CTAC2020
The 20th Biennial Computational Techniques and Applications Conference

30th Aug–2nd Sep 2020
University of New South Wales
Sydney, NSW, Australia

CTAC2020 Conference Abstracts

Contents

Welcome

We are pleased to host the 20th Biennial Computational Techniques and Applications Conference (CTAC2020) at the School of Mathematics and Statistics of the University of New South Wales, Sydney, Australia.

Due to the current COVID-19 pandemic, CTAC2020 this year will be conducted online via Zoom. There will be 8 invited talks, 81 contributed talks and 131 registered participants from Australia and overseas (USA, U.K., Canada, Italy, France, Japan, Netherlands, Austria, Poland, Germany, Norway, Nepal, India, Turkey, Kuwait, Nigeria) for the conference. Thank you to all invited speakers, contributed speakers, hosts and chairs of the sessions, members of scientific committee and members of the local organising committee that make the conference possible.

CTAC is organised by the special interest group in computational techniques and applications of ANZIAM, the Australian and New Zealand Industrial and Applied Mathematics Division of the Australian Mathematical Society. The meeting will provide an interactive forum for researchers interested in the development and use of computational methods applied to engineering, scientific and other problems. The CTAC meetings have been taking place biennially since 1981, the most recent being held in 2018 in Newcastle. Further information on past CTAC conferences can be found at https://www.anziam.org.au/Computational+Mathematics+Group.

A refereed proceedings will be published after the conference in the Electronic Supplement of the ANZIAM Journal. This will be subject to the usual rigorous ANZIAM J. refereeing process.

We hope you will enjoy the conference and meet many interesting colleagues.

The CTAC2020 organizing committee.

Sponsors

- School of Mathematics and Statistics, University of New South Wales, Sydney, Australia.
- The New South Wales Government.
- The Modelling and Simulation Society of Australia and New Zealand.
- The Mathematics of Computation and Optimisation (MoCaO), a special interest group of AustMS.

Committees

- Organising Committee

Member	Affiliation
Bishnu Lamichhane	University of Newcastle
Josef Dick	University of New South Wales
Ngan Le	Monash University
Quoc Thong Le Gia (chair)	University of New South Wales
Shev MacNamara	University of Technology Sydney
William McLean	University of New South Wales
Vera Roshchina	University of New South Wales
Thanh Tran	University of New South Wales

- Scientific Committee

Member	Affiliation
Steve Armfield	University of Sydney
Jerome Droniou	Monash University
Frances Kuo	University of New South Wales
Markus Hegland	Australian National University
Stephen Roberts	Australian National University
Ian H. Sloan (chair)	University of New South Wales
Ian Turner	Queensland University of Technology

Information

Conference venue

The conference will be hosted online on Zoom by the School of Mathematics and Statistics at the University of New South Wales, Sydney, Australia.

Presentations

All talks are 20 minutes long, plus 5 minutes for questions and discussion. The talks will be given online via Zoom. The session chair will give you a signal via the chatbox when you have 5 minutes remaining. Please do not exceed your time.

Zoom rooms

- Please check your email or email `mailto:ctac2020@unsw.edu.au`.

Student prizes

- The Modelling and Simulation Society of Australia and New Zealand is sponsoring an award for the best student presentation relating to modelling at CTAC2020. This prize will include free registration to the MODSIM2021 conference to be held in Sydney in December 2021.
- A prize worth A$500 sponsored by the Mathematics of Computation and Optimisation (MoCaO) special interest group of AustMS will be offered for the best student presentation.
- The co-ordinator for both prizes is Barry Croke (ANU).

Social events

On Sunday evening we will have virtual welcome reception at 18:00 Sydney time. If you are not familiar with Zoom, this is an excellent opportunity to get yourself comfortable with the software.

Sydney time vs. other time zones

Sydney	New Delhi	Tokyo	London	Paris/Vienna	New York	Los Angeles
09:00	04:30	08:00	00:00	01:00	19:00(-1)	16:00(-1)
10:00	05:30	09:00	01:00	02:00	20:00(-1)	17:00(-1)
11:00	06:30	10:00	02:00	03:00	21:00(-1)	18:00(-1)
12:00	07:30	11:00	03:00	04:00	22:00(-1)	19:00(-1)
13:00	08:30	12:00	04:00	05:00	23:00(-1)	20:00(-1)
14:00	09:30	13:00	05:00	06:00	00:00	21:00(-1)
15:00	10:30	14:00	06:00	07:00	01:00	22:00(-1)
16:00	11:30	15:00	07:00	08:00	02:00	23:00(-1)
17:00	12:30	16:00	08:00	09:00	03:00	00:00
18:00	13:30	17:00	09:00	10:00	04:00	01:00

Program

Sunday August 30th, 2020

17:30–18:00	How to use Zoom (a short tutorial for hosts and chairs) Zoom A
18:00–19:00	Welcome reception Zoom A

- The full conference program is listed in the next 3 pages, using Sydney time (Australian Eastern Standard Time).
- Please click on the speaker names to see the full title and abstract of the talk. If a name is emphasised, the speaker is a PhD student.
- At the end of the abstract, please click on the day (Monday/Tuesday/Wednesday) to go back to the conference program.
- The host of each session is responsible to start the Zoom meeting while the chair controls the schedule of the speakers and Q&A in the session.

Monday August 31st, 2020			
8:50–9:00	Opening by Bruce Henry (Zoom A)		
9:00–10:00	David Harvey - invited lecture Fast Fourier transforms of prime length Chair: Thong Le Gia Host: Lindon Roberts (Zoom A)		
	(Zoom A)	(Zoom B)	(Zoom C)
	Modelling Chair: Host: Thong Le Gia	Optimisation Chair: Vera Roshchina Host: Bill McLean	Fluid Dynamics Chair: Kenneth Duru Host: Josef Dick
10:00–10:25	Judy Bunder	Lourenço Bruno	*Nicholas Buttle*
10:25–10:50	John Maclean	Matthew Tam	*Aleksandar Badza*
10:50–11:15	Muhammad Shuaib Khan	*Vinesha Peiris*	*Joshua Hartigan*
11:15–11:40	Steven Psaltis	Lindon Roberts	Sudhir Singh
11:40–11:55	Morning tea		
	Modelling Chair: Rob Womersley Host: Thong Le Gia	Computational Math Chair: Kenneth Duru Host: Bill McLean	Approximation theory Chair: Markus Hegland Host: Josef Dick
11:55–12:20	Garry Newsam	*Luning Sun*	*Neil Dizon*
12:20–12:45	Simon Watt	Rimple Sandhu	*Manoj Kumar Palani*
12:45–13:45	Lunch		
	Modelling Chair: Kenneth Duru Host: Thong Le Gia	Computational Math Chair: Lindon Roberts Host: Bill McLean	Optimisation Chair: Matthew Tam Host: Josef Dick
13:45–14:10	*Solene Hegarty-Cremer*	Vivien Challis	Vera Roshchina
14:10–14:35	Ryan Murphy	*Riya Aggarwal*	Hoa Bui
14:35–15:00	*Tamara Tambyah*	*Layth Awin*	*Dinh Tran*
15:00–15:25	Paul Manuel	*Suleyman Cengizci*	Reinier Diaz Millan
15:25–16:00	Afternoon tea		
	Computational Math Chair: Kenneth Duru Host: Thong Le Gia	Computational Math Chair: Lindon Roberts Host: Bill McLean	Others Chair: Matthew Tam Host: Josef Dick
16:00–16:25	*Saleh Almuthaybiri*	*Abdul Hussain*	Chet Bahadur Adai Magar
16:25–16:50	*Michael Rehme*	*Suleyman Cengizci*	Francesco Strati
17:00–18:00	Aretha Teckentrup - invited lecture Convergence of Gaussian process emulators with estimated hyper-parameters Chair: Josef Dick Host: Thong Le Gia (Zoom A)		

19:00–20:00	Trevor McDougall - Public lecture Some mathematical aspects of physical oceanography Chair: Ian Sloan Host: Thong Le Gia (Zoom A)

Tuesday Sep 1st, 2020			
9:00–10:00	Kate Smith-Miles - invited lecture In search of algorithmic trust ... show us the stress-testing! Chair: Markus Hegland Host: Vera Roshchina Zoom A		
	(Zoom A)	(Zoom B)	(Zoom C)
	Computational Math Chair: Vera Roshchina Host: Thong Le Gia	Computational Math Chair: Markus Hegland Host: Bill McLean	Computational Math Chair: Matthew Tam Host: Josef Dick
10:00–10:25	*Andre Aquino*	Santiago Badia	Tiangang Cui
10:25–10:50	*Gleb Shabernev*	*Xifu Sun*	Arbaz Khan
10:50–11:15	Anju Chaurasia	Kenneth Duru	*Yuancheng Zhou*
11:15–11:40	Jerome Droniou	*Lishan Fang*	Abhijit Sarkar
11:40–11:55	Morning tea		
	Computational Math Chair: Vera Roshchina Host: Thong Le Gia	Computational Math Chair: Santiago Badia Host: Bill McLean	Computational Math Chair: Tiangang Cui Host: Josef Dick
11:55–12:20	*Christopher Williams*	Libo Feng	Zhongjian Wang
12:20–12:45	*Fillipe Georgiou*	*Benjamin Maldon*	Zhizhang Wu
12:45–13:45	Lunch		
	Computational Math Chair: Shev MacNamara Host: Thong Le Gia	Computational Math Chair: Santiago Badia Host: Bill McLean	Engineering Computations Chair: Tiangang Cui Host: Josef Dick
13:45–14:10	Bishnu Lamichhane	Ziad Ghauch	Yuka Hashimoto
14:10–14:35	Dave Lee	Thai Nhan	Jordan Pitt
14:35–15:00	Nathan March	*Roman Khotyachuk*	*Jordan Shaw-Carmody*
15:00–15:25	Hanz Martin Cheng	Markus Hegland	*Kenny Wiratama*
15:25–16:00	Afternoon tea		
	Computational Math Chair: Shev MacNamara Host: Thong Le Gia	Computational Math Chair: Santiago Badia Host: Bill McLean	Computational Math Chair: Matthew Tam Host: Josef Dick
16:00–16:25	Marcin Jurkiewicz	James Nichols	*Riley Whebell*
16:25–16:50	Vanenchii Peter Ayoo	*Matthew Colbrook*	Michele Ruggeri
17:00–18:00	Catherine Powell - invited lecture Adaptive & Multilevel Stochastic Galerkin Methods for PDEs with Uncertain Inputs Chair: Stephen Roberts Host: Shev MacNamara (Zoom A)		

18:30–19:30	Virtual conference dinner (Zoom A)

Wednesday September 2nd, 2020			
9:00–10:00	Alex Townsend - invited lecture The ultraspherical spectral method Chair: Bill McLean Host: Thong Le Gia (Zoom A)		
	(Zoom A)	(Zoom B)	(Zoom C)
	Modelling Chair: Host: Thong Le Gia	Data science Chair: Rob Womersley Host: Bill McLean	Computational Math Chair: Host: Josef Dick
10:00–10:25	Terry O'Kane	Christopher Tisdell	Masaji Watanabe
10:25–10:50	Rose Crocker	*Snigdha Mahanta*	*Khaled Mohammad*
10:50–11:15	Vassili Kitsios	Stuart Hawkins	*Michael Clarke*
11:15–11:40	Morning tea		
11:40–12:10	Discussion about CTAC proceedings Chair: Bill McLean (Zoom B)		
12:10–14:00	Lunch		
14:00–15:00	CMG meeting Chair: Bishnu Lamichhane (Zoom A)		
15:30–16:30	Konstantin Brenner - invited lecture Numerical modeling of two-phase flow in fractured porous media Chair: Jerome Droniou Host: Bill McLean (Zoom B)		
16:30–16:45	Afternoon tea		
16:45–17:45	Michael Feischl - invited lecture Numerical analysis and machine learning Chair: Thanh Tran Host: Josef Dick (Zoom C)		
17:45–18:00	Students' prizes presentation (Zoom A) Chair: Barry Croke		
18:00–18:05	Conference close		

Abstracts of invited presentations

Numerical modeling of two-phase flow in fractured porous media

Konstantin Brenner
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Understanding flow in heterogeneous, and in particular fractured porous media, is important for many industrial applications including for example oil and gas recovery, geothermal energy production, underground CO2 storage, or nuclear safety assertion. The fractured porous media are characterized by an extreme contrast of hydrodynamic properties at the interface between the fracture network and the surrounding matrix rock. For example, the fracture permeability can be several orders of magnitude greater than the permeability of the matrix. In the context of two-phase flows, the capillary pressure/saturation relation is also discontinuous across the matrix-fracture interface. Such discontinuity in the rock properties plays a key role in several important hydrogeological processes and therefore has to be accurately represented by the numerical model.

