AE646: SCIENTIFIC MACHINE LEARNING FOR FLUID MECHANICS

Course Website: https://hello.iitk.ac.in/studio/ae646sem12425

FIRST COURSE HANDOUT (FCH)

The aim of AE646 is to familiarize graduate and upper-level undergraduate students with the evolving field of scientific machine learning and to initiate them into research in physics informed machine learning surrogates as alternative flow prediction tools and for the possible construction of digital twins of engineered systems. The course will be project based requiring programming in python and evolving machine learning platforms to explore the frontier of AI as a complement to computational continuum mechanics.

Background Knowledge:
Mathematics: Linear Algebra, Probability, Optimization
Fluid Mechanics (Aerodynamics/Hydrodynamics), Programming Skills (Python)
and interest in exploring the potential of machine learning for continuum mechanics.

Instructors:
Principal Lecturer: Prof. Murali Damodaran (dmurali@iitk.ac.in)

Teaching assistants:
None

Classroom: Helicopter Building **Class hours:** Mondays and Fridays (1200 hrs-1300 hrs)
Classroom: Tutorial Block TB264: Class Hours: Tuesdays (1400 hrs-1600 hrs)
Office hours: To be arranged; Contact instructor via e-mail.

1.Course Modus Operandi

Mixture of Lectures, Self-Study, Review of Basic Concepts via Flipped Classes followed by Class Discussions. Group and Individual projects. Student Presentations of their projects. Invited Application Lectures.

2.Course Grade will be based on student effort in the following components.

Continual Assessment:Review Exercises at the end of each sub-Module and Quizzes: 20%
Group Projects and Presentations: 35%
Synopsis and Comments on Industrial Application Lectures: 5%
Individual Final Project and Presentation: 40%
No mid-term or final examinations for this course.

3.Student Effort towards learning via project work

As AE646 is a project-based course, students are expected to deliver on the Review Exercises, Group and Individual Projects as these components are geared towards grasping the essence of scientific machine learning for flow prediction and hone your skills in scientific machine learning. Review Exercises are to be wrapped up within a week by 2359 hrs Friday. Group Projects to be wrapped up on the date the group presentations are made. Individual Projects must be defined early and carried out as early as possible and presented during the 16th week before 14 Nov 2024. A brief synopsis must be submitted after attending the Invited Application Lectures delivered by practitioners in the field. Submission of all exercises, group projects and individual projects will be via *Jupyter* Notebooks or equivalent. IITK's code of conduct on academic integrity and honesty must be respected for this course.

4.Tentative Course Content:

Introduction to Scientific Machine Learning; Essential computational resources for developing Scientific Machine Learning Surrogates; Review of Basic Fluid Mechanics; Review of Essential Linear Algebra, Probability and Optimization; Shallow and Deep Neural Networks; Physics Informed Neural Networks (PINNs); Neural Networks with Delays; LSTM for Predicting Time-dependent Flows; Model Order Reduction; New developments in PINN/MOR- Operator Learning

5. REFERENCE BOOKS AND MATERIALS

- **Relevant References in this field include:**

1. Gil Strang's book on *Linear Algebra and Learning from Data* sets the tone for the development of AI in Applied Mathematics and provides motivation for the current effort.
2. Steven L. Brunton and J. Nathan Kutz, "*Data-Driven Science and Engineering: Machine Learning, Dynamics and Control*," Cambridge University Press, 2019,2022 http://databookuw.com/
3. Mark Asch, "*A Toolbox for Digital Twins: From Model-Based to Data-Driven*", SIAM 2022, https://markasch.github.io/DT-tbx-v1/
4. N. Thuerey, P. Holl, M. Mueller, P. Schnell, F. Trost, K. Um, "*Physics-based Deep Learning*", (2021) https://physicsbaseddeeplearning.org
5. A. Zhang, Z.C. Lipton, M. Li and A. J. Smola,"*Dive into Deep Learning*", An Interactive deep learning book with code, math, and discussions; *Implemented with PyTorch, NumPy/MXNet, JAX, and TensorFlow*; https://d2l.ai/index.html

- ***Relevant Internet Resources***

1. NPTEL-NOC-IITM Online Course on "Machine Learning for Engineering and Science Applications" by Balaji Srinivasan and Ganapathy Krishnamurthy. You can view these lectures in the YouTube Channel: https://www.youtube.com/playlist?list=PLyqSpQzTE6M-SISTunGRBRiZk7opYBf_K
2. Repository of Research Papers on Physics Informed Neural Networks, https://github.com/idrl-lab/PINNpapers
3. Resources on PINN at SISSA, Italy: https://mathlab.sissa.it/pina
4. R. Milk, S. Rave, F. Schindler, "pyMOR - Generic Algorithms and Interfaces for Model Order Reduction", *SIAM J. Sci. Comput.*, 38(5), pp. S194--S216, 2016; Website: pyMOR: Model Order Reduction with Python https://pymor.org/

6. Outcomes of this Course

1. To introduce students to the evolving field of Scientific Machine Learning which is an essential driver of AI in the development of a computational method which is trained to make predictions leveraging on computational physics and computer science.

