Introduction

02671 Data-Driven Methods for Computational Science and Engineering

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$$f(x+\Delta x)=\sum_{i=0}^{\infty}\frac{(\Delta x)^i}{i!}f^{(i)}(x)$$

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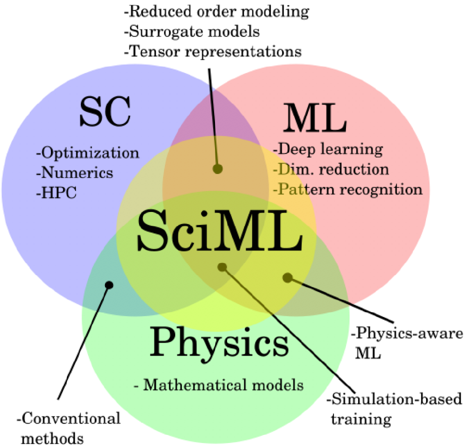
Course description

This course contributes to establishing a solid knowledge of theory and practice in Scientific Computing, complementing established numerical solution of differential equation systems based on ODEs/SDEs/PDEs. Data-driven discovery is revolutionising the modeling, prediction, and control of complex systems. This course draws on machine learning, engineering mathematics, and mathematical physics to integrate modeling and control of dynamical systems with modern methods in data science. The course emphasis fundamental techniques and tools behind recent advances in scientific computing and the emerging area scientific machine learning (SciML) that enable data-driven methods to be applied to a diverse range of complex systems across science and engineering. The range of topics help gain experience and understanding of state-of-the-art that is useful for advanced studies of mathematical problems arising in science and engineering applications.

Focus is primarily upon the application of techniques to different problems, with some introduction to mathematical foundations. Students will use the preferred programming language such as Python/Julia/Matlab to implement data-driven and other computational techniques. It is not necessary to know all details of a programming language prior to this course; however, familiarity of at least one programming language is assumed.

Scientific Machine Learning on the rise



- Areas of statistics, data-driven machine learning method and mathematical physics growing research area.
- Many opportunities for improving the scientific computing toolbox.

Scientific Machine Learning

With the help of ChatGPT[1] a description of Scientific Machine Learning is given...

Scientific machine learning is a subfield of machine learning that focuses on the development and application of machine learning algorithms and techniques to solve problems in the natural sciences, such as physics, chemistry, biology, fluid mechanics, and astronomy. This field draws on ideas from a wide range of disciplines, including scientific computing, computer science, statistics, and the natural sciences, and involves the use of advanced mathematical and computational methods to analyze and process large amounts of data. Some key challenges in scientific machine learning include developing algorithms that can accurately and efficiently process complex, high-dimensional data, and finding ways to apply these algorithms to solve real-world problems in the natural sciences.

Disclaimer: We live in a world with new technologies disrupting existing approaches. The chat robot ChatGPT and similar ones can be viewed as a productivity tools and cannot replace individual intellectual work. So, if you use ChatGPT in this course (fx. for building code templates), then mention this in your report and include snapshots/links of relevant solutions. Remark, ChatGPT has no build in guarantee that the results given are factually correct. Consult also info at `https://www.ai.dtu.dk/`DTU AI Hub.

[1] https://en.wikipedia.org/wiki/ChatGPT.

Dynamical Systems in Natural Sciences

Dynamical systems describe the evolution of phenomena occurring in nature, can be posed as initial value problems (IVPs) in terms of a differential equation system

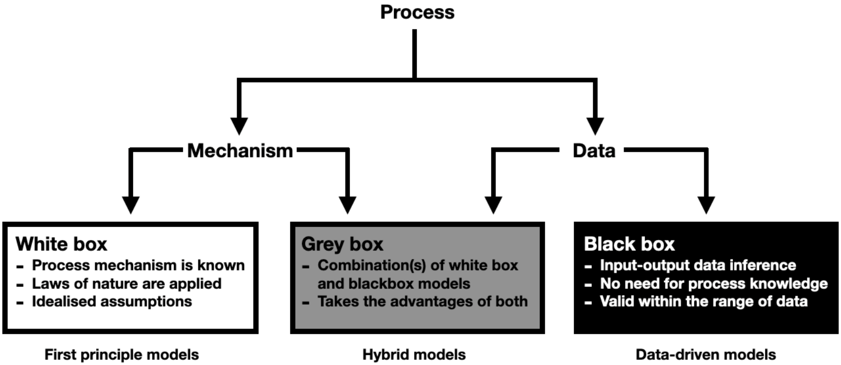
$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, t; \Theta), \quad \mathbf{y}(t_0) = \mathbf{y}_0, \quad t > t_0,$$

models the dynamics of $\mathbf{y} \in \mathbb{R}^d$. Here $\mathbf{f}(\mathbf{y}, t; \Theta) : \mathbb{R}^{d+1} \mapsto \mathbb{R}^d$ can be a nonlinear operator parameterized by parameters Θ.

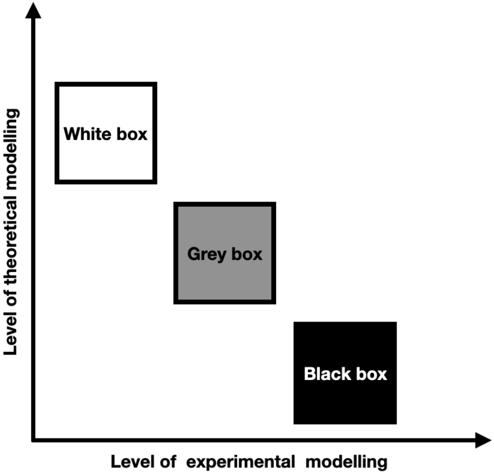
We can study and use such models in different scenarios, e.g.