The first part of this presentation will cover some common two-phase discrete fracture models with the associated finite volume schemes. The second part of the talk deals with the systems of nonlinear equations resulting from the discretization. Due to the stiff nonlinear terms arising at the matrix-fracture interface, the standard Newton's method is likely to break down. We will see how to improve the robustness and efficiency of the nonlinear solver by means of some relatively simple nonlinear preconditioning.

Wednesday 14:30–15:30 Zoom B

Numerical analysis and machine learning

Michael Feischl
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We illustrate the interaction between machine learning and numerical analysis in two examples: First, we show that a certain type of neural network can be trained to emulate optimal adaptive mesh refinement strategies for finite element methods. The network takes the current mesh and the approximate solution as an input and outputs information on where the mesh needs to be refined in order to decrease the approximation error of the finite element method in an optimal way. The result applies even to problems, for which no optimal classical mesh refinement strategy is currently known. Second, we propose a new method to train machine learning algorithms using data compression via quasi-Monte Carlo. The idea is to approximate the goal functional of the optimization algorithm by a quasi-Monte Carlo sum. Under certain assumptions, this allows us to construct an approximate goal functional, which can be evaluated with cost depending only on the desired accuracy but not on the number of data points.

Wednesday 15:30–16:30 Zoom C

Fast Fourier transforms of prime length

David Harvey
School of Mathematics and Statistics
University of New South Wales, Sydney, Australia
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Joris van der Hoeven and I recently proposed a new method for multiplying large integers that is asymptotically faster than all previously known algorithms for this problem. One of the main ingredients is a new technique for evaluating complex discrete Fourier transforms of prime length. This technique, which we call *Gaussian resampling*, is closely related to the Dutt-Rokhlin algorithms for transforms of non-equispaced data. In theory, Gaussian resampling gains a constant factor in time complexity compared to existing algorithms for transforms of prime length, such as Bluestein's algorithm and Rader's algorithm. In this talk, I will give an overview of all of these algorithms and mention a few open questions.

Monday 09:00–10:00 Zoom A

Some mathematical aspects of physical oceanography

Trevor McDougall
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University of New South Wales, Sydney, Australia
URL: https://research.unsw.edu.au/people/scientia-professor-trevor-mcdougall

The ocean's role in climate and climate change will be outlined, since these are the principle reasons for the need to better understand the physics of the ocean. The talk will then move onto some mathematical aspects of physical oceanography, and some puzzles that we are yet to figure out. One of the surprising things about the ocean is that mixing processes occur quasi-horizontally at a rate ten million times faster than vertically, and yet the vertical mixing processes are still vitally important for climate predictions. Also, the "density" surfaces along which the strong lateral mixing occurs are notoriously hard to define, both conceptually and numerically. These on-going puzzles will be described, along with a couple of recent advances we have published in (i) data interpolation, and (ii) an improvement to Newton's Method.

Monday 19:00–20:00 Zoom A

In search of algorithmic trust ... show us the stress-testing!

Kate Smith-Miles
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University of Melbourne, Australia
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Society is increasingly dependent on computational algorithms to drive decision making. But establishing trustworthiness of algorithms in the minds of skeptical humans is a challenge that relies on improvements in transparency and elimination of any perception of bias. Our trust is earned, or easily destroyed, when we test an algorithm's performance on instances with known expected responses. If an algorithm obtains reliable results for enough test instances, then we are likely to feel comfortable with its decision-making ability; if it produces poor responses for even just a few critically chosen instances, then it will be dismissed quickly as unreliable and therefore untrustworthy (and certainly not publishable!) The choice of test instances is clearly critical to gaining trust, but their quality and sufficiency is rarely examined comprehensively, with each study usually inheriting a collection of benchmarks from previous studies. Recent advances in Instance Space Analysis has now enabled the adequacy of test instances to be established, with consideration of key instance properties – diversity, unbiasedness, discriminatory power and real-world-likeness –offering visual evidence that gives confidence that an algorithm has been "stress-tested" under the widest range of scenarios. In this talk we revisit some prior work on algorithms for facial age estimation, but now from a new perspective offered by our Instance Space Analysis. The looming ethical implications of algorithms in fields such as image analysis will also be discussed, further justifying the urgency for methodologies to establish trustworthy algorithms.

Tuesday 09:00–10:00 Zoom A

Adaptive & Multilevel Stochastic Galerkin Methods for PDEs with Uncertain Inputs.

Catherine Powell
Department of Mathematics
University of Manchester, U.K.
URL: https://personalpages.manchester.ac.uk/staff/Catherine.Powell/

In this talk we will discuss recent advances in stochastic Galerkin approximation, a popular computational technique for performing forward uncertainty quantification (UQ) in PDE models with uncertain inputs. Starting with a standard scalar elliptic test problem, we describe in general terms, a strategy for performing a posteriori error estimation which can be used to drive adaptive solution algorithms with rigorous error control. We then demonstrate improvements in convergence that can be achieved using a so-called multilevel construction of the underlying approximation space. In the second part, we discuss how the computational methodology can be extended to more challenging physical models consisting of systems of PDEs, such as mixed formulations of linear elasticity problems with uncertain Young's modulus. Here, the right choice of norm is crucial. Working with the natural weighted norm with respect to which the weak problem is stable leads to an error estimator, as well as a solver for the associated discrete problems, that is robust in the incompressible limit.

Tuesday 17:00–18:00 Zoom A

Convergence of Gaussian process emulators with estimated hyper-parameters.

Aretha Teckentrup
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University of Edinburgh, U.K.
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We are interested in the task of estimating an unknown function from data given as a set of point evaluations. In this context, Gaussian process regression is often used as a Bayesian inference procedure, and we are interested in the convergence as the number of data points goes to infinity. Hyper-parameters appearing in the mean and covariance structure of the Gaussian process prior, such as smoothness of the function and typical lenght scales, are often unknown and learnt from the data, along with the posterior mean and covariance. We work in the framework of empirical Bayes, where a point estimate of the hyper-parameters is computed, using the data, and then used within the standard Gaussian process prior to posterior update. Using results from scattered data approximation, we provide a convergence analysis of the method applied to a fixed, unknown function of interest.

Monday 17:00–18:00 Zoom A

The ultraspherical spectral method

Alex Townsend
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Pseudospectral methods, based on high degree polynomials, have spectral accuracy when solving differential equations but typically lead to dense and ill-conditioned matrices. The ultraspherical spectral method is a numerical technique to solve ordinary and partial differential equations, leading to almost banded well-conditioned linear systems while maintaining spectral accuracy. In this talk, we introduce the ultraspherical spectral method and develop it into a spectral element method using a modification to a hierarchical Poincaré-Steklov domain decomposition method.

Wednesday 09:00–10:00 Zoom A

Abstracts of contributed presentations

Unified Methodology For Cloud Storage Providers' APIs

Chet Bahadur Adai Magar
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Many cloud users do not bother to register for the premium plans to get unlimited access to their storage services. We design and implement a unified API for cloud storage providers such as Dropbox, Google Drive and One Drive for resolving the issue of limited storage problem. We perform two experiments. We develop a simple web app that will be connected to all three cloud storage providers. Second experiment is the development of a core API enabling the storage functionality in all of the three drives. Both methodologies enable us uploading of the files on all of these drives or any one of them. If one service provider's server is down then we can upload and retrieve our files from the other storage service provider available via that unified API. PHP core language is used to develop the unified API. The results of the preferred approach are also justified by using the most accurate and open source tool J-meter enabling the validation of this research. Both methodologies results will be compared and conclusion will be directed with respect to the performance factor of the both methodologies. In this study, we highlight that how our research can be directed towards the future work of this study.

Monday 16:00 Zoom C

Bragg Edge Neutron Transmission Strain Tomography

Riya Aggarwal
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A wavelength resolved measurement technique used in neutron imaging applications is known as energy-resolved neutron transmission imaging. This technique of reconstructing residual strain maps is now a means for providing high spatial resolution measurements of strain distribution in the polycrystalline materials from the sets of Bragg edge measurement images. A comparison between the strain field reconstructions with different finite element meshes, i.e., triangular and quadrilateral, where neutron transmission revolves around the inversion of Longitudinal Ray Transform, which has uniqueness issues. We approach the reconstruction in the proposed algorithm via a least square method.

Monday 14:10 Zoom B

Sharper Existence and Uniqueness Results for Solutions to Third-Order Boundary Value Problems

Saleh Almuthaybiri
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The existence and uniqueness of solutions to third-order ordinary differential equations that are subjected to two- and three-point boundary conditions are obtained. The advancement is achieved in the following ways. Firstly, we provide sharp and sharpened estimates for integrals regarding various Green's functions. Secondly, we apply these sharper estimates to problems in conjunction with Banach's fixed point theorem. Thirdly, we apply Rus's contraction mapping theorem in a metric space, where two metrics are employed. Our new results improve a recent work of Smirnov by showing that a larger class of boundary value problems admit a unique solution.

The Youtube link for the presentation is https://www.youtube.com/watch?v=9NdS2K7kvWc.

Monday 16:00 Zoom A

Numerical Model To Investigate The Flow Instability Linked To Tiger-Striping In Inkjet Printers

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The existence of a flow instability in the print zone of inkjet printers induces a spatial-temporal periodic printing pattern known as tiger-stripes or wood-grain that is associated to the misplacement of satellite droplets. This flow instability is observed under specific conditions, but recurrent at elevated pen-to-paper spacing (PPS). The characteristics of this flow condition is relatively unknown, raising a major issue for the printing industry. A numerical methodology based on an average body-force approach rather than discrete phase modelling (DPM) is proposed here to characterize the vortex instability in a two-dimensional domain. A verification study that includes mesh and time-step independence analyses as well as boundary conditions set up is discussed. The predominant flow features existent within the printing zone are characterized and linked to the tiger-striping problem

Tuesday 10:00 Zoom A

Numerical Investigation Of Fountain Start-Up

Layth Awin
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Fountains are formed when the momentum of a jet is opposed by a buoyancy force. In the case of a rising jet, it penetrates to its maximum height and then forms a falling counterflow that surrounds the negatively buoyant rising jet and further decreases its momentum. This investigation examines the start-up of the rising jet before the returning counterflow is formed. A rectangular cube domain with open side and top boundaries, and a round jet source located at the centre of the otherwise impervious bottom boundary, is specified. The height of the domain is chosen to be less than the fountain penetration height, and the jet exits the domain through the upper boundary without the formation of a return flow. The governing Navier-Stokes equations, are normalised and solved by a finite volume method using the ULTRA-QUICK discretisation for the advection terms and standard second-order discretisations for all other spatial terms. Time integration uses the second-order Adams-Bashforth method for advection terms and Crank-Nicolson for the viscous terms, with the pressure obtained by enforcing continuity via a pressure correction approach. The numerical simulations for turbulent flow were performed on a computer cluster and obtained at three Froude numbers, Fr=10, Fr=20, Fr=30, at one Reynolds number, Re=2500. Results for entrained volume fluxes and centerline velocity are compared and analyzed to identify Fr based scaling relations.

