# Toward Understanding Misalignment in LLM Agents: A Survey of Taxonomy, Causes, Mitigation, and Evaluation

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## Abstract

Large language models are increasingly deployed as autonomous agents that interact with external environments to solve long-horizon tasks. As these systems move toward real-world deployment, misalignment in LLM agents has emerged as a distinct challenge. Unlike misalignment in stand-alone LLMs, it unfolds through multi-step interaction and may arise from mismatches with the environment, failures within the agent's own decision state, or breakdowns in inter-agent coordination. However, existing literature remains fragmented across agent-focused surveys and stand-alone LLM studies, leaving no unified account of misalignment in agentic systems. In this survey, we present a closed-loop perspective that frames misalignment in LLM agents as a systems-level problem shaped by interaction among the agent, the environment, and other agents. We organize the literature into three categories—agent–environment, intra-agent, and inter-agent misalignment—and review their causes, mitigation strategies, and evaluation practices. Finally, we highlight open challenges and future directions for building more reliable, robust, and trustworthy LLM-agent systems.

## 1 Introduction

Large language models (LLMs) are rapidly evolving from passive text generators into LLM agents that maintain context, access memory, invoke tools, and interact with external environments to solve long-horizon tasks (Yao et al., 2022; Park et al., 2023; Wang et al., 2024; Su et al., 2024a; Fang et al., 2025). This transition has broadened LLM applications from single-turn assistance to complex multi-step settings such as web automation (Zhou et al., 2024b; Ning et al., 2025), software engineering (Liu et al., 2024a; Novikov et al., 2025), scientific discovery (Ren et al., 2025; Lyu et al., 2026), embodied decision making (Xie et al., 2024; Liu et al., 2025b), and multi-agent collaboration (Du et al., 2024; Jin et al., 2025). With this growing autonomy, ensuring reliable and consistent behavior over extended interactions has become an increasingly important challenge (Yu et al., 2025).

As these systems move toward real-world deployment, agentic misalignment emerges as a distinct and critical problem (Lynch et al., 2025; Naik et al., 2025; Wang et al., 2026b). Broadly, agentic misalignment refers to situations in which the behavior of an LLM agent, or multiple interacting LLM agents, deviates from task goals, human intentions, internal consistency requirements, or environmental constraints over the course of multi-step interaction. Such misalignment may arise even when each local decision appears reasonable, because at every step the agent must interpret observations, update its internal state, choose actions, and respond to feedback (Lin et al., 2025), and errors in any of these processes can steer subsequent behavior away from what is intended (Yu et al., 2025). For example, an agent may rely on stale context, form misleading internal state, invoke unsuitable tools, misinterpret environmental signals, or coordinate poorly with other agents (Zhang et al., 2025c). Agentic misalignment is therefore not simply a matter of incorrect single outputs, but a systems-level challenge shaped by recurrent interaction and evolving state.

Existing literature fails to systematically characterize misalignment in LLM agents. On one hand, surveys on LLM agents mainly focused on components like architectures (Wang et al., 2024), planning (Huang et al., 2024), memory (Hu et al., 2025b), tool use (Jiang et al., 2025) and multi-agent collaboration (Khan et al., 2024). However, these studies are largely organized around what agents can do and how well they achieve that, rather than the misalignment dynamics that determine whether they remain reliable over long-horizon scenarios. On the other hand, related work on stand-alone

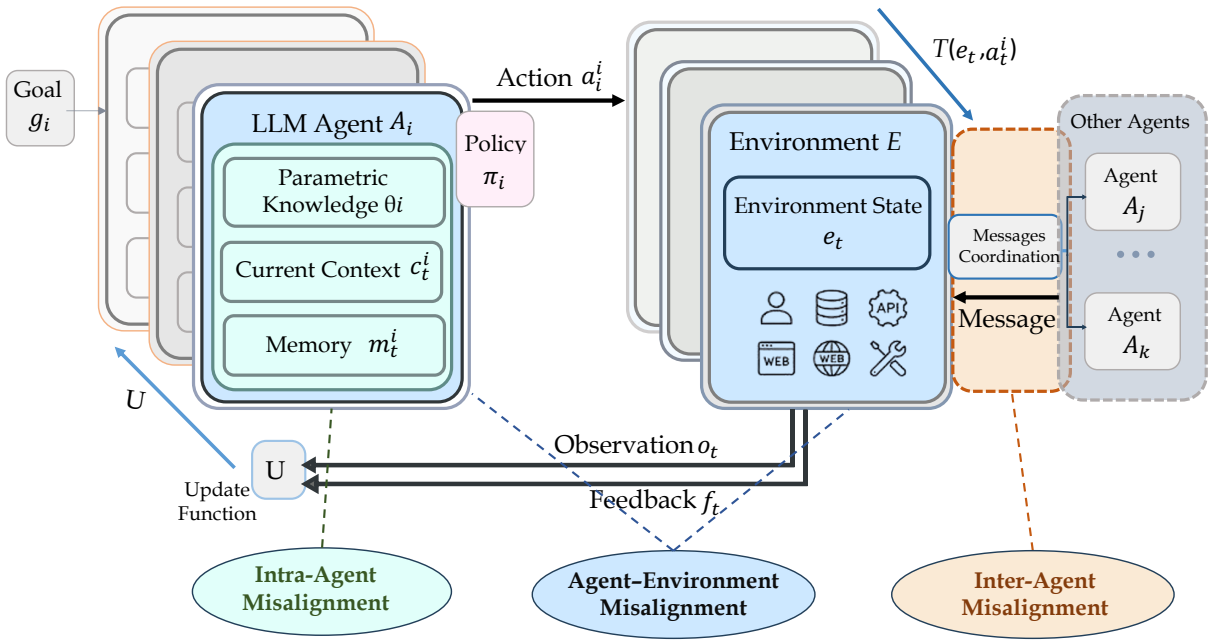


Figure 1: Three types of agentic misalignment between LLM agent, environment and other agents.

LLMs has examined misalignment-related phenomena such as knowledge conflicts (Xu et al., 2024), hallucination (Huang et al., 2025), and knowledge boundaries (Li et al., 2025). However, misalignment in agentic systems is fundamentally more challenging because of its nature of iterative interaction with the environment. Consequently, the field still lacks a unified framework for understanding where misalignment arises in LLM agents, how it propagates across interaction trajectories, and how to mitigate such misalignment behavior.

