: formalizing the mutual information under parametric encoding, identifying the computational obstacle posed by aggregate posterior marginalization, and deriving a tight variational upper bound through KL divergence.

Definition 7 (Parametric encoder and aggregate posterior). *The sender encodes its state S_i into message z through a stochastic encoder $q_\varphi(z|S_i)$ parameterized by neural network weights φ . The mutual information between state and message under this encoding is*

$$I_q(S_i; z) = \int p(S_i) \int q_\varphi(z|S_i) \log \frac{q_\varphi(z|S_i)}{q(z)} dz dS_i, \quad (\text{S48})$$

where $q(z) = \int p(S_i) q_\varphi(z|S_i) dS_i$ denotes the aggregate posterior—the marginal distribution of messages obtained by averaging encoder outputs over all possible sender states weighted by their occurrence probability $p(S_i)$ in the environment.

The computational obstacle arises from the aggregate posterior $q(z)$, which requires integrating over the entire data distribution $p(S_i)$ —an unknown, high-dimensional distribution of neural network hidden states. This integration is intractable both analytically (no closed form exists even for simple encoders) and numerically (Monte Carlo estimation suffers from exponential sample complexity in high dimensions and introduces high variance gradients unsuitable for optimization). We circumvent this obstacle by introducing a fixed prior distribution that serves as a tractable surrogate for the aggregate posterior.

Lemma 4 (Variational rate bound via prior substitution). *Let $p(z)$ be a fixed prior distribution over message space, typically chosen as an isotropic Gaussian $\mathcal{N}(0, I)$ for analytical tractability. The mutual information between sender state and message satisfies the upper bound*

$$I_q(S_i; z) \leq \mathbb{E}_{p(S_i)}[D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))], \quad (\text{S49})$$

where $D_{\text{KL}}(\cdot \| \cdot)$ denotes the Kullback-Leibler divergence and the right-hand side involves only pointwise encoder-prior comparisons, not the intractable aggregate posterior.

Proof. We establish the bound through algebraic manipulation exploiting KL divergence non-negativity. Expanding the expected KL divergence between encoder and prior yields

$$\mathbb{E}_{p(S_i)}[D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))] = \int p(S_i) \int q_\varphi(z|S_i) \log \frac{q_\varphi(z|S_i)}{p(z)} dz dS_i. \quad (\text{S50})$$

The key step is logarithmic decomposition: introducing and subtracting the aggregate posterior $q(z)$ in the numerator and denominator gives

$$\log \frac{q_\varphi(z|S_i)}{p(z)} = \log \frac{q_\varphi(z|S_i)}{q(z)} + \log \frac{q(z)}{p(z)}. \quad (\text{S51})$$

Substituting this decomposition into the expectation and separating integrals yields

$$\begin{aligned} \mathbb{E}_{p(S_i)}[D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))] &= \int p(S_i) \int q_\varphi(z|S_i) \left[\log \frac{q_\varphi(z|S_i)}{q(z)} + \log \frac{q(z)}{p(z)} \right] dz dS_i \\ &= \underbrace{\int p(S_i) \int q_\varphi(z|S_i) \log \frac{q_\varphi(z|S_i)}{q(z)} dz dS_i}_{I_q(S_i; z)} + \underbrace{\int q(z) \log \frac{q(z)}{p(z)} dz}_{D_{\text{KL}}(q(z) \| p(z)) \geq 0}, \end{aligned} \quad (\text{S52})$$

where the second term follows from $\int p(S_i) q_\varphi(z|S_i) dS_i = q(z)$ by definition of aggregate posterior. The fundamental property of KL divergence—non-negativity $D_{\text{KL}}(q(z) \| p(z)) \geq 0$ with equality if and only if $q(z) = p(z)$ almost everywhere—immediately yields inequality (S49). \square

Remark (Computational tractability and optimization implications). **Lemma 4** transforms an intractable mutual information into a tractable expectation of KL divergence. For Gaussian encoder $q_\varphi(z|S_i) = \mathcal{N}(\mathbf{m}_\varphi(S_i), \Sigma_\varphi(S_i))$ and Gaussian prior $p(z) = \mathcal{N}(0, I)$, the KL divergence admits closed form $D_{\text{KL}}(q_\varphi(z|S_i) \| p(z)) = \frac{1}{2}[\text{tr}(\Sigma_\varphi) + \mathbf{m}_\varphi^\top \mathbf{m}_\varphi - \log \det(\Sigma_\varphi) - d]$ where d is message dimensionality, enabling efficient gradient computation. Minimizing this upper bound during training explicitly penalizes the encoder for producing messages that deviate from the prior distribution, thereby enforcing compression: the encoder learns to allocate its limited information capacity only to features critical for the downstream prediction task, discarding sender-specific details irrelevant to the receiver.

S1.6.2 Deriving a tractable upper bound for the distortion

Having constructed a tractable upper bound for the communication rate, we now address the complementary challenge: bounding the distortion term $-I(z; O'_j | S_j)$ in the IB objective. The distortion quantifies the negative information the message provides about the receiver's future observations—minimizing distortion corresponds to maximizing predictive utility. We establish an upper bound amenable to optimization through a three-step derivation: entropy decomposition, identification of the optimization-relevant component, and variational approximation via a parametric decoder.

Proposition 2 (Entropy decomposition of conditional mutual information). *The conditional mutual information between message z and future observation O'_j given receiver state S_j admits the entropy decomposition*

$$I(z; O'_j | S_j) = H(O'_j | S_j) - H(O'_j | z, S_j), \quad (\text{S53})$$

where $H(O'_j | S_j)$ represents the receiver's baseline uncertainty about its future using only its current state, and $H(O'_j | z, S_j)$ represents the residual uncertainty after incorporating the message z .

Proof. This is a standard identity from information theory. By definition, conditional mutual information is $I(z; O'_j | S_j) = H(z | S_j) - H(z | O'_j, S_j)$. Equivalently, using the symmetric form, $I(z; O'_j | S_j) = H(O'_j | S_j) - H(O'_j | z, S_j)$. To verify: expanding using conditional entropy definitions, $H(O'_j | S_j) - H(O'_j | z, S_j) = [H(O'_j, S_j) - H(S_j)] - [H(O'_j, z, S_j) - H(z, S_j)] = H(O'_j, S_j) - H(S_j) - H(O'_j, z, S_j) + H(z, S_j)$. Using the chain rule $H(O'_j, z, S_j) = H(O'_j, S_j) + H(z | O'_j, S_j)$ and $H(z, S_j) = H(S_j) + H(z | S_j)$, we obtain $H(O'_j, S_j) - H(S_j) - [H(O'_j, S_j) + H(z | O'_j, S_j)] + [H(S_j) + H(z | S_j)] = H(z | S_j) - H(z | O'_j, S_j) = I(z; O'_j | S_j)$, confirming the identity. \square

Remark (Optimization-relevant component). *The first term $H(O'_j | S_j)$ in Eq. (S53) represents the baseline unpredictability of the receiver's future independent of the communication for the message z . Since this term is parameter-independent, it acts as an additive constant when optimizing \mathcal{L}_{IB} . Therefore, minimizing the distortion $-I(z; O'_j | S_j) = -H(O'_j | S_j) + H(O'_j | z, S_j)$ with respect to model parameters is equivalent to minimizing the conditional entropy $H(O'_j | z, S_j)$. Intuitively, minimizing distortion is equivalent to minimizing the receiver's residual uncertainty about its future after processing the message.*

The conditional entropy $H(O'_j | z, S_j) = -\mathbb{E}_{p(z, S_j)}[\int p(O'_j | z, S_j) \log p(O'_j | z, S_j) dO'_j]$ remains intractable because it requires the knowledge of the true conditional distribution $p(O'_j | z, S_j)$ governing how the receiver's future observations depend on both the message z and its current state. This distribution encodes complex environmental dynamics and is generally unknown. We resolve this through variational approximation, introducing a parametric decoder network $p_\vartheta(O'_j | z, S_j)$ that learns to predict future observations from the exchanged messages and receiver states.