Monday 14:35 Zoom B

Solution Of Systems Of Disjoint Fredholm-Volterra Integro-Differential Equations Using Bezier Curve Control Points

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Systems of disjoint Fredholm-Volterra integro-differential equations and the Bezier curves control-point-based algorithm are considered. Systems of two, three and four Fredholm-Volterra integro-differential equations are solved using the developed algorithm and convergence analysis for the Bezier curves method is also presented. The examples considered show the accuracy and efficiency of the proposed method.

Tuesday 16:25 Zoom A

H-Adaptive Unfitted Finite Element Methods

Santiago Badia
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A frequent hurdle in numerical simulation pipelines is the generation of meshes conforming to the geometry of the domain of analysis (a.k.a. body-fitted meshes). Current body-fitted mesh generators cannot scale up to a large number of CPUs and, often, require manual work to tune parameters. As a result, mesh generation is estimated to make 80main idea is to embed the complex physical domain into an artificial background domain with simple geometry. The background domain can then be efficiently meshed with, e.g., Cartesian grids. Adding to this setting a strategy to deal with the cells cut by the physical domain allows one to perform the analysis on the physical domain using a simple background mesh.

Even though unfitted methods circumvent the mesh generation bottleneck, they are prone to serious ill conditioning problems. The most prominent cause is the so-called small cut cell problem, arising when the condition number depends on the characteristic size of the cut cells. Small cuts can lead to arbitrarily high condition numbers and preclude efficient use of iterative Krylov methods and, thus, practical usage of unfitted methods for realistic large scale applications. To avoid this issue in the context of finite elements, we consider the aggregated unfitted finite element method, referred to as AgFEM. The technique is based on constructing enhanced finite element spaces by cell aggregation; shape functions on small cut cells are removed by enforcing suitable algebraic constraints. AgFEM has been introduced for elliptic [2] and Stokes [3] PDEs. For these problems, it retains good properties of standard finite element methods, independent on cut location, and exhibits good parallel performance and scalability on both uniform [4] and tree-based meshes.

This work presents the extension of AgFEM to interface elliptic boundary value problems. The Nitsche method is used to approximate the problem, whereas independent cell aggregation schemes are carried out at each subdomain to remove ill-posed degrees of freedom. Mathematical analysis proves well-posedness, approximation properties and a priori error estimates analogous to standard finite elements. Numerical experiments assess optimality and robustness of the method on tree-based meshes, regardless of cut location and material contrast. Good scaling properties are also retained.

References

[1] J A Cottrell, T J R Hughes, and Y Bazilevs. Isogeometric analysis: toward integration of CAD and FEA. Wiley, 2009.

[2] S Badia, F Verdugo, and A F Martín. The aggregated unfitted finite element method for elliptic problems. Comput Meth Appl Mech Engrg, 336, 533–553, 2018.

[3] S Badia, A F Martín, and F Verdugo. Mixed aggregated finite element methods for the unfitted discretization of the Stokes problem. SIAM Journal on Scientific Computing 40 (6), B1541–B1576, 2018.

[4] F Verdugo, A F Martín, and S Badia. Distributed-memory parallelization of the aggregated unfitted finite element method. Comput Meth Appl Mech Engrg, 357, 112583, 2019.

Tuesday 10:00 Zoom B

Sensitivity of Lagrangian Coherent Structure Detection Techniques To Numerical Noise or Uncertainty

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In two dimensional flow systems, Lagrangian coherent structures are objects which give an intrinsic idea into the general flow behaviour of a dynamic velocity system. These structures can take the form of one-dimensional flow barriers located along ridges where particle advection capability is much stronger, or two-dimensional shapes within which particle flow is more consistent. Many methods have been developed for generating these structures within various flow systems and in-depth evaluations of the functionality of these methods have been undertaken by several researchers. However, very few of these studies have examined the impact of numerical noise or uncertainty present within dynamic velocity data on the results produced by these methods. Hence for this talk, I shall briefly define four deterministic methods of Lagrangian coherent structure detection, and illustrate how these methods respond to the application of artificial stochastic noise to simulated computational fluid dynamics data.

Monday 10:25 Zoom C

Consistent Error Bounds And Convergence Rates In Convex Feasibility Problems

Lourenço Bruno
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We discuss the notion of consistent error bound functions, which provides a framework for the study of error bounds for convex feasibility problems (CFPs), especially in settings where constraint qualifications may fail to hold. Our main result is that the convergence rates of several algorithms for CFPs can be obtained directly from the underlying error bound function. Applications to conic feasibility problems will also be shown, where we establish further links between the singularity degree of the problem and the convergence rates of a number of algorithms. This is a joint work with Tianxiang Liu (RIKEN-AIP) and the preprint is available at Optimization Online: `http://www.optimization-online.org/DB_HTML/2020/07/7920.html`

Monday 10:00 Zoom B

Necessary Conditions for Non-Intersection of Collections of Sets

Hoa Bui
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We study elementary non-intersection properties of collections of sets, making the core of the conventional definitions of extremality and stationarity. In the setting of general Banach/Asplund spaces, we establish new primal (slope) and dual (generalized separation) necessary conditions for these non-intersection properties. The results are applied to convergence analysis of alternating projections.

Monday 14:10 Zoom C

Equation-Free Self-Adjoint Macroscale Modelling of Heterogeneous Diffusion

Judy Bunder
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Equation-free macroscale modelling is a systematic and rigorous computational methodology for efficiently predicting the dynamics of a microscale system at a desired macroscale system level. In this scheme, the given microscale model is computed in small patches spread across the space-time domain, with patch coupling conditions bridging the unsimulated space. The accuracy of the equation-free macroscale modelling is primarily dependent on the choice of patch coupling conditions. Recent work has developed a new patch coupling scheme which preserves translational invariance, rotational invariance, and self-adjoint symmetry, thus guaranteeing that conservation laws associated with these symmetries are preserved in the macroscale simulation. Here we discuss the accuracy of the equation-free modelling scheme in the context of heterogeneous diffusion.

Monday 10:00 Zoom A

Comparison Of Experimental And Numerical Ship Wakes Using Time-Frequency Analysis

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Ship wakes are the three-dimensional, V-shaped patterns generated by surface piercing objects moving on the surface of a fluid. These wakes are characterised by their relative composition of transverse waves, which travel in the same direction as the ship, and divergent waves, which travel at an angle to the ship. Analysis of the wakes generated by differently shaped vessels moving at different speeds is of interest, and a question is what amount of data needs to be collected. For example, accurately capturing the height of the surface of the fluid in the entire region of the waves is expensive in simulation and impractical in experiment. An alternative is to record just the time series of surface height values using a sensor fixed at a stationary point in space as the ship travels past. These time-dependent signal data can be analysed using windowed fast-Fourier transforms to extract the time-dependent frequencies of the waves that travel past the sensor. We use linear thin-ship theory to generate numerical signals and compare to experimental signals obtained for some simple hulls, and investigate the agreement between features predicted by the theory and those observed in practice.

Monday 10:00 Zoom C

A SUPG Formulation for Solving a Class of Singularly Perturbed Steady Problems in 2D

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Co-authors: Ömür Uğur (Middle East Technical University), Natesan Srinivasan (Indian Institute of Technology Guwahati).

In this presentation, approximate solutions of singularly perturbed partial differential equations are examined. It is a well-known fact that the standard Galerkin finite element method (GFEM) experiences some instability problems in obtaining accurate approximations to the solution of convection-dominated equations. Therefore, in this work, the Streamline-Upwind/Petrov-Galerkin (SUPG) method is employed to overcome the instability issues for the numerical solution of these kinds of problems. Furthermore, the stabilized scheme is supported by a shock-capturing technique. Two numerical experiments are provided to compare the results obtained by the GFEM and SUPG methods.

Monday 15:00 Zoom B

A Streamline-Upwind/ Petrov-Galerkin Formulation For Supersonic and Hypersonic Flow Simulations

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In this talk, we deal with a simplified version of chemically reactive multi-species hypersonic flow around a cylinder. For this purpose, it is assumed that the flow environment only consists of nitrogen gas (N_2), and no chemical reaction takes place in the flow field. Furthermore, the flow is assumed to be inviscid. A stabilized method is needed to prevent the numerical oscillations caused by the advection terms in the governing equations. Beyond that, a shock-capturing method is needed to obtain good solution profiles at the shocks. In this study, we use the compressible-flow Streamline-Upwind/Petrov-Galerkin method, complemented with the $YZ\beta$ shock-capturing. The zero-normal-velocity condition on the cylinder is enforced weakly. Numerical simulations are carried out in the FEniCS ecosystem for both supersonic and hypersonic freestream conditions.

Monday 16:25 Zoom B

Using Numerical Homogenisation To Understand The Anisotropic Elastic Properties Of A 3D-Printed Titanium Alloy

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Due to their low Young's Modulus, high strength and suitability for additive manufacturing, non-toxic beta-type titanium alloys are emerging as next-generation biomaterials. In this talk, I'll outline how we have used numerical homogenisation to explain the anisotropic elastic properties of selective laser melted Ti-24Nb-4Zr-8Sn. Selective laser melting (SLM) is an additive manufacturing (or 3d printing) process where metal powder is melted by a laser to make parts in a layer-by-layer fashion. Experimental electron backscatter diffraction measurements of the SLM manufactured Ti-24Nb-4Zr-8Sn were used to generate an appropriate finite element model. Our elastic homogenisation results qualitatively matched the measured anisotropic Young's modulus remarkably well.

This was joint work between computational mathematicians and materials engineers.

Monday 13:45 Zoom B

Hyperbolic spline approach to the solution of third-order boundary value problems

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A variety of problems are converted in boundary value problems for third order differential equations such as in physical oceanography, in the frame work of variational inequality theory, in the deflection of a curved beam, a three-layer beam, electromagnetic waves and so on. In this article, a novel numerical method, based on hyperbolic splines is presented to find the approximation to the solution of third order boundary value problems. Convergence of the method is also discussed to show the accuracy of the scheme. Numerical examples demonstrate the efficiency and validity of developed approach.

Tuesday 10:50 Zoom A

A Generalised Complete Flux Scheme For Anisotropic Advection-Diffusion Equations

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In this talk, we consider separating the discretisation of the diffusive and advective fluxes in the complete flux scheme. This allows the combination of several discretisation methods for the homogeneous flux with the complete flux (CF) method. In particular, we explore the combination of the hybrid mimetic mixed (HMM) method and the CF method, in order to utilize the advantages of each of these methods. The usage of HMM allows us to handle anisotropic diffusion tensors on generic polygonal (polytopal) grids; whereas the CF method provides a framework for the construction of a uniformly second order method, even when the problem is advection dominated.

