Sim2Science: ML with Imperfect Scientific Models

Georgia Channing, Noémi Éltető, Richard Gao, Daniel Gedon, Magdalena Lederbauer

1 Workshop summary

The core tenet of scientific discovery is the construction of knowledge that aligns with experimental observations. This knowledge often takes the form of mechanistic models or *simulators*, traditionally hand-crafted by domain experts and fit to experimental data [1, 2]. Such simulators underpin predictive simulation, parameter and state inference, uncertainty quantification, and decision-making across the sciences. The rapidly emerging field of AI4Science now plays a central role throughout simulator-based workflows [3], enabling breakthroughs across domains including protein folding [4] and genome modeling [5], drug discovery [6], materials discovery [7], plasma control [8], weather forecasting [9], and cognitive modeling [10]

Despite their utility, all simulators include simplifications and approximations of reality, inevitably inducing discrepancies between simulated and observed data. In other words, *"all models are wrong, some are useful"* [1, 11]. Understanding and addressing this mismatch is a fundamental challenge for both machine learning and the natural sciences. This challenge has broad relevance across machine learning and calls for integrated methodological responses: Examples include, inference from simulators under model misspecification (e.g., simulation-based inference) [12–16], learned augmentations of mechanistic models (e.g., surrogate or hybrid approaches) [17, 18], and experiment-in-the-loop scientific workflows (e.g., automated laboratories and closed-loop discovery) [19–21], and more. We expand the scope in Appendix A.

Workshop framing. The central question of this workshop is: *How can we best leverage imperfect scientific simulators when confronted with real-world data, and how can ML help account for and mitigate limitations in simulator-based workflows?* Towards this, the workshop pursues two complementary aims:
(i) to bridge communities across machine learning and the natural sciences by establishing a common understanding of how simulator discrepancies can be identified and quantified across fields; and
(ii) to clarify how machine learning methods can be used to learn from, account for, and reduce simulator discrepancies when integrating simulators with real-world data.

Topics. We invite contributions on theory and methods—including simulation-based inference, emulator learning, model and equation discovery, multi-fidelity modeling, generalized Bayesian inference, differentiable frameworks, LLM-assisted scientific reasoning, and automation in scientific workflow—as well as applications spanning biology, chemistry, physics, materials science, climate science, and related fields.

2 Activities and tentative schedule

Sim2Science is designed as interactive forum for the AI4Science community, which has recently seen rapid growth across many scientific domains [22]. We anticipate 150–200 participants. The program consists of six invited talks and a concluding panel, five contributed talks, two poster sessions, and a sponsored mentorship and networking lunch with a structured unconference component [23]. A draft website is available at `www.sim2science.github.io`, and the tentative schedule in Table 1.

Contributed works. We invite 5-page workshop papers and 2-page Tiny Papers (from under-represented, under-resourced, and/or budding researchers) on methodological advances and domain-specific applications that bridge simulators or emulators with real-world data using machine learning. We anticipate 100–120 submissions and expect to accept 50–60 papers, subject to room capacity to ensure space for poster presentation and discussion. Reciprocal reviewing will be implemented, where one author of each submitted paper is asked to review 2 other submissions, and supplemented by recruited program committee members and organizers as reviewers and area chairs. Five contributed talks will be selected based on review scores, topical fit, and diversity considerations, with all remaining accepted papers presented as posters.

Mentorship and networking unconference lunch. With confirmed sponsorship of approximately $4,000 from HuggingFace and DeepMind, we will organize a catered lunch with around 80 spots. Poster presenters will be invited to preregister first, with remaining spots allocated to other participants. The lunch has two goals: First, a **unconference session** to facilitate cross-disciplinary exchange, where participants propose and vote on topics (e.g., via Post-it notes) and are free to join and exit small group discussions. Second, workshop participants and presenters can network with invited speakers, scientific advisors, and organizers, who will serve as "mentors" in their respective fields of AI4Science. Further details in Appendix B.

Speaker panel. The workshop concludes with a panel that follows a structured format of lightning rounds of 45-second responses from each invited speaker to prepared questions, followed by moderated discussion. This both balances participation and maximizes engagement.