Lemma 5 (Variational entropy bound via decoder approximation). *Let $p_\vartheta(O'_j | z, S_j)$ be a parametric decoder approximating the true conditional distribution. The conditional entropy satisfies the upper bound*

$$H(O'_j | z, S_j) \leq -\mathbb{E}_{p(z, S_j, O'_j)}[\log p_\vartheta(O'_j | z, S_j)], \quad (\text{S54})$$

where the right-hand side is the expected negative log-likelihood (reconstruction error) under the decoder, a quantity tractable for gradient-based optimization.

Proof. The proof exploits KL divergence non-negativity between the true and approximate conditional distributions. For any fixed (z, S_j) pair, the KL divergence from true to approximate distribution satisfies

$$D_{\text{KL}}(p(O'_j | z, S_j) \| p_\vartheta(O'_j | z, S_j)) = \int p(O'_j | z, S_j) \log \frac{p(O'_j | z, S_j)}{p_\vartheta(O'_j | z, S_j)} dO'_j \geq 0. \quad (\text{S55})$$

Expanding the logarithm and separating integrals yields

$$\underbrace{\int p(O'_j | z, S_j) \log p(O'_j | z, S_j) dO'_j}_{-h(p(\cdot | z, S_j))} - \int p(O'_j | z, S_j) \log p_\vartheta(O'_j | z, S_j) dO'_j \geq 0. \quad (\text{S56})$$

where $h(p) := -\int p(x) \log p(x) dx$ denotes the Shannon entropy functional. Rearranging **Ineq. (S56)** gives $h(p(\cdot|z, S_j)) \leq -\int p(O'_j | z, S_j) \log p_\vartheta(O'_j | z, S_j) dO'_j$. Multiplying by -1 and taking expectations over $p(z, S_j)$ on both sides, we have

$$H(O'_j | z, S_j) = \mathbb{E}_{p(z, S_j)}[h(p(\cdot|z, S_j))] \leq -\mathbb{E}_{p(z, S_j, O'_j)}[\log p_\vartheta(O'_j | z, S_j)], \quad (\text{S57})$$

establishing **inequality (S54)**. \square

Corollary 4 (Variational upper bound on distortion). *Combining **Proposition 2** and **Lemma 5**, the distortion term satisfies the upper bound*

$$-I(z; O'_j | S_j) = -H(O'_j | S_j) + H(O'_j | z, S_j) \leq -H(O'_j | S_j) + \mathbb{E}_{p(z, S_j, O'_j)}[-\log p_\vartheta(O'_j | z, S_j)]. \quad (\text{S58})$$

Since $H(O'_j | S_j)$ is parameter-independent, minimizing this upper bound is equivalent to minimizing the expected negative log-likelihood (reconstruction error). Consequently, minimizing reconstruction error minimizes an upper bound on the distortion, ensuring messages become maximally predictive of receiver futures during training.

Proof. From **Proposition 2**, $-I(z; O'_j | S_j) = -H(O'_j | S_j) + H(O'_j | z, S_j)$. Applying **Lemma 5**'s upper bound on the conditional entropy gives the stated inequality. Since $H(O'_j | S_j)$ is constant with respect to model parameters, minimizing the bound reduces to minimizing $\mathbb{E}[-\log p_\vartheta(O'_j | z, S_j)]$ —the negative log-likelihood loss ubiquitous in supervised learning. \square

S1.6.3 Synthesis: Variational information bottleneck objective

Having derived tractable bounds for both rate and distortion, we now synthesize these components into a unified training objective. The preceding derivations resolved the fundamental computational obstacles in the IB principle through complementary variational approximations: an upper bound for the intractable rate term (**Lemma 4**) and an upper bound for the intractable distortion term (**Corollary 4**). We now demonstrate how these bounds combine to yield the variational information bottleneck (VIB) loss function—a fully tractable surrogate that preserves the essential feature of the original IB objective while enabling a tractable gradient-based optimization.

Theorem 3 (Variational information bottleneck bound). *The intractable Information Bottleneck objective $\mathcal{L}_{IB} = -I(z; O'_j | S_j) + \beta I(S_i; z)$ admits the tractable upper bound*

$$\mathcal{L}_{IB} \leq -H(O'_j | S_j) + \mathbb{E}_{p(S_i, S_j, O'_j)} \left[\mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)] + \beta D_{KL}(q_\varphi(z|S_i) \| p(z)) \right]. \quad (\text{S59})$$

Since $H(O'_j | S_j)$ is parameter-independent, minimizing this bound is equivalent to minimizing the Variational Information Bottleneck loss

$$\mathcal{L}_{VIB}(\varphi, \vartheta) := \mathbb{E}_{p(S_i, S_j, O'_j)} \left[\mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)] + \beta D_{KL}(q_\varphi(z|S_i) \| p(z)) \right]. \quad (\text{S60})$$

Minimizing \mathcal{L}_{VIB} with respect to encoder parameters φ and decoder parameters ϑ minimizes an upper bound on the original IB objective, providing principled approximate optimization.

Proof. We establish the bound through systematic substitution of the variational bounds derived for each term. From **Proposition 2**, the distortion term decomposes as

$$-I(z; O'_j | S_j) = -H(O'_j | S_j) + H(O'_j | z, S_j).$$

Thus, the original IB objective can be written as

$$\mathcal{L}_{IB} = -H(O'_j | S_j) + H(O'_j | z, S_j) + \beta I(S_i; z).$$

For the distortion component $H(O'_j | z, S_j)$, applying **Lemma 5**'s variational upper bound yields

$$H(O'_j | z, S_j) \leq \mathbb{E}_{q(z), p(S_j, O'_j)}[-\log p_\vartheta(O'_j | z, S_j)],$$

where $q(z) = \int q_\varphi(z|S_i)p(S_i) dS_i$ is the encoder-induced marginal. Expressing $q(z)$ via its definition:

$$\begin{aligned} \mathbb{E}_{q(z), p(S_j, O'_j)}[-\log p_\vartheta(O'_j | z, S_j)] &= \mathbb{E}_{p(S_j, O'_j)} \int q(z) [-\log p_\vartheta(O'_j | z, S_j)] dz \\ &= \mathbb{E}_{p(S_j, O'_j)} \int p(S_i) q_\varphi(z|S_i) [-\log p_\vartheta(O'_j | z, S_j)] dz dS_i \\ &= \mathbb{E}_{p(S_i, S_j, O'_j)} \mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)]. \end{aligned} \quad (\text{S61})$$

For the rate component, **Lemma 4** provides the upper bound

$$I(S_i; z) \leq \mathbb{E}_{p(S_i)}[D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))].$$

Combining these bounds:

$$\begin{aligned} \mathcal{L}_{\text{IB}} &= -H(O'_j | S_j) + H(O'_j | z, S_j) + \beta I(S_i; z) \\ &\leq -H(O'_j | S_j) + \mathbb{E}_{p(S_i, S_j, O'_j)} \mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)] + \beta \mathbb{E}_{p(S_i)}[D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))] \\ &= -H(O'_j | S_j) + \mathbb{E}_{p(S_i, S_j, O'_j)} \left[\mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)] + \beta D_{\text{KL}}(q_\varphi(z|S_i) \| p(z)) \right], \end{aligned} \quad (\text{S62})$$

establishing **inequality (S59)**. The definition of \mathcal{L}_{VIB} in **Eq. (S60)** follows by dropping the parameter-independent constant $-H(O'_j | S_j)$. \square

Corollary 5 (Practical VIB implementation). *For a single training sample (S_i, S_j, O'_j) , the VIB loss is simplified*

$$\mathcal{L}_{\text{VIB}}(\varphi, \vartheta; S_i, S_j, O'_j) = \mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)] + \beta D_{\text{KL}}(q_\varphi(z|S_i) \| p(z)). \quad (\text{S63})$$

The first term (reconstruction loss) is estimated via the reparameterization trick using a single Monte Carlo sample: parameterizing $q_\varphi(z|S_i) = \mathcal{N}(\mathbf{m}_\varphi(S_i), \Sigma_\varphi(S_i))$ and sampling $z = \mathbf{m}_\varphi(S_i) + \Sigma_\varphi^{1/2}(S_i)\epsilon$, where $\epsilon \sim \mathcal{N}(0, I)$, yielding differentiable gradients. The second term (KL regularizer) evaluates in closed form for Gaussian encoder and prior. Stochastic gradient descent over mini-batches provides scalable optimization.

