AI Methods for Science

CDS DS 595 · Spring 2026 · Boston University

Instructor:	Siddharth Mishra-Sharma	**Lecture:**	Mon/Wed 12:20–1:35pm
Email:	`smishras@bu.edu`	**Location:**	CAS 218
TF:	Wanli Cheng (`cwl1997@bu.edu`)	**Credits:**	4

Last updated: January 20, 2026

Discussion Section: Tuesdays 11:15am–12:05pm, MUG 205

Office Hours: Tue 3–4pm or by appointment, CDS 1528

Resources:

- Course website: `https://smsharma.io/teaching/ds595-ai4science.html`
- Discussion: Ed Discussion
- Assignment/lab submission: GitHub Classroom
- Computing: GPU access through the Shared Computing Cluster (SCC) and LLM API/finetuning credits will be provided for project work

There is no required textbook. Many readings reference *Understanding Deep Learning* by Simon J.D. Prince (MIT Press, 2023); the PDF is available on the website. Other readings are drawn from research papers and online resources.

About the Course

AI methods are increasingly central to how science gets done, spanning simulation, experiment, theory, and observation. This course aims to equip students with the methods to understand and carry out research at the intersection of AI and the natural sciences. Topics include probabilistic inference, neural networks that encode physical symmetries and domain knowledge, generative models for scientific data, and simulation-based inference. *While framed in terms of scientific applications, the methods discussed extend well beyond scientific research, with broad applicability across industry and general AI R&D.*

A major focus of the course is on large language models and their emerging role in science. As LLMs become more capable of scientific reasoning and operating autonomously, understanding how to evaluate, adapt, and collaborate with these systems is becoming essential. We explore what it means to work alongside AI scientists, and how to critically assess their capabilities as well as limitations.

Applications are drawn from domains including physics, materials science, and biology. The course involves two assignments emphasizing method design and critical analysis in collaboration with AI tools, plus two projects: a midterm applying AI methods to a scientific problem, and a final project finetuning an LLM to elicit a scientific capability.

Learning Objectives. By the end of this course, students will be able to:

- Apply probabilistic inference and sampling methods (e.g., MCMC) to scientific problems

- Design neural networks that encode scientific domain knowledge
- Train generative models (e.g., diffusion models) to emulate scientific data distributions
- Use simulation-based inference to connect simulators with observations
- Evaluate the edges and limitations of LLM capabilities for scientific reasoning
- Develop intuitions for how to collaborate effectively with AI systems on research tasks
- Read and understand AI-for-science research papers

Schedule

This schedule is tentative and subject to change as the course progresses.

	Date	**Topic**	**Notes**
Week 1			
L1	Wed, Jan 21	Science in the Era of Computation	
Week 2			
L2	Mon, Jan 26	Reasoning Under Uncertainty	
L3	Wed, Jan 28	Framing Scientific Problems as ML Tasks	
Week 3			
L4	Mon, Feb 2	Learning by Sampling and Optimization	
L5	Wed, Feb 4	Building Blocks of Learned Representations	A1 out
Week 4			
L6	Mon, Feb 9	Encoding Scientific Structure in Neural Networks I	
L7	Wed, Feb 11	Encoding Scientific Structure in Neural Networks II	
Week 5			
—	Mon, Feb 16	*No class*	Presidents' Day
L8	Tue, Feb 17	Encoding Scientific Structure in Neural Networks III	Substitute Monday
L9	Wed, Feb 18	Learning Distributions from Data I	A1 due; A2 out
Week 6			
L10	Mon, Feb 23	Learning Distributions from Data II	
L11	Wed, Feb 25	Learning Distributions from Data III	
Week 7			
L12	Mon, Mar 2	Guest Lecture (AI + bio)	Midterm out
L13	Wed, Mar 4	Differentiating Through Scientific Simulators	A2 due
Spring Recess: March 7–15			
Week 8			

	Date	Topic	Notes
L14	Mon, Mar 16	Learning Through Exploration	
L15	Wed, Mar 18	Inverting Simulators I	
Week 9			
L16	Mon, Mar 23	Inverting Simulators II	
L17	Wed, Mar 25	Discovering Equations from Data	
Week 10			
L18	Mon, Mar 30	Guest Lecture (AI + astro)	
L19	Wed, Apr 1	Guest Lecture (AI + particle collider physics)	Midterm due; Final out
Week 11			
L20	Mon, Apr 6	From Specialized to General Intelligence; Scaling	
L21	Wed, Apr 8	Quantifying and Predicting LLM Scientific Capabilities	
Week 12			
L22	Mon, Apr 13	LLM Building Blocks	
L23	Wed, Apr 15	Teaching LLMs to Science	
Week 13			
—	Mon, Apr 20	*No class*	Patriots' Day
L24	Wed, Apr 22	Learning Unified Representations Across Scientific Modalities	Proposal due Fri Apr 17
Week 14			
L25	Mon, Apr 27	Frontiers	
L26	Wed, Apr 29	Being a Human Scientist	
Finals			
—	Mon, May 4	**Final Project Due**	

Discussion Sections. Tuesdays 11:15am–12:05pm in MUG 205.