2. To develop an understanding of scientific machine learning and its potential application problems in applied aerodynamics and hydrodynamics. In the process students are expected to be motivated to learn, appreciate and hone their programming skills in a variety of enabling software and hardware platforms.

3. Develop a cohort of young researchers to explore the potential of building machine learning surrogates and digital twins and push this research frontier at IITK.

7. Course Audience:

PhD, MTech and MS students contemplating using elements of scientific machine learning for their research problems in computational aerodynamics and hydrodynamics.

Dual- BTech-MTech students and Senior BTech students looking to learn scientific machine learning for their academic development and to use it in their project work in continuum mechanics.

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L T P A

2 0 3 0 -*9 Credits*

TENTATIVE COURSE SYLLABUS

S/No.	Broad Title	Topics	No. of Lectures
1	Introduction to Scientific Machine Learning	**L01:** History, Motivation and Basic Ideas; Scientific Machine Learning;Forward and Inverse Problems in Fluid Mechanics; Model Order Reduction; Data Driven and Physics Informed Neural Networks and Neural Operator Learning.	1
2	Essential computational resources for developing Scientific Machine Learning Surrogates	Crash Course in *Python* on *Anaconda Platform* and/or *Julia*; *Jupyter* Notebook Interface. Machine Learning Tools using *TensorFlow, Keras, PyTorch, Sci-ML, Matlab, Julia; DeepXDE* Library, *Nvidia Modulus* for Scientific Machine Learning	3 hrs(Lab) *Self-Exploration*
3	Review of Basic Fluid Mechanics	**FM01:** Governing Equations for Potential, Euler, Boundary Layer and Navier-Stokes Equations; Notions of Scaling; Compressible & Incompressible flows; CFD Models as the Forward Problem in Fluid Mechanics; **FM02:** Boundary Conditions	2 *Self- Study*
4	Review of Essential Linear Algebra, Probability and Optimization	**LA01:** Vectors; Span, Linear Dependence; Matrix algebra, **LA02:** Eigenvalues/eigenvectors, SVD **P01:** Notions of Probability **OPT01**: Optimization Libraries	4
5	Shallow and Deep Neural Networks	**NN01:** Extreme Learning Machine (ELM) and Deep Neural Networks (DNN); Network Hyperparameters and Activation Functions. Regression. **NN02:** Loss Functions; Automatic Differentiation; **NN03:** Backpropagation Gradient Descent; Stochastic Gradient Descent	3
6	Physics Informed Neural Networks (PINN)	**PINN01:** Neural Differential Equations **PINN02:** Predicting Flow fields using PIELM and PINNS **PINN03:** Data and PINN driven Optimal Shape Designs	3
7	Neural Networks with Delays-RNN/LSTM for Flow Predictions	**PINN04-05:** RNN/LSTM/GRU/Physics Informed LSTM **PINN05**-06Unsteady flow prediction with LSTM and LSTM-PINN	3
8	Autoencoders	**PINN07:** Autoencoders and relationship to MOR **PINN08:** Variational Autoencoders	2
9	Model Order Reduction	**MOR01:** POD/SVD/Gappy POD/SPOD **MOR02-03:** DMD or DEIM for Nonlinear Systems **MOR04:** *SiNDY*	4
10	New developments in PINN/MOR: Operator Learning	**OL01-02:** Operator Learning: *DeepONet, Fourier Numerical Operator* (*FNO*) and *Physics Informed Neural Operator* (PINO)	2
11	*Invited Industrial/Application Lectures on the State of the Art SciML/DT*	*Topics in Scientific Machine Learning/Digital Twins*	2
		Total	26