Tuesday 15:00 Zoom A

Random Domains for Elliptic PDE's - the Shape Derivative Approach

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The role of uncertainty quantification has grown in scope and relevance particularly as it pertains to the theory of PDE's. One avenue of application involves the stochastic perturbation of the domain or boundary thereof, by way of a diffeomorphic mapping or perturbation method. In this work we take the Eulerian mapping approach which induces small $\mathcal{O}(\varepsilon)$ perturbations of the boundary ∂D_ε of our domain D. The goal is to examine the behaviour of the solutions as a function of their "shape derivatives" which relates to the concept of Lie derivatives for tensors in differential geometry. We derive the "shape-Taylor" expansion of the solution and corresponding weak and strong formulations for these derivatives. Ultimately, we can determine stastically meaningful quantities such as expectation, variance and two-point correlation via Karhunen-Loève expansions. This talk will focus on the background and general steps towards preliminary theoretical results, which will subsequently form the basis of future numerical investigations.

Wednesday 10:50 Zoom C

How To Compute Spectra With Error Control

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Computing and approximating spectra of operators (the generalisation of eigenvalues) is fundamental in the sciences, with wide-ranging applications in condensed-matter physics, quantum mechanics and chemistry, statistical mechanics, etc. However, the infinite-dimensional problem is notoriously difficult. While there are algorithms that in certain cases converge to the spectrum, no general procedure is known that (a) always converges and (b) provides bounds on the errors of approximation. This may lead to incorrect simulations in applications. It has been an open problem since the 1950s to decide whether such reliable methods exist at all.

We affirmatively resolve this question, and the algorithms provided are optimal, realising the boundary of what digital computers can achieve. The algorithms work for discrete operators and operators over the continuum such as PDEs. Moreover, they are easy to implement and parallelise, offer fundamental speed-ups, and allow problems that before, regardless of computing power, were out of reach. One surprising consequence is that the problem of computing spectra of compact operators, whose resolution has been known for decades, is strictly harder than the problem of computing spectra of Schrödinger operators on $L^2(R^d)$, which was open for more than half a century. Results are demonstrated on difficult problems such as the spectra of quasicrystals.

This algorithm forms part of a new class of algorithms that solve longstanding computational spectral problems for the first time, such as: computing spectra with error control; spectral measures, decompositions and the functional calculus; fractal dimensions, capacity and transport properties of spectra; discrete and essential spectra; and the spectral gap problem. The discussed computational problems are samples of what is likely to be a very rich classification theory, with applications beyond spectral theory.

Tuesday 16:25 Zoom B

Tackling Chaos In Geophysical Models Using Lagrangian Coherent Data Assimilation

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Data Assimilation (DA) is a key technique, primarily used in numerical weather prediction, which incorporates observational data into model forecasts to improve the computational modelling of dynamical systems. A key issue in using DA to make predictions about large-scale geophysical systems is that often both model and data exhibit chaotic, turbulent behaviour, severely impacting the prediction error. The topic of this talk is a very recent area of DA which attempts to incorporate Lagrangian Coherent Structures into DA schemes to tackle the issues associated with chaotic behaviour in geophysical models. Lagrangian Coherent Structures are objects frequently used in atmospheric and oceanographic modelling to track persistent, time-dependent fluid structures in complex flows.

I will give a brief introduction to DA in the context of geophysical models and how researchers have attempted to use Lagrangian Coherent Structures within DA schemes to improve predictive capabilities in challenging flow regimes. I will also discuss my own results using Lagrangian Coherent Structures within DA schemes to predict parameters in chaotic regimes of Rossby Wave Flow.

Wednesday 10:25 Zoom A

A Deep Inverse Rosenblatt Transformation Approach For Uncertaity Quantification

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Uncertainty quantification in many variables is a pressingly needed task, but the computation of desired quantities of interest involves a notoriously difficult high-dimensional integration over some intractable probability densities. Function approximations, in particular low-rank tensor product decompositions, have become popular for reducing this computational cost down to linear scaling in the number of variables.

However, tensor approximations rely on weak (in a certain sense) correlations between variables, which might not be the case for probability density functions in many practical applications. We present a nested approximation framework, where a sequence of functional tensor trains and numerically monotonic inverse Rosenblatt transforms are constructed to de-correlate change of coordinates to aid tensor approximation for more difficult problems. Similarly to deep neural networks, composing many layers of this procedure can significantly expand the class of feasible density functions. We demonstrate that the resulting deep inverse Rosenblatt transforms (DIRT) can produce efficient sampling procedures for several challenging problems in PDE constrained inverse problems and dynamical systems.

This is joint work with Dr. Sergey Dolgov.

Tuesday 10:00 Zoom C

Constructions And Applications Of Non-Separable Wavelets On The Plane

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The construction of compactly supported smooth orthonormal wavelets has been recently formulated as feasibility problems. This feasibility approach to wavelet construction has been successful in reproducing Daubechies' wavelets and in building non-separable examples of wavelets on the plane. Using the feasibility approach, we further construct non-separable wavelets on the plane with near symmetry or near cardinality properties. We apply these novel non-separable wavelets in image processing including edge detection, compression, and denoising of images corrupted by Gaussian noise.

Monday 11:55 Zoom C

A Fully Discrete Exact De Rahm Sequence, With Application To Magnetostatics

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Not all models can be attacked by brute force standard numerical methods. In certain cases, even with extremely fine refinement, the numerical approximation does not converge towards the exact solution. As shown in D. Arnold's book "Finite Element Exterior Calculus" (FEEC), this is for example the case for the eigenvalue problem of the vector Laplacian with magnetic boundary conditions. Standard finite element methods do not preserve at the discrete level the exactness of the de Rahm sequence corresponding to the operators grad/curl/div. This motivated the development of FEEC, whose purpose is to design FE spaces that preserve this exactness.

FEEC is however limited to standard-shape polygonal/polyhedral elements, and presents specific challenges when going for high-order (designing suitable unisolvent degrees of freedom is not straightforward).

In this talk, we will present the principles of a novel theory, the "fully discrete de Rahm sequence" (DDR), that designs discrete polynomial exact sequences on generic polygonal and polyhedral meshes. The theory allows for arbitrary order of approximation, and is based on discrete spaces made of polynomials on the edges, faces and elements. The interpolators are only made of L^2-projectors, which enables great freedom for the practical implementation of the polynomial spaces. On hexahedra, DDR has fewer degrees of freedom than FEEC. We also show the practical application of the method to the magnetostatics equations, for which stability is established using the exactness of the DDR sequence and discrete Poincare inequality for the discrete curl and div operators.

This is a joint work with D. A. Di Pietro (Univ. Montpellier, France) and F. Rapetti (Univ. Cote d'Azur, France).

Tuesday 11:15 Zoom A

On Energy-Stable Adaptive Discontinuous Galerkin Approximations For Scattering Problems In 3D Complex Elastic Media

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We present a physics-based numerical DG flux suitable for inter-element and boundary conditions in discontinuous Galerkin approximations of first order hyperbolic PDEs. Using this physics-based numerical penalty-flux, we will develop a provably energy-stable discontinuous Galerkin approximations of the elastic wave equation in complex geometries and heterogeneous media. By construction the numerical flux is upwind and yields a discrete energy estimate analogous to the continuous energy estimate. The discrete energy estimates hold for conforming and non-conforming curvilinear elements. The ability to handle non-conforming curvilinear meshes allows for flexible adaptive mesh refinement strategies. The numerical scheme have been implemented in ExaHyPE, a simulation engine for hyperbolic PDEs on adaptive structured meshes, for exa-scale supercomputers. We will show 3D numerical experiments demonstrating stability and high order accuracy. Finally, we present a large scale regional geophysical wave propagation problem in a heterogeneous earth model with geologically constrained media heterogeneity and geometrically complex free-surface topography.

Tuesday 10:50 Zoom B

Error Indicators And Adaptive Refinement Of Discrete Thin Plate Splines

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The thin plate spline technique is a data fitting and smoothing technique that captures important patterns of potentially noisy data. However, it is computationally expensive for large data sets and impractical for many applications. The finite element thin plate spline was developed to efficiently interpolate large data sets. It combines favourable properties of the thin plate spline and finite element method and produces sparse systems of equations with sizes no longer dependent on the size of the observed data.

Current research on the finite element thin plate spline uses uniform finite element grids, which often require a fine grid to achieve a certain accuracy. This leads to a large system of equations with the high computational cost. Adaptive refinement adapts the precision of the solution and refines only in sensitive regions. This reduces the computational costs and memory requirements while still retaining the required accuracy. The error indicator is an essential part of the adaptive refinement as it identifies whether certain regions should be refined. Many error indicators have been developed in the finite element method, but they may not be applicable for the finite element thin plate spline. In this talk, I will show four error indicators that I adapted and give some convergence results.

The YouTube link to the talk is `https://youtu.be/jdaKjZ9vJ4g`.

Tuesday 11:15 Zoom B

An Investigation Of Nonlinear Time-Fractional Anomalous Diffusion Models For Simulating Transport Processes In Heterogeneous Binary Media

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In this work, we consider two of the most frequently used two-dimensional nonlinear time-fractional anomalous sub-diffusion models for simulating transport phenomena in heterogeneous binary media—a variable-order model and a generalised transport equation based on the Riemann-Liouville fractional operator. Our computational modelling framework uses a second order modified weighted shifted Grunwald-Letnikov scheme with correction terms to approximate the time-fractional derivative and nonlinear source term, together with an unstructured mesh control volume method for the spatial discretisation that accommodates the heterogeneous model properties. The resulting nonlinear system of algebraic equations is then stepped in time using an efficient Jacobian-free, Newton-Krylov solver to determine the set of discrete solution unknowns. We derive a semi-analytical solution and mass balance equation for a class of two-layered problems to evaluate the accuracy of the different computational models. A key contribution of our work is to identify the correct form of the interfacial boundary conditions to impose for the flux terms within the time-fractional framework and to illustrate the significant impact that the time-fractional indices have on the mass transfer. We show that the generalised transport model not only exhibits the correct physical solution behaviour, it produces a more accurate overall mass balance in comparison to the variable-order time-fractional model which is unable to resolve the abrupt changes in the solution behaviour at the interface between two different media having contrasting diffusivity, fractional index and source term. This finding indicates that this generalised model is an effective tool for characterising anomalous transport processes in heterogeneous systems. Finally, a series of numerical examples are presented to verify the theoretical analysis and to highlight the capability of the generalised transport model.

Tuesday 11:55 Zoom B

A Finite Volume Scheme For Partial Integro-Differential Equations

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Modelling the interactions between locusts and their environment gives rise to some interesting Partial Integro-Differential Equations (PIDE). In this talk I will present a finite volume based numerical scheme for simulating PIDE, error and computation time analysis, as well as some of the more interesting results that were obtained.

Tuesday 12:20 Zoom A

Active Local Response Surface Approximation With Polynomial Chaos Techniques

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Metamodels have proven as an efficient mean for the approximation of response surfaces of engineered systems, particularly for resource-intensive experiment design. It is oftentimes the case in applications involving nonlinear response functions that interest is focused on a specific region of the parameter space. We propose an approach for local approximation of the response surface using polynomial chaos techniques. Our approach consists of two phases: an initial heuristic solution for parameter space exploration using an approximate global polynomial chaos metamodel, followed by an active local experiment design for efficiently evaluating a response surface locally. For engineered systems embedded in high-dimensional spaces, an adapted spectral representation is exploited for reducing the dimension of the local metamodel. The proposed methodology is examined on the problem of turbulent flow around an airfoil.

