
Position: Time to Close The Validation Gap in LLM Social Simulations

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Abstract

LLM-based social simulations—in which many language model agents interact over multiple turns—are rapidly proliferating across policy analysis, epidemiology, and computational social science. Yet the field lacks consensus on how to validate these simulations, with evaluation methods that are few, underdeveloped, fragmented, and rarely shared across disciplines. We argue this creates a serious risk: premature deployment of unvalidated simulators in high-stakes domains. Our position is that the field must pivot from expansion to consolidation, prioritizing methodological standardization—shared benchmarks, open data, and reproducible evaluation protocols grounded in social science and complex systems research. We outline a concrete research program organized around specific learning problems/benchmarks, providing a path toward answering the fundamental question: when are LLM social simulations useful modelling objects?

1. Introduction

The advent of Large Language Models (LLMs) has the potential to constitute an important step forward in the simulation of human social systems. They allow modelling human behaviour at a degree of social complexity and grounding that greatly exceeds existing modelling approaches, covering phenomena central to culture and society. A motivation to pursue such approaches comes from viewing LLMs as cultural technologies, providing access to large amounts of cultural information (Farrell et al., 2025). For such phenomena, they would supplant both traditional agent-based modeling, in which agent models with minimal complexity limit model expressivity, and deep reinforcement learning agent simulations, in which a blank-slate specification bur-

den limits model grounding to real social phenomena (Lake et al., 2017).

This technology promises to produce world models (Ding et al., 2025) (such as social world models), useful for understanding mechanisms, testing counter-factuals, and making predictions. Researchers from many disciplines are now developing LLM-based simulation approaches that build and run social world models for a variety of applications (e.g. generic (Zhou et al., 2025a; Ren et al., 2026), social media (Ng & Carley, 2025; Puelma Touzel et al., 2025), public health (Shi et al., 2026; Chopra et al., 2024; Kozłowski & Evans, 2025)). The seminal paper in the field explicitly proposed policy applications (Park et al., 2022) and policy analysts are starting to pay attention (e.g. (Orsi, 2024)). However, current research activity is scattered broadly over a range of disciplines, bringing heterogeneous goals and norms around quality and rigor.

There is a long tradition in social science of developing penetrating evaluations designed to interrogate complex social systems through the best, but still limited measurement of survey and observation. This toolkit is being brought to bear on LLM-based social simulations (Wallach et al., 2025; Cui et al., 2025).

In parallel and with access to unprecedented compute resources, software development technologies are being used to build general simulators with rich feature sets (e.g. (Piao et al., 2025a; Yang et al., 2024)). Many such products are advertised as general purpose, but are evaluated on a relatively narrow set of applications, leaving broader evaluation to domain-specific adopters.

A natural consequence of this discordant development is slow convergence towards consensus of what these models are capable of. For example, seemingly conflicting results regarding many core questions like the ability of LLMs to reproduce survey responses and the ability of groups of agents to produce genuine emergent behaviour. A likely cause in many of these cases, is divergent methodology and heterogeneous problem framing. Moreover, insufficient validation can lead to invalid conclusions about emergent behaviour (Barrie & Törnberg, 2025).

Evaluation-centric and feature-centric approaches are both

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necessary, but neither alone is sufficient. We argue that assessing the real utility of LLM-based social simulations requires their careful integration within a unified methodological framework. The natural vehicle for this integration is machine learning methodology: well-defined learning problems supported by shared data, open code, and standardized benchmarks.

Position: Validation of LLM-based social simulations has not kept pace with their proliferation. The field must pivot from expansion to consolidation—adopting shared benchmarks, open data, and reproducible evaluation grounded in social science—before these tools can responsibly inform high-stakes decisions.

Summarizing our paper’s contributions, we:

1. Provide a *modelling language* through which to ground discussions around the evaluation of a class of models we term Silicon Societies.
2. Express a list of *evaluation fallacies* made in the literature on silicon societies and phrase them in our language.
3. Outline a *frictionless reproducibility* approach that our position advocates for and provide an example simulator project to illustrate best practise.
4. Layout a set of *learning problems* inspired by a set of target properties and evaluations designed to measure them (stability, polarization, narratives)
5. Engage with *alternative views* and sketch a *call-to-action* about how researchers from different disciplines can participate in our proposed structured research community.