TENTATIVE AE646 COURSE SCHEDULE

AE646:SCIENTIFIC MACHINE LEARNING FOR FLUID MECHANICS					SciML4FM		
S1:AY2024-2025							
WEEK\HRS	1	1	1	1	1		
Week 01: 29.07.2024		X			X	HRS	
Week 02: 05.08.2024	L01-Intro	L02_CR(1)	L03_LA-01	CL	L04_FM-01	4	
Week 03: 12.08.2024	L05_FM-02	L06_LA-02	CL	CL	L07_OPT-01	3	
Week 04: 19.08.2024	L08_P-01	CL	CL	CL	L09_NN-01	2	
Week 05: 26.08.2024	L10_PINN-01	L11_PINN-02	CL	CL	L12_PINN-03	3	
Week 06: 02.09.2024	L13_NN-02	CL	CL	CL	L14_NN-03	2	
Week 07:09.09.2024	L15_PINN-04	L16_PINN-05	CL	CL	L17_PINN-06	3	
Week 08:16.09.2024	*Mid-Semester Exam (17-22 Sep)*						
Week 09:23.09.2024	L18_PINN-07	CL	CL	CL	L19_OL-1	2	
Week 10:30.09.2024	L20_MOR-01	CL	CL	CL	L21_MOR-2	2	
Week 11:07.10.2024	*Mid-Term Break(05-13 Oct)*						
Week 12:14.10.2024	L22_MOR-03	CL	CL	CL	L23_MOR-04	2	
Week 13:21.10.2024	L24_PINN-08	L25_IAL01	CL	CL	L26_IAL02	3	
Week 14:28.10.2024	CL	CL	CL	CL	CL		
Week 15:04.11.2024	CL	CL	CL	CL	CL		
Week 16:11.11.2024	CL	CL	CL	CL	CL		
Week 17:18.11.2024	*End-Semester Examination (17-26 Nov)*						

LEGEND

X: Cancelled

CL: Computational Lab Hours for Student Activities in Problem Solving and Projects in SciML4FM

IAL: Invited Application Lecture

Final Individual Project Presentation during Week 16.

LXX-Lecture Number

LA: Linear Algebra

FM: Fluid Mechanics

OPT: Optimization

P: Primer on Probability

NN: Neural Networks

PINN: Physics Informed Neural Networks

PIELM: Physics Informed Extreme Learning Machine

OL: Operator Learning

MOR: Model Order Reduction

ROM: Reduced Order Models

1	**L01**	**Introduction to the course**
2	**L02_CR(1)**	***Introduction to Computational Resources***
3	**L03_LA01**	**Linear Algebra Review 01-Basics- Given as Flipped Class**
4	**L04_FM01**	**Fluid Mechanics Models for the Direct Problem**
5	**L05_FM02**	**Boundary Conditions for Modelling Fluid Flows**
6	**L06_LA02**	**Linear Algebra 02 - Eigenvalues/Eigenvectors/Covariance/Eigen Decomposition/PCA/SVD**
7	**L07_OPT01**	**Optimization/Chain Rules/Backpropagation/Automatic Differentiation/ Steepest Descent and Variants**
8	**L08_P01**	**Essential Concepts of Probability for Machine Learning**
9	**L09_NN01**	**Shallow Neural Networks and ELM**
10	**L10_PINN01**	**PINNs and PIELM**
11	**L11_PINN02**	***DeepXDE***
12	**L12_PINN03**	**Methods to Improve Accuracy of PINNs**
13	**L13_NN02**	**Networks with Memory: RNN**
14	**L14_NN03**	**Networks with Memory: LSTM/GRU**
15	**L15_PINN04**	**Stacked and Bidirectional RNN;LSTM-PINN and Applications in Fluid Mechanics**
16	**L16_PINN05**	***Nvidia Modulus***
17	**L17_PINN06**	**Autoencoders**
18	**L18_PINN07**	**Convolutional Neural Networks and Applications in Fluid Mechanics**
19	**L19_OL-01**	**Operator Learning/DeepONet and FNO**
20	**L20_MOR01**	**Nonlinear Dynamical Systems and MOR**
21	**L21_MOR02**	**Proper Orthogonal Decompositions-POD**
22	**L22_MOR03**	**Dynamic Mode Decomposition-DMD**
23	**L23_MOR04**	**Nonlinear ROMs: SINDy&DEIM**
24	**L24_PINN08**	**Alternative ML Approaches/Digital Twins**
25	**L25_IAL01**	**Invited Application Lecture**
26	**L26_IAL02**	**Invited Application Lecture**

Note: All individual project presentation will be scheduled during Week 16 before or by 14 November 2024