Proof. The reparameterization trick parameterizes the stochastic encoder using deterministic neural networks \mathbf{m}_φ and Σ_φ , outputting mean and covariance, then externalizes randomness through $\epsilon \sim \mathcal{N}(0, I)$. This allows backpropagation through z despite stochasticity. For Gaussian distributions, the KL term admits closed form $D_{\text{KL}}(q_\varphi(z|S_i) \| \mathcal{N}(0, I)) = \frac{1}{2}[\text{tr}(\Sigma_\varphi(S_i)) + \|\mathbf{m}_\varphi(S_i)\|^2 - \log \det(\Sigma_\varphi(S_i)) - d]$ where $d = \dim(z)$, derived from standard Gaussian KL formulas. \square

Interpretation and trade-off control. The VIB objective achieves an elegant decomposition directly mirroring the rate-distortion framework from information theory: $\mathcal{L}_{\text{VIB}} = \text{Distortion} + \beta \cdot \text{Rate}$. The reconstruction term $\mathbb{E}_{q_\varphi(z|S_i)}[-\log p_\vartheta(O'_j | z, S_j)]$ corresponds to distortion: minimizing this term maximizes the decoder's accuracy in predicting the receiver's future observation from the message, directly implementing predictive utility maximization. The KL regularizer $D_{\text{KL}}(q_\varphi(z|S_i) \| p(z))$ corresponds to rate: minimizing this term constrains the encoder to produce compressed messages statistically indistinguishable from the prior, enforcing bandwidth efficiency and preventing information leakage about sender-specific details irrelevant to prediction. The hyperparameter $\beta > 0$ implements a Lagrange multiplier governing this trade-off: low β values prioritize distortion minimization over rate reduction, allowing the encoder to transmit more detailed, high-bandwidth messages that maximize the receiver's ability to predict future observations; high β values prioritize rate reduction over distortion minimization, forcing the emergence of abstract, highly-compressed symbolic mechanisms that minimize bandwidth usage while potentially sacrificing some prediction accuracy. This principled parameterization enables systematic exploration of the rate-distortion frontier, revealing how communication constraints shape emergent language structure for efficient communications—a central theme in our experimental investigations.

Theoretical guarantees and practical benefits. The VIB framework provides rigorous theoretical guarantees inherited from its variational foundation. **Theorem 3** ensures that optimizing the tractable surrogate \mathcal{L}_{VIB} drives down an upper bound on the true IB objective, guaranteeing improvement (under perfect optimization) toward the optimal rate-distortion trade-off. The tightness of this bound improves as the variational approximations become more accurate: when the encoder's aggregate posterior $q(z)$ approaches the prior $p(z)$ and the decoder $p_\vartheta(O'_j | z, S_j)$ approaches the true conditional distribution, the inequalities in **Lemmas 4** and **5** approach equality, yielding $\mathcal{L}_{\text{IB}} \rightarrow -H(O'_j | S_j) + \mathcal{L}_{\text{VIB}}$. Since the constant term $-H(O'_j | S_j)$ is parameter-independent, optimizing \mathcal{L}_{VIB} is equivalent to optimizing \mathcal{L}_{IB} regardless of bound tightness.. Practically, this framework enables end-to-end learning of communication mechanisms through standard deep learning infrastructure—gradient-based optimization, mini-batch training, and GPU acceleration—without requiring explicit symbolic grounding, hand-crafted message spaces, or task-specific communication engineering. The learned protocols emerge purely from the objective of collaborative prediction under bandwidth constraints, embodying the social predictive coding principle: agents learn to exchange information that is maximally novel and decision-relevant from the receiver's perspective, the essence of effective and efficient communication.