2. Silicon Societies

While LLMs are relatively recent, the research on simulating social systems with LLMs and on multi-agent AI systems is already vast. The position we argue here regards modeling social phenomena, which helps focus the scope onto works that aim toward Silicon Societies. We define *Silicon Societies* as simulations of human social interactions with a large amount of implicit (i.e. latent) cultural context selectively made explicit using LLMs. Works on task-oriented multi AI-agent systems (coding agents, web/computer agents, *etc.*), which typically do not explicitly model the larger human environment into which the agents will eventually be deployed and do not seek to model human behavior, are therefore out of scope (though some of their evaluation methods could still be of relevance, e.g. Vijayvargiya et al. (2025)). Phenomena in human society are typically strongly influenced by social reasoning about implicit and explicit social norms, or other aspects of social intelligence that emerge among

groups of agents. Emergent social intelligence then serves as a central topic in this scope and focuses model design on the *simulationist* design objective (Vezhnevets et al., 2025) in which the goal is empirical fidelity over a specified subset of social phenomena. While the aim is to match behaviours with the set of relevant phenomena, replicating microscopic detail is not necessary *a priori* as the details required depend on the phenomena of interest.

In pursuit of this simulationist objective, machine-readable (i.e. digital) environments are especially relevant as they offer large amounts of human interaction data to ground simulator behavior. Social media is a prime example of such an environment.

To reason clearly about the validity, limitations, and evaluation of silicon societies, we next introduce a minimal formal abstraction that captures what these systems have in common. In contrast to more general formulations (Ferrarotti et al., 2026), ours has the specificity to be able to state precisely a variety of important validation problems.

2.1. Formal Abstraction

In a high-level description, a silicon society induces a probability distribution over system trajectories. A trajectory records the evolution of the environment and agent interactions over time, including what agents observe and how they act.

Formally, let

$$\tau = (s_0, \{o_0^i, z_0^i, a_0^i\}_{i=1}^n, s_1, \dots, s_T),$$

denote a trajectory of length T , where s_t represents the environment state at time t , and o_t^i and a_t^i denote the observation and action of agent i .

A *silicon society* defines a distribution,

$$p(\tau \mid \mathcal{X}, \Theta),$$

where \mathcal{X} denotes the simulation specification (e.g., prompt templates, orchestration logic, environment rules), and Θ denotes model parameters (e.g., LLM weights, temperatures, and persona/environment initializations).

This abstraction is intentionally minimal. It hides architectural details and treats the simulator as a generative process over trajectories. Our critique applies to any system that induces such a distribution, regardless of whether agents are implemented via prompting, fine-tuning, tool use, explicit planning modules, or hybrid approaches.

Evaluations of silicon societies are then functions of trajectories,

$$\mathcal{L}(\tau),$$

which may assess properties such as behavioral realism, stability over time, coordination strength, or alignment with

empirical data. Learning or tuning a simulator—whether by adjusting prompts, model parameters, or environment design—can be understood as optimizing expected evaluation outcomes under this distribution.

Many claims made in the literature, including claims about emergence, coordination, or norm formation, are ultimately statements about statistical properties or dependencies within $p(\tau \mid \mathcal{X}, \Theta)$. Making this objective explicit allows such claims to be stated precisely and, in principle, tested.

2.2. A Representative Simulator Decomposition

We now describe one common instantiation of the abstract formulation above, using a machine learning–oriented formalism inspired by stochastic games and prior work on LLM-based agent simulations (e.g., Concordia (Vezhnevets et al., 2023)). This decomposition is representative rather than normative; many variants are possible.

A multi-agent simulation consists of n agents interacting within a shared environment. Each agent is implemented using a generative model (e.g., an LLM) that samples outputs conditioned on inputs and parameters. Given an input x (such as a prompt with context) and parameters θ , the model generates

$$y \sim p(\cdot \mid x, \theta),$$

where y can be text, structured data, or an action specification.

System Components At time t :

- s_t – environment state (locations, objects, social context)
- o_t^i – agent i ’s observation of the environment: $o_t^i = \mathcal{O}^i(s_t)$
- a_t^i – agent i ’s action (speech, movement, posts). Together, these actions form the joint action vector, \mathbf{a}_t .
- θ^i – LLM parameters for agent i (model type, weights, temperature, static+initial persona context)
- $\mathcal{A}^i(\cdot)$ – agent i ’s action generation function (prompt structure)
- θ_{Env} – environment parameters (model type, rules, static+initial environment context)
- $\mathcal{T}(\cdot)$ – environment state update function (prompt structure or rules)
- $\Theta = (\theta_{\text{Env}}, \theta^1, \dots, \theta^n)$ – all LLM model parameters

In addition to having implicit internal states (LLM activations), agent models can have explicit (e.g., natural language) internal states:

- z_t^i – agent i ’s internal state (beliefs, memories, goals, plans), and
- $\mathcal{Z}^i(\cdot)$ – agent i ’s internal state update function (prompt structure).

