Book of Abstracts

Indo-German Conference on Computational Mathematics

27-30 March 2023

CDS
Department of Computational and Data Sciences

भारतीय विज्ञान संस्थान

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Book of Abstracts

Indo-German Conference
on
Computational Mathematics

IISc Bangalore,
27-30 March 2023.

Foreword

The Indo-German Conference on Computational Mathematics 2023 is a collaborative event organized by the Department of Computational and Data Sciences (CDS) at Indian Institute of Science Bangalore (IISc) and the Interdisciplinary Center for Scientific Computing (IWR) at Heidelberg University, Germany. The conference is part of a four-year joint exchange program on "Hardware-aware algorithms in Scientific Computing" (HAASC), which was established in July 2020 and funded by the University Grants Commission (UGC) in India and the German Academic Exchange Service (DAAD) in Germany. The initiative includes several associated partners, including the Tata Institute of Fundamental Research, Centre for Applicable Mathematics (TIFR-CAM), Bangalore, the Jülich Supercomputing Centre, and NVIDIA India as an industrial partner.

The HAASC program aims to develop new algorithms and implementations that can adapt to the new hardware architectures available in the future, despite the slowdown and eventual end of Moore's law. The main objective of the program is to bring together research activities of the partners on hardware-aware scientific computing, develop young researchers, and initiate long-term collaborative projects in this challenging field.

The Indo-German Conference on Computational Mathematics 2023 is a platform to present and discuss challenges and opportunities in combining process and data-driven modelling. The conference topics include numerical analysis of partial differential equations (PDEs) & stochastic PDEs, physics-informed neural networks, efficient and robust numerical schemes for solving complex problems, optimal control and inverse problems, scalable parallel algorithms, and hardware-aware scientific computing. The conference is partially supported by the KIAC AI-ML centre

The conference has received more than 100 abstracts and will

feature 12 invited talks and 58 contributed talks, including 30 on numerical methods for PDEs, 21 on Scientific Machine Learning, and 7 on High Performance Computing. Among the 100 participants, 16 members are from foreign universities. The conference aims to foster interactions among the Scientific Computing and Machine Learning research communities and provide opportunities for collaboration and networking.

Prof. Peter Bastian
Prof. Sashikumaar Ganesan
Organisers, IGCM 2023

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27th March 2023 (Monday)

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-------- 2.15 PM to 2.30 PM: **Coffee Break** --------

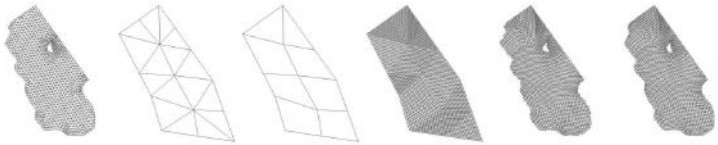
-------- 2.30 PM to 3.00 PM: **Closing Session** --------

Abstracts of Plenary Talks

Performance-optimized discontinuous Galerkin method on CPUs, GPUs, and FPGAs

Vadym Aizinger[1], Sara Faghih-Naini[1], Daniel Zint[2]
[1] University of Bayreuth, Germany
[2] Inria Sophia Antipolis, France

One of the most pressing challenges in creating exascale-ready PDE-simulation software is the difficulty of obtaining reasonable performance without sacrificing portability between hardware platforms. Meeting this challenge requires finding numerical and computational techniques suitable, on the one hand, for very general classes of applications and, on the other, running efficiently on a possibly wide variety of hardware.In our talk, we present a number of recent developments for the discontinuous Galerkin shallow-water model including generation of block-structured meshes for complex ocean domain, quadrature-free integration for non-linear PDE systems and p-adaptive hybrid execution modes. We also discuss the portability issues for CPU, GPU, FPGA, as well as hybrid computing architectures.



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Preconditioning Sparse Matrices with Alternating and Multiplicative Operator Splittings

Christoph Klein[1], Robert Strzodka[2]
[1,2] Institute of Computer Engineering (ZITI), Heidelberg University

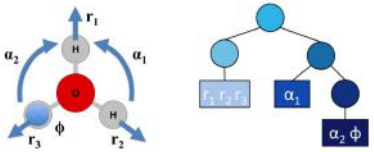
We present an algebraic framework for operator splitting preconditioners for general sparse matrices. The framework leads to four different approaches: two with alternating splittings and two with a multiplicative ansatz. The ansatz generalizes ADI and ILU methods to multiple factors and more general factor form. The factors may be computed directly from the matrix coefficients or adaptively by incomplete sparse inversions.

The special case of tridiagonal splittings is examined in more detail. We decompose the adjacency graph of the sparse matrix into multiple (almost) disjoint linear forests and each linear forest (union of disjoint paths) leads to a tridiagonal splitting. We obtain specialized variants of the four general approaches. Parallel implementations for all steps are provided on a GPU. We demonstrate the effectiveness and efficiency of these preconditioners combined with GMRES on various matrices.

The multiconfiguration time-dependent Hartree approach for quantum dynamics: theory, applications, and perspectives

Oriol Vendrell[1]
[1] Theoretical Chemistry, Institute of Physical Chemistry and Interdisciplinary Center for Scientific Computing, Heidelberg University

The multiconfiguration time-dependent Hartree (MCTDH) method is a powerful and a general algorithm for the efficient solution of the time-dependent Schrödinger equation, the computation of nuclear quantum dynamics. Its multilayer (ML-MCTDH) generalization, where the wavefunction Ansatz takes the form of a multilayered tensor tree, paves the way towards the accurate treatment of high-dimensional and highly correlated quantum mechanical systems. In this contribution, I introduce the theory behind the (ML-)MCTDH approach and its numerical implementation in the Heidelberg MCTDH package. I discuss some technical developments in our research group that have enabled recent applications to the spectroscopy and dynamics of complex quantum systems, both in the areas of nuclear and electronic quantum dynamics, and I close with some perspectives for further developments and standing challenges ahead.



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Neural networks with physical constraints, domain decomposition-based training strategies,and model order reduction

Alexander Heinlein[1]
[1] Delft Institute of Applied Mathematics, Delft University of Technology

Scientific machine learning (SciML) is a rapidly evolving field of research that combines techniques from scientific computing and machine learning. A major branch of SciML is the approximation of the solutions of partial differential equations (PDEs) using neural networks. The network models be can trained in a data-driven and/or physics-informed way, that is, using reference data (from simulations or measurements) or a loss function based on the PDE, respectively.

In physics-informed neural networks (PINNs) [4], simple feedforward neural networks are employed to discretize the PDEs, and a single network is trained to approximate the solution of one specific boundary value problem. The loss function may include a combination of data and the residual of the PDE. Chal lenging applications, such as multiscale problems, require neural networks with high capacity, and the training is often not robust and may take large iteration counts. Therefore, in the first part of the talk, domain decomposition-based training strategies improving the training performance using the finite basis physics-informed neural network (FBPINN) approach [3, 1] will be discussed.

In the second part of the talk, surrogate models for computational fluid dynamics (CFD) simulations based on convolutional neural networks (CNNs) [2] will be discussed. In particular, the network is trained to approximate a solution operator, taking a representation of the geometry as input and the solution field(s) as output. In contrast to the classical PINN approach, a single network is trained to approximate a variety of boundary value problems. This makes the approach potentially very efficient. As in the PINN approach, data

as well as PDE may be used in the loss function for training the network.

References

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Approximation Rates for Neural Operators

Jakob Zech[1]
[1] Heidelberg University

In this talk, we will discuss the use of neural network surrogates as approximations for smooth maps between infinite-dimensional Hilbert spaces. These surrogates have a wide range of applications and can be used in uncertainty quantification and parameter estimation problems in fields such as classical mechanics, fluid mechanics, electrodynamics, earth sciences etc. In this case, the operator input represents the problem configuration and models initial conditions, material properties, forcing terms and/or the domain of a partial differential equation (PDE) describing the underlying physics. The output of the operator is the corresponding PDE solution.

We will also present an alternative approach using interpolation, which allows for deterministic construction and eliminates the need for training the network weights. In both cases, algebraic and dimension-independent convergence rates are obtained.

Joint work with: Lukas Herrmann, Christoph Schwab

References

[1] Lukas Herrmann, Christoph Schwab and Jakob Zech. Neural and gpc operator surrogates: construction and expression rate bounds. arXiv:2207.04950, 2022.

Large scale PDE constrained optimization of cardiac defibrillation

Nagaiah Chamakuri
Indian Institutes of Science Education and Research, Trivandrum
(IISER TVM)

In this talk, we present a feasible study of optimal control techniques for cardiac defibrillation based on the bidomain equations posed on a rabbit ventricle geometry. The bidomain model consists of a system of elliptic partial differential equations coupled with a non-linear parabolic equation of reaction-diffusion type, where the reaction term, modeling ionic transport, is described by a set of ordinary differential equations. Since ODEs describe the ionic currents in the tissue, the PDE part dominates the solving effort. Thus, it is not clear if commonly used splitting methods can outperform a coupled approach by maintaining good accuracy. In the first part, the results will be presented based on a comparison of the coupled solver approach with commonly used splitting methods to solve more sophisticated physiological models. In this regard, the novel memory-efficient computational technique will be demonstrated to solve the coupled systems of equations. In the second part, the optimal control approach for successful cardiac defibrillation will be shown which is based on minimizing a properly chosen cost functional depending on the extracellular current as input at the boundary of the torso domain. This can be determined in such a way that wavefronts of transmembrane voltage in cardiac tissue is smoothed optimally.

Domain Specific Languages for Machine Learning and HPC: Challenges, Chances, and Tools

Artur Andrzejak[1], Diego Elias Costa, Paul Harris, Kevin Kiefer, Oliver Wenz
Heidelberg University, Institute of Computer Science and IWR

Domain-Specific Languages (DSLs) are programming languages which provide abstractions that are closely aligned with a specific domain, for example machine learning. They have proved useful in a variety of scenarios, from scientific computing (see Matlab) to databases (see SQL), and are recently becoming increasingly popular in the business domain as a part of low-code approaches. However, DSLs feature some non-trivial shortcomings. First, inherent limitations of the expressiveness of a particular DSL can increase overall project complexity due to need to integrate DSL and general-purpose code or due work-arounds. This problem is more severe in context of complex code or performance-critical code, as in HPC and machine learning. Second, designing, implementing and maintaining DSLs incurs a significant effort which limits their utility in context of smaller projects or frequently updated frameworks such as in data science. In this talk we describe two projects which attempt to address these challenges.

A first project proposes a tool for constructing DSLs for simplifying working with complex C++ code in context of performance optimization. Our DSL tool can be for example used to generate C++ function template instances for a large number of types and parameter combinations. The challenge of integrating DSL and the host code is approached by embedding DSL elements in C++ comments, and the ability to freely combine manually written and generated C++ code. We also provide a tooling based on CMake which simplifies the full stack build process. This approach uses internally the Python-based textX meta-programming library and can be extended to other DSL elements with a moderate effort.

The second project takes a more radical approach to the above challenges by multiple features incorporated in the tool NLDSL (https://bit.ly/nldsl-hd). We address the DSL integration problem by offering DSL expansion (i.e. target code generation) during the editing process and by embedding DSL in the comments. Simultaneously we support the developers in terms of the DSL syntax via intelligent code completions and in terms of the semantics via context-sensitive help. The challenge of facilitating DSL development and maintenance is targeted by constraining the structure of possible DSLs to chains of operations, which greatly simplifies implementation of DSL to target-code translation. We further simplify DSL creation by offering tools for template-based DSL specification and by wizards for generating DSLs from DSL/target-code examples.

NLDSL has been used to implement and deploy multiple DSLs in the domain of data science. The first and most popular DSLs cover processing and analysis of data frames/tables and allows a spectrum of queries similar to a relational algebra. Furthermore, by creating syntactically identical DSLs for Python/Pandas and for Apache PySpark we support porting the code between these libraries. Further DSLs for this framework cover deep learning frameworks PyTorch and TensorFlow, plotting libraries Matplotlib and Seaborn, and support templated data analysis studies in R. Our tool is publicly available as an extension for popular IDE Visual Studio Code at https://bit.ly/nldsl-vscode. Up to date it has been installed by more than 10,000 developers.

An interesting extension would be developing DSLs for scientific computing and HPC, in particular for C++ and MPI code generation. We will discuss these options with IGCM participants in order to explore future cooperation.

Exploring the Frontiers of Scientific Machine Learning

Subodh Madhav Joshi
Shell, India

Scientific Machine Learning has made great strides in the past decade, particularly with the advent of Physics-informed Neural Networks. This has revolutionized the fields of engineering and scientific simulations. During this talk, I will discuss two main concepts in Scientific Machine Learning: Physics-informed Neural Networks and the 'operator learning' paradigm. The former involves training artificial neural networks to solve differential equations that describe physical processes. The latter, specifically the DeepONet model, involves learning mathematical operators, including complex partial differential equations, by observing function-to-function mappings. Join me as we examine the "what, why, and how"of these innovative ideas in Scientific Machine Learning.