S2 Supplementary Results and Analyses

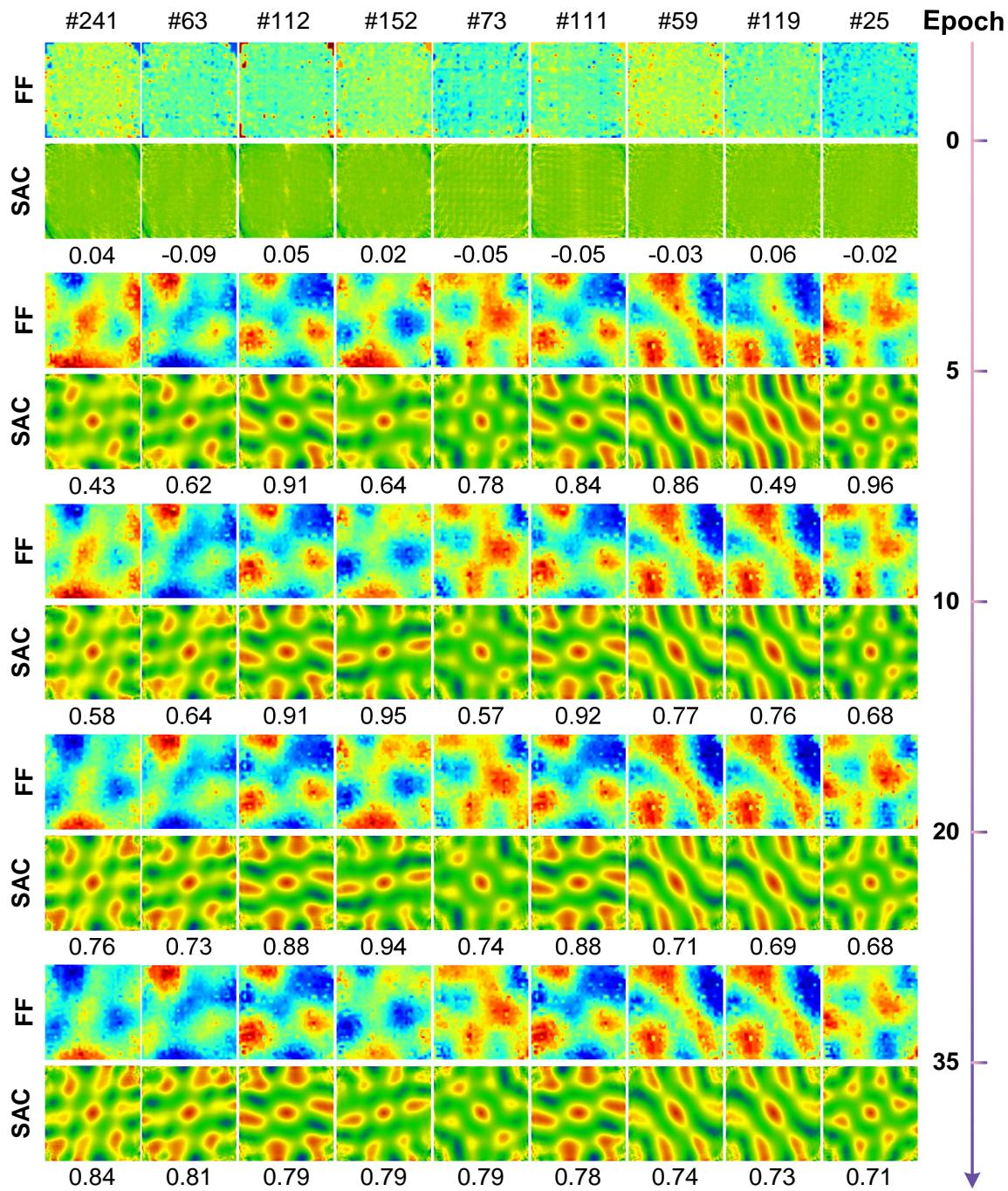


Figure S4. Emergence of grid-like neural representations through self-supervised training. This figure contrasts the neural activation patterns of four representative units from the path integrator's bottleneck layer before and after training, demonstrating the spontaneous formation of a grid-cell-like code. Before training, the units exhibit disorganized and non-periodic spatial firing fields (FF), as shown in their spatial rate maps (top row) and corresponding spatial autocorrelograms (SACs, bottom row). The gridness scores are low (close to zero or negative), indicating a lack of hexagonal symmetry. After training on the self-motion prediction task, the same units develop highly structured, periodic firing patterns that tile the environment. The gridness scores are now significantly positive, and the SACs reveal a clear six-fold rotational symmetry, a defining characteristic of biological grid cells. This transformation illustrates how the predictive learning objective drives the self-organization of a stable, metric neural code for space.

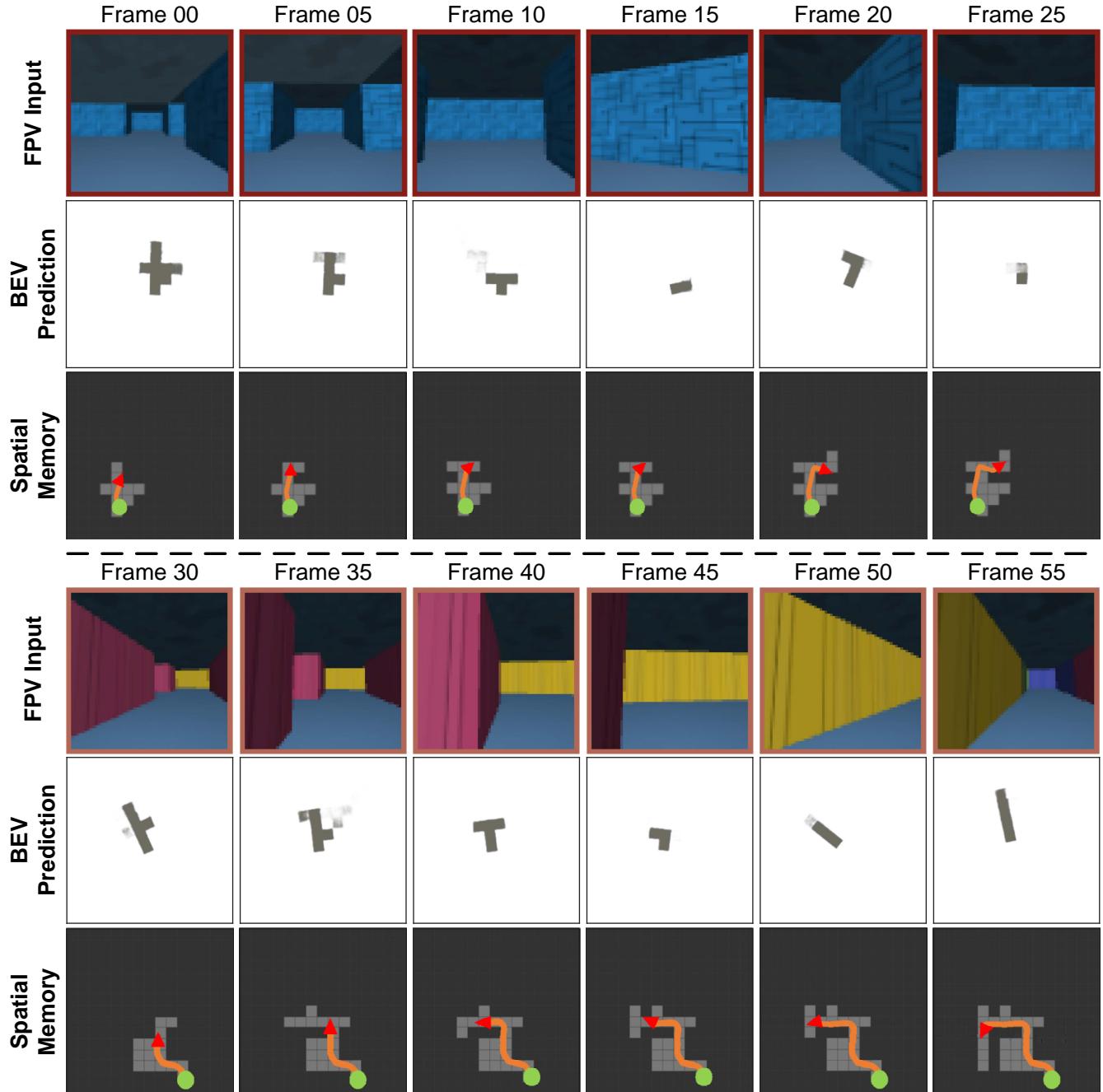
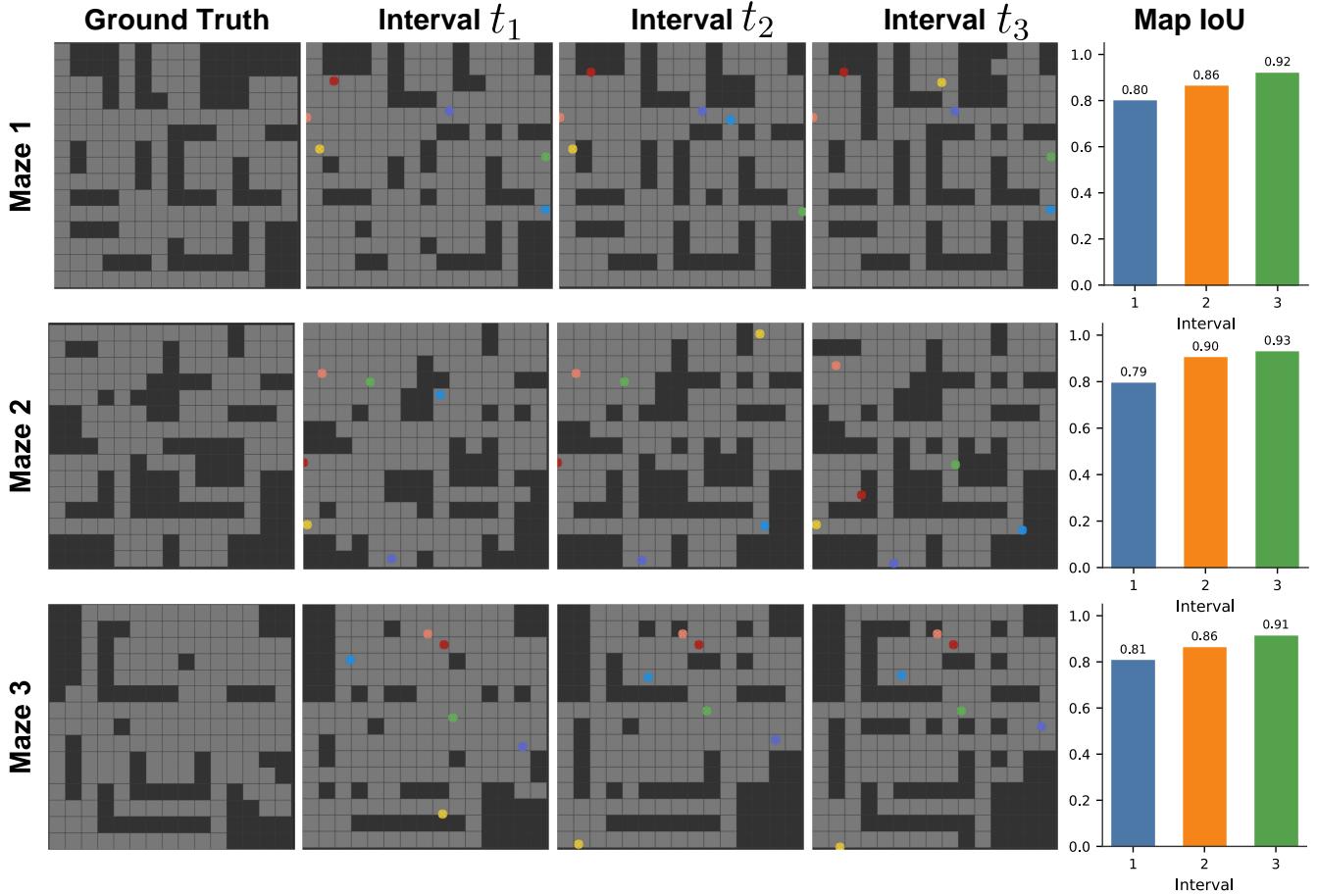