In this survey, we address this gap by studying agentic misalignment through the closed-loop interaction among the agent, the environment, and other agents. We begin by formalizing LLM agents (Sec. 2) and defining key concepts.. Then, we organize the literature into three categories: **agent-environment misalignment** (Sec. 3), which concerns failures at the interface between agents and the external world; **intra-agent misalignment** (Sec. 4), which concerns inconsistencies within the agent's own internal components; and **inter-agent misalignment** (Sec. 5), which concerns failures arising from communication, coordination, and heterogeneity in multi-agent setting. This taxonomy provides a unified lens for analyzing the origins, manifestations, mitigations or utilizations, and evaluations of agentic misalignment.

Our contributions are summarized as follows: i) We present a unified closed-loop perspective on misalignment in LLM agents, viewing it as a systems-level problem that emerges through iterative interaction among the agent, the environment, and other agents. ii) We propose a structured taxonomy that organizes the literature into three major categories: agent-environment misalignment, intra-agent misalignment, and inter-agent misalignment. iii) We systematically synthesize existing work within each category, covering its causes, mitigation and evaluation methods, thereby providing a comprehensive overview of the current research landscape. iv) We highlight open problems and future research directions that are critical for building more robust and trustworthy agentic systems.

## 2 Preliminaries

To ground the discussion in the remainder of this survey, we first define *LLM Agent*, the *environment* in which they operate, and the *interaction dynamics* between them. Based on this abstraction, we then introduce a unified notion of *misalignment* and later specialize it to three loci: agent-environment, intra-agent, and inter-agent settings with a unified view of the mitigation strategies.

### 2.1 Agent-Environment Formulation

**LLM Agent.** An *LLM agent* is a language-model-based system that pursues a goal through iterative, multi-step decision making. Unlike one-shot LLM usage, an agent continuously incorporates new information, takes actions that may affect the external world, and maintains state across steps. For-

mally, an agent $\mathcal{A}$ pursues a goal $g$, and at each step $t$ selects an action $a_t$ under policy $\pi$ based on three sources: parametric knowledge $\theta$ (encoded in model weights), current context $c_t$ (information available in the context window), and memory $m_t$ (cross-step information such as prior observations, intermediate reasoning, or interaction history).

**Environment.** We define the environment ($\mathcal{E}$) as the external system with which the agent interacts throughout the decision process. At step $t$, the environment is in state $e_t$, receives an action $a_t$, and returns to the agent an observation $o_t$ and feedback $f_t$ reflecting the consequence of that action. The environment may include task interfaces, users, tools, databases, webpages, or other external information sources. Importantly, the agent typically does not observe the full environment state $e_t$ directly, but instead reasons over partial, delayed, or otherwise mediated observations and feedback.

**Interaction Dynamics.** The interaction between an LLM agent and its environment can be viewed as a closed-loop sequential decision-making process. At each step $t$, the agent receives an observation $o_t$, combines it with its current context $c_t$ and memory $m_t$, and selects an action $a_t$ according to: $a_t \sim \pi(a \mid g, c_t, m_t; \theta)$. The executed action induces a new state and feedback from the environment in the formula: $e_{t+1} \sim \mathcal{T}(e_t, a_t)$ and $f_t \sim \Phi(e_t, a_t)$ where $\mathcal{T}$ denotes the environment transition function and $\Phi$ is the feedback function. The resulting observation and feedback are then incorporated into the agent's information for the next step: $(c_{t+1}, m_{t+1}) \sim \mathcal{U}(c_t, m_t, o_t, a_t, f_t)$, where $\mathcal{U}$ denotes the agent update function, which may append new context, revise memory or compress prior interaction history. It highlights that agent behavior is shaped by the interaction between internal information sources (e.g., $\theta$, $c_t$, and $m_t$) and external signals from $\mathcal{E}$. T, misalignment may arise from mismatches among internal information, decision policy, and environmental signals.

### 2.2 Misalignment Types and Mitigation

We use *misalignment* to denote a mismatch among the goals, information, states, or decision processes that must remain compatible for effective agent behavior. We distinguish three loci based on where such mismatches arise: *(a) Agent-Environment Misalignment* arises when the agent fails to remain aligned with the external environment in which it operates. *(b) Intra-Agent Misalignment* arises when a single agent fails to maintain coherence among its internal information or decision processes. *(c) Inter-Agent Misalignment* arises when multiple agents fail to maintain compatible goals, beliefs or communication during joint or related tasks. Under this view, mitigation methods can be summarized in a unified form according to their primary intervention mechanism, including prompt-based, supervised-fine-tuning (SFT)-based, inference-based, Reinforcement Learning (RL)-based, and architecture-based approaches as demonstrated in Table 1. This unified lens provides a common template for organizing prior work, while the later sections will examine how each misalignment type gives rise to its own specialized mitigation methods.

## 3 Agent-Environment Misalignment

As illustrated in Fig. 1, an LLM agent acts on the environment through its policy $\pi$, which maps goal $g$, parametric knowledge $\theta$, current context $c_t$, and memory $m_t$ to an action $a_t$. The environment then evolves according to its state $e_t$, transition function $T(e_t, a_t)$, and feedback function $\Phi(e_t, a_t)$, returning observation $o_t$ and feedback $f_t$ to the agent, which are incorporated through the update module $U(c_t, m_t, o_t, a_t, f_t)$. Agent–environment misalignment arises when these cross-boundary interactions do not match: the agent acts on incorrect assumptions about the environment, or it incorrectly interprets the signals the environment returns.

### 3.1 Underlying Causes

**Action: Transition Mismatch** Transition mismatch occurs when the agent's policy $\pi$ predicts action outcomes that do not match the environment's true transition function $T(e_t, a_t)$. It arises from two sources: deployment shift, where latency, noise, or physical constraints alter the real effect of actions (Yamagata and Santos-Rodriguez, 2024; Jonnarth et al., 2025); and partial observability, where the agent plans under incorrect assumptions about hidden state, delayed effects, or rare events. In agentic settings, this manifests as tool misuse, brittle plans, or optimization toward proxy behaviors (Chen et al., 2026a; Wang et al., 2026c).