Computational science and digital innovation for multi-physics and multi-scale energy systems modelling

Abhineet Gupta, Suranjan Sarkar, Suchismita Sanyal
Shell, India

Computational science augments the research methods by accelerating and guiding experimental work to provide physical insights which otherwise may not be possible by traditional routes. One of the most striking aspects of computational science projects is their breadth of scale that covers the interactions at the atomic and molecular levels to the design of reactors in industrial plants. By combining data-based models with physics/chemistry based computational models, we augment the power of both by integrating the speed and agility of AI with the interpretability and explainability of computational science.

System level modelling is one of the Shell's key capabilities to improve energy productivity while reducing greenhouse gas emissions. A deep physical understanding energy systems is critical to systematically develop accurate models for prediction, optimization and design of such systems at relevant scales. We primarily focus on three levers for decarbonizing our operations: improving energy efficiency, increasing the share of lower carbon energy sources, and deploying carbon sink technologies such as carbon capture, utilisation and storage.

In this talk, we will provide several examples where novel computational science techniques combined with data are being for used for multi-physics multi-scale energy systems modelling at Shell. Some of the application areas include energy systems optimization, windfarm modelling, CO2 sequestration and hydrogen transport, optimising fuel formulation, thermal runaway in battery packs, design of electrified crackers for chemicals production and modelling decarbonisation

pathways for hard-to-abate industries. We would also share our perspective on some of the emerging challenges and discuss the potential ways forward.

Multilevel spectral domain decomposition preconditioners

Peter Bastian
University of Heidelberg, Germany

Multilevel spectral domain decomposition methods are provably robust and efficient preconditioners as well as multiscale methods for solving heterogeneous elliptic partial differential equations. With respect to high performance computing they offer plenty of opportunities for parallel scalability and achieving high performance. In this talk we focus on the setup phase where multiple generalized eigenvalue problems need to be solved in parallel and randomized eigensolvers offer opportunities for increasing arithmetic intensity and using vectorization.

Generating metadata for the torso and tail of OTT videos using Machine Learning

Bharath Mohan
Sensara Technologies, Bangalore, India

Metadata (specially visually enriched metadata) is not just a necessity - but is a key differentiator in ensuring content is discovered. Entertainment video's head, torso and tail have had differential treatment to metadata. While movies like Interstellar have the most enriched metadata, the torso and tail get secondary treatment. This leads to a "rich become richer, poor stay poor" phenomenon in video too. Equity in discovery is directly related to the ability to generate metadata for the breadth of video. We present our work in automated metadata creation that takes a hybrid approach. A bottom-up video reasoning system generates several structural artifacts including poster art, trailers, cast information, promotions, brands, title credits, moods, and predict genre automatically. All this is fed into a graph database with global knowledge of TV, and from there on curated by metadata professionals. In total, we have an AI-assisted, metrics driven process and discipline to creation and maintenance of metadata. We have achieved early commercial success in demonstrating efficiency, SLAs and low costs - all extremely important in taking the metadata vision to reality.

Computational Engineering for High Throughput Scientific Computing

Chiranjib Sur
Shell, India

Computational science is about solving scientific problems numerically which is a very well-established field on its own. With the rapid growth in the field of computer science and related computing technology, there is a growing need to bring practises from engineering analysis and design into the field of scientific simulation. The primary driver behind the need is to develop a scalable scientific simulation software with which one can target for higher throughput, not just high performance. This is exactly why the field like computational engineering (CE) has emerged. CE is that area where computational mathematics, domain specific science, core computer science and software engineering converge.

In this presentation, we will be explaining different corners and the rationale behind developing the expertise in such a field with some real-life examples covering all the areas which are the foundation of computational engineering.

Abstracts of Paper Presentations

Numerical Methods for PDEs

Sum-of-products form of the molecular electronic Hamiltonian and its application within the MCTDH method

Sudip Sasmal[1], Oriol Vendrell[1,2]
[1] Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuneheimer Feld 229, 69120 Heidelberg, Germany
[1,2] Interdisciplinary Center for Scientific Computing, Universität Heidelberg, Im Neuneheimer Feld 205, 69120 Heidelberg, Germany

A first principles quantum formalism to describe the non-adiabatic dynamics of electrons and nuclei based on a second quantization representation (SQR) of the electronic motion combined with the usual representation of the nuclear coordinates is introduced. This procedure circumvents the introduction of potential energy surfaces and non-adiabatic couplings, providing an alternative to the Born–Oppenheimer approximation. However, the major problem of this method applied to ab initio studies of large molecular systems remains the enormous size of the electronic SQR Hamiltonian, whose number of terms increases with the fourth power of the number of spin-orbitals. We introduce three different approaches to represent the second-quantized electronic Hamiltonian in a sum-of-products form. These procedures aim at mitigating the quartic scaling of the number of terms in the Hamiltonian with respect to the number of spin orbitals, and thus enable applications to larger molecular systems. Here we describe the application of these approaches within the multi-configuration time-dependent Hartree framework.

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Sparse optimal control of the Monodomain model

Maria Robert

The work focuses on the optimal control problem subject to the monodomain equations. Monodomain equations are coupled equations which model the electrophysiological wave propagation of the action potential in the myocardium. They consist of a parabolic PDE which is of reaction-diffusion type and a set of ODEs. The objective of the optimal control problem contains the L1 - norm of the control, which produces sparsity in the solution. The existence of the optimal control, differentiability of the control-to-state operator, and the necessary condition for optimality were derived. Sparsity properties are analyzed for different regularizing parameters. Numerical solution of the problem is obtained using active sets.

Keywords: Reaction-diffusion equations, monodomain model, sparse optimal control, control constraints, primal-dual method, active sets

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A novel numeric scheme to study elastodynamic fracture at the interface between a layer and a half-plane

Avinash Gupta[1], Ranjith Kunnath[1]
[1] Mahindra University École Centrale School of Engineering, Hyderabad 500043, Telangana

We present a novel numerical scheme for 2D dynamic antiplane fracture problems at the interface between an elastic layer and an elastic half-plane. The scheme is based on the Fourier representation of the boundary integral equation method (BIEM), which relates the field quantities at the interface, i.e., the traction component of stress and resulting displacement discontinuity along the interface. The primary advantage of the current scheme is its numerical efficiency due to evaluating field quantities along the interface only, rather than computing them in the entire domain (i.e., an overall reduction in dimension by one). The BIEM involves the evaluation of a space-time convolution of the traction component along the interface. The spatial convolution is performed in the spectral domain, resulting in greater computational efficiency. The transformation between the spatial domain and the spectral domain is performed by the FFT (Fast Fourier Transform) algorithm. Since the formulation is spectral in nature, it is suited to parallel computing. The proposed scheme is illustrated by simulating frictional rupture propagation along the interface. Numerical results demonstrate types of rupture modes of frictional sliding, i.e., crack-like and pulse-like rupture propagation, depending on the nature of the prestress.

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A scalable asynchronous computing approach for discontinuous-Galerkin method based PDE solvers

Shubham K. Goswami, Konduri Aditya
FLAME Laboratory, Department of Computational and Data Sciences, Indian Institute of Science, Bengaluru, India

The discontinuous-Galerkin (DG) method has received a lot of interest in developing partial differential equation (PDE) solvers due to its ability to deliver high-order accurate solutions in complex geometries, especially for problems with hyperbolic nature. The method offers high arithmetic intensity and avoids global linear solves in an explicit formulation, and therefore, is suitable for high-performance computing platforms. However, massively parallel simulations based on the DG method display poor scalability of solvers at extreme scales. This is mainly attributed to data communication and synchronization between various processing elements (PEs). Recently, an asynchronous computing approach based on finite differences was proposed that relaxes communication/synchronization at a mathematical level. This approach improves the scalability of PDE solvers by allowing computations to continue independent of the communication status between PEs. In this work, we extend asynchronous computing to the DG method to improve its scalability at extreme scales. We investigate the numerical properties of standard DG methods under relaxed communication synchronization and show that their accuracy drops to the first order. Next, we develop new asynchrony-tolerant fluxes that produce solutions with any arbitrary order of accuracy. To demonstrate the accuracy of the asynchronous DG method, results from simulations of one-dimensional linear and nonlinear problems will be presented.

Keywords: Asynchronous computing, Partial differential equations, Massive computations, Discontinuous-Galerkin method

An computationally efficient numerical method based on domain decomposition approach for semilinear coupled system of singularly perturbed parabolic problems

Aakansha, Sunil Kumar
Department of Mathematical Sciences, Indian Institute of Technology (BHU) Varanasi India, 221005.

This work analyses a semilinear coupled system of singularly perturbed parabolic problems where the different magnitude parameters are multiplied with the diffusion term. A overlapping domain decomposition method is proposed to solve this system numerically. On each subdomain a classical central difference scheme in space and an Euler scheme along with splitting of components technique in time are employed. Then, we introduce an iterative process to solve the semilinear coupled system where the Dirichlet boundaries are used to exchange the information between the subdomains. The numerical schemes are proved to be parameter uniforms by including some auxiliary problems. Further, by establishing the discrete maximum principle we calculate the uniform error bounds and proved that the schemes are almost second order convergent in spatial direction and one in time. To support the theoretical findings we include the numerical results. Moreover, to show the efficiency of the proposed methods we compare the CPU time (in seconds) for the proposed methods and the classical Euler method.

An efficient numerical method based on Lucas polynomials to solve multi-dimensional stochastic Itô-Volterra integral equations

P. K. Singh, S. Saha Ray
Department of Mathematics, National Institute of Technology Rourkela, Rourkela-769008, India

In this work, the operational matrix method relying on Lucas polynomial has been investigated to find the solution of multi-dimensional stochastic Itô- Volterra integral equation. For that purpose, the properties of the Lucas polynomial and operational matrices have been investigated. Using functions approximations and operational matrices based on the Lucas polynomial along with collocation points, the multi-dimensional stochastic Itô-Volterra integral equation is converted into a linear or nonlinear system of algebraic equations. Numerical examples are examined to show their computational efficiency and accuracy.

Keywords: Multi-dimensional stochastic Itô -Volterra integral equation; Lucas operational matrix method; Lucas polynomial; Itô integral

Longwave modelling of thin film flow of a generalized second-grade fluid down a slanted plate

MAHESH T

The free surface dynamics of a thin film of a generalized second-grade fluid flowing down a slanted plate subjected to the action of gravity have been studied. A nonlinear evolution equation for the dynamics of the thin liquid film is derived using the long-wavelength approximation. The model allows to investigate the impact of fluid rheology and geometrical parameters on the thin film's height. The nonlinear dynamics equation is implicitly approximated on a uniform grid by applying the finite volume discretization method, which uses upwind discretization of the flux function and first-order discretization of the time differential term. The investigation reveals that the free surface deformation trends are similar for the Newtonian and non-Newtonian fluids but the non-Newtonian fluid properties substantially influenced the size and shape of the deformation. It is also found that the shear-thinning fluid moves faster down to the plate compared to the Newtonian and shear-thickening fluid.

Keywords: Thin liquid film, Generalized second-grade fluid, Finite volume method, Long-wavelength approximation.

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Bound on numerical rank of kernel functions in d dimensions

Ritesh Khan, V A Kandappan, Sivaram Ambikasaran

We study the rank of sub-matrices arising out of kernel functions, $F(\mathbf{x}, \mathbf{y}) \colon \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$, where $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ with $F(\mathbf{x}, \mathbf{y})$ is smooth everywhere except along the line $\mathbf{y} = \mathbf{x}$. Such kernel functions are frequently encountered in a wide range of applications such as N-body problems, Green's functions, integral equations [1, 4], electromagnetic scattering [6], Gaussian process regression [5], machine learning [2], radial basis function interpolation [3], kernel density estimation [7], etc. One of the challenges in dealing with these kernel functions is that the corresponding matrix associated with these kernels is large and dense and thereby, the computational cost of matrix operations is high. We prove a new theorem bounding the numerical rank of sub-matrices arising out of these kernel functions. Under reasonably mild assumptions, we prove that the rank of certain sub-matrices is rank-deficient in finite precision. This rank depends on the dimension of the ambient space and also on the type of interaction between the hyper-cubes containing the corresponding set of particles. This rank structure can be leveraged to reduce the computational cost of certain matrix operations such as matrix-vector products, solving linear systems, etc. We also present numerical results on the growth of rank of certain sub-matrices in 1D, 2D, 3D and 4D, which, not surprisingly, agrees with the theoretical results.

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An efficient operational matrices approach for solving integro-differential equations with weakly singular kernel of variable order.

Poonam Yadav[1], Vineet Kumar Singha[1]
[1] Department of Mathematical Sciences, Indian Institute of Technology (Banaras Hindu University), Varanasi, India.

The main purpose of this article is to present a numerical technique based on two basis functions namely Legendre wavelet (LW) and Interpolating scaling function (ISF) to deal with the variable-order (VO) integro-differential equation with the weakly singular kernel. First, we derive the operational matrices of Legendre wavelet and Interpolating scaling function. Moreover, we utilized the resulting operational matrices of LW and ISF to convert the proposed model into a system of algebraic equation along with the collocation method. We have also established error estimation and theoretical convergence analysis of the proposed schemes. Finally, the included experiments with the support of tables and graphs clearly show the reliability and computational efficiency of the formulated technique.

Keywords: Time-fractional derivative in Caputo sense, Legendre wavelet, Interpolating polynomial, Operational matrices, Collocation method, Theoretical convergence and Error estimation.

