The 21st Biennial Computational Techniques and Applications Conference

Queensland University of Technology

Brisbane, Australia

29 November – 2 December, 2022

Editors: Tim Moroney, Qianqian Yang

Acknowledgement of Traditional Owners

QUT acknowledges the Turrbal and Yugara, as the First Nations owners of the lands where QUT now stands. We pay respect to their Elders, lores, customs and creation spirits. We recognise that these lands have always been places of teaching, research and learning.

QUT acknowledges the important role Aboriginal and Torres Strait Islander people play within the QUT community.

Acknowledgements

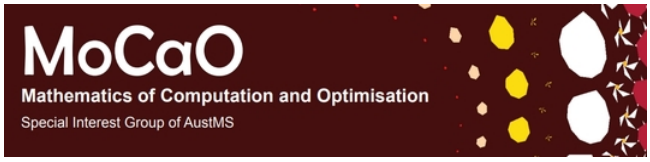
This conference was generously supported by

School of Mathematical Sciences, QUT

Centre for Data Science, QUT

Modelling and Simulation Society of Australia and New Zealand Inc.

Mathematics of Computation and Optimisation (MoCaO) special interest group of AustMS



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Plenary and Public Speakers

- **Chris Drovandi (Queensland University of Technology, Australia)**
- **Jennifer Flegg (The University of Melbourne, Australia)**
- **Frances Kuo (The University of New South Wales, Australia)**
- **Christian Lubich (University of Tuebingen, Germany)**
- **Marco Palombo (Cardiff University, UK)**
- **Emilie Sauret (Queensland University of Technology, Australia)**
- **Karen E Willcox (The University of Texas at Austin, USA)**
- **Andy Wilkins (CSIRO, Australia)** ***(Public Lecture speaker)***

Welcome

The 21st Biennial Computational Techniques and Applications Conference (CTAC2022) is hosted by the School of Mathematical Sciences and Centre for Data Science at Queensland University of Technology in Brisbane.

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 2020 online at the University of New South Wales.

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 will have two student prizes, one sponsored by Modelling and Simulation Society of Australia and New Zealand (MODSIM) and the other by the QUT Centre for Data Science. Student talks are denoted in the conference program and list of abstracts by an asterisk.

We hope you enjoy the conference.

Information

Conference venue

The conference is hosted at QUT, Gardens Point Campus.

Plenary talks are in S Block, level 4, room S403. (Level 4 is the main entrance level to the building.)

Contributed talks are in S Block, levels 4 and 3: S409, S405 which are just a few metres from the plenary room, and S307 which is directly opposite the main internal stairwell from level 4 to level 3.

The Public Lecture will be held in P Block, level 5, room P504, part of the Science and Engineering Centre.

The Computational Mathematics Group meeting will be held in S403 on Thursday 1 December from 1:30 – 2pm.

Presentations

All plenary talks are around 45 minutes long, followed by question time.

All contributed talks are 15 minutes long, plus 5 minutes for questions, discussion and changeover. The session chair will give you a signal when you have spoken for 10 minutes. Please do not exceed your time.

Each room is equipped with a projector and screen, and a desktop computer running Windows, with usual PowerPoint, PDF and web browsers. Please ensure your presentation is in one of these formats. Connecting your own laptop is possible, but this is only recommended if you really require it (e.g. if your presentation is not one of the formats above), and you are responsible for arranging this with the session chair ahead of time.

Internet access

QUT offers Free Public Wifi to guests and vistors to its campuses. Alternatively, you may use your home instution's login with Eduroam.

Social events

The welcome reception with drinks and canapés is in QUT's Room 360 from 5–7 pm on Tuesday, 29 November.

The public lecture with drinks and canapés beforehand is in P504 from 5:30–7:30 pm on Wednesday 30 November.

The conference dinner will be held in Room 360 from 6:30 pm on Thursday 1 December.

Dining

There are many good options for dining in and around QUT. For lunch on campus, QUT has a number of cafes and fast food options including Lady Harriet's Bar & Kitchen.

Right next door in 1 William St there are more options, and it's common to find QUT folks wandering over there at lunch time.

Walk over to South Bank to sample Brisbane's premier dining destination, including another QUT favourite The Ship Inn, just 10 minutes walk over the Goodwill Bridge.

Finally, you may stroll into the CBD proper where you'll find countless more options within 10 or 15 mintues walk.