Tuesday 13:45 Zoom B

High Resolution Simulations Of A Tornadic Storm Affecting Sydney

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On 16 December 2015 a severe thunderstorm with an associated tornado impacted Sydney causing widespread damage and insured losses of $205 million. Severe impacts occurred in Kurnell, with required repairs to Sydney's desalination plant, which supplies up to 15% of Sydney water during drought, not being completed until the end of 2018. Climatologically, this storm was unusual as it occurred during the morning and had developed over the ocean, rather than developing inland during the afternoon as is the case for many severe storms impacting the Sydney region. Simulations of the Kurnell storm will be conducted using the Weather Research and Forecasting (WRF) model on a triply nested domain in order to improve understanding of the environmental conditions and triggering mechanisms which led to the development of this storm, and elucidate the factors which influenced tornado development.

Monday 10:50 Zoom C

Preconditioning Technique Of Krylov Subspace Methods For Analyzing Nonlinear Dynamical Systems

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Krylov subspace methods for analyzing nonlinear dynamical systems attract attentions. The objective of these Krylov subspace methods are estimating Perron-Frobenius operators, which are linear operators describing time evolutions of dynamical systems, in RKHSs. In this talk, we propose a speed-up technique for the Krylov subspace methods for Perron-Frobenius operators in RKHSs by replacing positive definite kernels for RKHSs. In addition, we show this technique is equivalent to preconditioning the Perron-Frobenius operator by a certain linear operator.

Tuesday 13:45 Zoom C

A novel model and efficient data-driven framework for nowcasting SARS-CoV-2 transmission and impact

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Co-author: M. Ganesh (Colorado School of Mines, USA).

Compartmentalized differential equations (CDE) play a crucial role for modeling transmission of viruses, including SARS-CoV-2. Incorporating observed dynamic transmission and impact data (such as the active and recovered cases), and making the CDE models dynamic (with respect to the time-dependent data) is crucial for realistic nowcasting and forecasting of the transmission. In practice, uncertainties in the observed data are ubiquitous, and consequently it is crucial to identify and incorporate key variables that contribute to data-driven quantities of interest (QoI) in both modeling and simulation of the CDE.

In our stochastic continuous model for SARS-CoV-2 transmission and impact, uncertainties in the data-induced key variables are: detection rate; removal rate; and the basic reproduction number. Such uncertainties in our model induce uncertainties in the output stochastic process QoI (cumulative cases and deaths) modeled by the CDE system.

We develop an efficient data-driven discrete Bayesian framework to simulate our inverse stochastic continuous model. We first demonstrate (convergence and computational) efficiency of the framework using synthetic data to simulate the output QoI.

Subsequently, using several months of real COVID-19 data from several countries, we demonstrate the simulated impact of our model (by choosing several start time periods in conjunction with distinct levels of social-distancing rules) to accurately reproduce the known outcome in recent months and hence validate the efficacy of nowcasting of the pandemic.

Wednesday 10:50 Zoom B

Modelling Cell Guidance And Curvature Control In Evolving Biological Tissues

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Tissue geometry is an important influence on the evolution of many biological tissues. The local curvature of an evolving tissue induces tissue crowding or spreading, which leads to differential tissue growth rates, and to changes in cellular tension, which can influence cell behaviour. In this talk, I will present a cell-based mathematical model for the curvature control of evolving biological tissue to investigate how this control interacts with directed cell guidance mechanisms. I will first derive the mathematical model from conservation principles applied to the density of tissue synthesising cells at or near the tissue's moving boundary, and then present how the resulting partial differential equation on a moving boundary can be solved numerically using a hybrid front-tracking method called the cell-based particle method. I will illustrate how this model can be applied to understand how angled bone tissue formation may generate anisotropies in tissue material properties, as well as the role of tangential cell motion in the bone resorption process. Finally, I will present ongoing work on the application of the model to experimental bone pore infilling data available through collaboration with experimental bone biologists, and explore mechanisms which could cause irregular tissue growth behaviour.

Monday 13:45 Zoom A

Low rank approximation of positive semi-definite symmetric matrices using Gaussian elimination and volume sampling

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Positive semi-definite matrices commonly occur as normal matrices of least squares problems in statistics or as kernel matrices in machine learning and approximation theory. They are typically large and dense. Thus algorithms to solve systems with such a matrix can be very costly. A core idea to reduce computational complexity is to approximate the matrix by one with a low rank. The optimal and well understood choice is based on the singular value decomposition (SVD) of the matrix. Unfortunately, this is computationally very expensive.

Cheaper methods are based on Gaussian elimination but they require pivoting. We will show how invariant matrix theory provides explicit error formulas for an averaged error based on volume sampling and will compare them to the best error of the SVD based approach. We will then consider applications and error bounds.

Tuesday 15:00 Zoom B

Fitted Mesh B-Spline Collocation Method For Singularly Perturbed Multiple Boundary Turning Point Problems

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A singularly perturbed problem with a multiple turning point at a boundary is considered. The existence of bounds for the smooth and singular components of the analytical solution is given. These bounds are applied in the convergence analysis of the proposed B-Spline collocation scheme on fitted Shishkin mesh. Some numerical results are presented and compared with other existing methods that showed corroborating in practice the analytical values.

Monday 16:00 Zoom B

Bounds On Isolated Scattering Number

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The isolated scattering number is a parameter that measures the vulnerability of networks. This measure is bounded by formulas depending on the independence number. We present new bounds on the isolated scattering number that can be calculated in polynomial time. Furthermore, our upper bound is almost always better than the old one.

Tuesday 16:00 Zoom A

Mixed Finite Element Approximation For Poroelasticity: Deterministic And Stochastic Model

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Over the last couple of decades, models based on linear poroelasticity have attracted a lot of attention because of their applications in science and engineering. Although substantial work has been done in the engineering and mathematics communities on the formulation and numerical solution of deterministic poroelastic models, such as the Biot consolidation model, there has been little work to date on a posteriori error estimation and on stochastic modelling. The first part of this talk is to discuss some novel a posteriori error estimation for deterministic poroelastic models. The second part of this talk is to discuss a novel locking-free stochastic Galerkin mixed finite element method for a new five-field Biot consolidation model with uncertain Young's modulus and hydraulic conductivity field. Finally, we present specific numerical examples to validate the theoretical results.

The first part of this talk is joint work with Prof. David Silvester and the second part of this talk is joint work with Prof. Catherine Powell.

Tuesday 10:25 Zoom C

Poly-Exponential Weibull Distribution: Properties And Estimation

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In this research, we investigate the potential usefulness of the three parameter Poly-exponential Weibull distribution for modelling lifetime data. We obtain several mathematical properties of the Poly exponential Weibull distribution such as the expressions for the quantile function, moments, probability weighted moments, incomplete moments, Rényi and q-entropies, mean deviations, Bonferroni and Lorenz curves and the moments of order statistics. The method of maximum likelihood is used for estimating the model parameters. The Poly-exponential Weibull model has the potential to be alternatives to models currently available in the literature for modelling lifetime data, when classic distributions do not hold, and/ or when lifetime data is highly skewed.

Monday 10:50 Zoom A

Big Data And Machine Learning In Computational Fluid Dynamics

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In this work, the d3f software[1], based in the general-purpose PDE simulation software 'ug' [2], is used for numerically solving the problems from the Computational Fluid Dynamics. We have ported this software to the Spark cluster. Such a modification allowed implementing the mass parallel runs of d3f software, as well as efficient post-processing and further analysis of results using Big Data infrastructure and Machine Learning techniques. Specifically, our Spark-d3f setup used for simulation and analysis of the Elder problem [3]. For this problem, we achieved the following results.

1. We have created a tool for visual exploration of large solution sets of the Elder problem.

2. Using Principal Component Analysis from Spark MLlib, we have carefully analyzed solutions complexity with regards to time and solution types (so-called 1- and 2-fingers steady-state solutions).

3. We have developed predictive models for the Elder problem using classification methods [4]. Our models can be divided into three following types, depending on how the model's predictors (features) designed.

- Fully informed models.The models based on domain knowledge, i.e., using all possible information about the system.

- Partially informed models. The initial set of features designed using some knowledge about the system, then the feature selection techniques applied to select the most important features.

- "Black box" models. The models designed using purely data-driven approaches, i.e., without any knowledge about the system.

The best of our models are able able to predict a final state of the Elder problem (when time $t > 50$ years) with 95% of accuracy at $t = 10$ years.

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Tuesday 14:35 Zoom B

Improved Autoregressive Prediction Of Commodity Spot Prices Using Exogenous Climate Model Ensemble Forecasts Of The El Nino Southern Oscillation

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The physical and socio-economic environments in which we live are intrinsically linked over a wide range of timescales. With application to multi-year lead times, the production of certain agricultural commodities grown predominantly in tropics (e.g. coconut oil), covary with the dominant mode of climate variability in this region - the El Nino Southern Oscillation (ENSO). In the present study we develop autoregressive models with exogenous ENSO factors (ARX) for the anomalous coconut oil spot price log returns (relative change in price). We assess four types of coconut oil ARX models, using: no ENSO information as a lower bound; perfect future ENSO knowledge as an upper bound; autoregressive (AR) model of ENSO itself; and ensemble general circulation model climate forecasts of ENSO from the first generation CSIRO Climate Analysis Forecast Ensemble (CAFE) system. The climate forecasts couple together the atmosphere, ocean, and sea-ice, with their bred vector initial conditions specifically tailored to maximise forecast skill at multi-year time scales in the tropics. All econometric model coefficients are calculated from an historical period, with skill assessed in a future out-of-sample period. The lag extents of the ARX and AR models are determined by minimising measures of information entropy. ARX forecasts adopting exogenous ENSO factors outperform the econometric forecasts using no ENSO information. The most skilful forecasts of coconut oil price over multi-year lead times is produced when using the ensemble climate model forecasts of ENSO.

Wednesday 10:50 Zoom A

A Mixed Finite Element Method For The Poisson Problem Using A Biorthogonal System With Raviart-Thomas Elements

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We use a three-field mixed formulation of the Poisson equation to develop a mixed finite element method using Raviart-Thomas elements. We use a locally constructed biorthogonal system for Raviart-Thomas finite elements to improve the computational efficiency of the approach. We analyse the existence, uniqueness and stability of the discrete problem. We also develop an a posteriori error estimate for our formulation. Numerical results are presented to demonstrate the performance of our approach.

Tuesday 13:45 Zoom A

Structure Preserving Formulations For Atmospheric Simulation Using Mimetic Spectral Elements

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Structure preserving numerical methods have the potential to improve the long time statistics of climate models by mitigating against internal biases in the representation of dynamical processes. This talk will discuss spatial and temporal discretisations that satisfy the exact balance of energetic exchanges and the orthogonality of rotational and divergent flows for the rotating 3D compressible Euler equations on the sphere. This is achieved by preserving key identities of vector calculus as well as the skew-symmetric structure of the non-canonical Hamiltonian form of the equations of motion. Secondary topics essential to the efficient implementation of these methods, such as preconditioning and upwinding will also be discussed within the context of a mixed mimetic spectral element spatial discretisation, and results will be presented for the validation of these methods at both planetary and non-hydrostatic scales.