Figure S5. Visualization of the spatial memory construction pipeline. The agent's first-person visual (FPV) input (top row) is converted into an instantaneous bird's-eye view (BEV) prediction of the local surroundings (middle row). These predictions are sequentially integrated into a persistent and growing allocentric spatial memory map, which also tracks the agent's trajectory and current pose (bottom row).



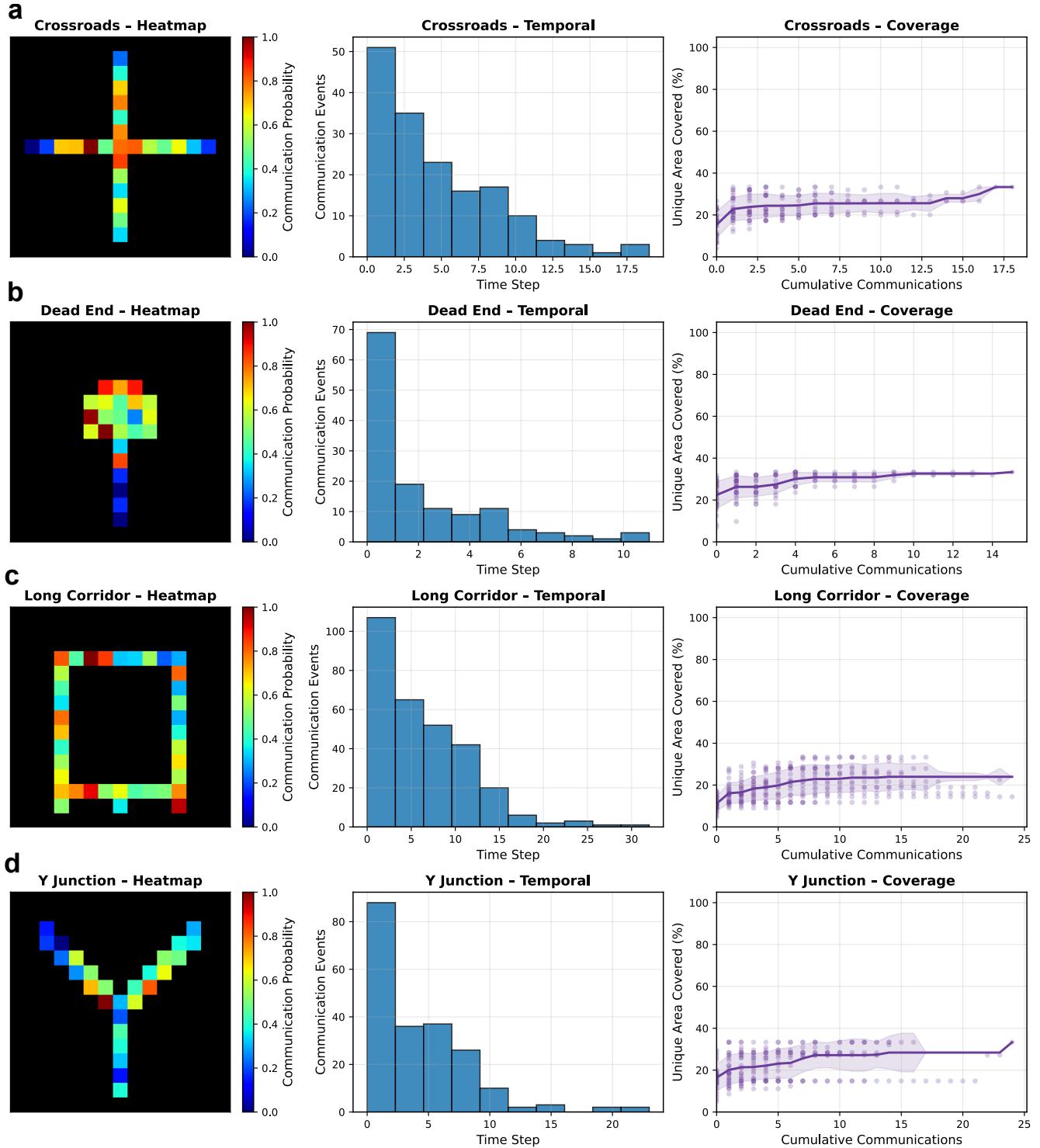
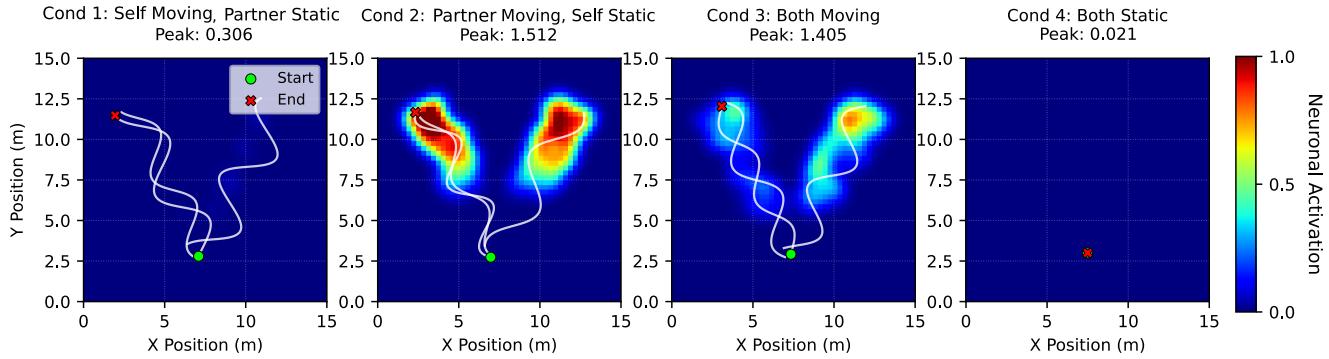
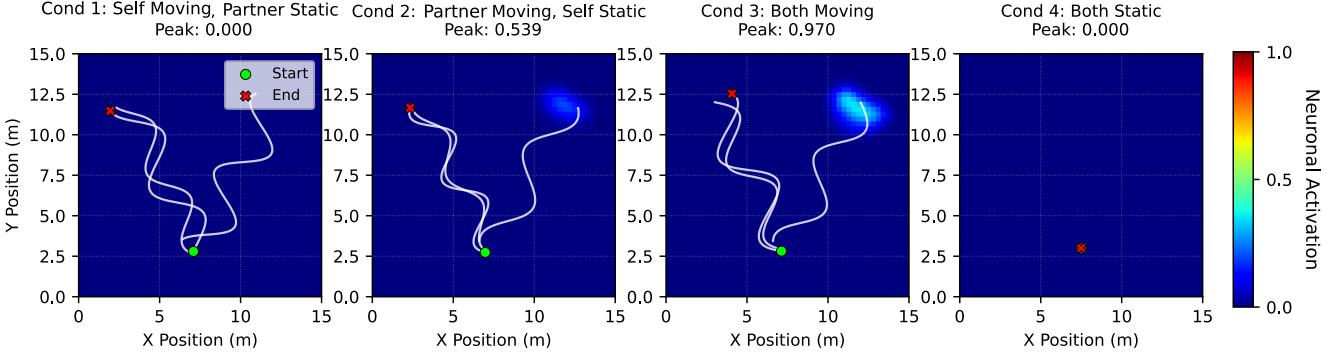