Gardens Point Wayfinding Map

City pedestrian entrance to Campus

Welcome reception & Conference Dinner held in Room 360, top level of Y Block

Public Lecture held in Room P514, Level 5, P Block

Goodwill Bridge to South Bank

Plenary and contributed talks held in S Block

Note: Ferry Terminal closed due to flood damage

Programme

Tuesday 29 November	
5.00-7.00pm	**Room 360**
	Welcome drinks & Registration

Wednesday 30 November			
8.20-8.45am	**Registration on Level 4 S Block**		
8.45-9.00am	**S403** **Welcome address by Professor Troy Farrell** **Executive Dean, Faculty of Science, QUT**		
S403: Plenary Chair	**Ian Turner**		
9.00-10:00am	Karen E Willcox (p.16) *Predictive Digital Twins: From Aerospace Engineering to Computational Oncology*		
	S409 Chairs: Stuart Hawkins	S405 Bishnu Lamichhane	S307 Vivien Challis
10.00-10.20am	Dylan Oliver* (p.27) *Adaptive dual-grid mapping method for solving the advection-diffusion-reaction equation in a heterogeneous medium*	Anthony Vine* (p.25) *Mathematical modelling of the drying of fruits and vegetables*	Jia Jia Qian* (p.31) *A polytopal discrete de Rham scheme for the Yang—Mills equations*
10.20-10:40am	Quanling Deng (p.41) *Multi-scale modelling of Arctic sea ice floes*	Olivier Dominique Y Huet* (p.38) *Simulation of surfactant-laden drops impacting on a flat surface: effect of Marangoni's stresses*	Sandra Jeyakumar* (p.44) *A structure-preserving approach to simulating Hamiltonian systems with dissipation*
10.40-11:00am	Tony Roberts (p.47) *Accurate and efficient multiscale simulation of a heterogeneous elastic beam via computation on small sparse patches*	Luke Patrick Filippini* (p.35) *Simplified models of diffusive transport in radially-symmetric media*	
11.00-11.30am	**Morning Tea**		
S403: Plenary Chair	**Markus Hegland**		
11.30-12.30pm	Frances Kuo (p.16) *Lattice Meets Lattice - Application of Lattice Cubature to Models in Lattice Gauge Theory*		
12.30-1.45pm	**Lunch**		

Wednesday 30 November			
	S409 Chairs: Megan Farquhar	S405 Tiangang Cui	S307 Quanling Deng
1.50-2.10pm	Riley Whebell* (p.42) *Modelling droplet dynamics without resolving interfaces using smoothed particle hydrodynamics*	David Ronald Jenkins (p.26) *Evaluation of maceral interface quality in 3D micro-CT images of metallurgical coke*	Jordan Shaw-Carmody* (p.33) *Optimal Hessian Recovery Using a Biorthogonal System with an Application to Adaptive Refinements*
2.10-2.30pm	Jiachen Zhao* (p.31) *Electrohydrodynamic control of viscous fingering during fluid displacement*	Edward Bissaker* (p.28) *A scalable two-point correlation and lineal path function computation method.*	Muhammad Awais Khan* (p.37) *Numerical analysis of stochastic Stefan problem using the gradient discretization method*
2.30-2.50pm	Jinshuai Bai* (p.32) *A physics-informed deep learning-based meshfree method for hydrodynamics modelling*	Yihan Nie* (p.49) *Resolving the dynamic properties of PCL by coarse grain simulations*	Ricardo Ruiz Baier (p.42) *Robust discretisations for poromechanics formulations using total pressure*
2.50-3.10pm	Gerald G Pereira (p.29) *Multi-component lattice Boltzmann for large density and viscosity ratio fluids*	Patrick Grant* (p.39) *Constructing Virtual Representations of Laminated Timber Products*	Frederick Fung* (p.29) *Resilience of Multigrid Method in Parallel Adaptive Mesh Refinment*
3.10-3.30pm	Samuel Stephen* (p.43) *Numerical analysis of the axisymmetric lattice Boltzmann method for steady and oscillatory flows in periodic geometries*	Amani Ahmed Otaif* (p.24) *Temperature field in fluids flowing through micro-channels in the slip regime*	Dean Muir* (p.27) *Stable and accurate method for simulating the Anisotropic Diffusion in toroidally confined magnetic fields*
3.30-4.00pm	**Afternoon Tea**		
S403: Plenary Chair	**Pascal Buenzli**		
4.00-5.00pm	Christian Lubich (p.17) *Convergent evolving surface finite element algorithms for geometric evolution equations*		
5.30-6.15pm	**P514** **Drinks and canapés**		
P514: Public Lecture	**Opening by Professor Tony Roberts** **Head of School, Mathematical Sciences, QUT**		
6.30-7.30pm	Andy Wilkins (p.17) *The Importance of Mathematics*		