Table 1: Tentative schedule for Sim2Science workshop

Time	**Event**	**Speaker**	**Affiliation**	**Domain**
08:00	**Invited Talk 1**	🔗 **Shirley Ho**	*Polymathic / NYU*	Astrophysics
08:30	Contributed Talk	2 × 15-minute orals		
09:00	**Invited Talk 2**	🔗 **Jonas Köhler**	*CuspAI*	Material Science
09:30	Coffee break			
09:45	**Invited Talk 3**	🔗 **Pablo Samuel Castro**	*Google DeepMind*	Cognitive Science
10:15	Contributed Talk	1 × 15-minute orals		
10:30	**Invited Talk 4**	🔗 **Marta Skreta**	*Mila*	Automated Laboratories
11:00	Posters			
12:00	Mentorship & networking unconference lunch			
14:00	**Invited Talk 5**	🔗 **Santiago Cadena**	*Proxima Fusion*	Nuclear Fusion
14:30	Contributed Talk	2 × 15-minute orals		
15:00	**Invited Talk 6**	🔗 **Petros Koumoutsakos**	*Harvard University*	Fluid Mechanics
15:30	Posters & coffee break			
16:30	**Speaker Panel**	*All Speakers*		
17:00	Closing Remarks			

Speakers. The speaker expertise spans a wide range of research topics across scientific domains, as well as backgrounds from both academic and industry labs. Diversity and inclusion were also central to our selection. Two of the six invited speakers identify as women, with representation from institutions in the EU, the UK, the US, and Canada. The speakers have each published recent work directly reflecting the workshop's focus on learning with imperfect scientific models [19, 24–30]. *All invited speakers have been confirmed and will be on-site.* More information on speakers is in Appendix C.

Scientific Advisors. Advisors are Prof. Jakob Macke (University of Tübingen), Prof. Cecilia Clementi (Freie Universität Berlin; Rice University), and Prof. Max Welling (University of Amsterdam; CuspAI).

3 History & previous related workshops

This is the first proposed iteration of Sim2Science. Related events include 🔗 Machine Learning for Astrophysics (ICML '22), 🔗 Synergy of Scientific and Machine Learning Modeling (ICML '23), 🔗 D3S3 (NeurIPS '24), and the ongoing 🔗 Machine Learning for the Physical Sciences series. While these workshops address simulation-based modeling in specific domains, Sim2Science targets imperfect scientific simulators across domains, emphasizing methods to quantify and mitigate simulator discrepancies and foster cross-disciplinary exchange.

4 Organizers

The organizing committee brings together researchers from academia and industry with complementary expertise across scientific machine learning disciplines, with a particular emphasis on applications to chemistry, neuroscience and material science. The team spans multiple career stages, including a PhD student, postdoctoral researchers, an assistant professor, and industry researchers, and includes organizers based in UK, Europe, and the United States. This composition enables us to balance methodological depth with applied perspectives, to design a program that is relevant to both foundational ML researchers and practitioners in scientific domains, and to ensure that no single institutional, disciplinary, or career-stage perspective dominates. Details on diversity are in Appendix D.

None of the organizers are part of other ICML workshop proposals, and all intend to participate in person.

1. **Georgia Channing.** Head of the AI for Science Team, Hugging Face.
   Email: `georgia.channing@huggingface.co` | Website | Google Scholar
   Her research focuses on accelerating scientific workflows with machine learning, including bespoke architecture design, high-throughput data processing, and automated decision-making [21, 22, 31, 32]. She has extensive experience organizing large open-source communities, most notably Hugging Science, a 7,000-member network of contributors building tools for AI-driven scientific discovery. She has also been deeply involved in organizing and leading major hackathons, including the Women's Longevity Hack, the Merck–Boltz Hackathon, the LLMs for Materials Science and Chemistry Hack, and the AI for Microscopy Hack. Finally, she has led initiatives across multiple institutions to support women in computer science and engineering, and has spoken on these efforts at the Grace Hopper Conference.