**Observation: Update Mismatch.** Update mismatch occurs after action execution, when observations $o_t$ and feedback $f_t$ are too sparse or ambiguous for the update module $U(\cdot)$ to correctly revise the agent's context and memory. It arises

from two main sources. First, generic error signals prevent the agent from diagnosing whether a failure is caused by an invalid action or a missing precondition (Lumer et al., 2025; Lu et al., 2025; Wang et al., 2025a). Second, unstated environmental dependencies—such as navigation requirements or tool configuration steps—are often not explicitly exposed to the agent (Udeshi et al., 2025; Zhou et al., 2026). In agentic settings, this leads the agent to update its internal state based on a distorted interpretation of the environment, causing it to persist with an invalid strategy.

### 3.2 Mitigation Strategies

**Exposing Transition Rules and Failure Signals.** One direct solution is to make the environment-facing interface more informative. Methods such as ALIGN augment the interaction loop by surfacing hidden constraints before acting and by converting vague outcomes into more diagnostic feedback after each step (Liu et al., 2025a). Related approaches similarly expose valid actions, state information, or execution traces through wrappers and auxiliary interfaces (Yang et al., 2023; Chen et al., 2024b; He et al., 2025; Sun et al., 2025; Zhou et al., 2024c). In terms of Fig. 1, these methods improve the quality of $o_t$ and $f_t$, reducing mismatch between environmental outcomes and agent updates.

**Grounding Policy and Update Through Interaction Trajectories.** A second direction is to adapt the agent itself from environment-specific trajectories. Reinforcement learning, meta-learning, and exploration-based methods help the policy $\pi$ and update process $U(\cdot)$ better reflect actual action consequences, failure patterns, and recovery behaviors observed during interaction (Qian and Liu, 2025; Zhang et al., 2025a; Mai et al., 2025; Luo et al., 2025b). Rather than generic adaptive training, the goal here is specifically to improve how agents choose actions and revise internal state from environment feedback.

**Learning Explicit Environment Models for Planning.** Another line of work reduces mismatch by making the agent's internal model of $T(e_t, a_t)$ and $\Phi(e_t, a_t)$ more explicit. WALL-E learns symbolic rules from observed trajectories, RWML learns action-conditioned world models, and RAP uses LLMs as predictive simulators for multi-step planning (Zhou et al., 2024c; Yu et al., 2026; Hao et al., 2023). These approaches directly target the cross-boundary prediction problem in Fig. 1: the agent should anticipate how the environment will transition before committing to an action.

**Standardizing Agent-Environment Protocols.** A complementary solution is to reduce ambiguity at the environment side. Formal languages such as RLang make preconditions and effects explicit, while Gym-style APIs and newer systems such as OpenEnv standardize action–observation protocols across tasks (Rodriguez-Sanchez et al., 2023; Towers et al., 2025; Brockman et al., 2016). Shared state representations, such as temporal knowledge graphs in Graphiti MCP, further help agents maintain a consistent view of environmental state across interactions (Rasmussen et al., 2025). These efforts reduce the need for the agent to infer basic environment semantics from weak signals alone.

### 3.3 Evaluation Frameworks

Existing relevant evaluation approaches can be broadly grouped into three categories: distributional generalization, interaction quality, and execution correctness. For distributional generalization, many works compare in-distribution (ID) and out-of-distribution (OOD) performance, where large gaps indicate poor robustness under changing environment dynamics. For example, RWML (Yu et al., 2026) is evaluated on both splits of ALFWorld (Shridhar et al., 2021), showing improved transfer through self-supervised world-model learning. For interaction quality, metrics such as invalid-action rates and interface reliance (IR) (Zhou et al., 2024a) capture whether agents depend on interface shortcuts rather than genuine understanding (Gu et al., 2026). For execution correctness in tool-using agents, benchmarks (Barres et al., 2025) show that failures often stem from malformed arguments or incorrect call ordering rather than wrong tool choice, making tool-selection accuracy, argument validity, and execution correctness key evaluation dimensions.

## 4 Intra-Agent Misalignment

Intra-agent misalignment refers to mismatches within the decision state of a single LLM agent. Concretely, it arises when the agent's parametric knowledge $\theta$, current context $c_t$, memory $m_t$, the update process $\mathcal{U}$, and the resulting policy $\pi(a \mid g, c_t, m_t; \theta)$ fail to remain mutually compatible during inference and action selection. Unlike agent–environment misalignment, which is defined at the boundary between the agent and the external

world, intra-agent misalignment concerns inconsistencies that are represented and must be resolved inside the agent itself. This paper organizes intra-agent misalignment into three forms: intrinsic misalignment, intrinsic-extrinsic misalignment, and extrinsic misalignment.

### 4.1 Underlying Causes

**Intrinsic Misalignment.** Intrinsic misalignment is generated primarily by the agent's intrinsic substrate, namely the parametric knowledge $\theta$ and the internal inference dynamics that instantiate the policy $\pi$. Typical cases include unstable outputs under the same input (Wang et al., 2022; Chen et al., 2026b), latent uncertainty (Xiong et al., 2024) among competing continuations, reasoning drift over multi-step inference (Zhang et al., 2026c), and divergence between high-level planning and downstream action (Erdogan et al., 2025). In these cases, even when $c_t$, $m_t$, and the update process $\mathcal{U}$ are held fixed, the induced policy may remain unstable or internally inconsistent. The core issue is therefore misalignment within what the model encodes and how it reasons from that encoding.

**Intrinsic-Extrinsic Misalignment.** Intrinsic-extrinsic misalignment arises when the agent's intrinsic knowledge $\theta$ conflicts with runtime information maintained in $c_t$ or $m_t$. Typical cases include disagreement between parametric knowledge and newly retrieved evidence, conflicts between prior beliefs and updated memory, or failures to decide whether information newly written into $c_t$ or $m_t$ should override what is already encoded in $\theta$ (Xu et al., 2024; Kortukov et al., 2024; Huo et al., 2025). This type of misalignment is closely tied to the update process $\mathcal{U}$, since the conflict often emerges when new observations or feedback are incorporated into the run-time state but are not reconciled properly with prior parametric knowledge.

