

Mathematical Foundations & Methodologies for Artificial Intelligence and Data-Driven Scientific Computing

Workshop on Data-Drive Scientific Computing

(11 Aug 2026–15 Aug 2026)



ORGANIZING COMMITTEE

Tan Minh Nguyen

National University of Singapore

Yang Liu

National University of Singapore

Richard Baraniuk

Rice University

Dong Bin

Peking University

Vincent Tan

National University of Singapore

Ji Hui

National University of Singapore

Li Qianxiao

National University of Singapore

Ren Weiqing

National University of Singapore

Venue

IMS Executive Seminar Room

Bock S17, Level 3

10 Lower Kent Ridge Rd Singapore 119076

For more information: <https://ims.nus.edu.sg/events/mathfoundationsai>

Workshop on Data-Drive Scientific Computing

(11 Aug 2026–15 Aug 2026)

Tuesday, 11 August 2026

Time	Title	Speaker
0900–0930	Registration	
0930–1030	Foundation Neural Operators and Diffusion Models over Function Spaces	Lu Lu <i>Yale University, USA</i>
1030–1045	Coffee Break	
1045–1145	Efficient Sampling, Optimization, and Targeted Diffusion Generation for Physical AI	Yueming Lyu <i>A*STAR, Singapore</i>
1145–1330	Lunch Break	
1330–1430	Foundation Models for Physics: From Transformers to Kinetic and Self-Warping Architectures	Maarten de Hoop <i>Rice University, USA</i>
1430–1530	In-Context Learning in Scientific Computing	Yulong Lu <i>University of Minnesota, USA</i>
1530–1600	Coffee Break	
1600–1700	When Does Scientific AI Actually Use Physics? From Causal Mechanism Audits to Executable Solver Semantics	Xinyu Yang <i>NUS, Singapore</i>

Wednesday, 12 August 2026

Time	Title	Speaker
0915–0930	Registration	
0930–1030	Deep Learning for Reynolds-Averaged Navier-Stokes Simulations of Turbulent Flows	Daniel Dehtyriov <i>University of Oxford, UK</i>
1030–1045	Coffee Break	
1045–1145	Neural Network Methods for Solving PDEs and Materials Design	Yang Xiang <i>HKUST, Hong Kong SAR</i>
1145–1330	Lunch Break	
1330–1430	Preconditioned One-step Generative Modelling for Bayesian Inverse Problems	Zhongjian Wang <i>NTU, Singapore</i>
1430–1530	Learning Mesoscopic Dynamics	Qianxiao Li <i>NUS, Singapore</i>
1530–1600	Coffee Break	

Wednesday, 12 August 2026		
Time	Title	Speaker
1600–1700	Flow-based Generative Models for Amortized Bayesian Inference in Regression and Inverse PDE Problems	Xuhui Meng <i>HUST, China</i>
Thursday, 13 August 2026		
Time	Title	Speaker
0915–0930	Registration	
0930–1030	Knowledge-Informed Machine Learning for Modelling and Simulation in Geomechanics	Pin Zhang <i>NUS, Singapore</i>
1030–1045	Group Photo & Coffee Break	
1045–1145	Mathematical and Computational Understanding of Neural Networks: From Representation to Learning, From Shallow to Deep, and Beyond	Hongkai Zhao <i>Duke University, USA</i>
1145–1330	Lunch Break	
1330–1430	ICON and EvE: Scientific Foundation Models and Self-Evolving Agents	Liu Yang <i>NUS, Singapore</i>
1430–1530	Curvature-Aware Optimization for High-Accuracy Physics-Informed Neural Networks	George Karniadakis <i>Brown University, USA</i>
1530–1615	Coffee Break	
1615–1715	Panel Discussion What will research be like in the era of AI?	George Karniadakis <i>Brown University, USA</i> Simon See <i>NVIDIA, Singapore</i> Sian Wee Tan <i>NUS Enterprise, Singapore</i>
Friday, 14 August 2026		
Time	Title	Speaker
0915–0930	Registration	
0930–1030	Accelerated Langevin Sampling of Complex Distribution using Variable Timestep and Friction	Benedict Leimkuhler <i>University of Edinburgh, UK</i>
1030–1045	Coffee Break	
1045–1145	Kolmogorov Superpositions: Construction, Approximation and Networks	Li-Lian Wang <i>NTU, Singapore</i>
1145–1430	Lunch Break	

Friday, 14 August 2026		
Time	Title	Speaker
1430–1530	Oppeinheim Lecture Agentic Scientific Machine Learning: Quo Vadimus?	George Karniadakis <i>Brown University, USA</i>
Saturday, 15 August 2026		
Time	Title	Speaker
0915–0930	Registration	
0930–1030	Benchmarking Neural Surrogates on Realistic Spatiotemporal Multiphysics Flows	Zhi Chen <i>Peking University, China</i>
1030–1045	Coffee Break	
1045–1145	Intelligent Scientific Computing: from Data-driven Modeling to Discovery	Hao Sun <i>Renmin University, China</i>
1145–1330	Lunch Break	
1330–1430	A Hybrid Two-level MCMC Framework to Accelerate Posterior Mean Estimation with Deep Learning Surrogates for Bayesian Inverse Problems	Juntao Yang <i>NVIDIA, Singapore</i>
1430–1530	Flow-based Bayesian Filtering for High-dimensional Nonlinear Stochastic Dynamical Systems	Ling Guo <i>Shanghai Normal University, China</i>
1530–1545	Short Break	
1545–1645	Autonomous Knowledge Distillation: Building an AI-Ready Infrastructure for Scientific Discovery	Yangshuai Wang <i>NUS, Singapore</i>

This schedule is accurate as of 11 Aug 2026 and is subjected to changes.