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Numerical investigation based on wavelet computational method to solve distributed order fractional financial mathematical model

Yashveer Kumar, Vineet Kumar Singh
Indian Institute of Technology (Banaras Hindu University), Varanasi, India

In this work, we have discussed the approximate solution of distributed order fractional mathematical model using a wavelet-based operational matrix. First, we construct the operational matrices for distributed order fractional derivative and integer order fractional derivative. After the construction of operational matrices, we apply the standard tau method and collocation points to convert the original problem into a system of linear algebraic equations. We obtained the approximate solution after solving the system of linear algebraic equations. For robustness and validation of the proposed method, we solve some test examples with error bounds.

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Generalization of Numerical Approaches for Fractional-order Differential Equations: A Review

Zaffar Mehdi Dar[1], Chandru Muthusamy[1], Sundararajan Natarajan[2], Arrutselvi Mouralidaran[2]

[1] Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India

[2] Department of Mechanical Engineering, Indian Institute of Technology, Madras-600036,Tamil Nadu, India

With the development of fractional-order models in various branches of science and engineering applications, such as diffusion, electrodynamics, control theory, structural engineering and biophysics, the researchers and scientists need an advanced and efficient analytical and numerical methods to solve these models. This paper provides a number of such choices of generalized analytical and numerical approaches to solve different kinds of fractional models. The existing developments in every generalized method presented has been provided and then efficiency and application of each model will help us to choose among these choices. In addition, an introduction of a very recent rigorous numerical approach namely Virtual Element Method (VEM), introduced and implemented in, [3, 2]. As, VEM has helped us with the complex geometries while solving partial differential equations of integer-order, the same concepts have been extended, so we can provide a solution of complex geometries of discretization in fractional partial differential equations, which has been presented here, where weak formulation, discrete form and stiffness matrix for fractional Laplacian model [1], given as:

$$(-\Delta)^s u = f \text{ in } \Omega, \text{ with } u = 0 \text{ on } \partial\Omega$$

where Ω is a domain, s is fractional order, has been produced. A numerical experiment for a fractional Poisson problem is also presented, which shows the efficiency of the method. As a result, this

method provides an efficient alternative choice when dealing with the complex geometries of finite element approximations. The goal is to provide with an alternative choice of methods to solve the growing fractional-order models in vast areas of Applied Sciences and Engineering.

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A hierarchy identification algorithm for translation of high-level models to low-levels models

Darpan Krishnakumar Shukla[1]
[1] MONK9 TECH PRIVATE LIMITED, Rajkot - 360005, Gujarat, India

Different system representation schemes can be divided into two categories, high-level models or low-level models. High-level models are considered to have the system representation close to the system while the system representation by low-level models can be considered to be far from the system. See the figure for pictorial description. Translation of the high-level model to low-level model would be useful in terms of user-friendly modeling feature provided by the high-level modeling schemes and mathematical foundations provided by the low-level modeling schemes. In this paper, a hierarchy identification algorithm is proposed to achieve the translation of one high-level model to a low-level model. This algorithm takes as input the high-level model in the form of a network. The steps of the hierarchy identification algorithm include identification of series connections, and parallel connections. This identified hierarchy is collapsed in series and in parallel direction. These two steps of identification and collapsing of hierarchies are performed iteratively till the complete collapse of the system. This algorithm is validated by a reliability application of a high-level and a low-level reliability modeling method. A high-level modeling method, smart component method (SCM), is considered that allows high-fidelity modeling of complex systems. A low-level modeling method, Petri Net (PN), is considered as target low-level model generation

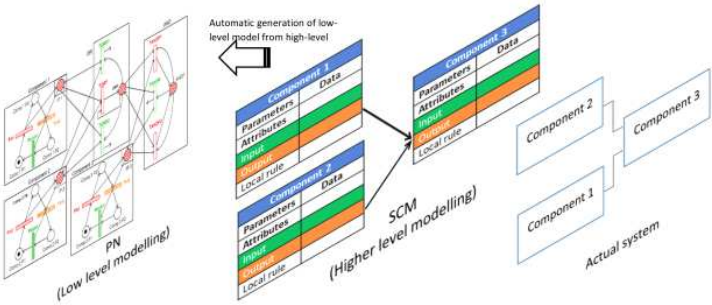

Fig. Illustration of the use of hierarchical identification algorithm. Smart component method as higher level model is automatically converted into its equivalent low-level model

A posteriori error estimation and dynamic adaptivity of a multi-scale cancer invasion model

Nishant Ranwan[1], Gopika P B[1], Nagaiah Chamakuri[2]

In this work, we analyze the residual-based a posteriori error estimation of the multi-scale cancer invasion model, which is a system of three non-stationary reaction-diffusion equations. We present the numerical results of a study on a posteriori error control strategies for FEM approximations of the model. In this paper, we derive a residual type error estimator for the cancer invasion model and illustrate its practical performance on a series of computational tests in three-dimensional spaces. We show that the error estimator is reliable and efficient with respect to the small perturbation parameters in the model.

A new two-level cubic spline scheme for the solution of a class of fourth-order nonlinear parabolic partial differential equations

Naina Sharma[1], Dr. Sachin Sharma[1]
[1] Netaji Subhas University of Technology, New Delhi, 110078

Fourth-order singular partial differential equations (PDEs) find application in a wide range of physical problems and are crucial. Owning to their vast importance, they are a point of interest for mathematicians and physicists. The closed-form solutions of fourth-order PDEs aid to determine the quali-tative behaviour of natural processes and physical phenomena. Solving PDEs to determine these solutions isn't possible in all cases unless they are linear or quasi-linear in nature. In other cases, approximate solutions are derived by constructing and using various numerical methods.

In the proposed work, a novel two-level implicit cubic spline scheme is derived at a uniform grid to solve a particular class of fourth-order time-dependent non-linear partial differential equations prescribed with initial and natural boundary conditions. Here, the proposed scheme is based on half-step discretization which includes a total of three-grid points: two half-step points $x_{l1/2}$ and a central point x_l. Using the properties of cubic spline equation and numerical approximations a fourth-order accurate implicit cubic spline scheme is developed. For the simplicity of the derived scheme, the original problem was transformed in a coupled system of two second-order partial differential equations along with initial and boundary conditions.

Further, the stability analysis of the proposed method is done for a class of fourth-order partial differential equations which is unconditionally stable using the characteristic equation. The proposed finite difference scheme is directly applicable to fourth-order singular equations whereas the method discussed in past studies involves a

special technique to tackle the singular points in the singular problem which involves a lot of complexity in the method. Also, the unconditional stability of the two-level method is an asset for solving singular problems with large time intervals. Additionally, the computational results obtained for the proposed work have been found to be better in comparison to the results of the known methodologies and have been implemented on various real-world problems.

Keywords: Finite Difference Method, Singular partial differential equation, Uniform Mesh, Half-step Discretization

Convective Stability In Modulated Non-Newtonian Fluid Filled Porous System

M . Meenasaranya[1], S. Saravanan[2]

[1] Assistant Professor, PSG College of Arts & Science, Coimbatore – 641 014, Tamil Nadu

[2] Professor and Head, Bharathiar University, Coimbatore – 641 046, Tamil Nadu

A three dimensional infinite horizontal non-newtonian fluid saturated porous system heated from below is considered. The system is subjected to gravity as well as thermal modulation. The Brinkman model and Boussinesq approximation are assumed to govern the fluid flow. The modulation and couple stress effects in the considered system has been determined using Energy method. The resulting Euler-Lagrange equations are solved using higher order Galerkin method. The increase in couple stress parameter is found to expand the stability region and decrease the value of critical wave number. An increase in the amplitude reduces the stability region for both thermal and gravity modulated systems. It has been found that the stabilisation or destabilisation of the system can be achieved by adjusting the values of modulated frequency and amplitude in appropriate form

L3 approximation of the Caputo fractional derivative and its applications

Nikhil Srivastava[1], Vineet Kumar Singh[1]
[1] Indian Institute of Technology (BHU) Varanasi-221005

In this talk, we will discuss about a novel L3 approximation of the Caputo fractional derivative of order $\alpha \in (1, 2)$. We have applied the Lagrange's cubic interpolating polynomial in the subinterval $[t_j, t_{j+1}]$ for $2 \leq j \leq k-1$ and quadratic interpolation in the first subinterval $[t_0, t_1]$ to develop this approximation. The L3 approximation is second order accurate and can be applicable to solve many fractional order partial differential equation involving Caputo fractional derivative of order $\alpha \in (1, 2)$. We have proposed a difference scheme to find the numerical solution of time-fractional wave equation. The difference scheme is also second order in time and space for all α. The approximation is validated on several test problem and a comparative study with the earlier existing scheme [2] is also provided the to show the effectiveness and accuracy of the proposed scheme.

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An efficient meshfree numerical technique to solve fractional Oskolkov-Benjamin-Bona-Mahony-Burgers equation describing propagation of long surface waves

B Sagar[1], S. Saha Ray[1]
[1] Department of Mathematics, National Institute of Technology Rourkela, Rourkela-769008, India

In this work, an efficient meshfree numerical scheme to solve the time-fractional Oskolkov-Benjamin-Bona-Mahony-Burgers equation has been proposed. This equation able to describe many nonlinear phenomena such as analysis of the long-wavelength surface waves in liquids, acoustic-gravity waves in compressible fluids and hydromagnetic waves in cold plasma. The proposed numerical scheme is based on finite difference and Kansa-radial basis function (Kansa-RBF) collocation approach. Firstly, the finite difference scheme has been used for temporal discretization and subsequently, the Kansa-RBF method is utilized for spatial discretization. The stability and convergence of the proposed numerical scheme are also demonstrated. Also, the Kudryashov technique has been used to obtain the soliton solutions for comparison with the numerical results. Finally, numerical simulations are performed to confirm the applicability and accuracy of the proposed method.

Keywords: Meshfree numerical scheme, Caputo fractional derivative, RBF method, Multiquadric

Adomian decomposition and homotopy perturbation method for the solution of time fractional partial integro-differential equations

A. Panda[1], S. Santra[1], J. Mohapatra[2]

The work deals with two different numerical methods to solve a time fractional partial integro-differential equation. The fractional derivatives are defined here in Caputo sense and the intgral considered is of Volterra type. The model problem is solved using the Adomian decomposition method [1] and homo-topy perturbation method [2]. Both the methods are effective in solving an extensive class of partial differential equations, fractional differential equations, and partial integro differential equations using the Adomian polynomials for treating the nonlinear operators and with the construction of perturbation equation by homotopy in topology. One may see [3] and references therein. Moreover, this study shows the uniqueness of the solution and proves the convergence analysis of the methods. Numerical evidences are illustrated in support of the theoretical analysis using figures and tabular data.

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Error based time stepping for Lax-Wendroff Flux Reconstruction

Arpit Babbar[1], Praveen Chandrashekar[2],
[1] Tata Institute of Fundamental Research Centre For Applicable Mathematics , India

The Lax-Wendroff method is a single step method for evolving time depen dent solutions governed by partial differential equations, in contrast to Runge Kutta methods that need multiple stages per time step. In [1], the authors presented a flux reconstruction version of the method in combination with a Jacobian-free Lax-Wendroff procedure that is applicable to general hyperbolic conservation laws with a special focus on construction of numerical flux to en hance Fourier CFL numbers and accuracy.

In this work, we present an error-based time step computation algorithm for the scheme in [1]. This algorithm has several benefits. First, it eliminates the need for manual time step size selection. Second, the error-based adaptive time stepping can run on larger time steps than the CFL restriction and decrease them as needed. Third, it can be applied to curvilinear meshes and viscous problems, where standard Fourier analysis may not be applicable. We demon strate the benefits of our proposed algorithm through numerical experiments of compressible Euler equations on curved meshes and Navier-Stokes equations. In the literature, error-based methods are available for Runge-Kutta schemes which have an embedded lower-order method. We present a novel approach to apply those ideas to Lax-Wendroff schemes without any overhead. To the best of our knowledge, this is the first error-based time stepping scheme for a single-step method.

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Multicomponent Multiphase Flow in Porous Media: Managing Phase Disappearance with Complementarity Constraints

Michal Toth[1], Peter Bastian[2],
[1] Heidelberg University

We investigate multicomponent multiphase transport in the porous medium. We model two phases liquid and gas, and several components that are present in both phases. We start with two components water and carbon dioxide, and later add additional components for the reactive transport model. Problem setting leads to situations when only one phase is present, with a possibility of having some part of the domain with only liquid, another with only gas phase, and the rest with both. In such situations, several physical quantities in mass balance equations are meaningless resp. undefined. For example, the variable representing water molar fraction when the liquid phase disappears. The solver has to be able to handle such degenerate states.

