Time	Monday	Tuesday	Wednesday	Thursday
9-10:30 am	From Machine Learning to AGI (I): The evolution of the "AI Scientist". Agent architectures: Planning, memory, tools, and action. Automating knowledge extraction and organization from unstructured sources (PDFs, lab notes). **L1**	Hands-on introduction to PyTorch (example application to fine-tuning a scientific LLM applied to protein molecular design; Hugging Face open-source tools and ecosystem). Vibe coding and vibe research. **L4**	Transforming AI for biology and healthcare (AlphaFold , Boltz, RFDiffusion, and applications to protein design, synthesis). Reasoning with foundation models. Fine-tuning Large Language Models (LLMs) for scientific tasks. Geometric deep learning. **L8**	Interpretability, scaling and deployment (inference engines, sandboxing, distributed agents, etc.). Model Distillation, Quantization, and SLMs (Small Language Models). Human-in-the-Loop Interfaces: How does a human scientist interact with a swarm? The UI/UX of agentic science. **L12**
10:30-10:45	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**
10:45-12:30:	From Machine Learning to AGI (II): (first-principles based multiscale modeling; synthetic datasets, experimental methods for data collection, self-driving labs). **L2**	Generative AI for materials: Diffusion & flow matching. Theory and application of diffusion models for inverse design. Generating 3D structures: Proteins, metamaterials, and crystal lattices. Practical guide to tensor algebra and other important math concepts needed. **L5**	Building, using and adapting LLMs and LRMs applied to materials (pre-training and fine-tuning, RL, PRefLexOR, reflective agents). Diffusion language models (DLMs) (applications of large language models to materials problems; category theory; time-dependent material phenomena). **L9**	**CLINIC #4:** Participant group project presentations & discussion, clarifications and feedback
12:30-1:00 pm	**LUNCH**	**LUNCH**	**LUNCH**	Concluding discussion Graduation ceremony & virtual certificates **L13**
1:00-2:30 pm	**CLINIC #1** Physics-aware vision models (from convolutional models to attention, multimodal AI). Example application to a data agent.	Responsible AI. Ensuring these systems are safe, reliable, and deployable in an enterprise environment. Data science, statistics and visualization (includes review of relevant Python toolkits). Collaborative research & open science practices **L6**	**CLINIC #3** Self-improving and adaptive AI models for inverse materials design and integration into agentic frameworks (AG2, CrewAI, MCPs, Skills, …). Using generative learning for protein design and synthesis planning. Translating biological mechanisms into synthetic material concepts. Active learning/negative data.	
2:30-2:45 pm	**COFFEE BREAK**	**COFFEE BREAK**	**COFFEE BREAK**	
2:45-4 pm	Digging deeper: Deep neural nets, loss functions, Stochastic optimization methods (e.g., stochastic gradient descent & variants), regularization. Introduction to Transformers and graph neural networks. **L3**	**LAB 1** *De novo* dataset construction and application to build a agentic workflows (covers computer vision tools, autonomous experimentation, robotics). Neural Interatomic Potentials and Neural Operators.	AI scientists and swarm intelligence. Agent development, orchestration, deployment, decentralized intelligence. Application to creative design tasks, protein design. Case study: Spawning multiple agent instances to explore a design space in parallel, critique each other's work, and converge on an optimal solution. **L10**	
4-5pm	**CLINIC #2:** Building your first reasoning agent for material failure analysis. Hands-on lab (constructing a basic agent to search literature, formulate hypothesis, and write code to test it). Graph reasoning; Memory/Retrieval-Augmented Generation. ***Feedback session*** *(participants can provide input or ask questions about the day's content)*	Introduction to graph neural networks (applications to molecular systems, truss systems, alloys, proteins, and healthcare; graph transformers). Connecting a generative agent to a physics simulator (e.g., LAMMPS or FEA) to automatically validate AI designs. ***Feedback session*** **L7**	Case study: AI in Manufacturing & Scale-up. Using AI to optimize processing parameters (3D printing, casting) based on limited data, real-time time series data collection and integration with LRMs. ***Feedback session*** **L11**	
5-7pm	**VIRTUAL RECEPTION** (includes participant introductions). Group formation for projects.	Optional: Time for Group Work and Assignments (can be arranged within groups at other times)	Optional: Time for Group Work and Assignments (can be arranged within groups at other times)	