Dynamics Each timestep involves agent computation following a perception-cognition-action cycle along with environment computation providing observations and resolving action effects:

1. **Think:** Update internal state based on observation and prior state

$$z_{t+1}^i \sim p(\cdot \mid \mathcal{Z}^i(o_{t+1}^i, z_t^i), \theta^i), \quad (1)$$

where $\mathcal{Z}^i(o_{t+1}^i, z_t^i)$ constructs the prompt, e.g. “Given {interaction} & {retrieved memories/beliefs}, what would {name} think?”.

2. **Act:** Generate action based on internal state

$$a_{t+1}^i \sim p(\cdot \mid \mathcal{A}^i(z_{t+1}^i), \theta^i), \quad (2)$$

where $\mathcal{A}^i(z_{t+1}^i)$ constructs the prompt, e.g. “Given {interaction} & {thoughts}, what would {name} do?”.

3. **Environment update:** An environment simulator is used to update the world based on all actions

$$s_{t+1} \sim p(\cdot \mid \mathcal{T}(s_t, \mathbf{a}_t), \theta_{\text{Env}}), \quad (3)$$

where $\mathcal{T}(s_t, \mathbf{a}_t)$ encodes update rules and/or constructs the prompt for LLM-based updating, e.g. “Given {the state}, and {names} attempted {actions}, what happens?”.

Simplified variants may omit explicit internal state and generate actions directly from observations and history, trading interpretability for computational efficiency.

Under this decomposition, the simulator induces the trajectory distribution introduced in Section 2.1. Different choices of prompts, parameters, or environment rules correspond to different distributions over trajectories and, consequently, different simulated social dynamics.

The benefit of this abstraction is not technical novelty but analytical clarity. By making the generative object explicit, it becomes possible to precisely formulate and evaluate claims about silicon societies. This perspective also clarifies what it means to validate, compare, or transfer simulations across settings—questions that motivate the critiques and fallacies discussed in the next section.

3. Common Evaluation Pitfalls in Silicon Societies

LLM-based agent simulations incur orders-of-magnitude higher computational costs than classical agent-based models (ABMs) (Samsi et al., 2023). To justify this expense, they must demonstrate clear advantages in explanatory power or empirical fidelity. However, recent *Silicon Society* literature has been accused of “failing to adequately evidence operational validity” (Larooij & Törnberg, 2025). Simulators

Axis	Fallacy	Framework Component	Core Issue
I. Distributional Validity	Face Validity	$p(\tau \mid \Theta) \approx p^*(\tau)$	Low-dimensional plausibility \neq full trajectory distribution
	Aggregate Validation	$\mathbb{E}[\psi(\tau)]$ vs. $p(\tau)$	Matching moments \neq matching distributions
	Cherry-Picking [†]	$p(E \mid \Theta)$ for event E	Post-hoc selection of favorable events
II. Agent–Human Correspondence	Human Proxy Assumption	$p(a \mid s)$	LLM behavior assumed human without evidence
	Social Desirability Bias	$p(a \mid \mathcal{A}, \theta)$	RLHF skews action distributions
	Demographic Representation	$\mathcal{A}^i(d^i)$	Prompting demographics \neq embodied agents
III. Design Justification	Untested Design Choices	\mathcal{X}, Θ	Complexity added without ablation or justification
	Prompt Sensitivity	$\mathcal{Z}^i, \mathcal{A}^i$	Semantic invariance violated under rephrasing
	Black-Box Gap	z_t^i	Internal reasoning unverifiable or uninterpretable
	Reproducibility Failure	$(\mathcal{Z}, \mathcal{A}, \mathcal{T}, \Theta, \dots)$	Key components underspecified or unstable
IV. Emergence & Diversity	Homogeneity	$\text{Var}[f(\tau)]$	Shared θ collapses agent diversity
	Single-Model Dependence [†]	Θ fixed	Model-specific artifacts mistaken for phenomena
	Circular Evaluation Sycophancy	$\theta^{\text{judge}} \approx \theta$ $p(a \mid \mathcal{A}, \theta, r)$	Shared biases inflate evaluation scores Researcher intent leaks into behavior
Generic ML Pitfalls [†]	Contamination	$\tau^* \in D_{\text{train}}$	Memorization mistaken for generalization
	Temporal Validity	$T_{\text{cutoff}} \in \theta$	Knowledge-time mismatch
	Causal Confounding	$p(U \mid s_t, T, \theta)$	Unconfoundedness assumptions violated

Table 1. Common evaluation fallacies in Silicon Society simulations, grouped by axis and mapped to components of the simulator formalism. [†]Denotes pitfalls not specific to multi-agent LLM simulations, but included for completeness.

are often engineered at impressive scale (e.g, thousands of agents (Yang et al., 2024)), yet remain difficult to use for scientific inference because their alignment with real-world behavior is weakly evidenced or entirely unknown.