Week	Date	Topic	Notes
—	Tue Jan 20	No discussion	First day of classes
2	Tue Jan 27	Lab: JAX, Autodiff, GitHub	
3	Tue Feb 3	Lab: Hamiltonian Monte Carlo	
4	Tue Feb 10	Lab: Training Neural Networks	
—	Tue Feb 17	No discussion	Substitute Monday schedule
6	Tue Feb 24	Lab: Diffusion Models	
7	Tue Mar 3	Midterm project intro + SCC setup	
—	Mar 7–15	No discussion	Spring Recess
8	Tue Mar 17	Lab: Differentiable Programming	
9	Tue Mar 24	Midterm project work	Midterm due Apr 1
10	Tue Mar 31	Lab: Simulation-Based Inference	
11–14	Apr	Final project work	Proposal due Apr 17 Report due May 4

Assessment

Deliverable	%	Out	Due
Discussion Labs	10%	Tue (select weeks)	Wed (select weeks)
Assignment 1: Inference	15%	Wed Feb 4	Wed Feb 18
Assignment 2: Architectures	15%	Wed Feb 18	Wed Mar 4
Midterm Project	25%	Mon Mar 2	Wed Apr 1
Final Project	35%	Wed Apr 1	Proposal: Fri Apr 17 Report: Mon May 4

- **Discussion Labs.** Weekly in-class labs reinforce lecture material through hands-on programming. Students work through a notebook during discussion, exploring implementations and comparing results. Graded on participation and completion. Labs are due end of day Wednesday.
- **Assignments.** Two assignments ask students to propose a novel method (or modification to an existing method) and then understand/critique it through theoretical analysis and empirical evaluation. AI tools may be used freely, but the analysis and interpretation require critically engaging with what was produced. The discussion labs build foundational skills for these assignments.
  - Assignment 1: Design and stress-test a novel sampling or variational inference method
  - Assignment 2: Design and stress-test a novel neural network architecture or inductive bias
- **Midterm Project.** Teams of 2–3 conduct a mini research project applying methods from the first half of the course (inference, architectures, generative models) to a scientific problem. Choose from a suggested list or propose your own. Deliverable is a ∼4 page workshop-style paper + code.
- **Final Project.** Teams of 2–3 identify a scientific capability that current large language models struggle with, then finetune a language model to improve that capability. This is a two-stage project:
  - Proposal: Demonstrate that LLMs struggle at a specific scientific capability by curating a dataset or benchmark
  - Final report (∼6 pages, NeurIPS format): Fine-tuned model and evaluation showing improvement, including artifacts used for fine-tuning (datasets, code, reinforcement learning environments)

Policies

Attendance. Regular attendance in lectures is expected. Please notify the instructor of planned absences.

Late Work. Late submissions are not accepted without prior arrangement. Extensions may be granted for documented emergencies.

Collaboration. Discussion of concepts and approaches is encouraged. However, all submitted code and written work must be your own. When collaborating, you must acknowledge your collaborators.

AI Tools. Learning to work effectively with AI is itself a course objective. Use AI tools freely to explore ideas, debug code, and deepen understanding. Focus on building genuine competence—understanding *why* something works, not just *that* it works. Disclose AI assistance in submissions, including its form and extent. See also the CDS GAIA policy.

Academic Conduct. All students are expected to read and abide by the BU Academic Code of Conduct. Plagiarism includes copying or restating work or ideas of another person or AI software without citing the source. In computing coursework, this includes sharing code, reusing code across courses without permission, and uploading assignments to external sites. Please review the examples of plagiarism provided by the BU Computer Science department. All suspected cases of plagiarism will be reported to the Academic Dean.

Accommodations. Boston University is committed to providing reasonable accommodations to students with documented disabilities. Students seeking accommodations should contact Disability & Access Services (25 Buick Street, Suite 300; 617-353-3658) as early as possible in the semester. A new Faculty Accommodation Letter (FAL) must be requested each semester; DAS will send this directly to instructors.

Religious Observance. Students observing a religious holiday during regularly scheduled class time are entitled to an excused absence. Please notify the instructor in advance to make arrangements for any missed work.

Recordings. Recording of lectures requires instructor permission. Students approved for recording as an accommodation must limit use to personal study and may not share recordings.