Figure S7. Strategic communication emerges across diverse maze topologies. This figure analyzes agents' emergent communication strategies across four canonical maze structures: (a) Crossroads, (b) Dead End, (c) Long Corridor, and (d) Y Junction. For each topology, we visualize message spatial distribution (Heatmap), timing (Temporal), and the relationship between communication and exploration (Coverage). The heatmaps reveal a consistent pattern of "strategic triggering": agents communicate at points of high predictive uncertainty for their partners. For instance, in the Crossroads (a) and Y Junction (d), communication peaks at the central intersection, an ambiguous location where information helps coordinate exploration. Conversely, in the Dead End (b), agents communicate from deep within the trap, acting as an efficient "prediction error" signal to inform teammates the path is not fruitful. These consistent patterns demonstrate that the social predictive objective drives agents to learn an implicit model of their partners' beliefs, sharing information when and where it best resolves uncertainty.

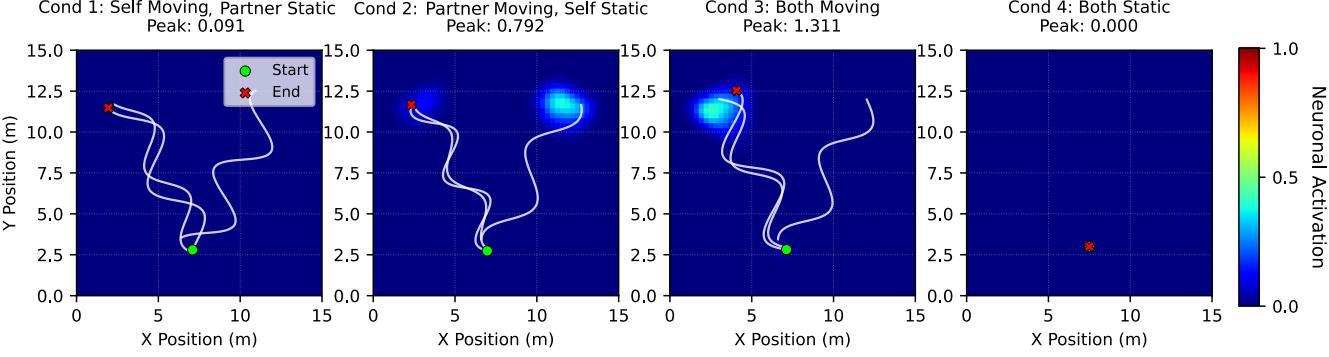
Bottleneck Neuron 27



Bottleneck Neuron 34



Bottleneck Neuron 62



Bottleneck Neuron 80

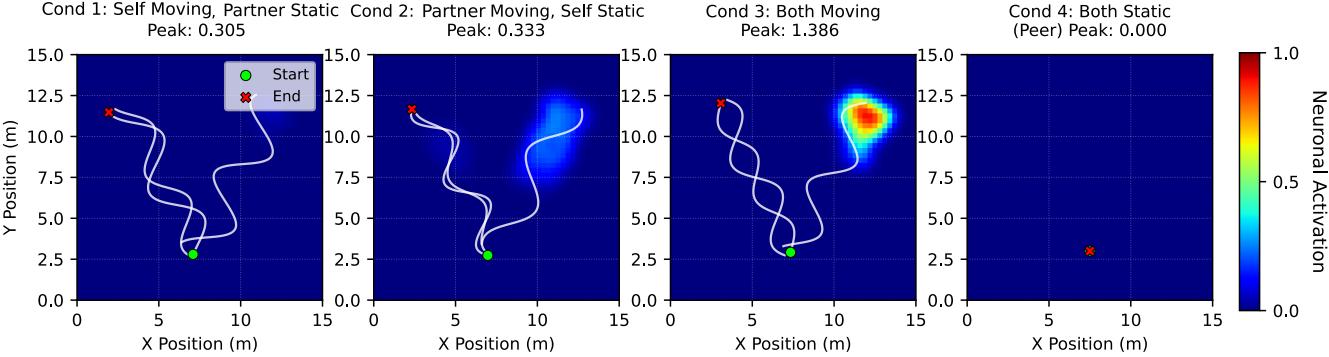
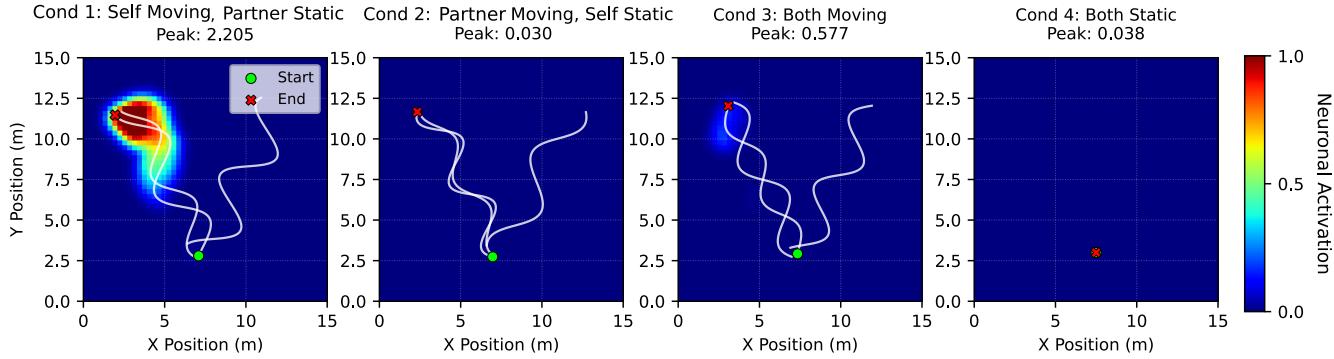
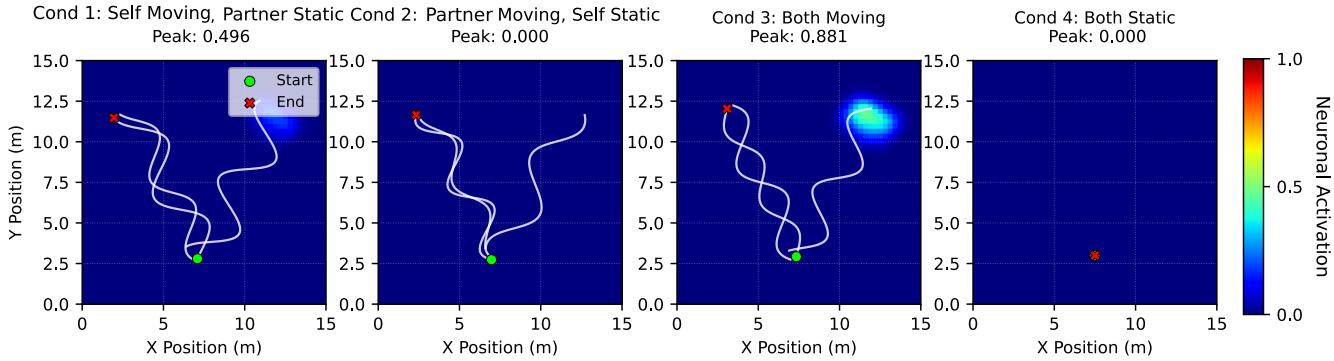


Figure S8. Gallery of emergent social place cells (SPCs). This figure shows representative units that selectively encode the partner's location. Each row displays a single neuron's activity across four conditions: (1) Self moving, peer static; (2) Peer moving, self static; (3) Both agents moving; (4) Both static. These SPCs exhibit strong, localized firing fields when the partner moves through a specific area (Condition 2), but remain largely silent in response to the agent's own movement (Condition 1). This selective tuning to another's position is the defining feature of social place cells.