Below, we group common pitfalls into four axes that are particularly salient. More general machine learning issues (e.g., cherry-picking / contamination) are acknowledged in Table 1 but not expanded upon, as they are not specific to this setting.

Axis I: Distributional Validity vs. Face Validity

A pervasive pitfall is equating qualitative plausibility with distributional correctness. Many works rely on anecdotal examples, hand-picked trajectories, or compelling visualizations as evidence of success, implicitly assuming that $p(\tau \mid \mathcal{X}, \Theta) \approx p^*(\tau)$, where $p^*(\tau)$ denotes the (unknown) real-world process.

In practice, evaluations often focus on low-dimensional projections (denoted ψ), such as individual conversations, summary statistics, or emergent narratives, rather than trajectory distribution itself. However, agreement on moments or marginal statistics does not imply agreement on the full distribution. This leads to *aggregate validation* fallacies,

where matching $\mathbb{E}[\psi(\tau)]$ is mistaken for matching $p(\tau)$.

Of course there are meaningful notions of matching that are not exact, e.g. distinguishability according to humans or a family of classifiers (Pagan et al., 2025), but these studies are rare. Matching issues are exacerbated by vague problem definitions “simulating society” or “modeling social media” (Yang et al., 2024; Piao et al., 2025b; Park et al., 2023; Surve et al., 2023; Vezhnevets et al., 2023; Kaiya et al., 2023; Park et al., 2022) and by ad-hoc metrics that prevent meaningful cross-paper comparison. In our formalism, this corresponds to validating isolated samples of τ , rather than defining and optimizing a principled evaluation function $\mathcal{L}(\tau)$.

Axis II: Agent–Human Correspondence

Many Silicon Society projects implicitly assume that LLM-based agents are reasonable proxies for human cognition and behavior. Yet empirical evidence paints a mixed picture. Studies comparing LLMs and humans across behavior (Bück-Kaeffer et al., 2025; Ma, 2025), neural representations (Holton et al., 2025; Pinier et al., 2025; Fedzechkina et al., 2025; Aw et al., 2024; Holton et al., 2026; Zhou et al., 2025b; Kwon et al., 2025), and psychological constructs (Schröder et al., 2025) yield inconsistent results.

Despite this, several works proceed as though the correspondence holds by default (Abdurahman et al., 2025; Piao et al., 2025b; Wang et al., 2023). In our notation, this amounts to assuming $p(a_i|s) = p_{\text{some human}}(a|s)$ without direct empirical support. Attempts to mitigate these gaps, either through alignment techniques or cognitive modeling, remain limited in adoption and are themselves contested (Binz et al., 2025; Chen et al., 2025b; Kong et al., 2026; Schröder et al., 2025; Namazova et al., 2025).

Without explicitly testing agent–human correspondence on the phenomena of interest, downstream conclusions about social dynamics rest on an unstable foundation. This has strong implications when investigating how LLMs would behave in the real world (Ren et al., 2026; Orlando et al., 2025) using simulated environments.

Axis III: Unjustified Simulator Design Choices

A distinct but closely related pitfall concerns simulator design itself. Silicon societies typically consist of many interacting components (e.g., persona initialization, memory systems, planning modules, environment, and orchestration logic), each adding complexity to \mathcal{X} and Θ .

A common fallacy is to treat this complexity as self-justifying. Components are often motivated by cognitive theories or narrative plausibility, but not validated through controlled experiments. While recent large-scale simulators demonstrate that ablations are almost always feasible even in complex computational models (Yang et al., 2024), such analysis remain rare.

This lack of validation leads to two complementary pathologies. Some works introduce elaborate mechanisms to address problems that are assumed, rather than demonstrated, to exist; others implicitly assume these mechanisms are unnecessary, again without testing the assumption. In both cases, \mathcal{X} and Θ are expanded without evidence of improvement under any evaluation function $\mathcal{L}(\tau)$, obscuring causal attribution and hindering principled comparison across simulators.

