Program for 2023 PhD Summer school @KTH
"Physics–Informed Neural Networks and Applications"

Arrival point:

Osquars backe 5, Stockholm

Architecture building KTH,

Digital Futures is located on the 1st floor

Digital Futures or DF: For registration on Sunday, June 18th, project work, Q&A sessions, all activities for week 2; welcome reception and other non–program activities.

F2: Lindstedtsvägen 26,28. For late registration on Monday, June 19th. For Lectures 1–8 during week 1

Hugin/Munin or H/M: Teknikringen 8. For Python Primer on Sunday, June 18th and Lectures 9 & 10 during week 1

R1: Drottning Kristinas väg 51. For final presentation week 2

Coffee breaks:
Week 1: coffee breaks will be served at 10:00 and 15:00 Monday till Saturday
Week 2: coffee will be available throughout the day at Digital Futures, In the afternoon some pastries will be served near the coffee.

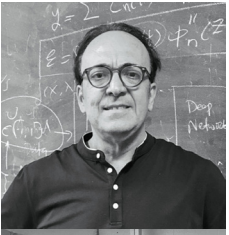
Lunch:
Lunch will be served at 12:00, except for Monday the 19th at 12:30.

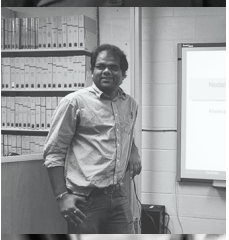
When & Where

19–30th of June 2023

KTH
Royal Institute of Technology

Stockholm, Sweden


George Em. Karniadakis

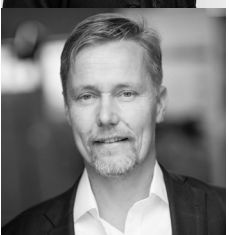

Khemraj Shukla


Kateryna Morozovska


Marco Laudato


Federica Bragone


Amritam Das


Karl Henrik Johansson

Sunday 18th of June, @Hugin/Munin

A primer on Python, NumPy, SciPy & jupyter notebooks

- Getting familiar with programming environment of the course
- Introduction of jupyter notebook and setting it up on your machine
- Basics of data structure and operation in NumpPy and SciPy
- Installation of deep learning frameworks TensorFlow and PyTorch
- Introduction to Nvidia's deep learning container and installation

Monday 19th of June, @F2 for lectures

Welcome to the course: (by organizers)

Brief overview of the course activities.
Introduction to KTH, Presentation of Digital Futures and The KTH Digitalization Platform

Lecture 1: History of Deep Learning, Introduction to Deep Learning Networks (George & Raj)

- History of Deep Learning
- Scientific Machine Learning
- Course objectives, Course Roadmap
- Different types of deep learning
- Workflow in training a deep neural network
- Basic concepts and terminology
- Regression versus classification
- Universal approximation theorem for functions and functionals (reduced, adapted to engineers)
- Example of a regression of a discontinuous/oscillatory function
- Fundamental approximation theory for shallow and deep neural networks (reduced, adapted to engineers)
- Activation functions and adaptivity
- Loss functions (simple and advanced)
- Forward/backpropagation and automatic differentiation
- Connecting neural networks with finite elements

Monday 19th of June, @F2 for lectures

Lecture 2: A primer Tensorflow, PyTorch, JAX (by Raj)

- Brief introduction of tensors and algebraic operations on tensors using TensorFlow, PyTorch and JAX.
- A brief introduction on preparing data for training and testing processes.
- An example of implementation of regression problem in python with and without TensorFlow, PyTorch and JAX.
- Demonstration on implementation of feed−forward fully−connected network in TensorFlow, PyTorch and JAX.
- Demonstration on implementation of AD process in TensorFlow, PyTorch and JAX.