The presented solution is the use of complementarity constraints. They in troduce branching on the equation level and the following discretization is standard. This makes them more straightforward than the variable switching or the equivalent primal-dual active set strategy. The cost for using complementarity constraints is the loss of regularity. Nevertheless, they fall into the category of functions for which the semismooth Newton method keeps the local quadratic convergence

A Posteriori Error Estimation and Adaptivity for Model Order Reduction of Large-Scale Systems

Sridhar Chellappa[1], Lihong Feng[2], Peter Benner[3]
[1] Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, 39106, Magdeburg, Germany

Model order reduction (MOR) has become a popular tool to speedup the repeated simulations of large scale systems that arise from the numerical discretization of partial differential equations [1]. To address the question of reliability of the resulting reduced order models (ROMs), it is critical to quantify the approximation error resulting from MOR. In this talk, we discuss our recent work on a posteriori error estimators for parametric steady/time-dependent systems. We first detail an inf-sup-constant-free error state error estimator for linear systems and then discuss a dual-based output error estimator for nonlinear systems. Using the error estimators, we perform adaptive model order reduction. Our adaptive approach is aimed at (a) bringing down the significant computational cost often associated with generating ROMs and (b) minimizing the user interference in obtaining efficient ROMs. We consider adaptive basis enrich ment [2, 3] and adaptive parameter sampling [4, 5]. We illustrate the benefits of the proposed approach through numerical examples arising from applications such as process engineering, computational elec tromagnetics and cardiac electrophysiology. Finally, we discuss future research avenues that incorporate machine-learning techniques for adaptive model order reduction.

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Data assimilation finite element method for the linearized Navier-Stokes equations with higher order polynomial approximations

Deepika Garg[1], Erik Burman[2], Janosch Preuss[3]
[1] Department of Mathematics, University College London, London, UK–WC1E 6BT, UK

In this talk, we design and analyze an arbitrary-order stabilized finite element method to approximate the unique continuation problem for laminar steady flow described by the linearized incompressible Navier–Stokes equation. We derive quantitative local error estimates for the velocity, which account for noise level and polynomial degree, using the stability of the continuous problem in the form of a conditional stability estimate. Numer ical examples illustrate the performances of the method with respect to the polynomial order and perturbations in the data. We observe that the higher order polynomials may be efficient for ill-posed problems, but are also more sensitive for problems with poor stability due to the ill-conditioning of the system.

Efficient & Scalable finite-element based computational methodologies for large-scale ab-initio modelling of energy storage materials

Kartick Ramakrishnan[1], Phani Motamarri[2]
[1] Department of Computational and Data Sciences, IISc, Bangalore-560012

Ab initio modelling of materials using density functional theory(DFT) is the modus operandi for predicting new-age materials for energy storage and design. The predictive capability can open a gateway for obtaining crucial insights into underlying mechanisms that govern the efficiency and safety of energy storage devices. However, this demands large-scale DFT simulations beyond the current high-throughput calculations routinely performed by employing plane-wave or atomic-orbital based approaches which are restrictive in terms of the nature of boundary conditions one can employ or the accuracy achieved. Furthermore, these approaches have limited parallel scalability and are restrictive in leveraging extreme scale computing architectures. To this end, the recently proposed finite-element-based methods for DFT (DFT-FE[1,2]) provide an efficient and scalable alternative while addressing these limitations. The current implementation of DFT-FE employs the norm conserving pseudopotentials and can handle system sizes with tens of thousands of electrons[3] (few nanometres in length scale). However, to gain an ab-initio understanding of a number of complex phenomenon in energy-storage devices, there is a need to target larger length scales (few hundreds of nanometers) and longer time-scales (few picoseconds). Towards this, we extend the current DFT-FE framework to incorporate Projector Augmented Wave (PAW[4]) formalism with an objective of significantly reducing the degrees of freedom required to achieve chemical accuracy, thereby pushing the limit of length and time-scales possible today with DFT calculations. In particular, we first propose a local real-space formulation amenable for spectral finite-element discretization of PAW formalism. Subsequently, we develop efficient

HPC-centric implementation methodologies combining the ideas of low rank perturbation of identity, mixed precision arithmetic in conjunction with nonlinear subspace iteration approaches to solve the underlying FE discretized generalized eigen problem on both multinode CPU and GPU architectures. We finally demonstrate the accuracy and performance of our proposed implementations on various representative benchmark examples using the current state-of-the-art plane-wave implementations available today.

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Higher order finite-element based methods for non-collinear magnetism and spin-orbit coupling in real-space density functional theory

Nikhil Kodali[1], Phani Motamarri[2]
[1] Department of Computational and Data Sciences, IISc, Bangalore-560012

Spin-orbit coupling is a fundamental and complex relativistic effect that plays a crucial role in a wide range of experimental phenomena[1], including magnetic anisotropy, phosphorescence, and spin-orbit torque. This effect is of significant importance in various active research areas, such as spintronics, low dimensional materials, and topological insulators. The utilization of pseudopotential Density Functional Theory (DFT), a widely adopted first-principles material simulation tool, has been shown to be effective in predicting various material properties when extended to account for non-collinear magnetism and spin-orbit coupling[2, 3]. Traditionally, these DFT calculations have been implemented using either a plane-wave basis or an atom-centered orbital basis set. However, the conventional implementations of DFT have several limitations, such as restrictions on simulation domains due to the need for periodic boundary conditions in the plane-wave basis set and a lack of systematic convergence when employing the atom-centered orbital basis set. Additionally, these basis sets exhibit poor scalability on massively parallel computing architectures.

Recently, a new computational methodology for DFT calculations based on a finite-element basis, incorporated in the open-source code DFT-FE[4], has emerged as a promising alternative. This method ology has demonstrated reduced computational pre-factor, thus delaying the onset of cubic scaling until system sizes of 30,000 electrons while maintaining accuracy comparable to existing plane-wave imple mentations and accommodating fully non-periodic, semi-periodic, and periodic boundary conditions. In this work, we will introduce

a real-space formulation for non-collinear magnetism with spin-orbit coupling and present an efficient, scalable finite-element-based implementation methodology within the framework of DFT-FE, suitable for use on both multinode CPU and GPU architectures. We also present a generalized force approach for evaluating atomic forces and unit-cell stresses in a unified computational framework for geometry optimization involving non-collinear magnetism with spin-orbit coupling.

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Stagnation point flow of Special third grade fluid over a vertical stretching/shrinking sheet and stability analysis

Sradharam Swain[1], Bikash Sahoo[2]
[1] Department of Mathematics, National Institute of Technology Rourkela, Rourkela, Odisha, 769008, India

A study is made to determine the similarity solutions for steady stagnation point flow of special third grade fluid over a permeable stretching/shrinking sheet. The Lie scaling group of transformations technique has been used for finding a new form of similarity transformations, which effectively transformed the governing momentum and energy equation into a new kind of coupled ordinary differential equations (ODEs). The transformed equations are then solved numerically using the shooting technique. It is observed that the similarity equations exhibit dual solutions in a certain range of shrinking strength. The interest lies in examining the effect of physical parameters on flow velocity, temperature distribution, skin friction coefficient and Nusselt number. Thus, emphasis has been given to carrying out a stability analysis to determine the physically reliable solution. The stability analysis shows that the upper branch solution is stable. It is observed that the suction parameter increases the range of dual solutions and the magnitude of the critical point from where the dual solutions bifurcate, however, the non-Newtonian parameter shows the opposite behavior. The momentum, thermal and concentration boundary layer thicknesses in the upper branch solution are lower than the lower branch solution.

Forced convective flows of magnetised Casson hybrid nano fluid exposed to Joule heating effects and variable thermo-physical properties - A Numerical Approach

K.Gnanaprasanna[1], Abhishek Kumar Singh[2]
[1] Mathematics Division, School of Advanced Sciences, VIT University, Chennai Campus, Chennai - 600127, India

The MHD flows of a chemically, radiative, electrically conducting temperature sensitive Casson hybrid nano fluid flows over diverging channel is studied in this work. The present study elucidates the suspension of copper and aluminium oxide nano particles in the non-newtonian base fluid ethylene glycol to interpret the variable thermo physical properties . Metallic oxides like titanium oxide(T io2), silver oxide(Ag20), copper oxides(Cuo) and carbon nano tubes posses good conductivity over heat and electricity and hence the applications of hybrid nanofluids include the industrial sectors like nuclear reactors, thermal power plants, etc. Varying values of the volume fractions of such hybrid nano particles along with the non-dimensional physical parameters influences more thermo-physical properties as compared with mono (single) nano fluids. The analysis of viscous dissipating parameter and the Non-Newtonian Casson fluid parameter is varied along with the varying values of volume fractions of copper and aluminium oxide nano particles and the graphs of the velocity, temperature and concentration profiles are monitored and their physical interpretations are explained in the results and discussion section. With the help of congenial non-similar transformations, the governing boundary layered equations are converted into dimensionless equations. Quasilinearization technique along with implicit finite difference scheme is applied to the transformed equations and finally the system of linearized dimensionless equations are solved using Varga's algorithm. It is observed that the velocity and temperature profiles are intensified for Al_2O_3 (aluminium oxide) nano particles than Cu (copper) nano particles, near the wall but the concentration profiles

is declined deeply for the same values. Surface plots for skin friction coefficient, Nusselt number and Sherwood number for varying values of Magnetic parameter and Brownian motion parameter are investigated and values are compared with previously existing literature has good agreement.

Numerical simulation of natural convection in a rectangular cavity with the Cattaneo effect

Muthumeena[1], S Saravana[2]
[1] Centre for Differential Equations and Fluid Dynamics,Department of Mathematics, Bharathiar University, Coimbatore-641046.

An incompressible flow of a Boussinesq fluid inside a vertical differentially heated square cavity is considered in which the vertical walls are isothermal and the horizontal walls are insulated. This set up is modeled through the unsteady Navier-Stokes equations and the energy equation with hyperbolic diffusion. In particular, the Cattaneo – Christov model of heat flux is incorporated into the energy equation. The numerical solution of the governing equations is obtained by the power law scheme of the finite volume method on a uniform staggered mesh. The resulting steady state results are obtained for different values of the Rayleigh and Prandtl numbers. Before carrying out an elaborate numerical simulation, the results were found to agree well with those predicted by the finite difference method. The isotherms and streamlines are plotted as a function of the relaxation parameter. It is found that the average Nusselt number across the cavity decreases and approaches the benchmark solution of the parabolic case (De Vahl Davis (1983)) as the relaxation parameter approaches zero.

Painlev´e integrability and new soliton solutions for (2 + 1)-dimensional Bogoyavlensky-Konopelchenko equation and generalized Bogoyavlensky-Konopelchenko equation with variable coefficients in fluid mechanics

Shailendra Singh[1], S. Saha Ray[2]
[1] National Institute of Technology Department of Mathematics, Rourkela-769008, India

The time-dependent variable coefficients of Bogoyavlensky-Konopelchenko (BK) equation and generalized Bogoyavlensky-Konopelchenko (gBK) equation are considered in this article. The integrability test by Painlev´e analysis is being implemented on both the considered equa tions. An auto-B¨acklund transformation has been generated with the help of Painlev´e analysis approach for both equations. Auto-B¨acklund transformation method has been used for obtaining the analytic solutions. By using auto-B¨acklund transformation method, three different analytic solution families have been derived for each of the considered equations. Both the methods are completely algorithmic and easy to implementable in computer algebra. All the results are expressed graphically in 3D by varying different functions and parametric values. These graphs revel the physical significance of the equations under consideration.

Centrifugal filtration convection in a bidisperse porous medium

S. Vigneshwaran[1], S. Saravanan[2]
Department of Mathematics, Bharathiar University, Coimbatore - 641 046, India.

Thermal dispersion through a rotating bidisperse porous layer subjected to alternating direction of centrifugal body force is studied. In particular, linear instability and nonlinear stability analyses are made to investigate centrifugation driven thermal convection in a bidisperse porous medium. The presence of micropores in the porous medium in addition to the usual macropores is considered. This allows the possibility of momentum exchange between these two families of pores. The linear analysis is performed through the normal modes whereas the nonlinear one is based on a suitably defined generalized energy functional. Sharp and unconditional nonlinear L2 stability limits are obtained through the variational principles.Compound matrix method based numerical solutions of the resulting eigenvalue problems are obtained and the usefulness of nonlinear results is established in most parts of the parametric space. It is found that an increase in momentum exchange delays the onset of convection,however, depending on the ratio of permeabilities in the two families of pores.

Natural convection in a partially heated and cooled square cavity in the presence of Cattaneo flux

M Manimekalai[1], S. Saravanan[2]
Centre for Differential Equations and Fluid Dynamics,Department of Mathematics, Bharathiar University, Coimbatore - 641 046, India.

A two-dimensional natural convection in a square cavity with partially heated and cooled vertical walls is considered. In particular, the bottom-top, top-bottom and middle-middle combinations of heating-cooling are considered while maintaining the horizontal walls insulated. The Navier-Stokes equations and the energy equation incorporating Cattaneo-Christov heat flux are used to model the heat and fluid flow within the cavity. A finite volume based numerical solution is obtained on a uniform staggered grid via the SIMPLE algorithm with the power law scheme. The steady-state results in terms of temperature, stream function, and heat transfer rates are obtained for different values of the relaxation parameter. The study compares the three heating-cooling combinations and addresses how the present results deviate from the classical parabolic theory.