Concrete examples illustrate this issue. Vezhnevets et al. (2023) and Wang et al. (2023) propose cognitively inspired agent frameworks, with Vezhnevets et al. (2023) grounding design choices in cognitive psychology. While theoretically motivated, such justification is insufficient absent evidence that these components improve task-relevant or societally meaningful metrics. Conversely, Yang et al. (2024) adopts a minimal, memory-based LLM agent design without ablation-based justification. To our knowledge, whether incorporating human-inspired cognitive components into LLM agents yields measurable improvements in simulation quality remains an open empirical question.

Axis IV: Emergence, Coupling, and Diversity

A defining motivation for Silicon Societies is the study of emergent social phenomena. However, many simulations inadvertently suppress emergence through architectural choices that induce excessive homogeneity. Shared model weights, similar prompts, and strong RLHF priors reduce variance across agents (Wu et al., 2025; Jiang et al., 2025), leading to collective behavior that reflects model bias rather than interaction-driven dynamics.

In formal terms, emergence requires violations of conditional independence: $p(a_t | s_t) \neq \prod_{i=1}^n p(a_t^i | s_t)$. Yet few works test this explicitly. While techniques to increase diversity exist (Nguyen et al., 2025), and its importance has been argued (Robertson et al., 2024), empirical demonstrations linking diversity to improved simulation fidelity remain scarce and have been contested (Barrie & Törnberg, 2025).

Towards proper validation

Recent work has begun to argue that persona simulation itself requires a scientific methodology (Li et al., 2025a). While these efforts focus primarily on individual agents, introducing environments and multi-agent interaction induces additional complexities and emergent effects (Orlando et al., 2025; Curvo et al., 2025; Schroeder et al., 2026) that demand additional, distinct validation strategies (Song et al., 2025).

Existing surveys and methodological critiques largely agree that current practices are insufficient (Larooij & Törnberg, 2025), and recent proposals offer some practical guardrails (Madden, 2025). What remains lacking is adoption and iterative improvement. Establishing shared standards for specifying simulators, justifying design choices, and evaluating trajectory-level behavior is essential if Silicon Societies are to mature into a reliable scientific tool rather than an exercise in plausible storytelling.

4. The solution is frictionless reproducibility

Machine learning has exhibited unprecedented growth compared with other disciplines. What explains this speed? Platt asked a similar question of molecular biology fifty years ago and pointed to rigorous hypothesis-based testing (Platt, 1964). But this “strong inference” approach is a weaker methodology for complex systems—particularly social ones—where causes cannot typically be isolated to individual components (Anderson, 1972). Donoho offers a more compelling answer for machine learning’s rapid progress: “frictionless reproducibility,” an interconnected set of research practices and incentives that make methodology explicit and efficiently leverage community consensus mechanisms (Donoho, 2023; Recht, 2024). In this section,

we contribute elements of this practise for the case of silicon society research.

4.1. Learning problems

Agent models Agent models are a primary target of machine learning. Here we list some non-mutually exclusive agent training paradigms:

1. *Model Training*: parameters can be fine-tuned from a base model $\theta^i = \theta_{\text{base}} + \Delta\theta^i$, using techniques such as Supervised Fine Tuning (SFT) or Reinforcement Learning (RL).
2. *Model Steering*: steering vectors Δx^i can be used to bias model activations x^i , controlling the value of the output logits of the model. This is used to structure the internal model representation (Chen et al., 2025a).
3. *Prompt engineering*: the structure of prompt functions can be trained, e.g., by
 - structure learning a component network (z now being a vector of natural language statements and \mathcal{Z} now updating all components with conditional dependence given by a component graph)
 - including data directly in the prompt, e.g. $\{a_j^i\}_{j=1}^D$ for D In-Context Learning (ICL) samples.
4. *Persona Learning*: Creating realistic agents may require grounding on real-world data. Personas can be condensed from existing human data and provided to the model via the above methods.

4.2. Core Learning Objectives

We now describe several learning problems that recur across silicon societies, ordered from most concrete to most structural.

Next-Action Prediction The most common and operationally convenient learning problem is next-action prediction. Given the environment state and interaction history, the agent predicts its next action:

$$\mathcal{L}_{NAP} = -\log p(a_{t+1}|s_t, a_t, \dots, s_1, a_1)$$

This framing collapses “thinking” and “acting” into a single observable step, aligning well with real-world datasets in which only actions and environment updates are logged. Social media platforms are a canonical example: users observe a post and may reply, react, repost, or ignore.