- **Known system**. When $\mathbf{f}$ and the parameters Θ are known, physics-based methods on numerical integration are commonly used to directly solve for $\mathbf{y}$, e.g. for scenario simulation where future states $\mathbf{y}_k$, $k = 1, ..., K$ are estimated.
- **Partially known system**. When $\mathbf{f}$ is known and the parameters Θ are unknown, physics-based methods on numerical integration are commonly used to directly solve for the unknown solution $\mathbf{y}$ and observations is used for parameter estimation of Θ to match predictions with such observations (data assimilation or system calibration).
- **Unknown system**. When $\mathbf{f}$ is unknown and data in the form of measurements of states $\mathbf{y}_k$ are available, one can seek to identify which differential equation model best describe data (system identification). It is possible to consider options for *learning a dynamical system* from observations, i.e. to search for a good model for a dynamical system in a hypothesis space guided by some criterion for performance.

Modelling Approaches



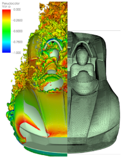
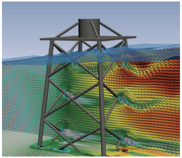
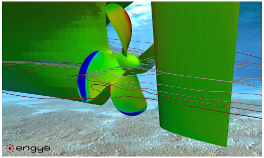
Modelling Approaches



- Black box machine learning is data "hungry".
- White box physics-based modelling requires little data, however, is often computationally expensive (fx. when solving PDEs).

Computational Modelling

Computational modelling and simulation is indispensable across science, engineering, virtual education and entertainment. High-fidelity typically implies large-scale computational physics-based models, cf. illustrations.

Consider a time-dependent PDE model (here in 1D, but can be any-D)

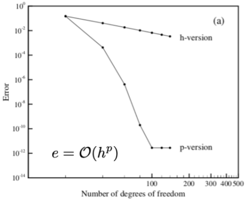
$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \mathcal{L}(u) + \mathcal{N}(u) + s, \quad \alpha < x < \beta \\
\mathcal{B}_- u(x,t) &= g_-, \quad x = \alpha \\
\mathcal{B}_+ u(x,t) &= g_+, \quad x = \beta \\
u(x,0) &= g_0, \quad \alpha < x < \beta
\end{aligned}
$$

Through a Method of lines discretization based on the Mean Weighted Residual (MWR) framework, we can arrive at a semi-discrete system of equations in the form of a IVP.

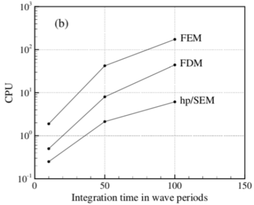
Computational Modelling

Decades of research and developments have led to many high-fidelity models that are *convergent*, *accurate*, *efficient* and $\mathcal{O}(n)$ or $\mathcal{O}(n \log n)$-*scalable*.

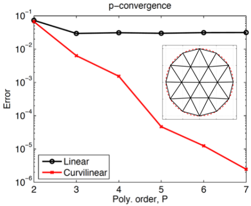
Algorithmic Efficiency



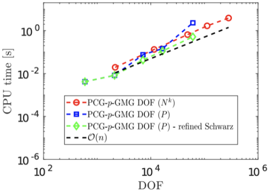
Numerical Efficiency



Geometric accuracy

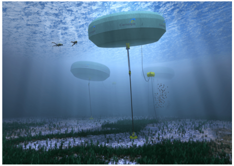
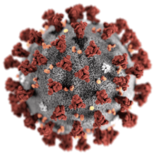


Scalability



Computational Modelling



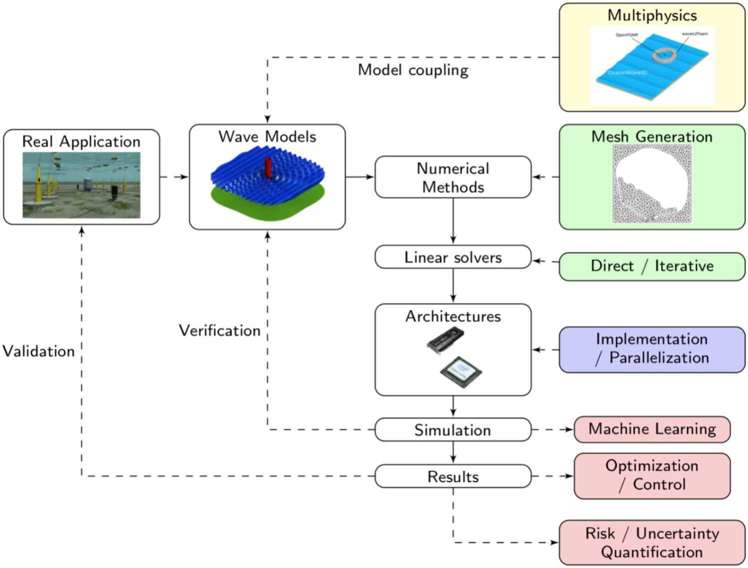



In many applications the computational expense is high resulting in a computational barrier for producing high-fidelity results fast and in *real-time*. Some applications are *time-critical* (restricted time window for solutions), fx.

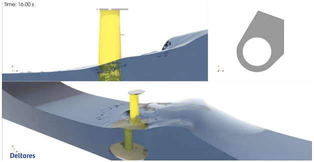
- **Interactive** virtual environments
- Model Predictive **Control**
- **Design** optimization
- Health **monitoring**
- **Interpretability** via mathematical models and **Visualization** (to support physical intuition)
- **Reliability** via **uncertainty quantification** along with predictions

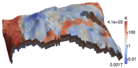
So what can be done?