Tuesday 14:10 Zoom A

Shocking Computational Homogenization: Patch Dynamics For Heterogeneous Multiscale Problems

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We adapt the 'Equation Free' modelling approach of patch dynamics to the simulation of systems that form or contain shocks, and that exhibit strongly varying advection and diffusion terms on fine spatial scales. Our approach is tested on a modified form of the one dimensional Burgers system in which the advection and diffusion coefficients vary on both fine and coarse spatial scales, and in which the shocks that form do not conserve energy and move significantly on simulation times.

Monday 10:25 Zoom A

An $M/G/1$ Feedback Queue With Repeated Service Under N-Policy And A Random Setup Time

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An $M/(\cdot(G_1 \quad G_2))/1$ queue with general server setup time under N- policy based on the case that the arrival rates vary according to the server's status is considered. A customer can repeat the same type of service. After completion of his/her service, a customer may depart from the system for taking the service again and again till his service becomes successful. The steady-state of this system, waiting time and expected busy period has been derived for this system. Analytical results for sensitivity analysis are also obtained. The behavior of system operational cost and optimal N are also analyzed by numerical study.

Wednesday 10:25 Zoom B

Numerical Methods For Solving Fractional Diffusion Equations Used In Modelling Dye-Sensitized Solar Cells

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With an academic profile spanning three decades, dye-sensitized solar cells (DSSCs) remain a competitive option for renewable energy. Improvements to efficiency and use of cheaper materials in DSSCs warrant comprehensive mathematical modelling. In particular, fractional diffusion models uniquely capture the random walk behaviour of the TiO_2 semiconductor. We solve the fractional diffusion model for DSSCs with a finite difference method, a spatial spline collocation method and a finite element method utilising finite difference iteration in time. In addition to calculating important performance benchmarks for DSSCs we also critique these numerical methods on their accuracy and computation time.

Tuesday 12:20 Zoom B

Revisiting Path-Type Covering And Partitioning Problems

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It is true that "covering problems" are the foundation of graph theory. There are several types of covering problems in graph theory such as covering the vertex set by stars (domination problem), covering the vertex set by cliques (clique covering problem), covering the vertex set by independent sets (coloring problem), and covering the vertex set by paths and cycles. A similar concept which is "partitioning problem" is also equally important in graph theory. Lately research in these topics has produced unprecedented growth because of its various applications in engineering and science. The covering and partitioning problem by paths itself have produced a sizable volume of literature. The research on these problems is expanding in multiple directions and the volume of research papers is exploding. A path-type means a path, an induced path or an isometric path. One of the objectives is to summarize the recent developments with related techniques on these problems, classify their literature and correlate the inter-relationship among the related concepts. The main objective of this research is to display the gap and open research problems under each topic and highlight the potential research topics. This article highlights that there is a plenty of open problems in this topic. In addition, this article will save time for young researchers to choose a right research topic in this domain and it may be a reference to apply common notations and appropriate terminologies in their research articles. Among all the six problems, we observe that the most attractive and interesting problem is the path partition problem. The literature on the path partition problem is huge. The reason may be due to the Gallai-Milgram theorem and Berge's path partition conjecture. The edge version of these problems is equally popular among the researchers. In the same way, covering and partitioning by cycles or trees are other challenging research topics in graph theory.

Monday 15:00 Zoom A

A Semi-Analytical Solution Method For Two-Dimensional Time-Dependent Diffusion Problems On Block Locally-Isotropic Heterogeneous Media

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We present a new semi-analytical method for the solution of a two-dimensional, time-dependent diffusion problem on block heterogeneous media. This method involves setting the flux across each interface between adjacent blocks to be unknown functions of space and time. The solution on each block is then expressed in terms of these unknown functions. We compare our new semi-analytical method to a benchmark finite volume method for a variety of test cases.

Tuesday 14:35 Zoom A

Alternating Conditional Gradient Method for Convex Feasibility Problems

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The classical convex feasibility problem in a finite dimensional Euclidean space is studied in the present paper. We are interested in two cases. First, we assume to know how to compute an exact project onto one of the sets involved and the other set is compact such that the conditional gradient (CondG) method can be used for computing efficiently an inexact projection on it. Second, we assume that both sets involved are compact such that the CondG method can be used for computing efficiently inexact projections on them. We combine alternating projection method with CondG method to design a new method, which can be seen as an inexact feasible version of alternate projection method. The proposed method generates two different sequences belonging to each involved set, which converge to a point in the intersection of them whenever it is not empty. If the intersection is empty, then the sequences converge to points in the respective sets whose distance is equal to the distance between the sets in consideration.

Monday 15:00 Zoom C

A Multirate Accelerated Schwarz Waveform Relaxation Method

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In this talk we describe an approach which combines a multirate method and domain decomposition in space and time. This approach uses the multirate splitting provided by Savcenco's multirate method to locate an appro- priate interface for the Schwarz Waveform relaxation method. We show that this initial guess has a dramatic effect

– reducing the number of Schwarz Waveform relaxation iterations to recover the single domain solution. In fact, in many cases only one SWR iteration is required to recover the global accuracy of the solution at the final time saving a lot of work and making the Multirate Schwarz Waveform relaxation (MR-SWR) algorithm efficient. The performance of the MR-SWR algorithm can be improved by increasing the number of subdomains resulting in a multi-domain multirate Schwarz Waveform relaxation algorithm (MD-MR-SWR). A corrected variant is possible using subsequent refinements of the interfaces between the fast and slow components.

Wednesday 10:25 Zoom C

Mechanical Cell Competition In Heterogeneous Epithelial Tissues

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Mechanical cell competition is important during tissue development, cancer invasion, and tissue ageing. Heterogeneity plays a key role in practical applications since cancer cells can have different cell stiffness and different proliferation rates than normal cells. To study this phenomenon, we propose a one-dimensional mechanical model of heterogeneous epithelial tissue dynamics that includes cell-length-dependent proliferation and death mechanisms. Proliferation and death are incorporated into the discrete model stochastically and arise as source/sink terms in the corresponding continuum model that we derive. Using the new discrete model and continuum description, we explore several applications including the evolution of homogeneous tissues experiencing proliferation and death, and competition in a heterogeneous setting with a cancerous tissue competing for space with an adjacent normal tissue. This framework allows us to postulate new mechanisms that explain the ability of cancer cells to outcompete healthy cells through mechanical differences rather than by having some intrinsic proliferative advantage. We advise when the continuum model is beneficial and demonstrate why naively adding source/sink terms to a continuum model without considering the underlying discrete model may lead to incorrect results.

Monday 14:10 Zoom A

A New Over-Complete Dictionary For Radar Imaging Of Sparse Rotating Objects

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When a helicopter in flight is illuminated by a continuous wave radar, its rotating blades induce a time-varying phase change on the radar returns. The relation between the phase change and the distribution of scattering elements in the rotor can be modelled as a first kind integral equation. The associated integral operator is severely ill-conditioned; nevertheless in practice, due to the rotor's simple structure, reasonable reconstructions can be generated by algorithms that model the rotor as a sparse collection of scattering atoms drawn from an over-complete dictionary whose components are lines of isotropic point scatterers. One big drawback of such a dictionary is the lack of a closed-form expression for atom-to-atom interactions, necessitating pre-computation and storage of very large look-up tables. The paper therefore presents a new dictionary whose atoms are anisotropic point scatterers: it has the advantages of having a closed form expression for atom-to-atom interactions while also adequately approximating the scattering generated by linear structures and allowing for anisotropic scattering structures. A corollary of the derivation of the closed form expression provides an interesting extension of Graf's addition theorem for Bessel functions to arbitrary complex arguments. Finally the paper considers possible thinning's of dictionaries and associated trade-offs between the degree of thinning and the resulting increase in the size of the sparse representation of the solution.

Monday 11:55 Zoom A

The Bakhvalov Mesh: A 50 Year History And Recent Results

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In 1969, Bakhvalov introduced the first layer-adapted mesh. We look back at his phenomenal idea of the mesh construction, discuss challenges in its analysis, and answer some open questions in the numerical analysis of singularly perturbed differential equations on the Bakhvalov mesh.

Tuesday 14:10 Zoom B

Nonlinear Reduced Modelling And State Estimation Of Parametric Pdes

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We examine the problem of state estimation, that is, reconstructing the solution of a known parametric PDE from m linear measurements. When linear reduced models are used, well known results in reconstruction stability and approximation errors can be used to give bounds of overall error of state estimation. We present some new results and schemes for the deployment of nonlinear reduced models for this task, specifically models that are locally linear for disjoint partitions of the parameter domain. One challenge in this task is sensing which locally linear model to apply, given some specific measurements. Our strategy for this is to consider the residuals, and chose local linear models according to which minimizes the residual associated with the PDE. We discuss results and some interesting dual-minimization strategies for parameter estimation that arise, and present a numerical study of this strategy.

Tuesday 16:00 Zoom B

Cafe60V1: The CSIRO Climate Retrospective Analysis And Forecast Ensemble System: Version 1

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We present a large ensemble retrospective analysis of the global climate system from 1960 to present with sufficiently many realizations and at spatio-temporal resolutions suitable to enable probabilistic climate studies. Specifically, we construct 96 climate trajectories (state estimates) over the most recent six decades derived from the assimilation of satellite altimetry, sea surface temperature and sea ice observations as well as in situ ocean temperature and salinity profiles with atmospheric observations sampled from the JRA55 atmospheric reanalysis. The CSIRO Climate retrospective Analysis and Forecast Ensemble system: version 1 (CAFE60v1) employs strongly coupled data assimilation with explicit cross domain covariances between ocean, atmosphere, sea ice and ocean biogeochemistry. Atmospheric and surface ocean fields are available at daily resolution and monthly resolution for the subsurface ocean and sea ice. In addition, the CAFE60v1 reanalysis provides a complete data archive of initial conditions potentially enabling individual forecasts for all 96 members each month over the 60 year period. CAFE60v1 provides a comprehensive and unique data resource for studying internal climate variability and predictability, including the climate response to anthropogenic forcing on multi-year to decadal time scales.

Wednesday 10:00 Zoom A

Using Monte Carlo tree search to find good generating vectors of lattice rules

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In the area of numerical integration known as Quasi Monte Carlo, lattice rules are widely studied as a means to achieve small integration error. The rules themselves are determined completely by so called generating vectors, so there is an interest in methods for constructing vectors that perform well. We start with the basic theory of Quasi Monte Carlo before discussing the classical component by component construction, which is one way to produce such vectors. The techniques for improving the computational cost of this construction are also discussed. Then we introduce a new approach to constructing generating vectors for rank 1 lattice rules that is modelled on Monte Carlo Tree Search. We consider the implementation and theoretical properties of the new construction, which is followed by an application of this new method to a computational problem.

Monday 12:20 Zoom C

Generalised Rational Approximation And Its Application To Improve Deep Learning Classifiers.

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A rational approximation by a ratio of polynomial functions is a flexible alternative to polynomial approximation. In particular, rational functions approximate nonsmooth and non-Lipschitz functions accurately, where polynomial approximations are not efficient. The optimisation problems appearing in the generalised rational (not restricted to polynomials) approximation are quasiconvex, and we use this fact develop an algorithm which is simple and robust at the same time. We apply our approximation as a preprocessing step to deep learning classifiers and demonstrate that the classification accuracy is significantly improved compared to the classification accuracy of the raw signals.