**Extrinsic Misalignment.** Extrinsic misalignment arises when the runtime substrate itself, namely $c_t$ and $m_t$, becomes unreliable after incorporating external information. This could include scenarios like contradictory context snippets, stale retrieved passages, noisy user instructions and memory write or revision errors (Liu et al., 2024b; Cheng et al., 2025; Hu et al., 2025a). This type of failure is most directly tied to the update process $\mathcal{U}(c_t, m_t, o_t, a_t, f_t)$, where the resulting context $c_t$ or memory $m_t$ may become corrupted, inconsistent, stale, or poorly synchronized with later reasoning. Here the source of the problem is external, but the mismatch is expressed inside the agent because subsequent decisions are conditioned on distorted context or memory.

### 4.2 Mitigation Strategies

**Reasoning Stabilization.** For intrinsic misalignment, the main mitigation objective is to stabilize how the policy $\pi$ is induced from the agent's intrinsic substrate. Existing methods mainly follow three directions. Self-verification methods, such as CoVe (Dhuliawala et al., 2024) and CRITIC (Gou et al., 2023), insert explicit checking or critique steps to validate intermediate reasoning or action candidates before commitment. Reflective refinement methods like Reflexion (Shinn et al., 2023) and Self-Refine (Madaan et al., 2023) iteratively use self-generated feedback to revise reasoning traces, memory, or outputs, reducing local drift. Plan-aware stabilization methods, such as Reflective Test-Time Planning (Hong et al., 2026) and EvoAgent (Feng et al., 2025), combine reflection with explicit planning or world-model guidance to keep action selection aligned with longer-horizon goals. Overall, these methods aim to regularize the mapping from intrinsic knowledge and memory to action, so that repeated or long-horizon inference yields a more coherent policy trajectory.

**Knowledge Reconciliation.** For intrinsic-extrinsic misalignment, the key mitigation challenge is to reconcile parametric knowledge $\theta$ with the run-time state $(c_t, m_t)$. A common strategy is to explicitly detect and arbitrate conflicts between internal knowledge and newly incorporated evidence. Self-RAG (Asai et al., 2023), CRAG (Yan et al., 2024), and CoV-RAG (He et al., 2024) improve this process by combining retrieval with critique and corrective retrieval. More conflict-centered methods such as FaithfulRAG (Zhang et al., 2025b) and Micro-Act (Huo et al., 2025) go further by modeling disagreements between parametric and retrieved knowledge and resolving them through structured self-reasoning. Overall, these methods improve how update function $\mathcal{U}$ incorporates new observations and feedback into context and memory.

**Run-Time State Governance.** For extrinsic misalignment, the main mitigation objective is to govern the construction and evolution of the run-time state itself, namely $c_t$ and $m_t$, through the up-

date process $\mathcal{U}$. Existing methods can be broadly viewed as memory architecture, memory management, and memory admission/control mechanisms. MemGPT (Packer et al., 2023), MemoryOS (Kang et al., 2025), Mem0 (Chhikara et al., 2025), and MIRIX (Wang and Chen, 2025) provide more structured memory architectures for long-horizon agents. A-MEM (Xu et al., 2025) and Reflective Memory Management (Tan et al., 2025) improve how memories are linked, summarized, and revised over time. TierMem (Zhu et al., 2026a) and A-MAC (Zhang et al., 2026a) further target specific governance failures such as lossy summarization and unreliable memory admission.

### 4.3 Evaluation Frameworks

Evaluation of intra-agent misalignment remains fragmented across benchmark families rather than unified under a single framework. Intrinsic misalignment is typically assessed through long-horizon evaluation of policy stability, with benchmarks such as DeepPlanning (Zhang et al., 2026b) and UltraHorizon (Luo et al., 2025a) exposing failures in planning consistency, long-range coherence, and trajectory stability. Intrinsic-extrinsic misalignment is best evaluated by testing whether the agent can reconcile parametric knowledge $\theta$ with runtime information in $c_t$ and $m_t$; representative benchmarks include ConflictBank (Su et al., 2024b) and MemoryAgentBench (Hu et al., 2025a), which focus on conflicts between encoded knowledge, retrieved knowledge, and their resolution. Extrinsic misalignment is best captured by benchmarks that stress the quality of the runtime state and the robustness of the update process $\mathcal{U}$ under noisy, stale, or evolving inputs, such as RealMem (Bian et al., 2026) and AgentNoiseBench (Wang et al., 2026a).

## 5 Inter-Agent Misalignment

Inter-agent misalignment refers to situations in which multiple agents, operating under shared or partially aligned goals, maintain incompatible informational states, reasoning trajectories, or final decisions during collaboration. Such misalignments originate from interaction among agents and arise from three structural asymmetries: differences in parametric knowledge $\theta$ induced by heterogeneous model backbones or role-conditioned prompts, differences in contextual information $c_t$ from asymmetric access to external evidence and differences in interaction structure that influence how agents update their context and memory $m_t$ during collaboration.

### 5.1 Underlying Causes

**Model Heterogeneity and Role Conditioning.** Differences in backbone architecture, pretraining, instruction tuning, or role-specific prompting constitute a fundamental source of inter-agent misalignment. Heterogeneous agents may encode distinct priors or privilege different decision criteria, producing persistent belief-level divergence that communication alone cannot resolve (Xiong et al., 2023; Wu and Ito, 2025; La Malfa et al.). Role-conditioned prompts further amplify this effect by selectively biasing attention and argumentative stance. Recent architectures such as Mixture-of-Agents explicitly exploit such heterogeneity to improve performance (Wang et al., 2025c), but complementary diversity also introduces representational misalignment as a structural byproduct.

**Information Asymmetry.** In retrieval augmented systems, agents accessing different evidence pools develop divergent beliefs even when model parameters are identical. Benchmarks such as ClashEval and Conflicting-RAG demonstrate that unresolved document contradictions systematically mislead collaborative reasoning (Wu et al., 2024; Wang et al., 2025b). Evidence selection thus becomes a structural driver of epistemic divergence, particularly when retrieval operates independently for each agent.

**Interaction Protocol Design.** Beyond agent and information differences, interaction protocol independently shapes collective outcomes. Debate-based, voting-based, or consensus-seeking designs impose different constraints on information exchange, causing identical agents to converge or diverge solely due to protocol structure (Choi et al., 2025; Chen et al., 2023). Aggregation rules determine whether minority-correct signals are preserved or suppressed, and systems lacking mechanisms for viewpoint diversity often collapse into majority voting dynamics (Zhu et al., 2026b; Li et al., 2026). Procedural design thus acts as a direct amplifier or dampener of inter-agent disagreement.