Welcome reception and networking, after 18:00 @DF

Tuesday 20th of June, @F2 for lectures

Lecture 3: Training and Optimization (by George & Raj)

- Definition of optimization problem; types of stationary points
- Bad minima and degenerate saddle points
- Gradient Descent (GD) versus stochastic GD (SGD)
- Effect of learning rate
- Practical tips in training a DNN
- Overfitting versus underfitting
- Vanishing and exploding gradients
- Xavier and He initializations
- Data normalization. Batch normalization
- What optimizer to use?
- First−order optimizers. Second−order optimizers
- Learning rate scheduling. Hybrid Least Squares {GD (LSGD)
- L2, L1 Regularization and Dropout
- Information bottleneck theory
- Dying ReLu DNN

Lecture 4: A few examples of PINNs and applications

- PINNs: data + physical laws
- Example: non−destructive evaluation of materials
- Example: Heat transfer
- Example: Hidden fluid mechanics
- Example: Rheology of shampoo
- Example: Reinforcement learning in fluids

FULL Course: Individual presentaions @DF

Brief 5 minute presentations of individual research interests of full course participants followed by short project group matchmaking

Wednesday 21st of June, @F2 for lectures

Lecture 5: Neural Network Architectures

- Convolution Neural Networks (CNN), Generative adversarial networks (GAN), Residual Neural Network (ResNet), Recurrent Neural Network (RNN), Long-short Time Memory Network (LSTM)
- Demonstration on implementation of CNN, GAN, ResNet and LSTM in PyTorch and TensorFlow

Lecture 6: Physics-Informed Neural Networks (PINNs) - Part I (by George)

- Data + Physical Laws. Data + Physical Laws + Neural Networks
- What is a PINN and Why PINNs
- PINN for Burgers Equation. PINN for Boundary Value Problems
- Soft Constraints and Weights.
- Hard Constraints: Boundary Conditions
- Linearly Constrained Neural Networks
- Hard Constraints: Design and Optimization
- Weighted Residual Methods

LUNCH BREAK

- hp-VPINNs: Domain Decomposition
- Variational Neural Networks
- Convergence Theory of PINNs. Convergence Theory of hp-VPINNs
- Error Decomposition. Error estimates of PINNs based on Quadrature
- PINNs vs DRM (Deep Ritz Method)

Guest Lecture: Potential of PINNs for industrial development

invited experts from Hitachi Energy Corporate Research

FULL Course: Project definition @DF

Find project group. Decide your project scope. Prepare short presentation. (supervised by organizers)

Thursday 22nd of June, @F2 for lectures, Full course start @DF

FULL Course: Project topic presentations @DF

Short 10 minute overview of the project scope: data, tasks, goals.

Lecture 7: Physics-Informed Neural Networks (PINNs) - Part II @F2

- An alphabet of PINNs – an overview
- Gradient-enhanced PINNs: gPINNs
- Conservative PINNs via domain decomposition: cPINNs
- Extended PINNs via domain decomposition: xPINNs
- PINNs for fractional PDEs: fPINNs
- PINNs for stochastic PDEs: sPINNs

Lecture 8: Deep Neural Operators (DeepONet) @F2

- Universal approximation theorem for functionals
- From function to operators

Thursday 22nd of June, @F2 for lectures

- Universal approximation theorem for operators
- DeepOnet: branch and trunk nets
- Theory of DeepOnet
- Learning integral and fractional operators
- Exponential convergence of DeepOnet
- Stochastic ODEs & PDEs
- DeepOnet as LSTM
- Multiscale DeepOnet
- Physics−informed DeepOnet.
- Variational physics−informed DeepOnet
- DeepOnet for high−speed flows
- Extensions of DeepOnet
- DeepM&Mnet concept

Guest Lecture: PINNs for fluid mechanics and sustainability given by KTH guest speaker.

FULL Course: Project work @DF (optional)

You can use DF premises all the time to work on the project alone or in a group.

Friday 23rd of June, Full course start @DF, Lectures @H/M

FULL Course: Project work @DF

Work on group projects, you can use course teachers to ask questions. Project work part is not constrained by the schedule. The schedule only indicates when TAs and teachers will be present to ask questions.