Monday 10:50 Zoom B

Modified Dispersive Wave Equations

Jordan Pitt
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In this talk, I present a new numerical method for a recently discovered class of equations that describe the behavior of water waves that are fully non-linear, weakly dispersive and include an additional surface tension like term. This class of equations is of interest to the wave modelling community because the added surface tension like term can be used to improve the linear dispersion relationship or produce equations that admit smooth solutions that approximate the solutions of the shallow water wave equations. This is the first well validated numerical method that robustly approximates the generalised form of this class of equations. The method has been validated against both analytic solutions of well understood members of this class of equations as well as forced solutions. The use of forced solutions extends the validation to include members of this class of equations for which there are currently no known analytic solutions. This class of equations presents many challenges and the success of this numerical method affirms the utility of the hybrid elliptic solver and finite volume methods we have developed previously for dispersive wave equations.

Tuesday 14:10 Zoom C

Prediction of sawn timber MOE from increment cores

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In this talk I will discuss work conducted as part of a large industry-led project on characterising the southern pine trees of southeast Queensland and northern New South Wales. I will focus on predicting the modulus of elasticity (MOE) of sawn timber boards, utilising data collected from diametrical cores. I will also discuss initial investigations into using functional data analysis to classify trees and plantations.

Monday 11:15 Zoom A

Uncertainty Quantification For The Hokkaido Nansei-Oki Tsunami Using B-Splines On Adaptive Sparse Grids

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Modeling uncertainties in the input parameters of computer simulations is an established way to account for inevitably limited knowledge. However, long run-times and high demand for computational resources can make using the simulation cumbersome. Instead, a surrogate model can be used to replace the original simulation, balancing accuracy and runtime appropriately. We use spatially adaptive Sparse Grids for the creation of this surrogate model. Sparse Grids are a discretization scheme designed to mitigate the curse of dimensionality, and spatial adaptivity further decreases the necessary number of expensive simulations. We further use B-spline basis functions which provide gradients and are exactly integrable, making them a favorable choice in the context of uncertainty quantification. We demonstrate the capability of this approach based on the investigation of a simulation of the Hokkaido Nansei-Oki Tsunami with ANUGA for which we develop a better understanding by calculating key quantities such as mean, percentiles and maximum run-up. We compare our approach to the Dakota toolbox and reach similar accuracy for the approximation but better results for optimization.

The Youtube link for the presentation is at https://www.youtube.com/watch?v=IKSdoM4kO54&t=1s.

Monday 16:25 Zoom A

Inexact Derivative-Free Optimisation For Bilevel Learning

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When variational regularisation methods are used to solve inverse problems, they suffer from the drawback of having potentially many parameters which the user must specify. A common approach to handle this is to learn these parameters from data. While mathematically appealing, this strategy leads to a bilevel optimisation problem which is difficult to solve computationally. Theoretically, algorithms for bilevel learning rely on access to exact solutions to the lower-level regularisation problem, but this condition is not guaranteed in practice. In this talk, we describe a novel approach using dynamic accuracy derivative-free optimisation for solving bilevel learning problems. This approach still retains convergence guarantees but allows the regularisation problem to be solved inexactly and hence is able to be implemented in practice. Using problems from image analysis, we demonstrate that our approach dramatically reduces the computational requirements of bilevel learning. This is joint work with Matthias Ehrhardt (Bath).

Monday 11:15 Zoom B

Facial structure of high dimensional convex sets

Vera Roshchina
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The structure of convex sets is determined by the relative arrangement of their faces. 'Good' facial structure ensures the absence of irregularities in optimisation problems modelled in terms of convex sets and functions, and in turn leads to efficient performance of numerical algorithms.

I will talk about several properties of convex sets that capture such good behaviours and will touch upon the benign implications of having such properties for both qualitative and quantitative analysis of optimisation techniques.

Monday 13:45 Zoom C

Error Estimation And Adaptive Algorithms For Multilevel Stochastic Galerkin Fem

Michele Ruggeri
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We consider a class of parametric elliptic PDEs, where the coefficients have affine dependence on infinitely many (uncertain) parameters. We introduce a two-level a posteriori estimator to control the energy error in multilevel stochastic Galerkin approximations. We show that the two-level estimator always provides a lower bound for the unknown approximation error, while the upper bound is equivalent to a saturation assumption. We propose and numerically compare adaptive algorithms, where the structure of the estimator is exploited to perform spatial refinement and parametric enrichment. This is joint work with Alex Bespalov (University of Birmingham, UK) and Dirk Praetorius (TU Wien, Austria).

Tuesday 16:25 Zoom C

Inference Of Model Sparsity In Nonlinear Dynamics Using Noisy Data

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This talk is concerned with the Bayesian calibration of nonlinear stochastic differential equations emulating physical phenomena using noisy and sparse observational data [1]. Due to the recent advances in data-driven model discovery techniques (aka machine learning), the laws-of-physics are being augmented with statistical elements to enhance the model predictive capabilities for unobserved physics. The Bayesian updating of unknown model parameters of such parametrically-flexible models can lead to overfitted models that lack generalizability. We proposed the semi-analytical algorithm of nonlinear sparse Bayesian learning (NSBL) to address this issue in an efficient and robust manner. NSBL is an extension of sparse Bayesian learning (SBL) to inverse problems involving 1) nonlinear mapping of observations and unknown parameters, and 2) significant prior knowledge of some parameters. In this talk, we will detail the mathematical details of NSBL and its application to nonlinear dynamics to demonstrate the effectiveness of NSBL.

References

[1] Sandhu, R., Khalil, M., Pettit, C., Poirel, D. and Sarkar, A., 2020, Nonlinear sparse Bayesian learning for physics-based models, Journal of Computational Physics (to appear).

1 Currently at National Renewable Energy Laboratory, Golden, Colorado, USA

2 Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Monday 12:20 Zoom B

Domain Decomposition Of Stochastic Pdes: Three-Dimensional And Time-Dependent Systems

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The intrusive spectral stochastic finite element method based domain decomposition (DD) solvers are developed for stochastic partial differential equations (SPDEs) which demonstrate scalable performances for high resolution spatial discretizations and large number of random variables [1, 2]. The two-level DD solvers equipped with vertex-based coarse grid corrections showed excellent numerical and parallel scalabilities for two-dimensional scalar SPDEs (i.e. Poisson equation) and coupled systems of SPDEs (i.e. equations of linear elasticity). Due to complex geometrical interface couplings among subdomains and block couplings in polynomial chaos space, the scalabilities of these algorithms degrade for three-dimensional SPDE systems. This issue is alleviated using a wirebasket-based enriched coarse grid corrections in the DD-based preconditioners. The scalabilities of the DD solvers are also demonstrated for time-dependent SPDEs (i.e. arising in acoustic wave propagation through random media).

References

[1] Desai, A., Khalil, M., Pettit, C., Poirel, D. and Sarkar, A., 2018, Scalable Domain Decom- position Solvers for Stochastic PDEs in High Performance Computing, Journal of Computer Methods in Applied Mechanics and Engineering, 335, 194-222.

[2] Desai, A., 2019, Scalable Domain Decomposition Algorithms for Uncertainty Quantification in High Performance Computing. Ph.D. thesis, Carleton University.

1 Currently at Bank of Canada, Ottawa, Ontario, Canada.

2 Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Tuesday 11:15 Zoom C

1D fractal image compression as a quadratic programming problem

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We introduce a new linear algebra formulation of the standard fractal image compression algorithm. We reformulate the core concepts of fractal image compression such as partitioned iterated functions systems, local Hutchinson operator, domain and range partitions in the linear algebra language and hence write the algorithm as a second order optimization problem. Special case of 1D image examples is considered and corresponding examples are given.

Tuesday 10:25 Zoom A

Testing For The Efficiency Of Economic Scenario Generators Under Different Random Number Generations

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Insurance policies with embedded options and guarantees are evaluated by means of Economic Scenario Generators (ESG), stochastic simulations developed via Monte Carlo techniques that span the evolution of risk factors proper to the insurer (financial and technical) in a way consistent with market data. The either pseudo or quasi-random number generator used in the model turns out to be of utmost importance for the precision of the valuation of the asset/liabilities process, playing a delicate role in the measure of the risk faced up by insurers. I shall compare five different random number generators in a G2++ model in order to assess the efficiency of the ESG by testing for the fulfillment of the martingale condition.

Monday 16:25 Zoom C

Projection Of The Non-Conforming Crouzeix-Raviart Finite Element Solution And Its Gradient Onto The Standard Conforming Finite Element Space

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In this talk, we will present the projection of the non-conforming Crouzeix-Raviart finite element solutions onto the standard conforming finite element space. We compare the errors in L2 and H1 norms for the projected solutions and the non-coforming solutions. In the next step, we will project the gradient of the non-conforming Crouzeix-Raviart solution on the standard finite element space and also on the Crouzeix-Raviart finite element space. We compare the errors in L2 norm for the projected gradient. We show an efficient way of projection using a biorthogonal system.

Tuesday 14:35 Zoom C

Dynamics Of Higher Order Rogue Waves In Boussinesq Equation

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In this work, we have discussed the rogue wave solutions of a new (2+1)-dimensional integrable Boussinesq model governing the evolution of high and steep gravity water waves. The evolution dynamics of obtained rogue waves along with the identification of their type, bright or dark type localized structures, and manipulation of their amplitude, depth, and width is also discussed. To construct rogue wave solutions, we used bilinear form and generalized polynomials. In particularly one, two and three order rogue wave solutions are obtained. The obtained results helps to demonstrate complete dynamics of rogue waves in higher dimension integrable systems and its various application over controlling mechanism of rogue waves in optical systems, atomic condensates, and deep water oceanic waves.

Monday 11:15 Zoom C

Investigation Of Determinism-Related Issues In The Sobol' Low-Discrepancy Sequence For Producing Sound Global Sensitivity Analysis Indices

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An efficient and robust sampling scheme can support sensitivity analysis (SA) of models to discover their behaviour through Monte Carlo approximation. This is especially useful for complex models as often occur in environmental domains when model runtime can be prohibitive. The Sobol' sequence is one of the most used quasi-random low-discrepancy sequences, as it can significantly explore the parameter space more evenly than pseudo-random sequences. It has been shown that the use of the Sobol' sequence yields higher accuracy than stratified sampling methods such as Latin-hypercube. The built-in determinism of the Sobol' sequence assists in achieving these attractive properties. However, at the same time, the Sobol' sequence tends to deteriorate in the sense that the estimated errors are distributed inconsistent across model parameters as the dimensions of a model increases. By testing multiple Sobol' sequence implementations in several python libraries, it is clear that the deterministic nature of the Sobol' sequence occasionally introduces relatively large errors in sensitivity indices produced by well-known global SA methods, and that the errors do not diminish by averaging through multiple replications. Problematic sensitivity indices may mistakenly guide modellers to make type I and II errors in trying to identify sensitive parameters, and this will potentially impact model reduction attempts based on these sensitivity measurements. This work will conduct a comprehensive analysis to investigate the cause of the Sobol' sequence's determinism-related issue and will provide suggestions and improvements that avoid this determinism-related issue.

