SciFM Summer School

July 8 - 26, 2024, 9 am - 5 pm Ann Arbor, MI







Agenda (all times ET)

Week 1

Monday, July 8

10:00 am	Welcome & Opening Remarks - Karthik Duraisamy (UM)
10:10 am	Summer School Goals - Venkat Viswanathan (UM)
10:30 am	Keynote: Foundation Models for Science - Ian Foster (ANL)

12:00 pm Open Discussion

Progress in Domain-specific Foundation Models

1:30 pm	Agents for Materials Discovery- Jan Jansen (Max Planck)
2:15 pm	Learning the Language of Chemistry - Philippe Schwaller (EPFL)
3:15 pm	Foundation Models for Drug Discovery - Bharath Ramsundar (Deep
	Forest Sciences)

4:00 pm Foundation Models for Climate - Aditya Grover (UCLA)

Tuesday, July 9

Foundation Models Programs @ DARPA

10:00 am	Overview - Erica Briscoe (DARPA)
10:20 am	Materials Synthesis - Jia Deng (Princeton)
10:40 am	Robot scientist - Boyuan Chen (Duke)
11:00 am	Measuring Creativity - Lav Varshney (UIUC)
11:20 am	Dynamic Multi-agent systems - Wei Wang (UCLA)
11:40 am	Hypothesis generation in Climate Science - Rose Yu (UCSD)

Visioning Session (Closed group) Existing attructures and institutes (discussion)

1:30 pm	Existing structures and institutes (discussion)
2:00 pm	Vision & SciFM Institute: Proposed Structure
2:30 pm	SciFM25 & Beyond : Future Conferences & Community building
	Working Breakout Session: Prompt: Produce a blueprint for SciFM
	Institute: Resources, Personnel, Structure

Wednesday, July 10

Tutorial 1

9:00 am Aurora: Foundation Model for the Atmosphere - Paris Perdikaris

(Microsoft/UPenn)

11:00 am PDE Foundation Models - Maximilian Herde (ETH)

1:30 pm Hackathon details and logistics

2:00 pm **Tutorial 2**

Data & Tokenization

Sequence data: Omics + Molecular (SMILES, SELFIES) - ANL Team

Tokenization - ANL + UM Team Discussion of Practical issues

Thursday, July 11

Tutorial 3

9:30 am **Training Models**

Training Infrastructure for Biological Sequence Models - **ANL Team**

Neural operators + other PDE architectures - Caltech Team

Vision Transformers & Foundation Models - Deep Forest Sciences

1:30 pm **Diffusion Models for PDEs - Tony Zhuang** (UM)

3:00 pm Scaling Laws (Discussion)

Overview of Scaling Laws - Alex Wadell (UM)

Scaling sequence models + compute optimal scaling

Vision scaling laws

Scaling laws of FNO, PDE

Friday, July 12

Tutorial 4

9:30 am Retrieval Augmented Generation - Ozan Gokdemir (ANL)

11:00 am **Agents: Part 1 (Biology)** - ANL Team

1:30 pm Agents: Part 2 (Chemistry) - ANL Team

External tooling, experimental data, Fine-tuning, preference:

3:00 pm LLMs and Autonomous Agents in Chemistry

4:00 pm Hackathon -Final team selection and goal setting for Hackathon

Week 2

Monday, July 15 & Tuesday July 16

Hackathon

Wednesday, July 17

Tutorial

Al Accelerators

9:30 Welcome & Goals

9:45 Cerebras

10:15 Sambanova

11:00 Graphcore

11:30 Grog

1:00 **NVIDIA**

1:30 Hands on session

3:15 Discussion

Thursday, July 18 & Friday, July 19

Tutorial

Federated Learning - **Ravi Madduri** (ANL) Hackathon

Week 3

Monday, July 22 & Tuesday, July 23 & Wednesday, July 24

Hackathon

Thursday, July 25

Hackathon teams presentation (industry present)

Materials

Biology

Agents

PDEs

Outlook for AI-assisted science in non-research settings

Friday, July 26

Open questions for Foundation Models for Science

Panel: Security, Equity, Safety

Ecosystem Gathering (University, Lab, DoD, Venture, Philanthropy)

Next steps and Closing discussion