Evaluation. Metrics can be defined at multiple granularities:

1. Individual level: action classification (e.g., F1-score), semantic similarity of generated content (cosine similarity of embeddings, Jaccard similarity over high-IDF terms), or divergence measures (e.g., Jensen–Shannon).
2. Population level: distributional alignment using aggregated statistics, kernel density estimates, or Monte

Carlo rollouts compared against historical data (e.g., KL or JS divergence).

Projects such as BluePrint (Bück-Kaeffer et al., 2025) instantiate this paradigm explicitly, emphasizing population-level fidelity rather than per-agent optimality. Matching here should cover both the content and action type (Gatta et al., 2026).

While next-action prediction is easy to train and evaluate, it is agnostic to internal reasoning structure and offers limited guarantees about long-horizon dynamics.

Component Structure Learning Beyond action prediction, some systems aim to learn or impose structure over agent internal state z_t^i . We distinguish two broad approaches:

1. Explicit structure learning, where internal state is represented in natural language or symbolic components (e.g., beliefs, goals, memories), possibly with learned dependency graphs and update rules.
2. Implicit structure learning, where internal structure is encoded in parameters (fine-tuned weights, steering vectors) without interpretable state variables.

These approaches correspond to different inductive biases:

1. bottom-up emergence versus top-down role or persona inference,
2. static versus dynamically updated internal state,
3. interpretable but brittle representations versus opaque but flexible ones.

Objectives in this regime are often indirect, such as narrative alignment, behavioral consistency, or constraint satisfaction, rather than likelihood maximization.

Environment Initialization and Orchestration Learning problems also arise at the level of the environment:

1. **Initialization**: choosing initial states s_0 (e.g., network structure, topic distribution, agent personas) that reproduce realistic downstream behavior.
2. **Interaction orchestration**: determining whether interactions are narration-driven, dialogue-driven, or event-driven, and how information propagates across agents.

Although these components are often treated as fixed design choices, they implicitly define strong priors over trajectories and can dominate downstream outcomes. One such design choice is whether agents update simultaneously or sequentially and in what order.

4.3. Stability and Long-Horizon Behavior

Silicon societies differ most from persona research (centering around one-shot settings, such as survey responses) in

that they admit interaction dynamics among agents. This temporally-extended simulation setting raises the question of long-horizon behavior. Even when local objectives (e.g., next-action prediction accuracy) are satisfied, small modeling errors may compound over time, leading to distributional drift or unrealistic equilibria.

This framing enables several important distinctions:

1. Local fidelity vs. global stability: a simulator may match empirical action distributions at short horizons while diverging over longer rollouts.
2. Training vs. deployment mismatch: objectives optimized under short trajectories may not control long-term population behavior.
3. Evaluation beyond snapshots: stability metrics depend on trajectories, not single-step predictions.

While most existing silicon societies do not explicitly optimize, let alone evaluate stability, making stability assumptions explicit clarifies what claims can—and cannot—be supported by current evaluation practices. While model complexity precludes the kind of mathematical control in dynamical systems research, the concepts of ergodic theory do provide a language to describe and classify long-term behaviour.

4.4. An Example Simulator

To illustrate what frictionless reproducible silicon society projects look like, we provide ScenSim¹, an example simulator project structured for training against evaluation objectives, with highly interoperable components. The simulator’s configuration has 5 main components:

- simulator (engine logging and execution)
- model (genAI models, model parameters, Θ)
- environment \mathcal{T} , θ_{Env} (interaction rules)
- scenario (agent models \mathcal{A}_i , \mathcal{Z}_i , shared knowledge)
- evaluation \mathcal{L} (metrics, probes, statistical operations)

Each component is configurable via schema-constrained plain text, with variants easily created through default overrides. The simulator outputs human- and LLM-readable action logs for evaluation. A probe system surveys agents longitudinally, feeding responses to evaluation function \mathcal{L} . We include two example scenarios (election and marketplace) with instructions for generating new ones..

The project follows open science practices: version-controlled with strict formatting and testing requirements, readable contribution guidelines, and emerging best practices for coding agents (e.g., context files for agent use). Project management is largely automated, letting researchers focus on model development and evaluation rather than tooling.