Physics-based simulation framework



Model validation





(a) Permeability field K_x

(b) Water injection wells are marked with red and production wells are marked with blue.

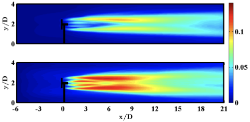


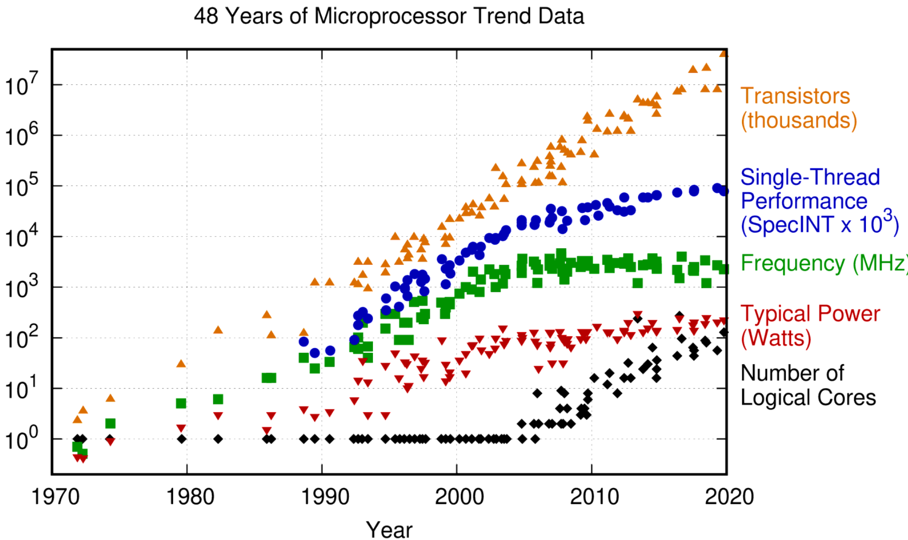
Figure 5.20: Contours of stream-wise turbulence intensity, $\frac{\sigma_u}{\bar{u}}$, at the middle vertical plane. Comparison Re-500 (Top), Re-2000 (Bottom)

Computational models should be validated against measurements to agree within, say 5% engineering accuracy, however, may require 100s of million cells and 1000s of time steps. This may lead to high simulation costs in weeks even when using 1000s of cores for parallel computing.

For engineering or time-critical applications there are often a computational barrier

- Design optimization
- Uncertainty quantification
- Model predictive control
- Robust design

Acceleration using High-Performance Computing



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

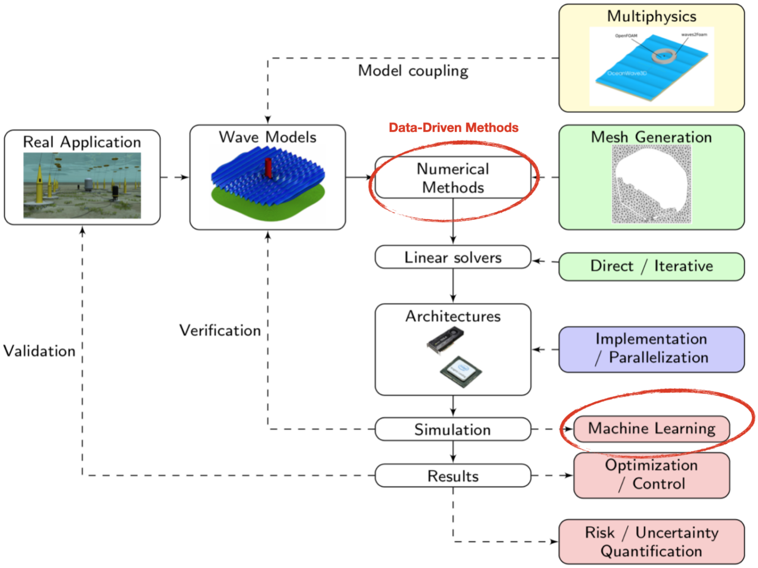
Acceleration using High-Performance Computing

DTU GPULAB (gpulab.compute.dtu.dk) established at Scientific Computing Section at DTU Compute, in **August 2008** as a unique national competence center and hardware laboratory with support from national FTP grant "Desktop Computing on Consumer Graphics Cards".

- ✦ Development of efficient algorithms for massively parallel computing
- ✦ High-performance scientific computing
- ✦ Performance profiling, auto-tuning and prediction
- ✦ Software engineering using parallel programming languages (fx. CUDA/OpenCL/MPI)
- ✦ Education and research in accelerator technology such as GPUs the core focus

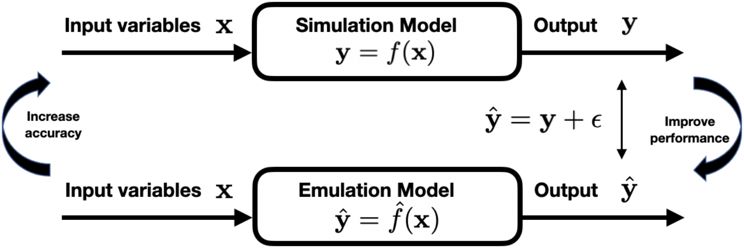
At DTU Compute there is **10+ years experience** with the proper mapping of algorithms and use of modern and emerging hardware accelerators.

Physics-based simulation framework



Simulation vs. Emulation

Complex computer codes (simulator) are used to make predictions about real-world systems in many fields of science and technology. Represent the simulator in the form of a function $\mathbf{y} = f(\mathbf{x})$, where a single run of the simulator is defined to be the process of producing one set of outputs $\mathbf{y}$ for a particular input configuration $\mathbf{x}$.