High Performance Computing

Matrix-free, memory-efficient parallel patch-smoothing for multigrid methods

Michal Wichrowski[1], Peter Munch[2], Martin Kronbichler[3], Cu Cui Guido Kanschat[4]

Efficient smoother is a crucial part of the multigrid method for solving partial differential equations. Patch smoothing has been shown to converge better than traditional point-wise smoothing techniques such as the Jacobi method. In this work, we focus on optimizing the matrix-free patch smoothing algorithm for modern computer architectures. We take advantage of the cache hierarchy in the CPU to minimize memory transfers, leading to improved performance. We start with a serial implementation where we adopt a patch ordering strategy that prioritizes data locality for efficient loop access. Unlike the global approach, we compute both the residual and solution correction in one step. Our evaluation of memory transfers is illustrated in Figure 1. In the parallel implementation, we resolve potential data races by coloring patches and partitioning them into chunks that fit into the L3 cache. The chunks are then sorted to maximize cache coherence. We demonstrate with hardware counters that the proposed method results in improved cache usage and increased throughput for the patch-smoothing application. Our experiments show that by organizing the smoother's execution so that memory transfers are minimized, we can significantly improve its performance.

Overall, this work provides a comprehensive approach to optimizing the patch-smoothing operation and highlights the trade-off between data locality and parallel execution. The results show that the proposed method is a promising approach for high-performance numerical simulations.

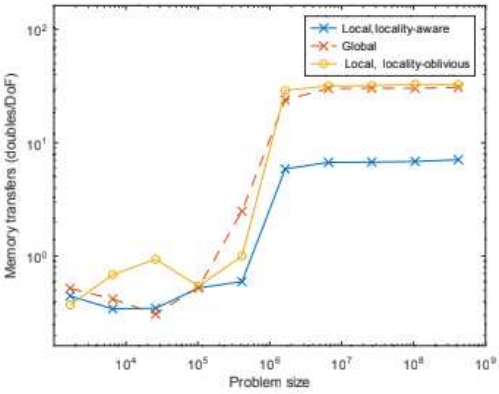

Figure 1: Comparison of memory transfers in serial implementation of a patch smoother

Implementation of the asynchronous discontinuous-Galerkin method in deal.II: accuracy and scalability

Vidyesh Rajendra Dapse[1] Shubham K. Goswami[1] Konduri Aditya[1]
FLAME Laboratory, Department of Computational and Data Sciences Indian Institute of Science, Bengaluru, India

The discontinuous-Galerkin (DG) method has drawn wide interest in developing partial differential equation(PDE) solvers, particularly for problems involving shocks/discontinuities governed by hyperbolic equations. Our interest is in time-dependent partial differential equations, where the DG method discretizes the domain into several elements and approximates the solution there using basis functions that are discontinuous across the elements. For the time derivative, an explicit time integration scheme is used. In a parallel implementation, the discretized spatial domain is decomposed into multiple subdomains and assigned to different processing elements (PEs). To compute the solution at a PE boundary element, the PE requires the ghost element values from a neighbouring PE. This communication overhead affects the scalability of the solver at extreme scales [2]. An asynchronous DG (ADG) method is proposed to overcome this communication bottleneck. The ADG method relaxes communication at a mathematical level and uses previous time-level values available in the ghost elements. It is implemented using the communication-avoiding algorithm (CAA) in the finite element library deal.II [1], which solves the compressible Euler equations using the DG method. The accuracy of the ADG method with the standard numerical flux is restricted to first-order. Therefore, we developed new asynchrony-tolerant (AT) fluxes that provide high-order accurate solutions despite relaxed communication/synchronization. The accuracy results of numerical simulations of one-dimensional linear and non-linear PDEs are presented. The strong scalability results show an improvement in the scalability of the DG solver with the

ADG method compared to the standard DG method.

Keywords: Asynchronous computing, Partial differential equations, Massive computations, Discontinuous Galerkin method,deal.II

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Performance Comparison of Multigrid Implementationson Accelerators

Paul Grosse-Bley[1], Robert Strzodka[1]
[1] Institute of Computer Engineering (ZITI), Heidelberg University

Multigrid (MG) methods are an important tool for efficiently solving large, sparsely occupied linear systems that arise e.g. when discretizing and solving partial differential equations (PDEs). Due to the prevalence of graphics accelerators in the HPC space, this poster compares the performance of different multigrid algorithms in existing implementations on an Nvidia A100 accelerator. Due to their general applicability the well-known sparse solver/preconditioner libraries PETSc[4] and hypre[1] implement algebraic multigrid (AMG) algorithms which can work with any sparsity pattern. Another contestant is the AMGX[2] library developed at Nvidia. For matrices with regular sparsity patterns as they appear when discretizing PDEs on a structured grid, geometric multigrid (GMG) schemes are in theory much more efficient as they make use of the inherent geometry of the discretization. In contrast to AMG there are few broadly used, production-grade libraries that implement GMG efficiently on accelerators, i.e. using stencils instead of general sparse matrix-vector products. In addtion to the GMG implementation in PETSc, we therefore take a slightly modified version of the hpgmg-cuda benchmark and the experimental ExaStencils[3] code generation framework as GMG implementations.

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Recent advances in streaming (hyper)graph partitioning

Marcelo Fonseca Faraj
Heidelberg University

Partitioning a (hyper)graph into balanced blocks such that few edges run between blocks is a key problem for large-scale distributed processing. Currently, there is a gap observed in the space of available partitioning algorithms. On the one hand, there are streaming algorithms that have been adopted to partition massive graph data on small machines. In the streaming model, vertices arrive one at a time including their neighborhood, and then have to be assigned directly to a block. These algorithms can partition huge graphs quickly with little memory, but they produce partitions with low solution quality. On the other hand, there are offline (shared-memory) multilevel algorithms that produce partitions with high quality but also need a machine with enough memory to partition huge networks. In this talk, we present recent advances in the area of streaming algorithms for the problem. First, we present a buffered streaming approach: this model allows to read more than one node and its neighborhood at the time. This enables our algorithm to leverage multilevel techniques, and thus significantly improve solution quality while surprisingly also enhancing the overall complexity of the algorithm. [1]

On the other hand, we present a shared-memory streaming multi-recursive partitioning scheme that performs recursive multi-sections on the fly without knowing the overall input graph to compute hierarchical partitionings. If the topology of a distributed system is known, it is possible to further optimize the communication costs by mapping partitions onto processing elements. [2]

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Matrix-free computations of higher-order finite-element discretized matrix multi-vector products on GPU architectures

Gourab Panigrahi, Phani Motamarri
Computational & Data Sciences, Indian Institute of Science
Bengaluru, India

The finite-element (FE) discretization of a partial differential equation usually involves the construction of a FE discretized operator and computing its action on trial FE discretized fields for the solution of a linear system of equations or eigenvalue problems and is traditionally computed using global sparse-vector multiplication modules. Furthermore, it has also been noted that the evaluation of such sparse matrix-vector products can be done more efficiently on parallel architectures using cell-level dense matrix-vector multiplications followed by the assembly of cell-level product vectors. However, recent hardware-aware algorithms for evaluating such matrix-vector multiplications suggest that on-the-fly matrix-vector products without building and storing the cell-level dense matrices reduce both arithmetic complexity and memory footprint and are referred to as matrix-free approaches. These approaches exploit the tensor-structured nature of the FE polynomial basis for evaluating the underlying integrals. The current state-of-the-art matrix-free implementations deal with the action of the FE discretized matrix on a single vector [1]. These are neither optimal nor readily applicable for matrix multi-vector products involving many vectors. Such situations are often encountered in solving FE discretized eigenvalue problems using iterative orthogonal projection approaches or solving linear systems of equations arising from FE discretizations with multipleRHS vectors. These problems arise in the areas of real-space quantum modeling of materials [2], scientific machine learning to train ML models with the solutions of FE discretized partial differential equations with multiple forcing vectors.

The current work proposes an efficient hardware-aware implementation procedure for the matrix-free algorithm to compute such FE discretized matrix multi-vector products on GPU architectures. We present a data layout for storing the FE discretized global multi-vector to minimize the non-contiguous data accesses during the extraction of the FE cell-level vector from the global vector resulting in efficient parallelization. On GPU-based architectures, the proposed matrix-free implementation utilizes the concept of kernel fusion to minimize data access. It also efficiently utilizes the GPU-shared memory to overlap data access and computation. Further, our implementation takes advantage of a broadcast feature of constant memory to reduce memory transactions and also utilizes registers to decrease bank conflicts. Additionally, it also uses texture memory to reduce pressure on shared memory and better utilize the GPU pipelines.Finally, we assess the accuracy and performance of our implementation to compute FE discretized matrix multi-vector multiplications corresponding to the Laplacian and Helmholtz operators as representative benchmark examples, and we report the superior performance of our matrix-free implementation compared to state-of-the-art implementations using cell-level dense matrix-multi-vector multiplications.

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Multithreaded Finite Elements in DUNE

Santiago Ospina De Los Ríos, Peter Bastian

In this talk, we will discuss the use of a multithreading strategy to assemble vectors and matrices for grid-based methods. These assembly operations are typical in many numerical methods for partial differential equations (e.g. finite elements, finite differences, and finite volumes) and often take a considerable part of the total run-time. Because of irregular shared regions and synchronization costs, multithreading assembly implementations are challenging and can easily perform worse than a simpler private memory model (e.g., MPI). In this case, we will show distinctive aspects related to hardware and grid-based methods that make our implementation amortize the synchronization costs of the shared memory model and be an appropriate and efficient alternative to the private memory model.

Towards accelerating high-fidelity reacting flow simulations using GPUs

Subhajit Safui, Ravikiran Anapagaddi, Sayantan Mitra, Ramsatish Kaluri

The urgent demand to cut down carbon footprint necessitates developing novel combustion concepts that can achieve higher efficiencies and lower emissions. This has led to a growing interest in the combustion community to accurately predict combustion processes depending on realistic chemical kinetic models. The primary challenge in realistic reacting flow simulation is the massive scale of the detailed chemical reaction kinetics. Such detailed mechanisms may contain tens of thousands of reactions and a much larger number of species. A full-scale simulation using such mechanisms is largely out of scope even with the current state-of-the-art computing hardware. This is the reason that a majority of the existing works focus on 'skeletal mechanisms' that contain a much smaller number of reactions and species. In the goal of accelerating chemical kinetics, researchers have followed different approaches. Broadly, the approaches can be classified into two different categories. The first approach involves developing novel algorithms for the simulations, such as more advanced integration algorithms, matrix-based formulations, and more. The second approach involves novel implementations of the existing algorithms that exploit features of the target hardware such as GPUs to expose the inherent concurrency in large-scale simulations. In many scenarios these two approaches are not mutually exclusive, where the aim is to develop novel algorithms that conform to the architecture of the target hardware. In the present work, the aim is to accelerate small to moderate sized reaction mechanisms on different granularity of grids using GPUs. For this purpose, the governing PDEs involving the spatial and temporal derivatives have been converted to a set of ODEs by use of suitable discretization. Thus, the system is transformed into solving a single ODE at each computational cell. This

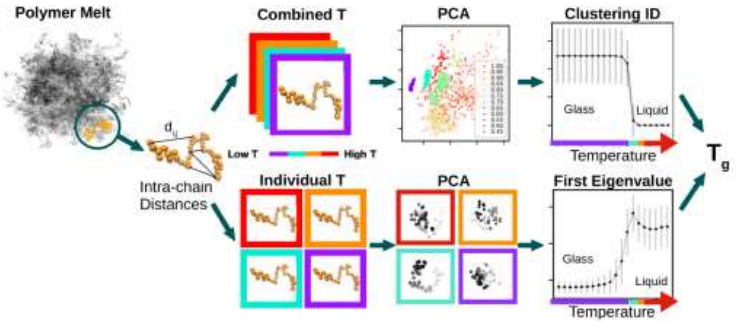
is performed on GPU by assigning each ODE to a GPU thread. An operator-splitting technique is used to decouple the chemical kinetics equations from the convective and diffusive transport equations. Further, host-device data movement is minimized by porting the entire application involving both the species transport as well as the chemical kinetics parts onto the GPU. The correctness of the GPU implementation is tested by comparing the results with the CPU implementation. Initial comparison with a one-reaction mechanism reveals up to 125x speedup over single threaded CPU implementation for 2D grids with 250k cells. Further, some of the GPU kernels are observed to achieve up to 66 percent of the peak theoretical bandwidth of a NVIDIA Tesla V100 GPU.

Scientific Machine Learning

Data-driven identification and analysis of the glass transition in polymer melts

Atreyee Banerjee[1]

On cooling, the dynamical properties of many polymer melts slow down exponentially, leading to a glassy state without any drastic change in static structure. Understanding the nature of glass transition, as well as precise estimation of the glass transition temperature (Tg) for polymeric materials, remain open questions in both experimental and theoretical polymer sciences. We propose a data-driven approach, which utilises the high-resolution details accessible through the molecular dynamics simulation and considers the structural information of individual chains. It clearly identifies the glass transition temperature of polymer melts of semiflexible chains. By combining principal component analysis (PCA) and clustering (shown in the schematic), we identify glass transition temperature at the asymptotic limit even from relatively short-time trajectories, which just reach into the Rouse-like monomer displacement regime [1]. We demonstrate that fluctuations captured by the principal component analysis reflect the change in a chain's behaviour: from conformational rearrangement above to small vibrations below the glass transition temperature. We demonstrate the generality of the approach by using different dimensionality reduction and clustering approaches. The method can be applied to a wide range of systems with microscopic/atomistic information. More recently we applied this methodology to all-atom acrylic paint systems [2]. Our study reveals the explicit role of backbone and side chain residues to determine the glass transition temperature.