### 5.2 Mitigation and Utilization Strategies

Because inter-agent misalignment arises from structural asymmetries in collaborative systems, practical system design focuses not on eliminating it

entirely but on shaping how it influences collaborative reasoning. Recent research therefore explores two complementary directions: regulating harmful misalignment that destabilizes coordination or propagates incorrect assumptions, and leveraging the reasoning diversity it introduces to improve collective problem solving (Wu and Ito, 2025; Cemri et al., 2025; La Malfa et al.).

**Mitigate Harmful Misalignment.** A first line of mitigation targets the structural and epistemic sources of misalignment. At the architectural level, optimization frameworks such as MASS treat agent roles and communication topology as jointly tunable variables, demonstrating that co-optimizing these elements reduces persistent divergence across reasoning processes (Zhou et al., 2025). Structured reconciliation protocols further stabilize heterogeneous agent groups by encouraging explicit justification and cross-agent comparison (Chen et al., 2024a; Wu and Ito, 2025). At the epistemic level, contradiction-aware retrieval pipelines and provenance-sensitive reasoning protocols reduce the likelihood that inconsistent documents propagate through collaborative reasoning chains (Wang et al., 2025b; Wu et al., 2024). Hybrid mechanisms combine debate-style reasoning exchange with confidence-weighted voting and protocols that explicitly preserve minority signals (Choi et al., 2025; Kaesberg et al., 2025).

**Utilize Misalignment for Exploration.** Rather than suppressing all divergence, a complementary line of work treats reasoning heterogeneity as a resource. Mixture-of-Agents architectures organize heterogeneous LLMs into layered structures in which agents iteratively refine each other's outputs, exploiting complementary capabilities while requiring coordination mechanisms to prevent inconsistent beliefs from propagating (Wang et al., 2025c). Debate-based protocols regulate this process by encouraging agents to critique intermediate steps and refine hypotheses through iterative interaction, though effective collaboration requires both viewpoint diversity and calibrated confidence communication to avoid collapsing into majority voting (Du et al., 2024; Liang et al., 2024; Zhu et al., 2026b). Dynamic debate architectures address this by explicitly generating diverse reasoning paths and specialized agent roles to sustain exploration during deliberation (Li et al., 2026). Reversible reasoning further complements these approaches by introducing rollback mechanisms that allow agents to backtrack when intermediate reasoning becomes inconsistent (Zhao et al., 2025).

**Adaptive Optimization Across Episodes.** Beyond single-episode coordination, misalignment can serve as a diagnostic signal for long-term system improvement. Evaluation-in-the-loop frameworks treat coordination structures themselves as optimization targets, refining prompts, agent roles, and communication protocols based on observed failures. MASS exemplifies structural co-optimization across episodes (Zhou et al., 2025), while evolutionary frameworks such as AlphaEvolve iteratively refine solution strategies through generation–evaluation–selection cycles (Novikov et al., 2025). By systematically analyzing recurring failure modes, such approaches transform misalignment from a problem to eliminate into a driver of sustained coordination improvement (Cemri et al., 2025; La Malfa et al.).

### 5.3 Evaluation of Inter-Agent Misalignment

Evaluating inter-agent misalignment requires going beyond task accuracy to capture interaction dynamics. Recent work suggests that effective evaluation should consider coordination stability, reasoning consistency, and robustness under conflicting evidence. Empirical studies show that different coordination protocols can yield substantially different outcomes even with identical agents, highlighting the importance of evaluating aggregation behavior and convergence dynamics (Radeva et al., 2025). Comparative analyses further reveal that multi-agent collaboration may introduce performance trade-offs due to coordination overhead and inconsistent information flow (Zhu et al., 2025). At the reasoning level, debate-based evaluation frameworks such as ChatEval explicitly model disagreement and reconciliation to better align with human judgments (Chan et al., 2024), while recent benchmarks extend evaluation to social dynamics such as consensus formation and role-induced bias (Reza).

## 6 Challenges and Future Directions

**Attribution and Localization of Misalignment.** A central open challenge is attribution: determining where misalignment originates and how it propagates through the agent loop. Recent work has begun to study failure attribution, error diagnosis, and modular debugging, but these efforts are still mostly post hoc and benchmark-specific. They rarely provide a unified way to localize misalign-

ment across perception, state update, policy formation, and coordination. Future work should therefore develop finer-grained attribution methods that can identify not only where failure appears, but also how local errors cascade into later reasoning and action.

**Realistic and Process-Level Evaluation.** Another major challenge is benchmark design. Existing evaluation studies repeatedly show that current agent benchmarks often overemphasize final success while under-measuring process quality, robustness, and recovery. Although recent benchmarks have started to cover long-horizon planning, memory evolution, and noisy interaction, each still captures only part of the problem. Future benchmarks should jointly evaluate long-horizon reasoning, partial observability, memory updates, perturbation robustness, and process-level quality so that misalignment can be studied as a dynamic systems problem.

**Balancing Autonomy and Controllability.** As LLM agents become more autonomous, a key challenge is to preserve controllability without overly constraining useful agent behavior. Existing work often improves autonomy through stronger planning, memory, or reflection, but these same mechanisms can also make agent behavior harder to predict, supervise, or redirect. This tension becomes especially important when agents update their own state, revise plans, or act over long horizons with limited human intervention. Future research should therefore study how to balance agent autonomy with explicit mechanisms for intervention, correction, and controllable behavior under realistic deployment settings.

**Cross-Modal Misalignment in Multimodal Agents.** An emerging challenge is cross-modal misalignment in multimodal agents. As agents increasingly combine language with visual, auditory, spatial, or embodied inputs, failures may arise when information across modalities is inconsistent, incomplete, or interpreted unevenly. Existing multimodal agent work has mostly focused on improving capability and task performance, while the question of how conflicts across modalities affect memory, reasoning, and action remains less explored. Future work should therefore investigate how multimodal evidence is fused, updated, and verified over time, and how modality-specific errors propagate into broader agent misalignment.