To turn an expensive dynamic simulation into a cheaper process that can replace the simulation model through an emulation model that mimic the results of the simulation. Seek an inexpensive albeit sufficiently accurate map $\hat{f}(\mathbf{x}) \simeq f(\mathbf{x})$. This way, accuracy can be traded for performance using this algorithmic approach.

Simulation using dynamical systems

Simulation is a means to predict future states from the current or past states using a model.

A linear dynamical system is expressed in terms of the dynamics (or update) equation

$$x_{t+1} = A_t x_t, \quad t = 1, 2, ...$$

where A_t are the dynamics matrices, and x_t is the state of the system at time t.

A nonlinear dynamical system can be formulated as

$$y_t = F(y_{t-1}, y_{t-2}, y_{t-3}, \dots, u_t, u_{t-1}, u_{t-2}, u_{t-3}, \dots) + \varepsilon_t$$

where ε_t is a noise term accounting for errors in the update.

By iterating we can find the future trajectory $x_{t+1}, x_{t+2}, ...$. This is called simulating the system dynamics. Here $F(\cdot)$ can be a nonlinear function of single or multiple past future states and inputs $u_t, u_{t-1}, ...$.

Remark, models of this form are often used in time series analysis and econometrics, where they are called auto-regressive (AR) models.

Emulation

So, emulation is a means to improve performance over expensive simulation.

Most often emulation techniques are applied to dynamic simulators in two different ways.

- Emulate output of full simulation (many sequential steps wrt. time)

  $$\mathbf{y} = \hat{f}(\mathbf{x})$$

  Con: after model is generated it cannot extrapolate outside parameter domain.
  Pro: model can execute very fast

- Emulate a change in state in one step of a simulation to be able to use this iteratively for many steps

  $$\mathbf{y}_{k+1} = \hat{f}(\mathbf{y}_k)$$

  Con: after model is generated varying boundary conditions needs to be handled.
  Pro: model can generalize to predict future states

Error contributions

When models are produced they come with errors. This can be understood through the lens of function approximation as

$$\hat{\mathbf{y}} = \mathbf{y} + \epsilon$$

Employing the triangle equality, one can derive a bound for the error between the true model against the surrogate model (emulator)

$$\underbrace{||f - \hat{f}||}_{\substack{\text{surrogate} \\ \text{modelling} \\ \text{error}}} \leq \underbrace{||f - f_{HF}||}_{\substack{\text{high fidelity} \\ \text{modelling} \\ \text{error}}} + \underbrace{||f_{HF} - \hat{f}||}_{\substack{\text{surrogate} \\ \text{approximation} \\ \text{error}}}$$

Artificial Intelligence

Artificial Intelligence (AI) will strongly determine our future prosperity and well-being. Due to its generic nature, AI will have an impact on all sciences and business sectors, our private lives and society as a whole. AI is pre-eminently a multidisciplinary technology that connects scientists from a wide variety of research areas, from behavioural science and ethics to mathematics and computer science.

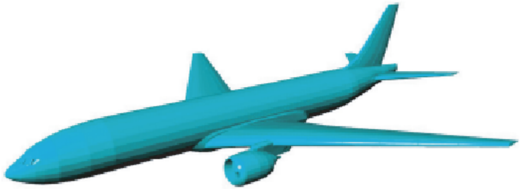
> *"Artificial intelligence is in its adolescent phase, characterised by trial and error, self-aggrandisement, credulity and lack of systematic understanding."*
> - Robert Dijkgraaf (2019)

Mathematics can contribute to the much-needed systematic understanding of AI, for example, greatly improving reliability and robustness of AI algorithms, understanding the operation and sensitivity of networks, reducing the need for abundant data sets, or incorporating physical properties into neural networks needed for superfast and accurate simulations in the context of digital twinning.

Source: MATHEMATICS: KEY ENABLING TECHNOLOGY FOR SCIENTIFIC MACHINE LEARNING (2021)

Digital Prototypes and Digital Simulation for Design Optimization

"Scientific computing enabled the prototyping of aircraft design through physics-based emulators that resulted in substantial cost savings to aerospace manufacturers. The Boeing 777 was the first aircraft to have been designed completely from simulation without a mock-up.", cf. Brunton et al. (2020).



"Emerging methods in machine learning may be thought of as data-driven optimization techniques that are ideal for high-dimensional, non-convex, and constrained, multi-objective optimization problems, and that improve with increasing volumes of data. "

See also NASA Common Research Model:
`https://commonresearchmodel.larc.nasa.gov/`.

Digital Twins and history

Renewable and Sustainable Energy Reviews 161 (2022) 112407

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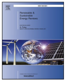
Renewable and Sustainable Energy Reviews

journal homepage: www.elsevier.com/locate/rser



Energy digital twin technology for industrial energy management: Classification, challenges and future

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A R T I C L E I N F O

Keywords:
Digital twin
Industry 4.0
Energy engineering
Sustainable energy
Renewable energy
Process systems engineering

A B S T R A C T

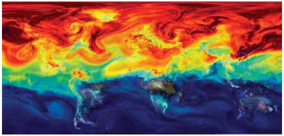
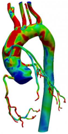
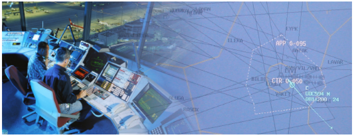
Digitalisation of the process and energy industries through energy digital twin technology promises step-improvements in energy management and optimisation, better servicing and maintenance, energy-efficient design and evolution of existing sites, and integration with locally and regionally generated renewable energy. This systematic and critical review aims to accelerate the understanding, classification, and application of energy digital twin technology. It adds to the literature by developing an original multi-dimensional digital twin classification framework, summarising the applications of energy digital twins throughout a site's lifecycle, and constructing a proposal of how to apply the technology to industrial sites and local areas to enable a reduction in carbon and other environmental footprints. The review concludes by identifying key challenges that face uptake of energy digital twins and a framework to apply the energy digital twins.