¹<https://anonymous.4open.science/r/scensim-0558>

5. Alternative Views

Our position is constructive: we not only identify the dilemma but propose a timely solution. Alternative views to our position can take a few forms:

Arguments against benchmarking. A common objection is that benchmarks are inherently gameable. This concern is valid, but incentive structures are improving rapidly. For example, PeerBench (Cheng et al., 2025) combines sealed execution, item banking with rolling renewal, and delayed transparency, and operates alongside open benchmarks to reduce strategic overfitting.

A deeper critique is that ML benchmarks are ill-suited to large, complex social systems, where ground truth is often ambiguous or unavailable. It is unclear, for instance, how to objectively rank a simulated response to a policy intervention or global event. From this perspective, benchmarking risks imposing a false precision that misrepresents the epistemic status of social science. We agree that naïve ranking is inappropriate. However, evaluation need not reduce to scalar scores. Instead, it can characterize model behavior, surface sensitivities, and clarify which assumptions drive outcomes. Social science already operates productively without definitive ground truth, relying on comparative analysis and typologies; the framework we propose explicitly draws on these traditions.

The real problem is deployment, not methodology. Another view holds that the primary risk is not the absence of benchmarks, but the uncritical deployment of these simulators by decision-makers. The remedy, on this account, is governance and stakeholder education rather than additional ML infrastructure. We agree that standards alone cannot prevent misuse. However, shared evaluation norms are themselves communicative: they make limitations legible, create common reference points for critique, and signal appropriate use to downstream stakeholders.

Ethical and technical challenges of obtaining ground truth. A key motivation for *Silicon Societies* is the ability to study scenarios that would be costly, impractical, or unethical to examine with human subjects. In such cases, relevant datasets may be sparse, sensitive, or altogether unavailable, making validation against real-world ground truth infeasible. We acknowledge this limitation, but caution that deploying unvalidated models in high-stakes domains is itself problematic. When grounding is impossible, this should be stated explicitly and the strength of resulting claims attenuated accordingly. Where feasible, ethical data frameworks should be developed and preferred (Bück-Kaeffer et al., 2025).

Validation is premature and may stifle development. A related argument is that the field is too young to know which

assumptions matter, and that early validation risks locking in the wrong abstractions. We agree that exploratory work is essential. Nonetheless, some degree of evaluation is necessary even at early stages to ensure progress is cumulative rather than idiosyncratic. Provisional and lightweight evaluation frameworks can evolve alongside the field without foreclosing future methodological shifts.

Are social simulations a good use case for LLMs? Given the cost and complexity of LLMs, it is important to clarify when LLM-based social simulations are well motivated. Traditional agent-based models capture diffusion processes such as social contagion and epidemics (Guilbeault et al., 2017; Sambaturu et al., 2020), but struggle with phenomena rich in social meaning. Deep reinforcement learning agents exhibit general coordination capabilities (Stooke et al., 2021), yet remain far from human social complexity. One-shot or few-turn LLM persona studies probe implicit social knowledge (Li et al., 2025a), and are informative when interaction and dynamics are not central.

We argue that LLM-based social simulations are a truly novel and useful approach to modelling, and are especially valuable for phenomena characterized by:

- *Collective network effects* emerging from many interacting agents;
- *Social norms and sanctioning* shaping behavior (e.g., family planning, public health compliance, political participation);
- A central role for *language*, including semantic abstraction and linguistic ambiguity.

6. Call to Action

Realizing this vision requires coordinated action. ML researchers should adopt validation frameworks, report sensitivity and variance metrics, and build on community standards rather than ad hoc procedures. Social scientists can identify suitable benchmark datasets, advise on domain-appropriate evaluation criteria, and challenge oversimplified claims about simulation capabilities. Venues (NeurIPS, ICML, AAMAS) should require validation protocols for acceptance and create tracks for methodological work. Funding agencies can include validation requirements in proposals and prioritize interdisciplinary teams and methodological rigor. Industry labs should adopt validation benchmarks internally, contribute to open infrastructure, and be transparent about model limitations for social simulation. To catalyze this transition, we propose forming an interdisciplinary working group to deliver three foundational resources:

1. A benchmark suite spanning survey response prediction, economic games, opinion dynamics, and crisis

behavior, with held-out test sets and contamination controls;

2. An open-source evaluation toolkit implementing standardized metrics for distributional validity, variance calibration, and sensitivity analysis; and
3. An author checklist and reviewer guidelines for LLM social simulation papers.

These resources would provide the shared infrastructure necessary to transform a fragmented literature into a cumulative research program capable of answering the fundamental question: when, if ever, can LLM social simulations be trusted?