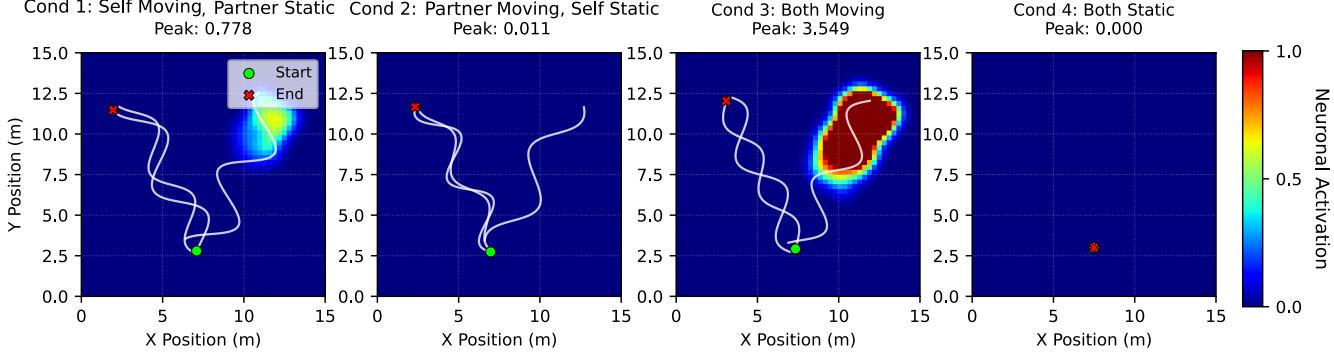
Bottleneck Neuron 102



Bottleneck Neuron 118



Bottleneck Neuron 139



Bottleneck Neuron 208

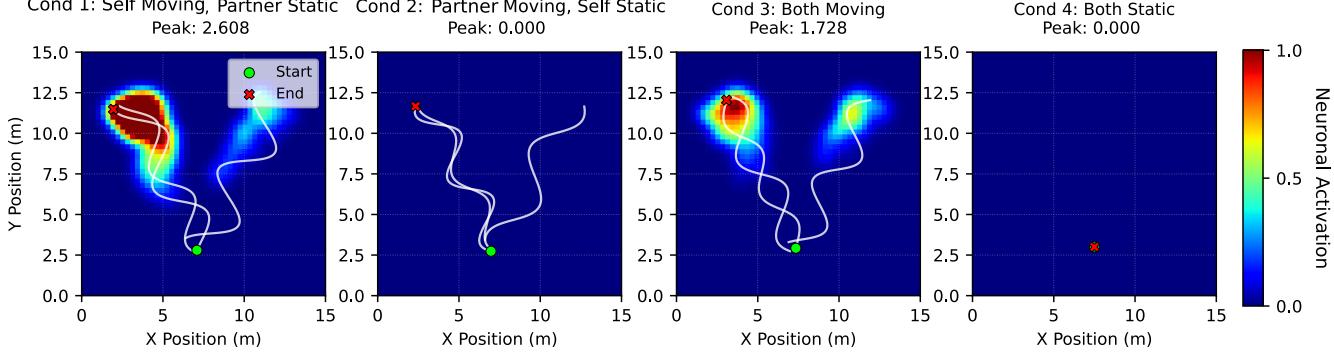
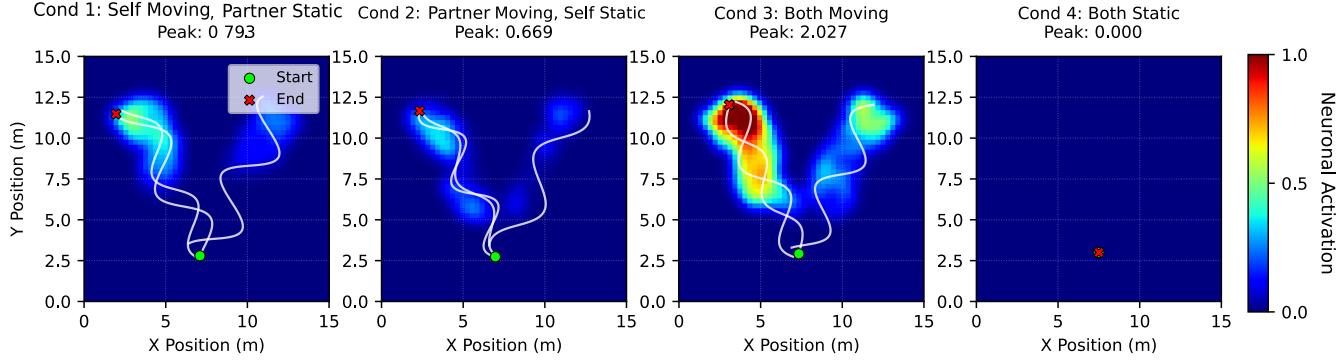
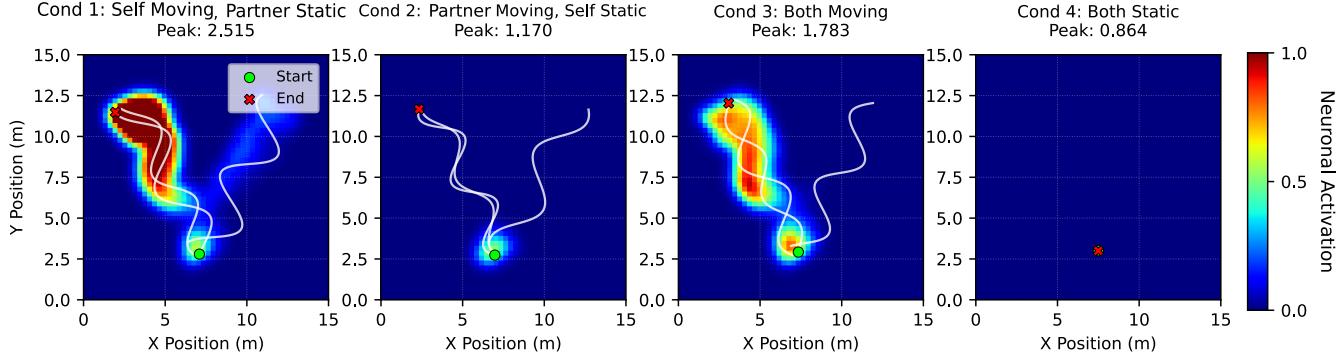


Figure S9. Gallery of emergent place cells (PCs). This figure shows representative units that function as classical place cells, selectively encoding the agent's own location. The four conditions are shown for each neuron. These units display strong, stable firing fields when the agent itself traverses a specific location (Condition 1), but show negligible activation in response to the partner's movement (Condition 2). This demonstrates a clear encoding of self-position, providing a stable allocentric representation for the agent.

