### **PhD** Course Description

We offer a one week PhD course/workshop on "Scientific Machine Learning".

The PhD course is offered as a part of activities and with support from the DTU Compute PhD School and the Danish Center for Applied Mathematics and Mechanics (DCAMM) at Technical University of Denmark, see www.dcamm.dk.

## PhD Course objective

The aim of the course is to introduce the students to some of the methods and algorithms used in scientific machine learning (SciML), and let the students experience these methods on elementary computer experiments. The PhD course covers several topics in SciML: neural differential equations, universal differential equations, physicsinformed neural networks (PINN), automatic differentiation (AD) / differentiable programming, neural operators, symbolic regression, and more. The objective is to give the student an overview of the "tools" available and how they can be modified for particular SciML applications.

- ✓ Understand problems and questions addressed by SciML methods.
- ✓ Understand how methods are used as building blocks to address SciML questions.
- ✓ Be able to choose a suitable method depending on the situation and problem.
- $\checkmark$  Implement some of these methods in Julia.
- ✓ Skillfully perform numerical experiments and interpret the results.
- ✓ Setup and train neural differential equations and physics-informed neural networks.
- ✓ Identify and exploit the properties and structure of scientific knowledge within machine learning applications.
- ✓ Independently solve a special topics problem offered in the course.
- $\checkmark$  Written presentation of results in a report or a poster.

# PhD Course Homepage

http://www2.compute.dtu.dk/~apek/SCIML2022/

## **Organizers and Lecturers**

- Ph.D. Chris Rackauckas, Research Affiliate and Co-PI of the Julia Lab at the Massachusetts Institute of Technology, United States.
- Associate Professor Allan P. Engsig-Karup Dept. Applied Mathematics and Computer Science, DTU Compute, Technical University of Denmark. E-mail: apek@dtu.dk

# Participants

The course is intended for PhD students, PostDocs and MSc students with a fundamental knowledge of programming and scientific computing, linear algebra, and must be able to program in some high level language (R, MATLAB, Python, Julia, C++, C, etc.).

# Work Load

Approximately 20 scheduled hours (lectures, discussions and computer exercises) during the course and approximately 20 hours for the completion of an assignment problem after the duration of the workshop. Also, to prepare for the course it is required that participants read the literature proposed below in advance.

# Literature

The course is partly based on the lecture notes from MIT's 18.337 Parallel Computing and Scientific Machine Learning. <u>https://book.sciml.ai/</u>

# Language

All lectures will be given in English.

# Registration

Sign up by sending an E-mail to the DTU organizer.

# **Registration Fee**

There is no registration fee for students enrolled at Danish universities and public research institutions. For other PhD students the fee is  $\notin$ 200. For researchers employed at universities and public research institutions the registration fee is  $\notin$ 400. For all other participants the registration fee is  $\notin$ 1050. Payment information will be given upon signing up for the workshop.

### Deadline

The submitted request for registration must be received by the course secretariat no later than May 29<sup>th</sup>, 2022 (limited seats, so sign up early is recommended). Information on enrollment will be posted within a week after this date. Signup is on a first-come first-serve due to limited seats.

Sign up via <a href="https://forms.gle/kyUE4RH1FWUzJBjC6">https://forms.gle/kyUE4RH1FWUzJBjC6</a> .

# **Evaluation and Diplomas**

To pass the course, active participation and the satisfactory completion of an assignment problem after the duration of the course are required. **ETCS points: 2.5** (equivalent to 1.5 week effective full time work).

# **Course Contents**

The following topics will be covered in the course

- 1. Introduction to Scientific Machine Learning (SciML)
- 2. Physics-Informed Neural Networks
- 3. Automatic Differentiation and Differentiable Programming
- 4. Neural Differential Equations
- 5. Universal Differential Equations and Symbolic Regression
- 6. Neural Operators

Visit the PhD course homepage and materials or talk to the DTU advisor for more details.

### Lunch

The DTU Compute PhD School and DCAMM are sponsoring a daily lunch for participants that are enrolled at universities and public research institutions.

### Housing

Accommodation in hostels/hotels can also be arranged by the participants themselves, see e.g. the Wonderful Copenhagen website at <u>www.wonderfulcopenhagen.com/</u> and course webpage.

#### **Internet Resources**

For facts on the Technical University of Denmark and visitors' information: See <u>http://www.dtu.dk</u>. Information about teaching and research at DTU Compute can be found at <u>http://www.compute.dtu.dk</u>, and for DCAMM at <u>http://www.dcamm.dk</u>. The DTU Computing Center (DCC) <u>https://www.hpc.dtu.dk/</u> and GPULAB provide general access to hardware and support high performance computing for modern scientific computing applications.

#### About the DTU Compute PhD School

The DTU Compute PhD School administers the PhD program at DTU Compute. The school promotes crossdisciplinary research, matching information technology and mathematical modelling with other disciplines, often in collaboration with external collaborators: Other research institutions and private companies.

The DTU Compute PhD aims to strengthen research education through a series of initiatives: Specialized PhD courses and summer schools, quality assurance of supervision, PhD processes and procedures, research environment, implementation of a mentor program, help with IPR, social activities, etc.



#### DANISH CENTER FOR APPLIED MATHEMATICS AND MECHANICS

The Danish Centre for Applied Mathematics and Mechanics, DCAMM, is an informal framework for internationally oriented scientific collaboration between staff members at a number of departments at the Technical University of Denmark (DTU), Aalborg University (AAU), Aarhus University (AU) and University of Southern Denmark (SDU). The Departments cooperating within DCAMM are:

- Dept. of Applied Mathematics and Computer Science, DTU
- Dept. of Civil and Mechanical Engineering, DTU
- Dept. of Wind and Energy Systems, DTU
- Dept. of the Built Environment, AAU
- Dept. of Mathematical Sciences, AAU
- Dept. of Mechanical and Manufacturing Engineering, AAU
- Dept. of Civil and Architectural Engineering, AU
- Dept. of Mechanical and Production Engineering, AU
- Dept. of Mechanical and Electrical Engineering, SDU

DCAMM is an informal construction that was founded October 27, 1969. The day to day activities are coordinated by the chairman of the Center (pt. Associate Professor Niels Leergaard Pedersen Department of Civil and Mechanical Engineering, Solid Mechanics), while the formal governing body of DCAMM is the Scientific Council.

## The Technical University of Denmark DTU Compute

Section for Scientific Computing & DTU Compute PhD School





# PhD School on Scientific Machine Learning

Kgs. Lyngby, Denmark June 13<sup>th</sup> to June 17<sup>th</sup>, 2022 DDSA DANISH DATA SCIENCE ACADEMY



EuroTech Universities

DTU Compute Department of Applied Mathematics and Computer Science

Center for Energy Resources Engineering CERE