"Digitalisation of the process and energy industries through energy digital twin technology promises step-improvements in energy management and optimisation, better servicing and maintenance, energy-efficient design and evolution of existing sites, and integration with locally and regionally generated renewable energy."

See also the DTU Compute Mathematics of Data Science seminar talk by Dirk Hartman, Siemens Technology, Feb 6, 2024, on "Executable Digital Twins".

Scientific Machine Learning Applications

There are many use cases for physics-based and data-driven modelling...

"Numerical methods are prevalent in science to improve the understanding of our world, with applications ranging from climate modeling over simulating the efficiency of airplane wings to analyzing blood flow in a human body. These applications are extremely costly to compute due to the fine spatial and temporal resolutions required in real-world scenarios."

Refs: 'Solver-in-the-Loop: Learning from Differentiable Physics to Interact with Iterative PDE-Solvers'. Ses 'Skilful precipitation nowcasting using deep generative models of radar'. Se also weather forecasting news on twittter (Nov. 2023).

To develop improved physics-based modelling at reduced cost or improved fidelity, it is possible to utilize data-driven approaches (fx. many use cases for *function approximation* and *applied regression techniques*) that rely on mathematical optimization.

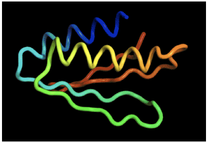
Scientific Machine Learning Applications

Why Machine Learning within science and engineering?

Big data analysis and computational science. In 2019, the first image of a black hole was done using machine learning

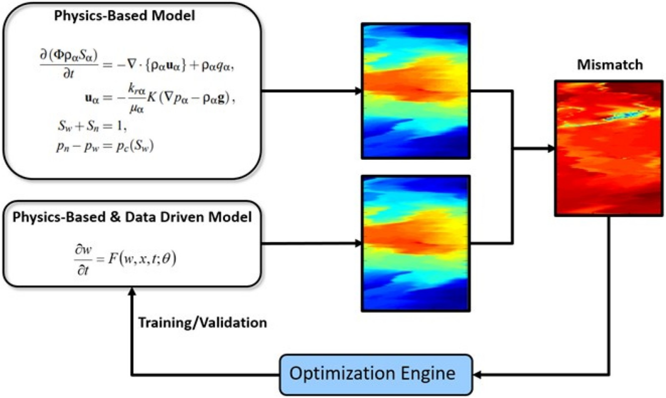
Read the NumFocus story on how open source software was used.

Scientific discovery. The most accurate predictions of protein structures of high relevance for drug discovery was done using machine learning



Scientific Machine Learning Applications

A concept for training a physics-based data-driven model for improved and/or accelerated predictive modelling of complex real-world problem (here reservoir simulation) can be presented as



where the objective is to learn the right hand side function of the physics-based model using data-driven, physics-based principles and math techniques.

Scientific Machine Learning - research and applications

Inspirational work: physics-informed neural networks for parametrized boundary conditions and real-time room acoustics.

JASA EXPRESS LETTERS ARTICLE asa.scitation.org/journal/jel CrossMark

Physics-informed neural networks for one-dimensional sound field predictions with parameterized sources and impedance boundaries

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Abstract: Realistic sound is essential in virtual environments, such as computer games and mixed reality. Efficient and accurate numerical methods for pre-calculating acoustics have been developed over the last decade; however, pre-calculating acoustics makes handling dynamic scenes with moving sources challenging, requiring intractable memory storage. A physics-informed neural network (PINN) method in one dimension is presented, which learns a compact and efficient surrogate model with parameterized moving Gaussian sources and impedance boundaries and satisfies a system of coupled equations. The model shows relative mean errors below 2%/0.2 dB and proposes a first step in developing PINNs for realistic three-dimensional scenes.

[Editor: D. Keith Wilson] https://doi.org/10.1121/10.0009057

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1. Introduction

In computer games and mixed reality, realistic sound is essential for an immersive user experience. The impulse responses (IR) can be obtained accurately and efficiently by numerically solving the wave equation using traditional numerical methods, such as finite element methods,[1] spectral element methods (SEM),[2] discontinuous Galerkin finite element method,[3] and finite-difference time-domain methods.[4,5] For real-time applications spanning a broad frequency range, the IRs are calculated offline due to the computational requirements. However, for dynamic, interactive scenes with numerous moving sources and receivers, the computation time and storage requirement for a lookup database become intractable (in the range of gigabytes) since the IR is calculated for each source-receiver pair. When covering the whole audible frequency range, these challenges become even more extensive. Previous attempts to overcome the storage requirements of the IRs include work for lossy compression,[6] and lately, a novel portal search method has been proposed as a drop-in solution to pre-computed IRs to adapt to flexible scenes, e.g., when doors and windows are opened and closed.[7] A recent technique for handling parameter parameterization and model order reduction for acceleration of numerical models is the reduced basis method (RBM).[8,9] Although very efficient, RBM cannot meet the runtime requirements regarding computation time for virtual acoustics.

In this paper, we consider a new approach using physics-informed neural networks (PINNs)[10–12] including knowledge of the underlying physics (in contrary to traditional "black box" neural networks[13]) to learn a surrogate model for a one-dimensional (1D) domain that can be executed very efficiently at runtime (in the range of ms) and takes up little storage due to their intrinsic interpolation properties in grid-less domains. The applications of PINNs in virtual acoustics are very limited,[14,15] and the main contribution of this work is the development of frequency-dependent and independent impedance boundary conditions with parameterized moving Gaussian sources, making it possible to model sound propagation taking boundary materials properly into account. This work investigated PINNs for virtual acoustics in a 1D domain—still taking the necessary physics into account—making it a possible stepping stone to model realistic and complex 3D scenes for applications, such as games and mixed reality, where the computation and storage requirements are very strict.