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Improving the physics of heating in climate models using deep learning

Ayantika Dey Choudhury[1], Vishnu Dev Tripathi[1,2], Manmeet Singh[1], Vaisakh S.B[1], Yogeshwar Singh[2], Manisha Nene[2], R. Krishnan[1]

[1] Indian Institute of Tropical Meteorology, Ministry of Earth Sciences, Pune, India

[2] Defence Institute Of Advanced Technology, Ministry of Defence, Pune, India

Precipitation is vital for different sectors of societal development, including agriculture, infrastructure, water supplies, industries, transport, among others, and is an essential part of the Earth's weather and climate. Accurate and reliable predictions of precipitation distribution across space and time scales remains a major challenge in weather and climate models. Over the tropics, the release of latent heat by the condensation of water vapor into liquid or solid during the formation of clouds is a key process that drives thunderstorms, tropical cyclones and large-scale circulation. Latent heating must be accurately represented in weather and climate models for skillful precipitation forecasts, but this process is challenging due to its intricate and nonlinear connections among several meteorological variables. This research utilizes a data-science model to construct 3-dimensional fields of time-mean latent heating using meteorological fields. To provide the best possible results, the model is trained using cutting-edge machine learning methods and subjected to extensive hyperparameter optimization. Improved representation of latent heating in weather and climate models has the potential for improving rainfall predictions over the tropics.

Characterization of ANN-based reconstruction methodology for one-dimensional laminar premixed flames in the CoK-PCA framework

Dibyajyoti Nayak[1], Anirudh Jonnalagadda[1], Uma Balakrishnan[2], Hemanth Kolla[2], Konduri Aditya[1]

[1] Department of Computational and Data Sciences, Indian Institute of Science, Bengaluru, Karnataka, 560012, India

[2] Sandia National Laboratories, Livermore, CA 94550, United States

Dimensionality reduction seeks to reduce the feature space of high-dimensional data while effectively retaining the information and dynamics of the original system. The widely used principal component analysis (PCA) achieves this for combustion data by transforming the original thermo-chemical state space into a low-dimensional manifold with eigenvectors of the covariance matrix of the input data. However, this may not effectively capture the stiff chemical dynamics when the reaction zones are localized in space and time. Alternatively, a co-kurtosis PCA (CoK-PCA), wherein the principal components are obtained from the singular value decomposition (SVD) of the matricized co-kurtosis tensor, demonstrated greater accuracy in capturing the stiff dynamics. However, both methods incur significant errors due to a linear reconstruction of data onto the original manifold. Nonlinear methods such as artificial neural networks (ANNs) can greatly improve reconstruction accuracy over linear methods, thereby allowing further dimensionality reduction of the original manifold. We investigate the efficacy of our approach, i.e., CoK-PCA-ANN, relative to PCA-ANN in two cases, namely, homogeneous reactor data of premixed ethylene-air and ethylene-air freely-propagating premixed laminar one-dimensional flame by comparing errors in the reconstruction of the thermo-chemical state, species production rates, and heat release rates. Our results show that, while ANN outperforms linear reconstruction in general, the proposed CoK-PCA-ANN captures the stiff dynamics better than PCA-ANN.

Keywords: dimensionality reduction, thermo-chemical state, extreme events, eigenvalue decomposition, flashbacks, co-kurtosis, singular value decomposition, deep neural networks, activations, regularisation

Transport-based sampling using polynomial density surrogates

Josephine Westermann[1], Jakob Zech[1]
[1] University of Heidelberg, Germany

Generating samples from arbitrary probability distributions is a central task in several areas of modern applied mathematics, such as parameter inference and uncertainty quantification. Transport-based sampling [1] can overcome problems such as burn-in phases and sample correlation that arise in common sampling methods such as Markov Chain Monte Carlo. However, in most practical applications, the target probability density is not analytically accessible and transport methods cannot be readily applied. We describe how the Knothe-Rosenblatt transport can be constructed from polynomial density surrogates of target densities on the d-dimensional unit cube [0, 1]d . Such a transport can then be used to generate samples that are approximately distributed according to the desired target distribution. We discuss efficient implementation schemes and derive error convergence rates for target densities belonging to different smoothness classes.

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Modeling of Electric Discharge Trepanned Hole Circularity using Machine Learning Technique

Surendra Kumar Saini[1]
[1] Mechanical Engineering Department, Poornima College of Engineering Jaipur, Rajasthan (India)

Machine learning technique is best suited to establish the engagement between quality and design factors of a nonconventional machining process. In this study wire electric discharge trepanning/circular cutting in to thick die steel plate is performed. Wire electric discharge trepanned hole surface roughness is measured using Feret's diameter. Four variables pulse on, pulse off time, wire feed and current are taken as design factor while surface roughness is considered as quality parameter. Total twenty seven experiments conducted on work material using orthogonal array. Artificial neural network (ANN) is used to develop a mathematical model. Improved weights and biases values are obtained at minimum mean square error. The validation of developed ANN mathematical model is done by computing average percentage prediction error (APPE) that is found less than five percentage.

Keywords: Wire electrical discharge trepanning; Steel; orthogonal array; artificial neural network.

$$Y_p = \frac{1}{\left[1+e^{\left[-\left(w_{pj}\ x_j+\ b_p\right)\right]}\right]} \qquad (1)$$

$$Y = \sum_{i=1}^{p} Y_p\ \ w_p + b \qquad (2)$$

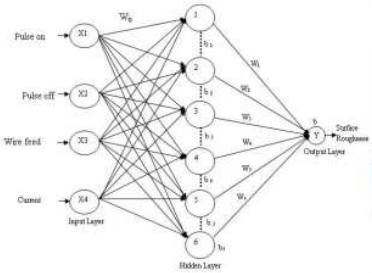

Fig. 1 Artificial Neural Network architecture 4-6-1 for surface roughness
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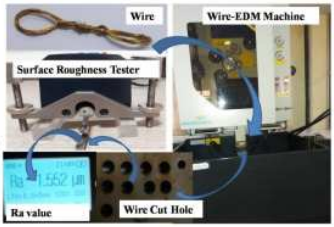

Fig. 2 Experimental Setup of Electrical Discharge Trepanning

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Plant-wide Leak Detection for Targeted Maintenance in LNG plants

Stephen Varghese[1], Arvind Ravi[1], Rihab Abdul Razak[1], Shirish Nanda[1], Jose M. Gonzalez-Martinez[1]

[1] Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India

[2] Department of Mechanical Engineering, Indian Institute of Technology, Madras-600036,Tamil Nadu, India

LNG (liquified natural gas) has emerged in the world market as a viable contender for transportation fuel, especially in hard-to-abate sectors like shipping where it could serve as a replacement to traditional fuel oils due to LNG's environmental, operational, and economic advantages. Methane (CH4), which is a major component in the natural gas, plays a vital role in the greenhouse gas (GHG) effect and global warming. Shell has committed to keep the CH4 emission intensity below 0.2% by 2025 as part of its sustainability strategy. In this context, identifying a natural gas leak as and when it develops in LNG liquefaction terminals, help take pro-active measures to plan maintenance and carry out repair in a targeted manner, thereby contributing towards a reduced GHG footprint.

Various monitoring and leak detection techniques are available such as placement of analyzers (e.g., flame ionization detector, remote methane leak detector) in critical locations in the plant to identify leaks in the surrounding area. This usually involves less coverage area and cost limitations hinder installing analyzers at multiple locations in the plant [1]. To overcome this limitation, a data-driven framework has been developed using existing sensor data for leak localization and leak quantification, for cases in which the leak intensity is well below sensor noise levels, based on data reconciliation [2], Kalman filters [3] and Multivariate Statistics-based FDI techniques [4], [5]. A robust algorithm capable of handling various leak scenarios

relative to sensor errors and process / operational changes has been implemented. To illustrate the performance of this novel leak detection and localization algorithm, synthetic data from a quasi-steady simulation of a simple LNG plant [6] is used, which takes into consideration different scenarios of leaks, sensor noise, and plant operations.

Preliminary results indicate that the developed algorithms can detect and localize leak well below the sensor noise level for the simulated dataset. Future work would include extending the ability of algorithms to detect leak in case there is a drift / bias in sensor or in case instrumentation is not rich enough or available at all desired points. Based on the performance of different developed algorithms, the best performing algorithm will be chosen for further development into an online tool, to enable near real-time leak detection to enable targeted repair and reduce GHG impact.

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Random forest surrogate model for viscoelasticity prediction of MWCNT-based advanced nanocomposites

Salur Srikant Patnaik[1], Haritha Kallamadi[1]
[1] Assistant Professor, uGDX Institute of Technology, L77, 315 work avenue, HSR Layout, Sector- 6, Bengaluru- 560102

In the present work, a supervised machine learning algorithm based on random forest surrogate (RFS) model has been used for the prediction of viscoelastic properties of multi-walled carbon nanotubes (MWCNT) reinforced advanced nanocomposites. The experimental approach using dynamic mechanical analyser for the nanocomposite, is expensive and requires skilled scientists and is laborious as well. The upgradation of experimenting process and calculating/predicting the viscoelastic properties using RFS model is cost effective and saves time. The nanocomposite samples with different weight fractions of MWCNTs were fabricated and tested on dynamic mechanical analyser to capture the creep strain behaviour in time domain. Further, these are utilised in the Laplace transform to compute the viscoelastic properties of nanocomposites in terms of storage modulus and loss modulus in frequency domain. Using the viscoelastic properties obtained from the experiments, we build a machine learning model using RFS algorithm. The proposed machine learning model reduces the experimentation cost and predict the viscoelastic properties of nanocomposites accurately.

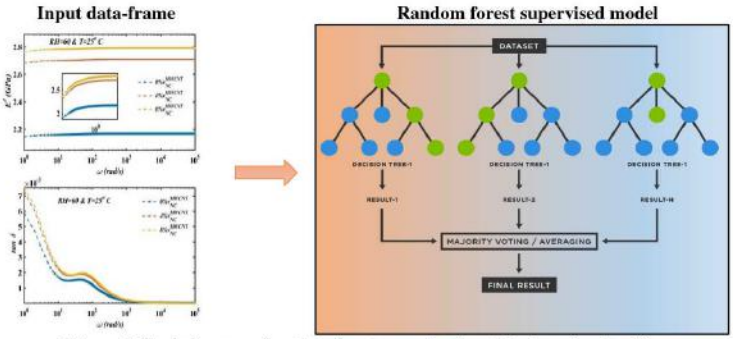

Figure 1 Block diagram of random forest supervised machine learning algorithm

Keywords: MWCNT; advanced nanocomposite; viscoelastic properties; machine learning; random forest supervised model

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Structural analysis of screw compressor block using Bayesian Machine Learning

Abhishek Kumar[1]

Due to the increasing demand of screw compressors in the industry, the design and construction of these compressors becomes a challenging task. Numerical simulations using Computational Fluid Dynamics (CFD) and Finite Element Analysis (FEA) are the most common and validated tools for solving the fluid flow or performing structural analysis. The benefit of these simulations is replicating the real life scenario and understanding the failure criteria without executing these experiments which saves a lot of effort and manpower. In this paper structural analysis of a screw compressor block is carried out using Ansys and SCORG (commercial licensed software tools available for the finite element modeling package & screw compressor analysis). The data generated from this analysis are being used to train the Machine Learning algorithms for different working conditions. Hyperparameters tuning of the best suited Machine Learning algorithm is being carried out using Bayesian Optimisation to improve the accuracy. The tuned ML model is used to predict the principal stress and deformation at given nodal points of the given compressor block without the dependency on any physics solver with low computational effort, minimum time and with high accuracy. In the future study, the computational fluid dynamics of the screw compressor block is to be carried out using Machine Learning and to be validated experimentally.

Keywords: Finite Element Analysis (FEA), SCORG, Ansys, Bayesian Optimisation and Machine Learning

A Novel Reduced Order Model for Uncertainty Quantification in Earthquake Engineering

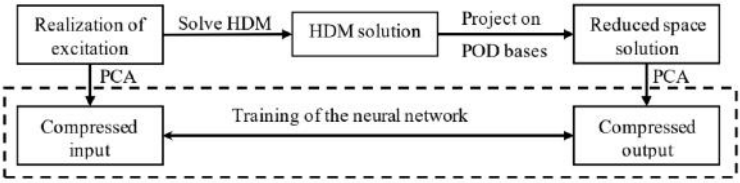
Chandan Bharti[1], Debraj Ghosh[1]
[1] Department of Civil Engineering, IISc Bangalore, Bengaluru, India-560012

Solving a large-scale dynamical system can be computationally challenging. Uncertainty quantification of such a system further increasesthe cost as it requires repeated solutions for large numbers of realizations. In the current work, this computational issue is addressed by developing a novel proper orthogonal decomposition (POD)-based non-intrusive reduced-order model (ROM) for a random process. Generally, in a POD-based non-intrusive ROM, the high dimensional model (HDM) is solved for a few realizations of the parameters, and a set of POD bases is computed. The space spanned by these bases is referred to as reduced space. The HDM solution is then projected on these bases, and the reduced space solution is found. This projection leads to a reduction in the dimension of the model. For a new realization of the parameters, these reduced space solutions are approximated or interpolated in the reduced space. Accordingly, the computational cost reduces.