Lecture 9: Discovering Differential Equations @H/M

- Problem Setup
- Neural ODEs
- Multistep neural networks. Recurrent neural networks {comparisons
- Seq2Seq
- Structure−preserving neural networks
- Symplectic and Poisson nets
- The GENERIC framework

Individual sessions: You can use DF premises and several other locations around campus.

Individual Q&A for groups and individuals who need some pointers and ideas on PINN implementation to their research.

Midsommer Celebration & Course Dinner, @Skansen

Sweden has a longstanding tradition of celbrating the longest day in the year or as we call it Midsummer. We will start the evening with a re−ception and dinner at Skansen (oldest open air museum) and see where the night takes us

Saturday 24th of June, @H/M

Lecture 10: Uncertainty Quantification(UQ) in Scientific Machine Learning

- Total uncertainty. Bayes' theorem. Bayesian model average
- Methods for UQ. BNNs and BPINNs. Multifidelity BPINNs
- Functional priors
- UQ in Scientic Machine Learning: A unified view
- Deep Ensembles (DEns). Snapshot Ensembles (SEns)
- Stochastic Weight Averaging Gaussian (SWAG)
- Methods for UQ: Functional Prior
- A Unied view of UQ for neural networks
- Metrics of comparison. Calibration
- Function approximation with unknown and varying noise
- UQ in PINNs. UQ in DeepOnet
- Detection of Out-Of-Distribution (OOD)
- NeuralUQ in TensorFlow and JAX

Individual sessions: @DF and KTH campus.

Individual Q&A for groups and individuals who need some pointers and ideas on PINN implementation to their research.

Sunday 25th of June, @DF

Lecture 11: Implementation of PINNs and DeepOnet @DF

- DeepXDE: Introduction
- DeepXDE: Capabilities
- Workflow for PINNs using DeepXDE
- Complex domains using DeepXDE
- Demo 1: 1D Poisson equation
- Demo 2: Diffusion equation
- Demo 3: Poisson equation over a L-shaped domain
- Demo 4: Inverse problem
- Workflow for DeepONet using DeepXDE
- Demo 5: Learning the antiderivative operator
- Workflow for Multi-fidelity Neural Network (MFNN) using DeepXDE

Lecture 12: Multi-GPU Scientific Machine Learning @DF

- Introduction of data parallel approach for PINN on distributed (multi-GPU) computing platform
- Introduction of domain decomposition methods: Conservative PINN (cPINN) and Extended PINN (XPINN)
- Sampling of training and testing data for PINNs on simple, complex and irregular geometries
- Implementation of multi-GPU PINNs using data parallel approach in SimNet (TensorFlow) and PyTorch and MODULUS
- Demonstration on implementation of multi-GPU cPINN and XPINN using PyTorch and TensorFlow

Lecture 13: MODULUS Library @DF

- Introduction to NVIDIAs MODULUS package for PINNs
- Building MODULUS by using NVIDIA GPU CLOUD (NGC) containers
- Demonstration on implementation of PINNs
- Implementation of computational graph compilation, XLA based compilation, choice of precision for floats (TF32, BF16 (bFloat), FP16, FP32, FP.) vis−a−vis training cost on Nividas latest GPU based on Ampere architecture (A100 and RTX3090)

Monday 26th of June, @DF

FULL Course: Project work @DF

Q&A Session, @DF

Tuesday 27th of June, @DF

FULL Course: Project work @DF

Q&A Session, @DF

FULL Course: Project work @DF

Wednesday 28th of June, @DF

FULL Course: Project work @DF

Q&A Session, @DF

FULL Course: Project work @DF

Thursday 29th of June, @DF

FULL Course: Project work @DF

Q&A Session, @DF

FULL Course: Project work @DF

Friday 30th of June, @R1

Project Presentations

Each group will have a 20 minute presentation slot, which will be followed by questions and suggestions from the audience.