**Scaling Misalignment Mitigation to Multi-Agent Systems.** Another open problem is how to scale mitigation strategies from single-agent settings to multi-agent systems. Many current methods for reflection, memory management, and conflict resolution are designed for one agent with one decision state, but collaborative systems introduce additional challenges such as role mismatch, protocol ambiguity, and divergent local beliefs. As the number of interacting agents grows, local misalignment can also spread more quickly across communication and coordination channels. Future work should therefore study how mitigation mechanisms can be extended from individual reasoning and memory control to distributed settings with shared tasks, evolving roles, and heterogeneous agents.

**Scalable Coordination under Human and Resource Constraints.** A final challenge is to make alignment mechanisms effective under practical deployment constraints. Existing multi-agent and value-alignment work highlights that coordination quality depends not only on reasoning accuracy, but also on communication efficiency, oversight cost, latency, and social compatibility. At the same time, current evaluation still tends to emphasize technical performance more than human-centered, economic, or safety-related considerations. Future research should therefore move beyond asking whether an alignment method improves task success, and instead ask whether it remains controllable, cost-effective, and socially compatible in realistic human-in-the-loop and resource-constrained deployments.

## 7 Conclusion

In this survey, we present a unified view of misalignment in LLM agents across agent–environment, intra-agent, and inter-agent settings. Grounded in a common formulation of LLM agents as sequential decision-making systems with parametric knowledge, run-time context, memory, policy, and state update, we organize the literature around how misalignment arises, propagates, is mitigated, and is evaluated. By bringing these previously fragmented lines of work under a shared framework, we highlight misalignment as a systems-level challenge for increasingly autonomous, interactive, and collaborative agents. We hope this survey provides a useful foundation for future research on building more reliable, coherent, and controllable LLM-agent systems.

## 8 Limitations

This survey has several limitations. First, given page constraints and the rapid growth of the literature, we necessarily make selective choices about coverage, emphasis, and granularity. Some related topics, benchmarks, and methodological variants are therefore discussed only briefly. Second, while we organize the field into agent–environment, intra-agent, and inter-agent misalignment, these categories are intended as an analytical framework rather than a rigid partition, and some works naturally cut across multiple loci. Third, LLM-agent research is evolving quickly, so any survey can provide only a partial snapshot of a moving landscape. New benchmarks, memory systems, and multi-agent frameworks may extend or reshape the taxonomy over time. Finally, our emphasis is on conceptual synthesis and organization of the field, rather than exhaustive empirical comparison. We hope this survey provides a useful starting point for future refinement as the study of misalignment in LLM agents continues to mature.

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## A Main Paper Collections

As shown in Table 1, the papers can be grouped by category, subcategory, mitigation strategy, evaluation setting, and domain.