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Scientific Machine Learning - research and applications

Inspirational work: Surrogate modelling using generalised residual networks for urban drainage systems.

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Accelerating hydrodynamic simulations of urban drainage systems with physics-guided machine learning

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A R T I C L E I N F O

Keywords:
Hydrodynamic simulation
Scientific machine learning
Surrogate model
Urban drainage

A B S T R A C T

We propose and demonstrate a new approach for fast and accurate surrogate modelling of urban drainage system hydraulics based on physics-guided machine learning. The surrogates are trained against a limited set of simulation results from a hydrodynamic (HiFi) model. Our approach reduces simulation times by one to two orders of magnitude compared to a HiFi model. It is thus slower than e.g. conceptual hydrological models, but it enables simulations of water levels, flows and surcharges in all nodes and links of a drainage network and thus largely preserves the level of detail provided by HiFi models. Comparing time series simulated by the surrogate and the HiFi model, R^2 values in the order of 0.9 are achieved. Surrogate training times are currently in the order of one hour. However, they can likely be reduced through the application of transfer learning and graph neural networks. Our surrogate approach will be useful for interactive workshops in initial design phases of urban drainage systems, as well as for real time applications. In addition, our model formulation is generic and future research should investigate its application for simulating other water systems.

1. Introduction

Computational modelling is essential in all phases of managing urban drainage systems (UDS), from design to monitoring and control. Physics-based deterministic models are widely used around the world. These models solve Saint Venant's system of equations in small time steps for each pipe element (Abbott and Ionescu, 1967). We will refer to this approach as "high-fidelity models". High-fidelity (Hifi) models are directly linked to physical system characteristics such as pipe diameter and length, and both water levels and flows are simulated in a realistic manner which makes them attractive to practitioners. However, high simulation times limit stakeholder involvement in the design phase (Leskens et al., 2014), as well as the exploration of impacts of deep uncertainties about future climates and urban developments (Löwe et al., 2020). In addition, real-time applications such as warning and control usually require shorter simulation times than what is feasible with HiFi models.

To circumvent these problems, hydrologists have developed a number of so-called lower-fidelity surrogates (Razavi et al., 2012). In particular, a variety of conceptual (or lumped) hydrological models were developed for UDS (Burger et al., 2016; Kroll et al., 2017; Moreno-Rodenas et al., 2018; Thrysøe et al., 2019). All these approaches reduce computation times by orders of magnitude. However, they achieve speedup at the cost of simplifying the simulated processes or lowering the spatiotemporal resolution. Typically, only flows are simulated (not water levels), and only few selected locations in the pipe network are considered. The practical consequences are that the existing surrogates are valid only for a limited range of purposes (e.g. sewer overflow but not flood risk), are not straightforward to set up automatically from pipe databases, and extrapolate poorly to a changing drainage system structure. This limitation is not present for cellular automata approaches that only simplify the mathematical description of the processes but preserve the level of detail of the model (Austin et al., 2014). However, similarly small simulation time steps as with a numerical simulator must be selected. Limited speed-ups in the order of factor 5 where therefore achieved.

Machine learning approaches have gained traction in hydrology. They are frequently applied in an input-output setting, including

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Scientific Machine Learning - research and applications

Inspirational work: reduced basis method for accelerated room acoustics.

JASA ARTICLE

Reduced basis methods for numerical room acoustic simulations with parametrized boundaries

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ABSTRACT:
The use of model-based numerical simulations of wave propagation in rooms for engineering applications requires that acoustic conditions for multiple parameters are evaluated iteratively, which is computationally expensive. We present a reduced basis method (RBM) to achieve a computational cost reduction relative to a traditional full-order model (FOM) for wave-based room acoustic simulations with parametrized boundaries. The FOM solver is based on the spectral-element method; however, other numerical methods could be applied. The RBM reduces the computational burden by solving the problem in a low-dimensional subspace for parametrized frequency-independent and frequency-dependent boundary conditions. The problem is formulated in the Laplace domain, which ensures the stability of the reduced-order model (ROM). We study the potential of the proposed RBM in terms of computational efficiency, accuracy, and storage requirements, and we show that the RBM leads to 100-fold speedups for a two-dimensional case and 1000-fold speedups for a three-dimensional case with an upper frequency of 2 and 1 kHz, respectively. While the FOM simulations needed to construct the ROM are expensive, we demonstrate that the ROM has the potential of being 3 orders of magnitude faster than the FOM when four different boundary conditions are simulated per room surface. © *2022 Acoustical Society of America*. https://doi.org/10.1121/10.0012696

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[Editor: Steffen Marburg] Pages: 851–865

I. INTRODUCTION

Room acoustic simulations are used for various purposes, e.g., building design, music, hearing research, entertainment, and virtual reality (VR). Historically, these simulations have mostly been carried out by means of geometrical acoustics (GA) methods,[1,2] such as ray tracing, which approximate the sound propagation to ensure a manageable computational cost but fail to simulate the correct wave nature of sound, resulting in diffraction and interference at low frequencies. The geometric approximation is known to cause a considerable degradation of the simulation accuracy in many cases.[3] Another approach is to numerically solve the governing equations, i.e., the wave equation in the time domain (TD) or the Helmholtz equation in the frequency domain, using numerical discretization methods. Different numerical methods have been applied to the room acoustics problem in the past, e.g., the finite element method (FEM),[4,5] the spectral element method (SEM),[6] the finite difference method (FDTD),[7] the boundary element method (BEM),[8] and the discontinuous Galerkin finite element method (DG-FEM).[9] These numerical methods are, in principle, more accurate than GA, as no approximation on the wave propagation is introduced except for numerical errors by the discretization.