However, for a random excitation, the approximation needs to be performed in a high parametric dimension. Here the issue is two-fold (i) efficient mathematical representation and (ii) approximation or interpolation in the high dimensional space. The first issue is addressed by compressing the random excitation using principal component analysis (PCA). This simple yet important transformation of the data extracts the dominant features of the excitation and thus reduces the parametric dimension. Approximation in the high dimension is handled using an artificial neural network. Neural networks have been successfully used for various high-dimension regressions in

recent years.

In the proposed method, a set of random excitations is generated, and then the HDM is solved for each excitation. Subsequently, POD bases are computed, and the reduced space solutions are found for each excitation. The PCA is then performed separately on both the excitations and reduced space solutions. These compressed data pairs are used to train the neural network in the reduced space. The schematic of the methodology is shown in the following figure.



Once the training is completed, the reduced space response for a new realization is found by evaluating the trained network. This newly computed response is projected back on the POD bases to find the corresponding HDM solution.

The accuracy and efficiency of the proposed ROM are tested for a beam on Winkler foundation under earthquake excitation. A spectrum-compatible random excitation is considered here to simulate the earthquake. The numerical results show that the proposed method is accurate in capturing the entire time history of the response. Besides, it is efficient in performing uncertainty quantification as well. The numerical experiments show that the frequency bandwidth of the excitations governs the size of the training sample. A wider bandwidth requires a larger sample size. The numerical studies are performed for the Gaussian and stationary excitations. However, an earthquake excitation is essentially a non-Gaussian and non-stationary process. The performance of the proposed method for such a process remains to be explored.

Simulation and Model Order Reduction of Thermal Electrohydrodynamical Convection in Annular Geometry

J. Roller[1], A.Meyer2[2], M. Meier[2], V. Heuveline[1]

[1] Engineering Mathematics and Computing Lab, Interdisciplinary Center for Scientific Computing, Heidelberg University, Mathematikon, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany

[2] Dep. Aerodynamics and Fluid Mechanics, Brandenburg University of Technology Cottbus Senftenberg, Siemens-Halske-Ring 15a, 03046 Cottbus, Germany

We consider the hydrodynamical behavior of a dielectric fluid contained in a cylinder annulus under applied voltage and temperature gradient between inner and outer wall. This setting gives rise to a resulting body force, being a superposition of buoyancy and dielectrophoretic force (DEP). The situation can be modeled by means of thermal electrohydrodynamical (TEHD) Boussinesq equations. Due to its multiphysical nonlinear dynamics, finite element simulation of this model is computationally expensive. We propose a data-driven reduced order model (ROM) based on the well-known proper orthogonal decomposition (POD) to tackle this problem.

In the typical scenario with Earth's gravity acting upon a horizontal annulus, steady or time-periodic solutions are obtained. The former are characterized by increased temperature at the top of the annulus, the latter by periods of rising and falling temperature at the top and bottom, respectively. We investigate the effects of a range of thermal and electric Rayleigh numbers on flow stability in this scenario. In addition, we examine the capability of the POD-ROM to replicate the qualitative flow behavior and compare our results quantitatively with experimental data.

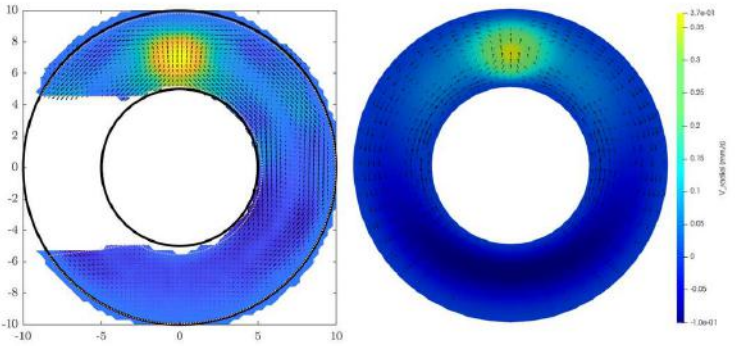


Figure 1: Experimentally measured radial velocity (left), steady finite element solution (right) for $\Delta T = 2$ K and $V_{peak} = 8$kV.

Using the Cone Method with Minmax Robustness to Solve Uncertain Multiobjective Optimization Problems

Nand Kishor[1] , Dr. Debdas Ghosh[1],

[1] Department of Mathematical Sciences IIT BHU, Varanasi, India, 221005

It is often hard to find optimal solutions to real-world optimization problems, which is due to the uncertainties that can deteriorate the quality of an optimal solution or even render it infeasible. Robust optimization, which aims to find solutions that are feasible for all possible scenarios of uncertain input data, is one way of dealing with uncertainty. For problems with a single-objective function, robust optimization has been very well developed to address decision-making under uncertainty. Typically, most real-world decision making problems have multiple decisions or goals. Therefore, researchers have recently acknowledged the necessity of finding robust solutions to multiobjective problems and presented some preliminary results on this subject.

In this talk, we extends the use of the cone method for robust multiobjective optimization problems. Next, we propose the robust counterpart of an uncertain multiobjective optimization problem and analyse the concept of robust efficiency for uncertain multiobjective optimization problem. Further, we describe an interpretation of robust counterpart of an uncertain multiobjective optimization problem using the idea of objective-wise worst case.

The applicability of our proposed work can be seen to obtain all the robust efficient solutions of an uncertain multiobjective optimization problem having robust counterpart which may not be possible by the implementation of weighted sum and ϵ-constraint methods. The primary reason that supports the recommendation of the cone

method for uncertain multiobjective optimization problems is its appropriacy for deterministic non-convex optimization problems. If the robust counterpart of an uncertain multiobjective optimization problem is non-convex, then the cone method may be a better alternative than other existing scalarization methods.

Keywords: Uncertainty Set, Multiobjective Optimization, Robust Efficient Solution, Cone Method.

Fractal interpolation: A data-driven approach for reconstruction

T.M.C. Priyanka[1]

[1] Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu – 632014

While there are a variety of conventional interpolation methods tailored for the interpolation of regular data sets, fractal interpolation is introduced as an advanced interpolation technique for the irregular data approximation and reconstruction [1]. As many of the real-time data sets like EEG data, temperature anomalies, stock price fluctuations, etc., are highly non-smooth when plotted and erroneous with missing data, traditional interpolation approaches are insufficient to reconstruct such data sets. This phenomenon is being addressed by fractal interpolation functions, which are constructed using the notion of iterated function systems, as a result, the number of data points increase at each iteration, thereby, improves the accuracy of aforesaid irregular data sets. With an aim of enhancing the flexibility and diversity in approximation, in sequel to the linear fractal interpolation function of Barnsley, types of fractal interpolants have been developed to reconstruct both regular and irregular data sets (and functions). Moreover, the continuity and non-differentiable nature of fractal functions have interestingly connected the field of fractal analysis with the quite popular field of fractional calculus [2]. To highlight the practical significance of fractal functions, a linear fractal interpolation function is used for reconstructing the sample data of greenhouse gas emissions, refer [3].

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Classification of Epileptic EEG Signals based on Bonferroni mean (BM) Operator

Gowtham Reddy N[1], Debashree Guha[1], Manjunatha Mahadevappa[1]
[1] School of Medical Science and Technology, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India

Globally, according to WHO, almost 60-70 million people are suffering from epilepsy disease. It is a chronic non-communicable neurological malady that affects the nervous system due to irregular discharge of brain neurons, and makes disturbance of motion, jerks in the movement of arms and legs, behavior. An Electroencephalogram (EEG) is the most effective tool for studying epileptic seizure brain activity. The analysis of EEG recordings by neurologists takes a long time to examine epileptic abnormalities in EEG signals visually. In this study, a novel data-driven machine learning algorithm is proposed to detect epileptic seizures automatically from continuous EEG signals.

The EEG data features are extracted using the discrete wavelet transform (DWT) technique. By decomposing the EEG signals into time-frequency sub-bands levels, 8 different meaningful statistical features are extracted. Finally, these features are fed to the Bonferroni aggregation operator based fuzzy pattern tree algorithm that utilizes the Bonferroni mean (BM) operator to capture the inter-relationships between the data features while constructing a classifier model. We term the new method as Bonferroni mean-based fuzzy pattern tree (BM-FPT) classifier.

The proposed BM-FPT algorithm achieves 98.2% accuracy, 97.05% specificity, 98.49% sensitivity and 95.65% F1-score on the Bonn university EEG database. The proposed model outperformed some existing studies in terms of performance metric.

Keywords: Epilepsy, Electroencephalogram, Discrete wavelet transform, Bonferroni mean, Pattern tree, Classification

Computational and statistical complexities of learning algorithm for non-linear dynamical systems

Lakshman Mahto[1]

[1] Indian Institute of Information Technology Dharwad, India

We study and analyse improvement of the statistical and computational complexities of the learning algorithms for non-linear dynamical systems with the betterment of optimization algorithms as well as additional statistical assumptions. We demonstrate that the optimization algorithm reaches a final statistical radius of convergence around the true parameter after logarithmic number of iterations in terms of the sample size. Our analysis has two key components: i) an improved generalization gap based on the optimization algorithm for computationally efficient recovery of dynamics, and ii) an improved concentration bounds for approximation error under additional statistical assumptions setting for sample complexity of recovery of dynamics. Finally, we illustrate our theory to apply few embedded linear and generalized linear regression models.

Uncertainty and Stability Analysis of Perturbed Interval-valued Value Function in Interval Optimization Problems

Anshika[1], Dr. Debdas Ghosh[1]
[1] Department of Mathematical Sciences Indian Institute of Technology, BHU, Varanasi, India, 221005

The uncertainty in the perturbation functions is found in the study of variational analysis which includes problems based on well-posedness, sensitivity, and stability. With the development of quantum mechanics in atomic and subatomic physics, several perturbation methods were adopted during the 20th century to estimate the changes observed in a particle with the emission in radioactive elements. Several theories and methods have been developed for finding an approximate solution to a perturbed problem. This includes proposing the optimality conditions in various problems of optimization and equilibria, viscosity solutions of partial differential equations, etc. For instance, see [1, 2, 3, 4].

Uncertainty analysis is related to the study of the stability of solution behavior concerning changes in a given problem. In this talk, we discuss the concept of perturbed interval-valued value function. To develop the results, the notion of a Lagrangian interval-valued function (IVF) plays a key role. Therefore, we analyse a characterization of the gH-subdifferential set of perturbed interval-valued functions. After that, we present a saddle point efficiency interpretation of the perturbed interval-valued function based on a saddle point criterion of the Lagrangian IVF. Next, we discuss the stability of a solution to an Interval optimization problem (IOP) with the help of gH-subdifferential set of perturbed interval-valued functions. Furthermore, the gH-subdifferential set of an interval-valued value function is used to estimate the efficient solution of an Interval optimization problem (IOP) under certain restrictions. Lastly, an exam-

ple to show an application of the interval-valued value function in a practical phenomenon will be performed.

Keywords: Interval uncertainty, interval-valued value function, Interval-valued functions, Interval optimization

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Environment temperature variation error compensation at Tool Centre Point (TCP) using ML/AI module on Vertical Milling Machine (VMC) - C-frame type machines.

Dr. Harshad Sonawane[1], Shreedhar Nayak[1], Shubham Mali[1]
[1] Bharat Fritz Werner Limited, Bangalore

Computer Numerical Control (CNC) machine plays a vital role in the manufacturing industry. Metal parts manufactured with the help of CNC machines are accurate and precise. Despite all the technological devolvement and advancements in the manufacturing process, there is still scope for improvements as far as accuracy is concerned. CNC machine encompasses of variety of metal parts with different physical attributes. These materials respond differently to temperature variations occurring on and by machines. When it comes to ambient temperature variation, the temperature change is gradual and slow as compared to temperature variation caused by any other means. Despite the slow and gradual change in ambient temperature, metal parts of CNC machines still react to this variation. This response from the metal parts causes an error in accuracy as it distorts the Tool Centre Point (TCP) of the machine. The error caused by temperature variation is predominant which is about 75% of the total error, under this it is very important to eliminate or reduce the ambient temperature variation error that occurred on TCP. This paper elucidates the approach to bringing down the ambient temperature variation error with experimentation and results. The Machine learning module named Environment Temperature Variation Error (ETVE) is developed to compensate for ambient temperature variation on TCP. Data collected from experiment is used as training and testing for machine learning model. After splitting the experimental data in training and testing, machine learning model learns from the data and predicts the error caused by ambient temperature variation on machine components and ultimately at TCP and compensates

the same. For experimentation purposes, an RTD PT100 temperature sensor is used to collect the ambient temperature, an IOT device named Raspberry pi 4 is used to collect this real-time temperature and CNC data. Displacement measuring devices like Eddy Current sensors are used for collecting the data for measuring TCP distortion using data acquisition system and Accumeasure software. The results received from experimentation are compared with machine learning model results and inference has been taken out. Raspberry Pi 4 an IOT platform is used as a data acquisition system and as a control device which gives the flexibility of remote control. The inference from the machine learning module results shows that the model is effective in controlling the ambient temperature variation and significantly reduces the TCP distortion, which ultimately improves the accuracy and precision of final component.