Table 1: Main Paper Collections

| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| Safe and Robust Reinforcement Learning: Principles and Practice | arXiv 2024 | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Principles to ensure the responsible deployment of RL systems | System-level, Single-agent | Safety, RL Systems, Principles |
| Sim-to-Real Transfer of Deep Reinforcement Learning Agents for Online Coverage Path Planning | arXiv 2024 | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Continuous-space Reinforcement Learning | System-level, Single-agent | Continuous-space RL, Planning |
| The Shadow Self: Intrinsic Value Misalignment in Large Language Model Agents | arXiv 2026 | Agent-Environment | Representation (Intrinsic Value Misalignment) | Carefully filtered and constructed benchmark and human verification | System-level, Single-agent, Multi-step | Framework, Safety, Ethic |
| From Helpfulness to Toxic Proactivity: Diagnosing Behavioral Misalignment in LLM Agents | arXiv 2026 | Agent-Environment | Representation (over-refusal) | Benchmark by multi-turn interactions between dual models | System-level, Single-agent, Multi-step | Framework, Safety, Planning, Tool-use |
| Graph RAG-Tool Fusion | arXiv 2025 | Agent-Environment | Representation (dataset for improving tool-use) | Dataset, Fine-tuning (SFT) | System-level, Single-agent | Dataset, Tool-use, Graph Computation |
| ToolSandbox: A Stateful, Conversational, Interactive Evaluation Benchmark for LLM Tool Use Capabilities | ACL 2025 Findings | Agent-Environment | Structural (Single-turn Interaction) | Benchmark/Framework, Interactive Prompting | Step-level, Single-agent | Benchmark, Tool-use |
| WISE-Flow: Workflow-Induced Structured Experience for Self-Evolving Conversational Service Agents | arXiv 2026 | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Self-evolving, Prompting | System-level, Single-agent/Multi-agent | Framework, Self-evolving |
| Agent-Environment Alignment via Automated Interface Generation | arXiv 2025 | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Lightweight wrapper for model editing, Incontext-learning (generating adapter) | System-level, Single-agent/Multi-agent | Framework, Automated Interface Generation |
| Failures Pave the Way: Enhancing Large Language Models through Tuning-free Rule Accumulation | EMNLP 2023 | Agent-Environment | Representation (Intrinsic Repeating Issues) | Manually Rules Collection and then Incontext learning | Step-level, Single-agent | Tuning-free (prompting) |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| AutoManual: Constructing Instruction Manuals by LLM Agents via Interactive Environmental Learning | NeurIPS 2024 | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Prompting, Multi-turn interaction | System-level, Single-agent | New environment adaption, general improvements on agent tasks |
| IDEA: Enhancing the Rule Learning Ability of Large Language Model Agent through Induction, Deduction, and Abduction | ACL 2025 Findings | Agent-Environment | Structural (Transition Mismatch, Actions from the agent to environments) | Benchmark, Evaluating instruction following by multi-stage interaction (prompting) | System-level, Single-agent | Benchmark, Instruction Following |
| OS-Genesis: Automating GUI Agent Trajectory Construction via Reverse Task Synthesis | ACL 2025 | Agent-Environment | Structural (Mismatch between real-world and synthetic training data) | RL + Prompting | System-level, Single-agent | Framework, Synthetic Data Generation, RL |
| WALL-E: World Alignment by Rule Learning Improves World Model-based LLM Agents | NeurIPS 2025 | Agent-Environment | Representation (mismatch between real-world environment and agent's knowledge) | World Model Fine-tuning | System-level, Single-agent | World Model, RL |
| MetaAgent: Toward Self-Evolving Agent via Tool Meta-Learning | arXiv 2025 | Agent-Environment | Representation (knowledge mismatch between real-world environment and agents) | Self-evolving + Meta Learning | System-level, Single-agent | Self-evolving, Meta Learning, Tool Use |
| AgentRL: Scaling Agentic Reinforcement Learning with a Multi-Turn, Multi-Task Framework | arXiv 2025 | Agent-Environment | Structural (Scaling RL-based Agent to diverse environments) | Multi-turn RL | System-level, Single-agent | Scaling RL-based agents for diverse environments |
| Agent RL Scaling Law: Agent RL with Spontaneous Code Execution for Mathematical Problem Solving | arXiv 2025 | Agent-Environment | Structural (RL policies for reasoning tasks) | RL + Incontext Learning | System-level, Single-agent | RL, Reasoning Tasks, Tool-use |
| Agent Lightning: Train ANY AI Agents with Reinforcement Learning | arXiv 2025 | Agent-Environment | Structural (lightweight RL training pipelines for agents) | RL + Incontext Learning (Long-chain Thinking) | System-level, Single-agent | RL, Lightweight Training Pipelines |
| Reinforcement World Model Learning for LLM-based Agents | arXiv 2026 | Agent-Environment | Process (RL-based world model for better planning strategies) | RL + World Model | Step-level, Single-agent | RL, World Model, Planning |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| Reasoning with Language Model is Planning with World Model | EMNLP 2023 | Agent-Environment | Process (RL-based world model for better planning strategies) | RL + World Model | Step-level, Single-agent | RL, World Model, Planning |
| RLang: A Declarative Language for Describing Partial World Knowledge to Reinforcement Learning Agents | ICML 2023 | Agent-Environment | Representation (mismatch between real-world environment and agent's knowledge) | RL + Multi-turn Conversation | System-level, Single-agent | RL, Planning |
| Gymnasium: A Standard Interface for Reinforcement Learning Environments | arXiv 2024 | Agent-Environment | Representation (mismatch between real-world environment and agent's knowledge) | Benchmark/Resources for designing RL-based agent systems | System-level, Single-agent | RL, Resources |
| ALFWorld: Aligning Text and Embodied Environments for Interactive Learning | ICLR 2021 | Agent-Environment | Representation (abstract knowledge augmentation) | SFT + Prompting | System-level, Single-agent | Framework, SFT, Incontext Learning |
| $\tau^2$-Bench: Evaluating Conversational Agents in a Dual-Control Environment | ICLR 2025 | Agent-Environment | Structural (measuring agents' performance in following rules) | Benchmark, Human Rules/Realistic Simulation | System-level, Single-agent | Benchmark, Datasets, Instruction Following |
| Measuring and Improving Consistency in Pretrained Language Models | Publication | Intra-Agent | Representation (Belief conflict) | Parameter Editing (Weight modification at specific layers) | Episode-level (single edit), Single-agent | |
| Self-Consistency Improves CoT Reasoning | TACL 2021 | Intra-Agent | Representation (Belief conflict) | Learned Gradient-based Editing (Meta-editor network) | Episode-level, Single-agent | |
| Chain-of-Verification | ICLR 2023 | Intra-Agent | Representation (Evidence assimilation conflict) | Architectural + Inference (Multi-agent aggregation over contradictory retrieved evidence) | Episode-level, Multi-agent | |
| Self-Refine | EMNLP 2023 | Intra-Agent | Representation (Tool-induced belief inconsistency) | Prompt Optimization (Tool instruction refinement) | Episode-level | |
| STaR: Bootstrapping Reasoning with Reasoning | NeurIPS 2023 | Intra-Agent | | | | |
| LET'S VERIFY STEP BY STEP | NeurIPS 2022 | Intra-Agent | Structural (Topology / Role Design) | Prompt + Topology Co-optimization | Episode-level, Multi-agent | |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| Adaptive Chameleon or Stubborn Sloth: Revealing the Behavior of LLMs in Knowledge Conflicts | ICLR 2024 | Intra-Agent | Structural (Aggregation protocol comparison) | Protocol Ablation (Debate vs Voting) | Episode-level, Multi-agent | |
| Measuring and Enhancing Trustworthiness of LLMs in RAG through Grounded Attributions and Learning to Refuse | ICLR 2025 | Intra-Agent | Structural (Decision rule comparison) | Protocol-level Aggregation Design | Episode-level, Multi-agent | |
| Taming Knowledge Conflicts in Language Models | EMNLP 2024 | Intra-Agent | Structural (Bias mitigation in consensus) | Dynamic Prompt Refinement + Sycophancy Mitigation | Episode-level, Multi-agent | |
| Steering Knowledge Selection Behaviours in LLMs via SAE-Based Representation Engineering | NAACL 2025 | Intra-Agent | Structural (Judging architecture) | Multi-agent Debate-based Evaluation | Episode-level, Multi-agent | |
| Rich Knowledge Sources Bring Complex Conflicts | ICML 2023 | Intra-Agent | | | | |
| Large LMs Can Be Easily Distracted by Irrelevant Context | arXiv 2025 | Intra-Agent | Process (Search trajectory divergence) | Multi-round Debate (Inference-time protocol) | Episode-level, Multi-agent | |
| Control Illusion: The Failure of Instruction Hierarchies in LLM | arXiv 2025 | Intra-Agent | Process (Diverse reasoning strategies) | Tit-for-Tat Debate Prompting | Episode-level, Multi-agent | |
| Retrieval-Augmented Generation with Conflicting Evidence | NAACL 2025 | Intra-Agent | Process (Cognitive diversity induction) | Role-diversified Debate | Episode-level, Multi-agent | |
| PA-RAG: RAG Alignment via Multi-Perspective Preference Optimization | arXiv 2025 | Intra-Agent | Process (Irreversibility mitigation) | Rollback / Backtracking Mechanism | Episode-level, Multi-agent | |
| Mem0: Building Production-Ready AI Agents with Scalable Long-Term Memory | ACL 2025 | Intra-Agent | Structural (Across-episodes refinement) | Evolutionary Generation–Evaluation–Selection | Across-episodes | |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| Large LMs Can Be Easily Distracted by Irrelevant Context | arXiv 2025 | Intra-Agent | Structural diagnostics informing mitigation | Failure Mode Taxonomy (Motivates structural refinement) | Episode-level, Multi-agent | |
| MemGPT: Towards LLMs as Operating Systems | | Intra-Agent | Structural critique | Systems-level audit (Conceptual guidance) | System-level | |
| Locating and Editing Factual Associations in GPT | NeurIPS 2022 | Inter-Agent | Representation (Belief conflict) | Parameter Editing (Weight modification at specific layers) | Episode-level (single edit), Single-agent | Model Editing / Factual Knowledge |
| Fast Model Editing at Scale | ICLR 2022 | Inter-Agent | Representation (Belief conflict) | Learned Gradient-based Editing (Meta-editor network) | Episode-level, Single-agent | Scalable Model Editing |
| Retrieval-Augmented Generation with Conflicting Evidence | COLM 2025 | Inter-Agent | Representation (Evidence assimilation conflict) | Architectural + Inference (Multi-agent aggregation over contradictory retrieved evidence) | Episode-level, Multi-agent | RAG under contradictory evidence |
| PLAY2PROMPT: Zero-shot Tool Instruction Optimization for LLM Agents via Tool Play | arXiv 2025 | Inter-Agent | Representation (Tool-induced belief inconsistency) | Prompt Optimization (Tool instruction refinement) | Episode-level | Tool-augmented Agents |
| Multi-Agent Design: Optimizing Agents with Better Prompts and Topologies | arXiv 2025 | Inter-Agent | Structural (Topology / Role Design) | Prompt + Topology Co-optimization | Episode-level, Multi-agent | MAS coordination optimization |
| RECONCILE: Round-Table Conference Improves Reasoning via Consensus among Diverse LLMs | ACL 2024 | Inter-Agent | Structural (Consensus protocol) | Structured Debate + Confidence-weighted Voting | Episode-level, Multi-agent | Multi-model consensus reasoning |
| Debate or Vote: Which Yields Better Decisions in Multi-Agent Large Language Models? | NeurIPS 2025 | Inter-Agent | Structural (Aggregation protocol comparison) | Protocol Ablation (Debate vs Voting) | Episode-level, Multi-agent | Decision protocol analysis |
| Voting or Consensus? Decision-Making in Multi-Agent Debate | ACL 2025 Findings | Inter-Agent | Structural (Decision rule comparison) | Protocol-level Aggregation Design | Episode-level, Multi-agent | Aggregation dynamics |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| CONSENSAGENT: Towards Efficient and Effective Consensus in Multi-Agent LLM Interactions Through Sycophancy Mitigation | ACL 2025 Findings | Inter-Agent | Structural (Bias mitigation in consensus) | Dynamic Prompt Refinement + Sycophancy Mitigation | Episode-level, Multi-agent | Consensus stability |
| ChatEval: Towards Better LLM-based Evaluators through Multi-Agent Debate | ICLR 2024 | Inter-Agent | Structural (Judging architecture) | Multi-agent Debate-based Evaluation | Episode-level, Multi-agent | LLM-as-judge |
| Multi-Agent Debate for LLM Judges with Adaptive Stability Detection | NeurIPS 2025 | Inter-Agent | Structural (Judging + stopping criteria) | Adaptive Stopping + Debate Arbitration | Episode-level, Multi-agent | Reliable arbitration |
| Improving Factuality and Reasoning in Language Models through Multiagent Debate | ICLR 2024 | Inter-Agent | Process (Search trajectory divergence) | Multi-round Debate (Inference-time protocol) | Episode-level, Multi-agent | Factual QA / reasoning |
| Encouraging Divergent Thinking in Large Language Models through Multi-Agent Debate | EMNLP 2024 | Inter-Agent | Process (Diverse reasoning strategies) | Tit-for-Tat Debate Prompting | Episode-level, Multi-agent | Logical reasoning |
| Breaking Mental Set to Improve Reasoning through Diverse Multi-Agent Debate | ICLR 2025 | Inter-Agent | Process (Cognitive diversity induction) | Role-diversified Debate | Episode-level, Multi-agent | Mathematical / logical reasoning |
| ReAgent: Reversible Multi-Agent Reasoning for Knowledge-Enhanced Multi-Hop QA | EMNLP 2025 | Inter-Agent | Process (Irreversibility mitigation) | Rollback / Backtracking Mechanism | Episode-level, Multi-agent | Multi-hop QA |
| The Hidden Strength of Disagreement: Unraveling the Consensus-Diversity Tradeoff in Adaptive Multi-Agent Systems | EMNLP 2025 | Inter-Agent | Process–Structural interface | Implicit Consensus via In-Context Learning | Episode-level + Dynamic Environments | Adaptive MAS |
| AlphaEvolve: A Coding Agent for Scientific and Algorithmic Discovery | arXiv 2025 | Inter-Agent | Structural (Across-episodes refinement) | Evolutionary Generation–Evaluation–Selection | Across-episodes | Coding agent |