The main drawback of a wave-based modeling approach is the high computational cost, especially when modeling large spaces at higher frequencies. This makes it difficult to apply them to scenarios where the full audible spectrum and large room dimensions must be considered, e.g., simulating a large hall from 20 Hz to 20 kHz. A wave-based simulation of a large hall up to 20 kHz remains very challenging, and the goal of this study is not to propose a methodology that enables this. Instead, we consider the case where the same room is simulated multiple times under varying boundary conditions. This type of use case is very common in, e.g., building design, where different surface materials are tested to identify desired acoustic conditions. Thus, reducing the computation time for the parameterized boundary condition case is of utmost importance for many applications.

We propose a computational framework to reduce the computational cost compared to traditional *full-order* numerical solutions. The framework is based on a reduced basis method (RBM) for the acoustics problem that includes

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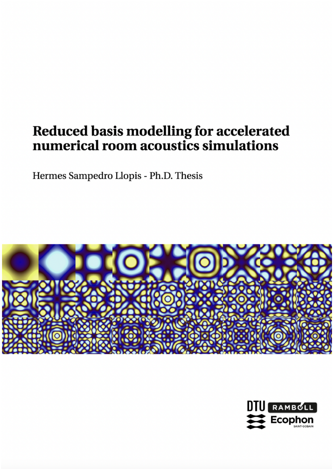

Proof-of-concept: youtube video

On Sustainability in Computing

The carbon footprint of activities across product cycles is of increasing concern and computing has an impact on CO2e measures. For example,

- Carbon footprint of training NLP models
- Carbon Emissions and Large Neural Network Training
- AI transforming financial ecosystem
- The role of artificial intelligence in achieving the Sustainable Development Goals
- The carbon impact of artificial intelligence
- Green AI
- Towards the Systematic Reporting of the Energy and Carbon Footprints of Machine Learning
- The dilemma of digitalization versus energy consumption

Remark, there is two sides of the 'coin' here. One part is the (offline) training part that can be excessively expensive. The other one is the (online) inference part and cost. Thus, it is attractive to build models that can execute a low cost and/or be re-used many times fit for purpose while addressing sustainability aspects as the outcome.

Generative AI for Science - Large Language Models for Programming

HPC wire

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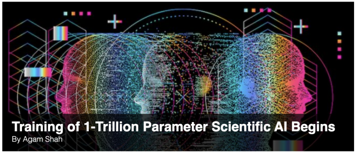


November 13, 2023

A US national lab has started training a massive AI brain that could ultimately become the must-have computing resource for scientific researchers.

Argonne National Laboratory (ANL) is creating a generative AI model called AuroraGPT and is pouring a giant mass of scientific information into creating the brain.

The model is being trained on its Aurora supercomputer, which delivers more than an half an exaflop performance at ANL. The system has Intel's Ponte Vecchio GPUs, which provide the main computing power.

Intel and ANL are partnering with other labs in the US and worldwide to make scientific AI a reality.

"It combines all the text, codes, specific scientific results, papers, into the model that science can use to speed up research," said Ogi Brkic, vice president and general manager for data center and HPC solutions, in a press briefing.

Brkic called the model "ScienceGPT," indicating it will have a chatbot interface, and researchers can submit questions and get responses.

Chatbots could help in a wide range of scientific research, including biology, cancer research, and climate change.

Generative AI for Science - Co-Pilots

DTU Makes artificial intelligence available to students, Feb 1, 2024

If you use large language models (fx. Co-pilots / ChatGPT / Claude / Gemini) in this course, then please state how it was used (e.g. for producing code), and what the outcome of the use. If a model such as Co-pilots / ChatGPT / Claude / Gemini solved the problem for you, please state so and discuss in the reports why this is the correct solution using references to expectations grounded in the theory presented in the course (cf. book/slides).

Feel free to discuss in class how you benefit from using large language models.

DECLARATION OF USE OF GENERATIVE AI

A student using any unacknowledged content generated by artificial intelligence within a summative assessment[2] as though it is their own work constitutes academic misconduct, unless explicitly stated otherwise in the assessment brief. The use of generative AI may lead to unintended plagiarism due to the reproduction of existing sources, the generation of text that closely mirrors copyrighted or previously published material, and the inability to reliably verify the originality or provenance of AI-generated content.

DTU Rules

- DTU Code of honour
- Cheating at exams and other forms of assessment

[2] A summative assessment is an evaluation that measures a learner's achievement at the end of a learning period (such as a course, unit, or module).

DECLARATION OF USE OF GENERATIVE AI

Please include a section in your reporting stating:

DECLARATION OF USE OF GENERATIVE AI

This declaration must be filled out and included as the final page of the document. The questions apply to all parts of the work, including research, project writing, and coding.

- I/we have used generative AI tools: yes/no

If you answered yes, please complete the following sections.

List the generative AI tools you have used:

Describe how the tools were used:

What did you use the tool(s) for?

At what stage(s) of the process did you use the tool(s)?