2. **Noémi Éltető.** Research Scientist, Google DeepMind.
   Email: `noemielteto@google.com` | Website | Google Scholar
   Her research centers on data-driven scientific discovery within neuroscience. She has experience with interpretable theory generation in the form of Python programs [26], as well as probabilistic grammars and disentangled neural networks. Currently, she is applying deep ensemble active learning to advance automated experiment design. Beyond her research, she organized the external seminar series at the Max Planck Institute for Biological Cybernetics and served on the program committee for COSYNE.

3. **Richard Gao.** Assistant (W1) Professor, Institute of Computer Science, Goethe University Frankfurt.
   Email: `r.gao@em.uni-frankfurt.de` | Website | Google Scholar
   His research focuses on developing ML and other computational modeling approaches to understand brain dynamics at the cellular and network levels. Relevant to the workshop, he has extensive experience developing simulator-based workflows that combine biophysical models of neural circuits with deep generative models (e.g., in simulation-based inference [33, 34]), in addition to methodological contributions that leverage generalized Bayesian inference to handle simulator discrepancy or misspecification [14]. He has previously co-organized multiple workshops, most recently at NeurIPS 2025 (Data on the Brain and Mind), and also at computational neuroscience conference such as COSYNE and Bernstein Computational Neuroscience.
   He will act as a contact person for workshop communications.

4. **Daniel Gedon.** Postdoctoral Fellow, University of Tübingen.
   Email: `daniel.gedon@uni-tuebingen.de` | Website | Google Scholar
   His research centers on developing probabilistic machine learning tools for scientific discovery and mechanistic modeling. This work encompasses simulation-based inference methods [16] as well as automated approaches for model discovery. Applications of these methods include neuroscience,

pharmacology, medical modeling, and related areas. Daniel has organized an SBI hackathon (2025) and a combined SBI hackathon–tutorial (2026).
He will act as a contact person for workshop communications.

5. **Magdalena Lederbauer.** PhD Student, MIT.
   Email: `magled@mit.edu` | Website | Google Scholar
   Her research focuses on machine learning for chemical discovery, including molecular structure elucidation using physics-constrained neural networks and multimodal learning approaches for extracting synthesis procedures from scientific literature at scale. She is advised by Connor Coley and received her BSc and MSc in Chemistry from ETH Zurich.

5 Contact information

Daniel Gedon: `daniel.gedon@uni-tuebingen.de`
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A Expanded workshop summary

The Sim2Science workshop is concerned with how scientific knowledge is constructed and updated when simulators, i.e., mechanistic models of natural systems, are necessarily imperfect. Across scientific domains, simulators encode simplifying assumptions, partial mechanistic understanding, or unknown parameters, yet remain central to prediction, inference, and decision-making. The workshop adopts a broad perspective on how machine learning can interact with such simulators, not as replacements, but as tools for understanding their limitations, integrating them with data, and supporting scientific reasoning under uncertainty.

A central aim of the workshop is to bring together researchers developing general-purpose ML methodology with scientists who work with simulators in practice, and to foster a shared vocabulary across domains. Topics span a wide range of approaches, including:

- simulation-based inference and related parameter inference methods;
- understanding and mitigating model misspecification, including simulator diagnostics, and discrepancy modeling;
- emulator and surrogate modeling, as well as hybrid and physics-informed approaches;
- analysis of simulator structure, degeneracy, simplifications, and identifiability;
- simulator pipelines, including data handling, preprocessing, and integration with downstream ML models;
- active learning and Bayesian optimization for fitting parameters or model components;
- closed-loop and experiment-in-the-loop scientific workflows;
- multi-fidelity and multi-resolution modeling;
- application-driven studies across biology, chemistry, neuroscience, materials science, physics, astronomy, and related fields.

The relevant topics are intentionally broad and inclusive, reflecting the many ways in which imperfect simulators arise and are used across scientific disciplines.

B Mentorship & unconference lunch

The mentorship and unconference lunch is designed to be explicitly *participant- and junior-led*, with senior researchers serving as mobile mentors rather than fixed discussion leaders. The session follows the well-established unconference model of participant-driven discussion [23]. In this format, early-career participants identify and shape the scientific, methodological, or career questions most relevant to them, while receiving targeted feedback from both peers and senior researchers in an informal setting.