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| Paper | Pub. | Category | Subcategory | Mitigation | Evaluation | Domain |
|---|---|---|---|---|---|---|
| Why Do Multi-Agent LLM Systems Fail? | NeurIPS 2025 | Inter-Agent | Structural diagnostics informing mitigation | Failure Mode Taxonomy (Motivates structural refinement) | Episode-level, Multi-agent | MAS failure analysis |
| Large Language Models Miss the Multi-Agent Mark | arXiv 2025 | Inter-Agent | Structural critique | Systems-level audit (Conceptual guidance) | System-level | MAS theory vs LLM systems |
| Demystifying Multi-Agent Debate: The Role of Confidence and Diversity | arXiv 2026 | Inter-Agent | Structural (Debate dynamics: diversity & confidence) | Diversity-aware initialization + Confidence-modulated debate updates | Episode-level, Multi-agent | Debate dynamics / collective reasoning |
| Mixture-of-Agents Enhances Large Language Model Capabilities | ICLR 2025 | Inter-Agent | Structural (Layered agent aggregation architecture) | Architectural aggregation (Layered Mixture-of-Agents inference) | Episode-level, Multi-agent | Multi-model collaboration |
| DynaDebate: Breaking Homogeneity in Multi-Agent Debate with Dynamic Path Generation | arXiv 2026 | Inter-Agent | Process (Reasoning path homogeneity / trajectory collapse) | Dynamic Path Generation + Process-centric debate + Verification agent | Episode-level, Multi-agent | Debate-based reasoning |