SpiNet QSM: Model-based Deep Learning with Schatten p-norm regularization for QSM reconstruction

Venkatesh Vaddadi[1], Phaneendra K. Yalavarthy[1]

[1] Computational and Data Sciences, Indian Institute of Science, Bengaluru

Quantitative susceptibility mapping (QSM) is a recent approach that estimates the magnetic susceptibility values of the tissues from magnetic resonance (MR) phase measurements. QSM has significant clinical relevance as bulk tissue magnetic susceptibility provides essential information about tissue composition and microstructure, such as myelin content in white matter and iron deposition in gray matter. Pathological changes in tissue susceptibility values are closely related to neurodegenerative diseases, such as Multiple Sclerosis and Alzheimer's Disease. The estimation of the tissue magnetic susceptibility (source) from the measured magnetic field distribution/local tissue field (effect) inherent in the MR phase images is achieved by numerically solving the inverse source-effect problem. In essence, this utilizes the established relation connecting source and effect using the dipole kernel, and hence the susceptibility map reconstruction is called dipole deconvolution. The advent of deep learning-based methods has shown promising results in deconvolving the susceptibility distribution from the phase information of the MR signal. However, most of the existing deep learning approaches are solely dependent on data and do not utilize the underlying physical model of dipole deconvolution. This work presents a Schatten p-norm-driven model-based deep learning framework for quantitative susceptibility mapping. As opposed to other model-based architectures that enforce either l2-norm or l1-norm for the denoiser, the proposed approach can enforce any p-norm ($0 < p \leq 2$) on the denoiser. The comparison of the proposed method was performed with conventional methods, deep learning based approaches such as QSMnet, and model-based

deep learning approaches such as learned proximal convolutional neural network (LP-CNN). Reconstructions performed across 97 imaging volumes with different noise levels, acquisition protocols, and clinical conditions such as hemorrhage and multiple sclerosis showed that the proposed approach outperforms existing state-of-the-art methods by a significant margin in quantitative merits.

Physics Informed Neural Networks for Approximating the Solutions of Vibration Equation of Large Membranes

Arup Kumar Sahoo[1], S. Chakraverty[1]
[1] Department of Mathematics, National Institute of Technology Rourkela, Rourkela-769008, India

Artificial intelligence (AI) has been a subject of intense media hype in the 21st century. However, modeling and forecasting multi-physical systems remain a challenge due to scarcity of data and noise. Most of the implementation of neural networks are to perform non-linear mapping from input space to target space. However, prior physical information in the form of a differential equation is not utilized in most of the traditional neural models. In this paper, **Physics-Informed Neural Network (PINN)** is implemented to solve vibration of large membranes considering the physics of the system [1]. Vibration analysis of large membranes has a great importance due to its broad applications in areas such as music, biomechanics and acoustics [2]. The trainable parameters between the layers can be learnt by minimizing mean squared error loss: $MSE = MSE_u + MSE_f$. Here the loss MSE_u corresponds to the initial and/or boundary conditions and MSE_f enforces the structure imposed by given differential equation at a finite set of collocation points. Sample points are generated randomly inside the given domain in order to train and test the PINN model. Adam optimizer has been used for hyperparameter tuning along with the Swish activation function, to increase the robustness of the present model [3].

It is worth mentioning that there exist other numerical methods to solve the titled problem. But all of these traditional methods have their own intrinsic worth, applicability, and limitations. Additionally, these methods are sometimes problem dependent and require repetitions of the simulations. In most of the numerical techniques, the

solution is discrete in nature and/or a solution of finite differentiability where the ANN model-based solution is continuous over the given domain of integration [4]. Also, once the NN is well-established, it can be used as a black box. Furthermore, to examine the accuracy of the PINN algorithm, the L2 and L1 errors are considered. The physical significance of the obtained neural results has been shown by graphical depictions. This neural algorithm can be useful for solving relevant problems emerging in various other engineering applications.

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Solving a (2+1) Dimensional Partial Differential Equations Using Five Point Stencil Convolutional Neural Networks

Jain M Francis[1], Chandhini G[1]
[1] Department of Mathematical and Computational Sciences, National Institute of Technology Karnataka, Srinivasanagar, Mangalore-575025

In recent years neural networks have been widely used to solve model problems involving partial differential equations (PDEs). Most of the methods train the given initial/boundary value problems individually to predict the solution. To overcome this issue a neural network inspired by the finite difference method has been introduced by [1], having named five-point stencil CNNs (FCNNs) as in Figure 1, and applied this network to solve second order reaction-diffusion equation. In this work, we try to extend this network and try to evaluate the efficiency of the method to solve a class of PDEs having different initial conditions.

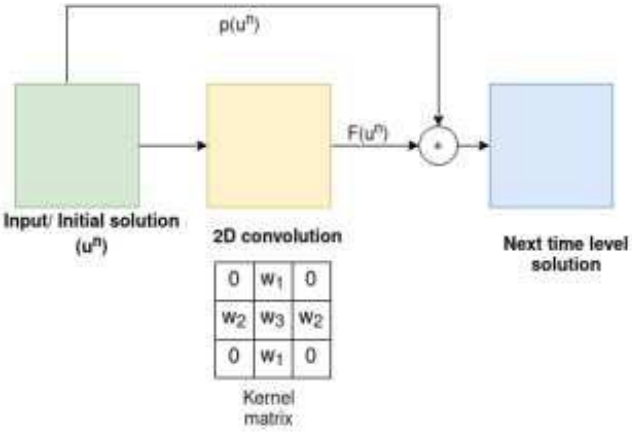

Figure 1: FCNN

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Deep operator network (DeepONets) for system identification

Vijay Kag[1], Birupaksha Pal[1]
[1] Bosch research and Technology Center, Bangalore

The mathematical basis of neural networks is based on the universal approximation theorem for functions. There is another powerful but comparatively lesser-known result called the universal approximation theorem for operators, which says that a neural network with one hidden layer can accurately approximate any continuous non-linear operator. George Karniadakis, one of the founders of the physics informed neural network (PINNs), has recently proposed the method called Deep Operator Networks to realize the universal approximation theorem for operators in practice[1]. Here we present a brief about this novel method, look at some test examples and discuss the potential it holds in system identification and scientific machine learning.

Let us consider (U, V and S) to be a triplet of Banach spaces and N to be a Differential operator (linear or non-linear). If we consider a system to be modelled by the PDE N (u, x) where u is the input and x the state of the system, then the objective of the method DeepONet is to find the state x in terms of u. In other words, it strives to find an operator/functional G which takes u to x i.e. G(u) = x. The architecture of DeepONet consists of two neural networks one the branch and the other the trunk network. The function of the branch network is to approximate the transformation of the input function u while the trunk network encodes the point y where the output of u through the branch network will be evaluated i.e. G(u)(y), G(u) be the output of u through the branch network and G(u)(y) is the evaluation of the function G(u) at y. The main function of the trunk network is to encode y in a shape where a dot product of it's output with the output of the branch network will hold good, and this is done

to realize the universal approximation theorem for operators. Now, as the branch network takes in a function as the input hence it's represented discretely by the function evaluation at finite locations called the sensor points. Below is a pictorial representation of the architecture of the unstacked DeepONet.

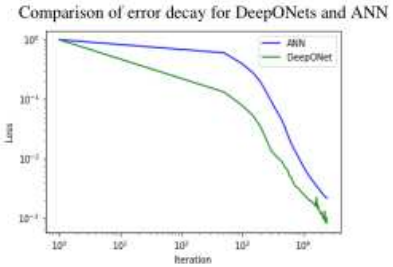
One of the strengths of this method vis a vis existing ML methods for system identification is that once trained the model gives much better prediction for unseen inputs as compared to other methods. This becomes very crucial for many black box identification problems, in engineering and science, where in almost all practical applications once deployed the model may face inputs of unseen types. Here we show with an example the potential of this method wrt generalization error vis a vis ANN (artificial neural network) which is a very popular method for black box modeling and system identification. We consider the black box system to be a reaction diffusion system and use the exact solution of the equation as synthetic data for training a DeepONet architecture. We use part of the data to train the model and predict back the remaining data. Further, we make a comparison between the DeepONet prediction, the ANN prediction (using the same training data) and the exact solution, to show the efficacy of the method.

The governing differential equation (reaction – diffusion)

$$\frac{\partial s}{\partial t} = D\frac{\partial^2 s}{\partial x^2} + Ks^2 + u(x) \text{ for } x \in [0,1] \ \& \ t \in [0,1],$$
$$D = 10^{-2}, K = 10^{-2}$$

We evaluate the solution of the equation at 256X100 grid points. This data we consider as exact/reference solution. For training the DeepONet and ANN we consider 100 points out of these 256X100 as training data (trunk network) corresponds to each input functions. For the branch network we consider 100 random functions and further each of the functions are evaluated at 50 sensor points. Once the model has been trained then predictions are made for unseen

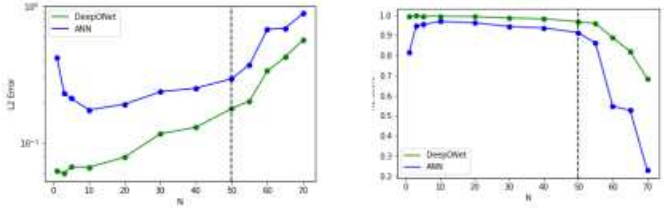
functions. We have shown an extensive hypermeter tuning (number of hidden layers and number of neurons per layer). The optimal results for DeepONet is obtained for one with Branch network of size [50,50,50] and the Trunk network of size[2,50,50] and has 7800 total parameters. Likewise for ANN the optimal network is one of size [52,50,50,50,1] and total 7801 parameters. The minimum relative L2 Error for the optimal DeepONet is 0.111 & for the optimal ANN is 0.312. Below plot shows the error decay for the optimal DeepONet and ANN.



The random periodic functions which we consider as inputs are of the following form:

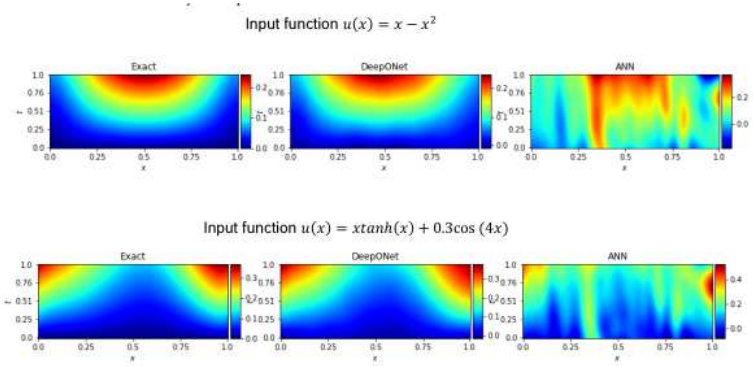
$$u(x) = \sum_{n=1}^{N} A_n \cos(nx + nlogn) + B_n \sin(nx + nlogn)$$

where A_n , B_n are random coefficients which uniquely define the input functions. N being the order of the functions.



Model trained for input functions of order 50 and tested on similar functions from order 1 to 70. The plot clearly shows that both in terms of the error and R2 score DeepONet performs better. We further test the generalizability property of DeepONets by considering two different unseen input functions. It's important to remember

we trained the model with input functions of linear combination of sinusoidal type. Here we show that the trained model can make good predictions when given input functions other than sinusoidal type like algebraic and hyperbolic as shown below. And in both cases it's shows better accuracy as compared to ANN.



Currently ANN is a popular method of choice for system identification and black box modelling, Deep Operator Networks holds a great promise as an alternative to ANN with better generalization properties. Further, this method can also be combined with Physics informed neural networks (PINNs) to form Physics informed Deep Operator networks[2] which could potentially show higher efficiency. The above results showcase the promise of this novel method of scientific machine learning for system identification. This holds a great potential for utilization for engineering and scientific applications in both industry and academia.

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Bonferroni mean-based pooling function in Convolutional Neural Networks

Pragya Gupta[1], Debashree Guha[2], Nihar Domala[3], Debjani Chakraborty[1]

[1] Department of Mathematics, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India

[2] School of Medical Science and Technology, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India

[3] Department of Electrical Engineering, Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India

In the domain of Deep Learning, Convolutional neural networks (CNNs) are used to operate the data where local feature information is applicable, such as image or video. CNN comprises convolutional layers that function consecutively over the input image data and generate feature kernels stacked together. Afterward, the pooling layer of CNNs employs the classical maximum or arithmetic mean function to suppress the convolutional layer's extracted features in the down-sampling procedure. The maximum pooling prefers sparser feature characteristics in CNNs, but arithmetic mean pooling also demonstrates adequate interpretation for some modern architectures. However, both arithmetic mean and maximum pooling functions ignore all possible dependencies between the significant data values to be reduced in the process. With this view, in this study, the classical pooling aggregation is replaced with the Bonferroni mean (BM) type aggregation function in the polling layer, which considers the conjunction between the data values and includes the pairwise contribution of significant data values required to assess the data dependency on their neighborhood information. The use of different variations of Bonferroni mean functions are analyzed, which not only consider all the characteristics of maximum and arithmetic mean functions but also model the dependencies among the data values. To empirically show the interpretation of BM aggregation in the pooling layer, experiments on various models of different complexity are performed

by choosing real and medical datasets and comparing them with the classical pooling functions. It is observed that the utilization of the BM-type pooling aggregation function outperforms most of them.

Keywords: Convolutional Neural Networks, Bonferroni mean, Pooling function

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CDS
Department of Computational and Data Sciences

DAAD
Deutscher Akademischer Austauschdienst
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