Farewell and departure

Saturday 1st of July

Farewell and departure

	Sun 18th	Mon 19th	Tue 20th	Wed 21st	Thu 22nd	Fri 23rd	Sat 24th
8:00	Arrival & Registration 10:00–18:00 DF lobby	Registration	Start 8:30	Lecture 5, F2	Presentation of project topics, DF	Project work, DF	Lecture 10, H/M
8:30		Welcome lecture	Lecture 3, F2				
9:00		Lecture 1, F2				Lecture 9, H/M	
9:30							
10:00			Coffee	Coffee	Coffee		Coffee
10:30			Lecture 3, F2	Lecture 6, F2	Lecture 7, F2		Lecture 10, H/M
11:00		Coffee					
11:30		Lecture 1					
12:00			Lunch, near F2	Lunch, near F2	Lunch, near F2	Lunch, near DF	Lunch, near DF
12:30		Lunch, near F2					
13:00					Lecture 8, F2	Individual work with Q&A Session, DF	Individual sessions, Project work, DF and around campus
13:30			Lecture 4, F2	Lecture 6, F2			
14:00	Python primer, H/M	Lecture 2, F2					
14:30							
15:00		Fika	Fika	Fika	Fika		
15:30		Lecture 2, F2	Individual presentations, DF	Guest Lecture, F2	Guest Lecture, F2	Free time	
16:00							
16:30				Project definition, DF	Lecture 8, F2		
17:00						Course dinner, Skansen till 23:00	
17:30					Project work, DF or city tour		
18:00 <		Course Mingle, DF till 23:00	City tour				City tour

	Sun 25th	Mon 26th	Tue 27th	Wed 28th	Thu 29th	Fri 30th	Sat 1st
8:00			Project work, DF	Project work, DF	Project work, DF		Farewell
8:30	Lecture 11, DF	Project work, DF					
9:00						Presentations of project results	
9:30							
10:00							
10:30	Lecture 12, DF						
11:00							
12:00	Lunch, DF	Lunch, DF	Lunch, DF	Lunch, DF	Lunch, DF	Lunch, R1	
13:00	Lecture 12, DF	Q&A Session, DF	Q&A Session, DF	Q&A Session, DF	Q&A Session, DF	Presentations of project results	
14:00	Lecture 13, DF						
15:00		Project work, DF	Project work, DF	Project work, DF	Project work, DF		
16:00	Project work, DF						
17:00							
18:00 <	Own time	Own time	Own time	Own time	Own time	Farewell	

Full course, Project work

Lectures

Common workshops

Arrival, departure

Meals, coffee

Useful Information

Travel in Stockholm:
– Public transport operates under one ticket system, covering: subway, trains, trams, busses and even several ferry connections
– To use public transport you should purchase your ticket using Sl.se look for respective applications for android and iPhone.
– Ticket can also be purchased at the chasier in the subway station or at the train station or you can pay directly with your VISA or MasterCard by using it to enter any of the abovementioned transports.

KTH Main Capmus is located in the city of Stockholm, therefore many locations can be considered a walking distance away from the course location.

Internet, WiFi:

Eduroam: Most of the participants who come from abroad can continue using eduroam around KTH campus.
If your university does not have Eduroam connection please notify the organizers and we will provide you with access to KTH open WiFi network.