7. Responsible Research

This research program centers around advancing LLM simulations. Like all powerful technologies, LLMs have dual-use nature. Here, an accurate social simulator could be misused to design manipulation campaigns, persuasive advertising, engineered misinformation, or content exploiting social media algorithms. Early work on design iteration using these technologies suggests such applications may be credible (Li et al., 2025b; Duetting et al., 2025). Simulations might also train manipulator agents or generate fake engagement.

These concerns align with existing literature on LLM social risks. Researchers have already used LLM simulations to study AI-coordinated influence campaigns (Orlando et al., 2025), build influential social media bots (Jin & Guo, 2025), and model adversarial bot dynamics (Le et al., 2022). Evidence shows LLMs are highly persuasive, even regarding elections (Lin et al., 2025) or conspiracy theories (Costello et al., 2026), while LLM-generated disinformation—a documented threat to democracies (McKay & Tenove, 2020; Badawy et al., 2018; Givi et al., 2024)—was already difficult to detect in 2023 (Chen & Shu, 2024). These concrete risks add to the AI safety risks of multi-agent AI systems (Hammond et al., 2025).

We share these concerns. However, malicious actors can freely test tactics on real people, while safety researchers face ethical constraints. These simulators would provide safe testing environments for developing defenses without harming anyone. Pursued responsibly, this tool could level the playing field, though risks should be systematically measured and limited.

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A. Full Trajectory Factorization

For completeness, we provide the explicit factorization of the trajectory distribution induced by the simulator described in Section 2.2.

Let \mathcal{X} denote the set of prompt constructors and orchestration logic, and let initial states be drawn from $p(s_0, z_0^1, \dots, z_0^n)$. The joint distribution over a trajectory τ of length T factorizes as:

$$p(\tau \mid \mathcal{X}, \Theta) = p(s_0, z_0^1, \dots, z_0^n) \prod_{t=0}^{T-1} \left[\underbrace{p(s_{t+1} \mid \mathcal{T}(s_t, \mathbf{a}_t), \theta_{\text{Env}})}_{\text{environment}} \times \prod_{i=1}^n \underbrace{p(o_t^i \mid s_t)}_{\text{observe}} \cdot \underbrace{p(z_{t+1}^i \mid \mathcal{Z}^i(o_{t+1}^i, z_t^i), \theta^i)}_{\text{think}} \cdot \underbrace{p(a_{t+1}^i \mid \mathcal{A}^i(z_{t+1}^i), \theta^i)}_{\text{act}} \right]$$

This factorization makes explicit the conditional dependencies between environment dynamics, agent observations, internal state updates, and action generation. While not required for the conceptual arguments in the main text, it enables precise reasoning about independence assumptions, intervention effects, and evaluation metrics.

B. Simulation Visualization

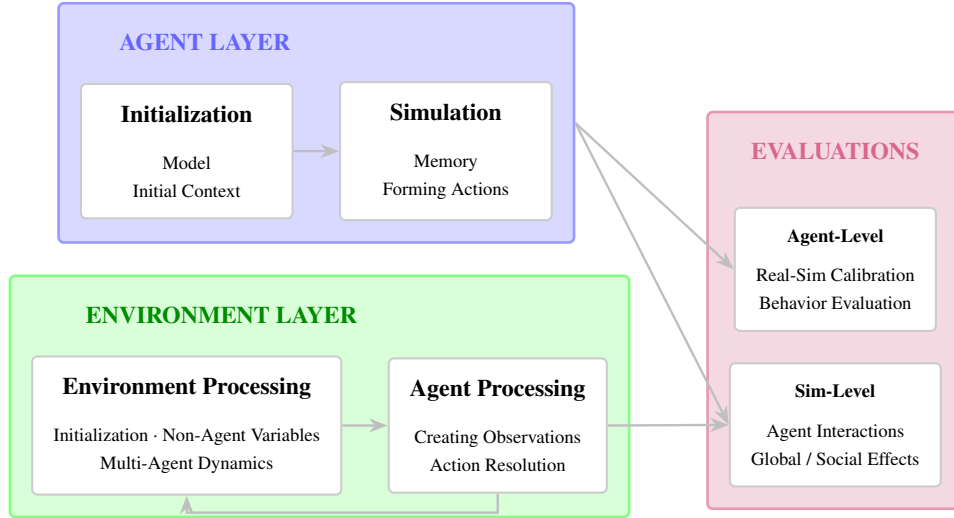


Figure 1. A visualization of the components involved in the simulation task. Arrows depict flow of information/computation.