- **Topic generation.** During the morning sessions, coffee breaks, and poster session, participants are invited to propose discussion topics by adding post-it notes to a shared wall. Topics may span scientific questions, methodological challenges, career paths, or broader issues in AI4Science (e.g.,“calibrating simulators with sparse data”, “career paths in AI4Science”, or “failure modes of surrogates”).
- **Interest signaling and selection.** Participants can indicate interest by placing pins on topics they would like to join. Around midday, organizers identify the most popular and complementary topics, while leaving space for additional ad hoc discussions to form organically.

- **Mentor circulation.** Invited speakers, and organizers are encouraged to intentionally circulate across topics so that each discussion group is joined by at least one mentor for a substantial portion of the lunch. This ensures mentoring depth without constraining discussion flow.
- **Structure and facilitation.** Discussions are informal and participant-driven. Organizers act as light-touch facilitators to help manage time, encourage inclusive participation, and support movement between groups if interests shift.

This format emphasizes agency for junior participants, lowers barriers to interaction with senior researchers, and supports cross-domain exchange driven by concrete questions rather than pre-defined agendas.

C Speaker details and relevance

Shirley Ho. *Polymathic / New York University.* Shirley Ho is an astrophysicist with a long track record of combining large-scale cosmological and galaxy simulations with modern machine learning. Her work spans surrogate modeling, simulation acceleration, and statistical inference in astronomy. She brings a domain perspective where simulators are computationally expensive, scientifically central, and inevitably approximate, making her experience directly relevant to discussions of learning with imperfect simulators.

Jonas Köhler. *CuspAI.* Jonas Köhler is a machine learning scientist working at CuspAI on ML-driven methods for materials science. His work focuses on bottlenecks of traditional scientific simulators by developing scalable ML systems that accelerate and augment simulation pipelines. With a background spanning quantum chemistry, biophysics, and materials, he contributes a strongly engineering-oriented perspective on deploying ML for simulation-heavy scientific applications.

Pablo Samuel Castro. *Google DeepMind.* Pablo Samuel Castro's research lies at the intersection of machine learning, cognitive science, and behavioral modeling. He works on discovering and comparing interpretable, often symbolic, models from human and animal behavior, where mechanistic explanations are partial and contested. His perspective highlights how ML can support model discovery, evaluation, and revision when simulators are abstract or incomplete.

Marta Skreta. *University of Toronto.* Marta Skreta's research sits at the intersection of AI, chemistry, generative modeling, and self-driving laboratories. Her work explores how learned models, simulators, and automated experimentation can be combined in closed-loop discovery pipelines, making her expertise directly relevant to discussions of experiment-in-the-loop workflows and simulator-driven decision making.

Santiago Cadena. *Proxima Fusion.* Santiago Cadena works on plasma physics and fusion-related optimization problems, including the construction of benchmarks and datasets derived from complex simulators. His experience reflects real-world challenges of multi-fidelity modeling, constrained optimization, and decision-making under simulator uncertainty in high-stakes scientific applications.

Petros Koumoutsakos. *Harvard University.* Petros Koumoutsakos is a leading researcher in computational science and scientific machine learning, with contributions spanning fluid dynamics, multiscale modeling, optimization, and AI-driven modeling of physical systems. His work focuses on integrating mechanistic models with data-driven and learning-based methods to understand and control complex dynamical systems. He brings a unifying, cross-domain perspective on how learning can augment, correct, and extend traditional simulators in high-dimensional and multi-physics settings.

D Diversity and inclusion

Diversity and inclusion considerations inform all aspects of the workshop design, including speaker selection, organizing roles, and participant engagement. The invited speakers span academia and industry, multiple scientific domains, and institutions across Europe and North America, with deliberate attention to gender and career-stage representation. The organizing team similarly reflects a mix of seniority levels, disciplinary backgrounds, sectors, and geographic locations.

To broaden participation, we conduct targeted outreach beyond established AI4Science networks, including to early-career researchers and groups traditionally underrepresented at major ML venues. Complementary registrations are used to support participation by students, particularly those with limited access to travel funding. The mentorship and unconference lunch is explicitly structured to lower barriers for junior participants by giving them control over discussion topics and direct access to senior mentors. Together, these measures aim to foster an inclusive environment that values diverse perspectives, scientific backgrounds, and career trajectories.