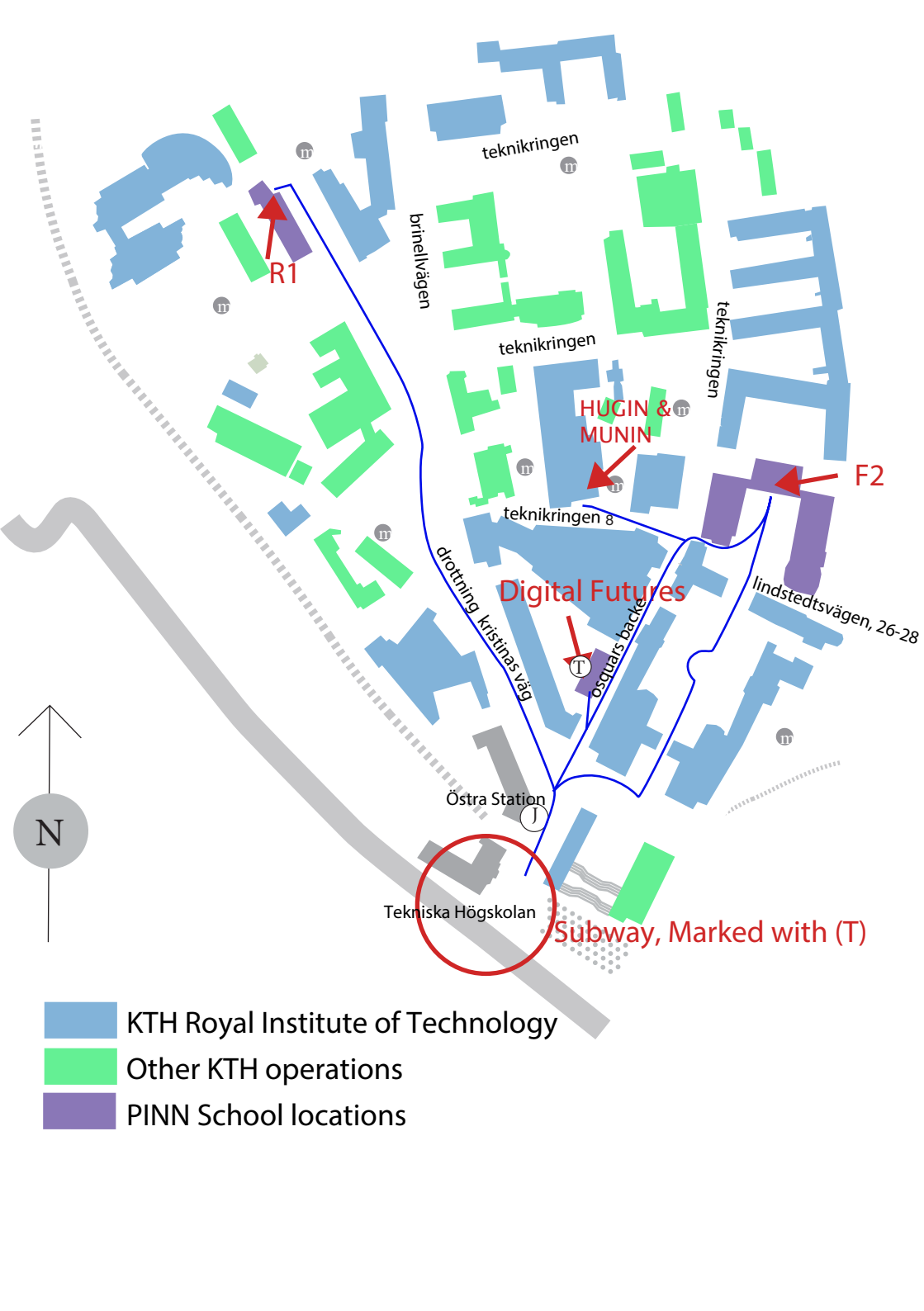
Course Dinner:

The course Dinner will take place in Skansen at Gustavianska våningen. We will go as a group from KTH starting from Main campus.

If you wish to travel to the venue alone you can plan your journey using SL.se app. To reach Skansen from KTH take bus 67 till stop Skansen.

Emergency number Sweden:

If you experience emergency use universal emerency number 112, for police, healthcare, fire department etc.


R1
brinellvägen
teknikringen
teknikringen
teknikringen
HUGIN &
MUNIN
F2
teknikringen 8
drottning kristinas väg
Digital Futures
osquars backe
lindstedtsvägen, 26-28
Östra Station
Tekniska Högskolan
Subway, Marked with (T)
N
KTH Royal Institute of Technology
Other KTH operations
PINN School locations

Course assistants:

Nicole Rosi,
DTU

For general questions & help around campus

Lorenzo Branca,
SNS Pisa

Questions on software instalaltions, using HPC resources, tech. support

Contact Information:

Use Slack channel for questions to both organizers and participants.

For certificates of participation, other questions: 2023@pinns.se

Emergency and Urgent situations:

Call: +46 762552977, Kateryna
+46 724425313, Marco
+46 723550100, Federica