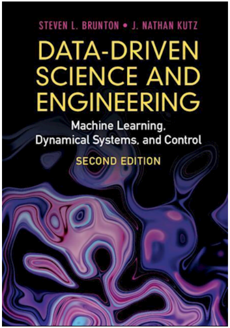
Overview (tentative plan)

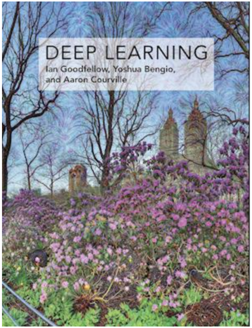
- 01 Introduction : motivation for the use of data-driven methods and scientific machine learning
- 02a Learn from data : singular value decomposition and regression
- 02b A bit about coding practices [Niels]
- 03 Sparse Identification of Nonlinear Dynamics : SInDy, Discovering governing equations from data by sparse identification of nonlinear dynamical systems
- 04 Numerical solution of dynamical systems : finite difference methods for solving boundary value problems and dynamical systems
- 05 Reduced Order Models (ROMs) : reduce dimensionality of high-fidelity models and accelerate time to solution
- 06 Neural Networks and Deep Learning : universal function approximation and dynamic systems modelling
- 07 Physics-Informed Neural Networks : A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations systems
- 08 Neural Operator Learning : a framework for learning the solution operators of parametric PDES
- 09 Independent projects : Applications of techniques

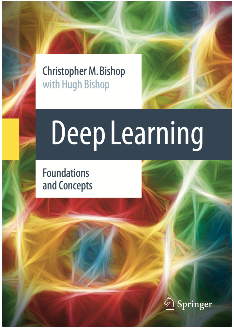
Remark: I allow pursuing independent topics during the course if we agree on content, e.g. exchange exercises with other exercises etc.

Material

Make good use of...







- Book: Steven Brunton & Nathan Kutz (2022) Data-Driven Science and Engineering - Machine Learning, Dynamical Systems and Control, Cambridge.
- Book: Deep Learning (2016).
- Book: Deep Learning - Foundations and Concepts (2024), Bischop & Bishop
- Symbolic manipulation: Mathematica/Maple/Sage.
- Programming environment: Python/Matlab/Jax/PyTorch.
- Slides

Large Language Models for Code Generation

You are permitted to use large language models for code generation in this course.

It is always you responsibility to understand what the code does and test the code to establish that the results are correct in a proper scientific way.

If models such as Github Co-pilot, ChatGPT, Claude, Gemini, etc. has been used, then you MUST state this as a part of your reporting. Describe how your process was with the LLM and how you verified that the code was working through testing etc.

AI Tools

Claude desktop: Claude: `https://claude.ai/login`

Claude Code: Best practices for agentic coding: `https://code.claude.com/docs`

GitHub Co-pilot + VS Code: It is possible to get a student license for Github Co-pilot and this can be used in an extension through VS code through the following installation guide line...

`https://docs.github.com/en/copilot/quickstart`

LM Studio:

LM Studio - Local AI on your computer : `https://lmstudio.ai/`

Ollama: Ollama works with favorite tool and run locally : `https://ollama.com`

How to hand in solutions to exercises / assignments

Throughout the course there will be weekly exercises that focus on doing things hands-on and getting experiences with programming, linking the details in the materials to codes that actually work. The following is to be handed in to count towards assessment of the work

- Short reports that describe the problem and its solution in sufficient detail to understand theory used, methods applied and what results were achieved. Remember to discuss pros/cons. Quality over quantify. Give attention to the methods and recipes used to solve a problem rather than the outcomes alone.
- Zipped well-structured code with reelvant comments that is setup to produce the figures that are presented and discussed in the exercises reports.

For the last approx. 4 week assignment on an agreed topic that meets course objectives, the requirement are

- Short report incl. declaration of AI (cf. above).
- Zipped code (cf. above)
- Poster to be presented for other participants to learn about your study.

All written work count towards final assessment with grade according to the Danish 7-scale.

Scientific Machine Learning : what is new?

Discuss/brain storm [5 mins]: What is really new here in your mind within the emerging area of 'scientific machine learning'?

Scientific Machine Learning : what is new?

What is new?

- Access to HPC, parallel computing
- Improved methods allow learning from data and combine with modelling (fx. SINDY / PINNs / etc.)
- Open source software (fx. PyTorch/Julia/Jax/Etc.)
- Increasing availability and need for utilization of data sources

How is scientific machine learning useful?

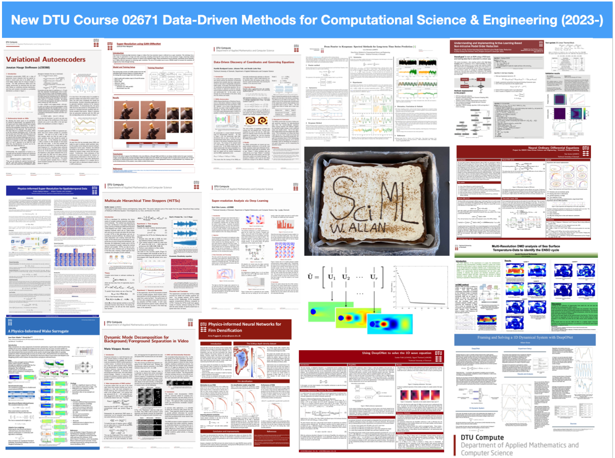
- Learning from data and combine with mathematical-physical modelling (physics-informed modelling / grey box modeling)
- Acceleration (surrogate modelling, reduced order modelling)
- Addressing curse of dimensionality (dimensionality reduction)

For practical applications, we need

- Theory-based approaches for reproducibility, interpretability and robustness
- Ability to compute at increasing scale and modelling fidelities
- Ability to generalise on unseen data
- Ability to interpret outcomes and models obtained using data

02671: Past party poster outcomes...

At the end of the course you are to present a poster with results of a project:



Examples of posters can be found here:
`https://www2.compute.dtu.dk/~apek/ScientificComputingPosters/`