Keywords: Sobol' sequence, low-discrepancy, Monte Carlo, Sensitivity Analysis

Tuesday 10:25 Zoom B

Physics-Constrained Bayesian Neural Network For Fluid Flow Reconstruction With Sparse And Noisy Data

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In many applications, flow measurements are usually sparse and possibly noisy. The reconstruction of a high-resolution flow field from limited and imperfect flow information is significant yet challenging. In this work, we propose an innovative physics-constrained Bayesian deep learning approach to reconstruct flow fields from sparse, noisy velocity data, where equation-based constraints are imposed through the likelihood function and uncertainty of the reconstructed flow can be estimated. Specifically, a Bayesian deep neural network is trained on sparse measurement data to capture the flow field. In the meantime, the violation of physical laws will be penalized on a large number of spatiotemporal points where measurements are not available. A non-parametric variational inference approach is applied to enable efficient physics-constrained Bayesian learning. Several test cases on idealized vascular flows with synthetic measurement data are studied to demonstrate the merit of the proposed method.

Monday 11:55 Zoom B

Analysing Iterative Algorithms Without Monotoncitiy

Matthew Tam
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The first step in the convergence analysis of many algorithms in nonlinear optimisation involves establishing that some measure of the distance between the current iterate and the solution set is monotone nonincreasing. Two common examples of such as a measure are: (i) the gap between the current and optimal objective function values, and (ii) the Euclidean distance between the current iterate and a fixed solution of the problem. Although knowing a sequence is monotone can greatly simplify analyses, mandating this can place restrictions on other properties of an algorithm might possess. In this talk, I will discuss a number iterative schemes, each having a different favourable algorithmic property, which do not generate monotone nonincreasing sequences in either of the above senses.

Monday 10:25 Zoom B

A Free Boundary Mechanobiological Model Of Epithelial Tissues

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In this presentation, we couple intracellular signalling and cell-based mechanical properties to develop a novel free boundary mechanobiological model of epithelial tissue dynamics. Mechanobiological coupling is introduced at the cell level in a discrete modelling framework, and new reaction-diffusion equations are derived to describe tissue-level outcomes. The free boundary evolves as a result of the underlying biological mechanisms included in the discrete model. To demonstrate the accuracy of the continuum model, we compare numerical solutions from the discrete and continuum models relating to two different signalling pathways. First we study the Rac-Rho pathway where cell- and tissue-level mechanics are directly related to intracellular signalling. We then study an activator-inhibitor system which gives rise to spatial and temporal patterning related to Turing patterns. In all cases, the continuum model and free boundary condition accurately reflect the cell-level processes included in the discrete model.

Monday 14:35 Zoom A

No, Professor: You Don't Need To Reverse The Order of Integration!

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Many of us teach multi-variable calculus courses and discuss examples where the order of integration is reversed in double integrals. Moreover, the narrative associated with these examples is that the reversal is necessary in order to solve the problem.

I illustrate that the method of integration by parts can be directly applied to many of the classic pedagogical problems in the literature concerning double integrals, without taking the well-worn steps associated with reversing the order of integration. I advocate for integration by parts to be a part of the pedagogical conversation in the learning and teaching of double integral methods; and call for more debate around its use in the learning and teaching of other areas of mathematics. Finally, I emphasize the need for critical approaches in the pedagogy of mathematics more broadly
.

YouTube video presentation: https://youtu.be/mkh3fr0ji5M

Wednesday 10:00 Zoom B

New Regularization For Sparse Optimization

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Penalized regression is a popular method due to its simplicity and bias-variance tradeoff. In many applications, a sparsity-induced penalty is used to perform variable selection and to obtain a simpler model. Some well-known examples of sparsity-induced penalties are the ℓ_0 penalty and its convex relaxation, the ℓ_1-norm. However, penalized regression with ℓ_0 penalty can be unstable due to its intrinsic discontinuity while ℓ_1-norm regularization performs worse in high-dimensional problems. Thus, non-convex and non-smooth penalties such as the ℓ_q penalty, with $q \in (0, 1)$, have been investigated and numerical experiments show positive results in high-dimensional setting.

In this talk, we will introduce a new non-convex, non-smooth penalty and compare the numerical results with the ℓ_q penalty. The algorithm to solve the problem and the convergence analysis will be described briefly. Finally, we will provide some possible future directions for the topic in this presentation.

Monday 14:35 Zoom C

Robust Lagrangian Numerical Schemes In Computing Effective Diffusivities For Chaotic And Random Flows

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Effective diffusivities of passive scalars diffusion in incompressible velocity fields have theoretical and practical importance. In this thesis, efforts have been made to develop a Lagrangian approach to calculate effective diffusivities and to analyze the error and physic phenomenons based on numerical results. Our approach is to integrate the stochastic differential equations of the particles by proposed discrete schemes via Monte Carlo methods. To compute the effective diffusivities, we take the variance of the sampled positions divided by computational time. The computational time should be longer than the mixing time of dynamics, so the discrete schemes should preserve the inherent structures of the dynamics. Via backward error analysis techniques, we proved the proposed schemes converge asymptotically with respect to the timestep. Later on, we developed a new proof to show the convergence is uniform in computational time. The key ingredient of the proof is to propose discrete type cell problems, which are analogs to cell problems in traditional parabolic homogenization theory. And we concluded the schemes should preserve the invariant measure on torus space introduced by the periodicity of velocity fields. We generalized the proof to time-dependent cases and random cases. Numerical examples were presented to verify the convergence in each case. We calculated the effective diffusivities of chaotic and random flows, including the Taylor Green field in two dimensions, the Arnold-Beltrami-Childress flow and Kolmogorov flow in three dimensions and also their generalizations to time-dependent and random cases. We investigated the convection-enhanced diffusion phenomenon in the large Peclet number regime. Our results showed that the diffusion enhancement has a strong correlation to mixing time and Lyapunov exponent.

Tuesday 11:55 Zoom C

Application Of Iterative Method To Construction Of Underwater Topography

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Techniques to generate a surface appropriate for given data points are introduced. A piecewise linear function over a triangular mesh represents a surface. A least square approximation updates the values of a piecewise linear function at vertices of an element with data including three vertex data. Once those processes are carried out over all the elements, a mapping on nodal values is defined, and a fixed point of the mapping represents a desired surface. Our techniques are applied to underwater topographical data obtained with an RTK-GPS and an echo sounder.

Wednesday 10:00 Zoom C

Chaotic Flow In Competitive Exothermic-Endothermic Reaction Systems

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We study the effects of chaotic advection in a two-dimensional competitive reaction system with an exothermic reaction and an endothermic reaction and investigate the formation of the filament structure. In previous studies, two distinct behaviours have been observed in the system. The first is when the stirring is fast and the reaction is slow. In this case, flame quenching occurs. The other is when the stirring is slow and the reaction is fast. In this case, local temperature perturbations lead to a stationary flame with a complex filament structure. In both of these behaviours, the advective flow and reaction processes dominates the diffusion process. There is a third behaviour, where the diffusion process dominates the advective flow and an expanding swirling travelling wave develops. We will explore the parameter values which separate these different behaviours.

Monday 12:20 Zoom A

Implicit Reconstructions Of Thin Leaf Surfaces From Large, Noisy Point Clouds

Riley Whebell
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We consider how to mathematically reconstruct the surfaces of leaves from a hand-scanned point cloud data set. Our motivation is to build mathematical representations of whole plants for use in agrichemical droplet impaction and spreading simulations. A surface reconstruction from such a point cloud should preserve key characteristics of each leaf, including possessing a continuous mean curvature, which is important for use in future droplet spreading models. We use regularised polyharmonic splines to form an approximate implicit interpolant from a point cloud augmented with off-surface points. While implicit surface reconstruction techniques typically assume a closed, orientable surface, we show that by restricting the evaluation of the interpolant to a tight domain around the point cloud, we can just as easily reconstruct open surfaces. For large point clouds, ($N > 10^4$) we use a partition of unity method to turn the global interpolation problem into many local subproblems, with an octree-like strategy for choosing subdomains. We present reconstructions of a capsicum plant and demonstrate the impact of the degree of spline smoothness on the continuity of surface curvature.

Tuesday 16:00 Zoom C

3D Numerical Simulations Of Elastic Waves And Dynamic Earthquake Ruptures In Complex Geometries Using High Order Accurate Upwind Finite Difference Methods

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High-order accurate finite difference operators based on the summation-by-parts (SBP) framework constitute efficient numerical methods for simulating large-scale hyperbolic wave propagation problems. Traditional SBP finite difference operators that use standard central difference stencils for approximating spatial derivatives often have spurious unresolved wave-modes in their numerical solutions. For marginally resolved solutions, these spurious wave-modes have the potential to destroy the accuracy of numerical solutions for first order hyperbolic partial differential equation, such as the elastic wave equation. To improve the accuracy of numerical solutions of elastic wave equations in complex geometries, we discretise the 3D elastic wave equation with a pair of non-central (upwind) finite difference stencils [Ken Mattsson 2017], on boundary-conforming curvilinear meshes. Using the energy method, we prove that our scheme is numerically stable and computationally demonstrate robustness. The simulation of nonlinear dynamic earthquake ruptures and propagation of elastic waves in heterogeneous media with free surface topography are presented, including simulation of community developed seismological benchmark problems. Our results show that the upwind SBP operators are more robust and less dispersive on marginally resolved meshes, when compared to traditional operators.

Tuesday 11:55 Zoom A

Weak Imposition Of Boundary Conditions For The Gauge Formulation Of The Incompressible Navier-Stokes Equations

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The projection method was first introduced by Chorin and Temam as a computationally efficient numerical method to solve the incompressible Navier-Stokes equations. Despite its success in decoupling the computations of velocity and pressure, it suffers from inaccurate numerical boundary layers. As an effort to resolve this inaccuracy, E and Liu proposed the gauge method, which is a reformulation of the Navier-Stokes equations in terms of an auxiliary vector field and a gauge variable. This method utilizes the freedom of choosing a boundary condition of the gauge variable to reduce the numerical coupling between the considered variables. Nevertheless, the computational implementation of the boundary conditions for the auxiliary vector field is difficult in the context of finite elements since they involve either normal or tangential derivative of the gauge variable. In order to circumvent this issue, we propose a weak formulation of the boundary conditions based on the Nitsche's method. Computational results are presented to illustrate the accuracy of the proposed method.

Tuesday 15:00 Zoom C

Numerical Computation Of Schrodinger Equations With Random Potentials

Zhizhang Wu
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In this talk, the numerical computation of the linear Schrodinger equation with random potentials is considered. The randomness is formalized as random variables and hence the random equation is converted into a parameterized one. The stochastic regularity is first investigated. By combining the time-splitting spectral method and the stochastic collocation method, a numerical scheme is given and the relevant convergence analysis is presented based on theories of polynomial interpolation. Subsequently, the Schrodinger equation with a periodic potential and a random external potential is considered. A Bloch decomposition based stochastic Galerkin method is presented. The advantage of higher temporal accuaracy and stability is proved and shown via numerical experiments.

Tuesday 12:20 Zoom C

Combination Technique Applied To Quantities Of Interest

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Functionals related to a solution of a problem, usually modelled by partial differential equations can be important quantities used to capture features of the problem. When a high dimensional problem is considered, the computational cost of the functionals can be large since the numerical solution of a high dimensional partial differential equation is usually expensive to compute. We apply the sparse grid combination technique to reducing the cost of computation of important functionals. Our method is based on the error splitting models of the functionals. We build the error splitting models for some special types of functionls when numerical schemes used to compute the PDEs and the functionals are known. We show the connection between the decay of the surpluses and the error splitting models. By using the connection, we can also apply our combination technique to functionals when we only know their surpluses. Numerical experiments are provided to illustrate error splitting models for the functionals and the performance of our method,

Tuesday 10:50 Zoom C

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