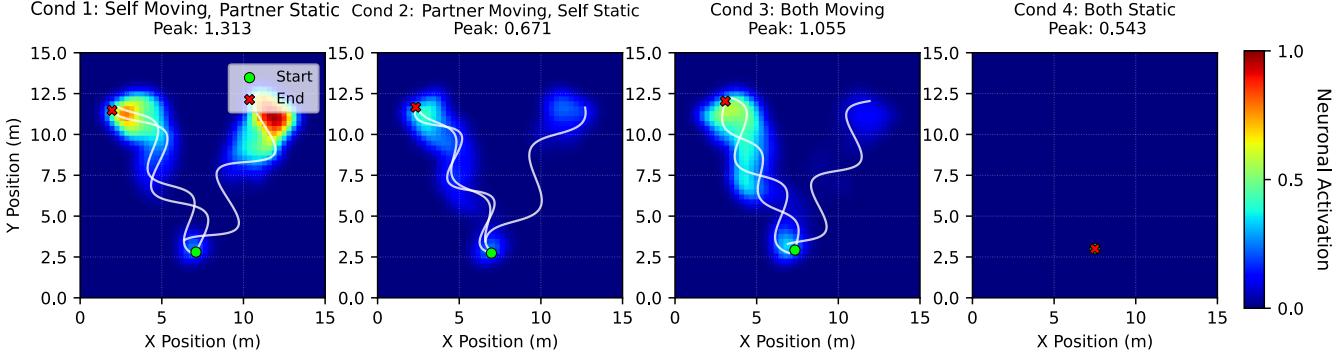
Bottleneck Neuron 145



Relational Neuron 3



Relational Neuron 30



Relational Neuron 35

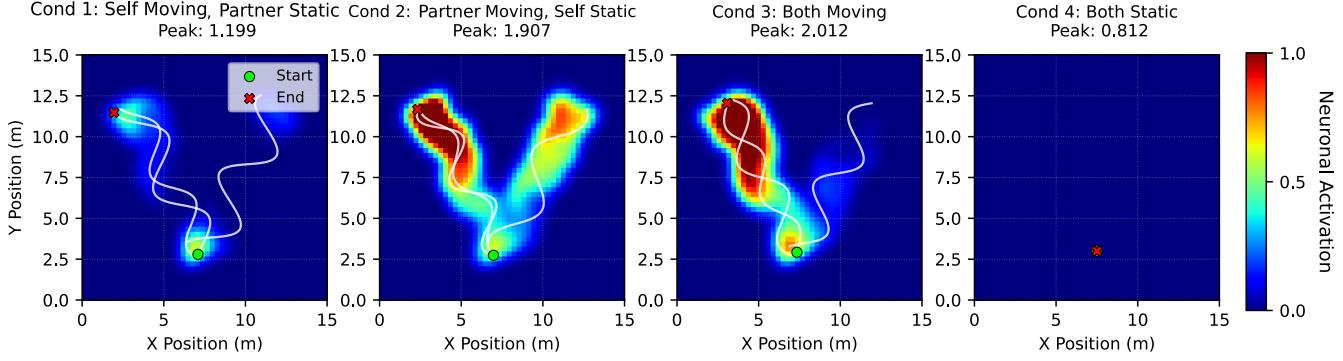


Figure S10. Gallery of special SPCs with mixed selectivity. This figure shows representative units, including “Relational Neurons”, that conjunctively encode both self and partner information. The four conditions are displayed for each unit. Unlike pure PCs or SPCs, these neurons show significant activation in response to both the agent’s own movement (Condition 1) and the partner’s movement (Condition 2). Firing is often maximal when both agents are moving (Condition 3), indicating that these cells encode a higher-order relational variable between the agents rather than a simple location.

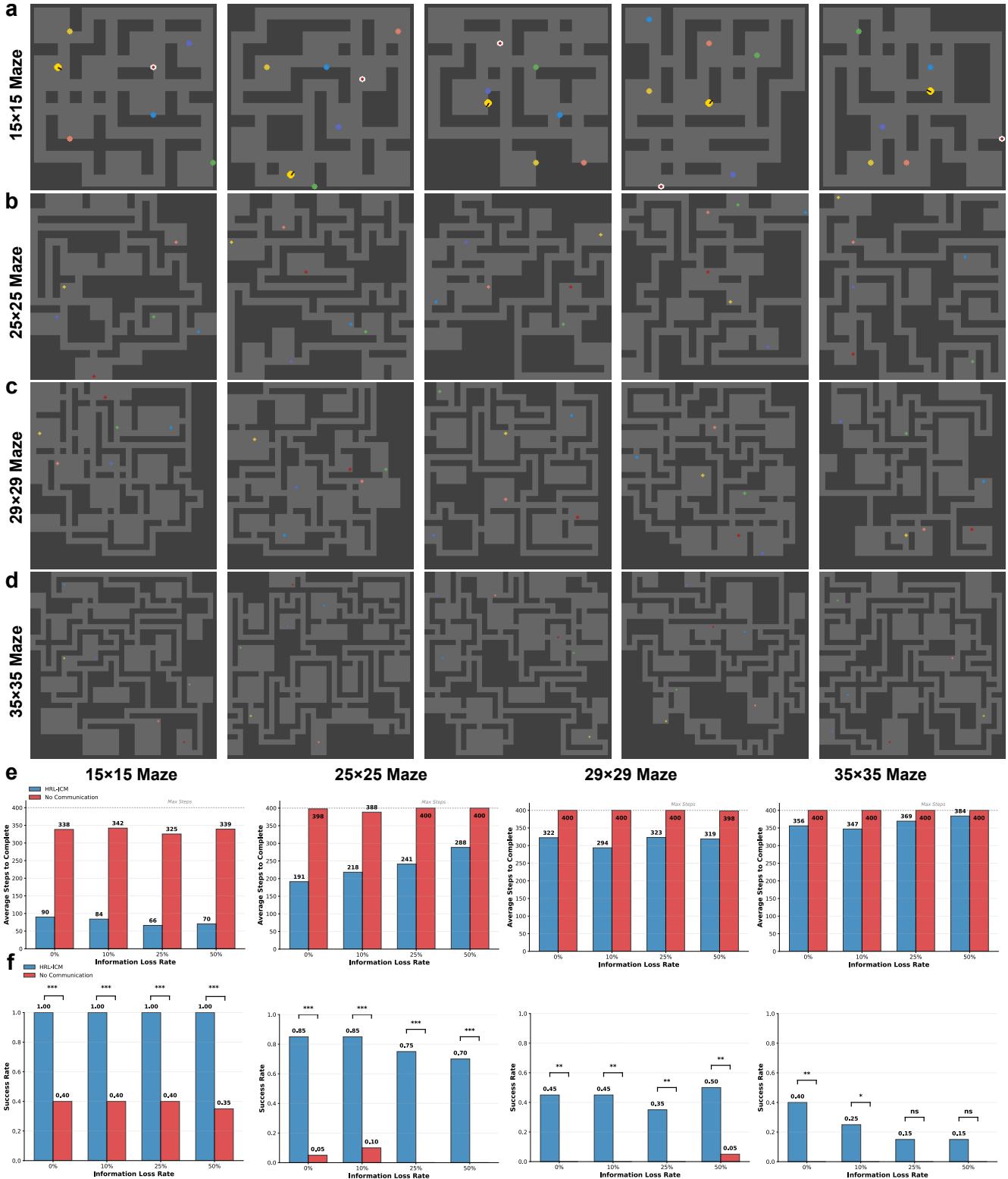


Figure S11. Robustness of the learned communication protocol to noise and scaling environmental complexity. This figure evaluates the HRL-ICM framework's robustness to communication noise across a suite of procedurally generated mazes of increasing scale and complexity, shown in panels (a-d). Performance is compared against a “No Communication” baseline by measuring the average steps to completion (e) and the task success rate (f) under varying information loss rates (0-50%). The results demonstrate that HRL-ICM (blue) consistently solves tasks with higher efficiency and a significantly greater success rate. Crucially, its performance degrades gracefully as noise increases, whereas the baseline consistently fails. This robust advantage persists even in larger, more complex environments, highlighting the scalability of the learned protocol. Statistical significance is denoted as: * $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$.

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