Thursday 1 December			
8.50-9.00am	**S403**		
	Conference Update		
S403: Plenary Chair	**Qianqian Yang**		
9.00-10:00am	Marco Palombo (p.17) *Perspectives on AI-powered brain microstructure imaging*		
	S409 Chairs: Nathan March	S405 Kenneth Duru	S307 Megan Farquhar
10.00-10.20am	Matthew Adams (p.36) *Normally-distributed compositional data: a review of computational methods*	David Bee Olmedo* (p.26) *Laminar flow through rectangular channels with walls of different permeabilities: a contraction mapping approach*	Yi Liu* (p.48) *The unstructured finite element method for the magnetohydrodynamic flow and heat transfer on a two-dimensional irregular convex domain*
10.20-10:40am	Sarah Vollert* (p.44) *A sequential method for efficiently parameterising ecosystem models*	Steven Kedda* (p.46) *Self-similarity and Fractalisation in Interfacial Hydrodynamics*	Mengchen Zhang* (p.37) *Fractional Diffusion Model Generalised by the Distributed-order Operator Involving Variable Diffusion Coefficients*
10.40-11:00am	Joanne Liu* (p.32) *Dynamic equations on time scales and some foundational biological models*	Simon Watt (p.45) *Chaotic flow in competitive exothermic-endothermic reaction systems*	Xingyu An* (p.48) *Empirical investigation for the fractional Black-Scholes models with S&P 500 index options*
11.00-11.30am	**Morning Tea**		
S403: Plenary Chair	**Matthew Adams**		
11.30-12.30pm	Jennifer Flegg (p.18) *Mathematical Modelling of Avascular Tumour Growth*		
12.30-1.30pm	**Lunch**		

Thursday 1 December			
1.30-2.00pm	**S403**		
	CMG meeting		
	S409 Chairs: Qianqian Yang	S405 Ricardo Ruiz Baier	S307 Brodie Lawson
2.10-2.30pm	Adrianne Jenner (p.24) *What insight computational mathematical modelling brings to Multiple Sclerosis*	Tiangang Cui (p.47) *DIRT: Tensorised Rosenblatt Transport for High-Dimensional Stochastic Computation*	Seunghoon Ji* (p.45) *Ship wake analysis using machine learning*
2.30-2.50pm	Hasitha N Weerasinghe* (p.30) *The Effect of Immune Cells as a Treatment for Cancer Using an Agent-based Model*	Abi Srikumar* (p.23) *Approximating distribution functions in uncertainty quantification using quasi-Monte Carlo methods*	Rudi Adha Prihandoko* (p.43) *Summation by Parts Analysis with Finite Volume: Linearized Shallow Water Wave Equation with*
2.50-3.10pm	Adel Mehrpooya* (p.24) *Random Walks on Irregular Spatial Networks and their Advection-Diffusion-Reaction Continuum Limit*	Markus Hegland (p.35) *Computing expected moments of the Rényi parking problem on the circle*	Yijia Liu* (p.49) *Optimal PML parameters for efficient numerical simulation of waves in unbounded domain*
3.10-3.30pm	Peter Humphreys* (p.39) *A comprehensive approach and solution techniques for operating theatre scheduling*	Elizabeth Harris* (p.28) *Adaptive batch strategy using a leverage score based initialisation for calculating the minimum volume covering ellipsoid*	Kenny Wiratama* (p.34) *An Energy Stable Discontinuous Galerkin Spectral Element Method for the Linearized Serre Equations*
3.30-4.00pm	**Afternoon Tea**		
S403: Plenary Chair	**Tim Moroney**		
4.00-5.00pm	Chris Drovandi (p.18) *Likelihood-Free Bayesian Inference and Model Misspecification*		
6.30-10pm	**Room 360**		
	Conference Dinner		

Friday 2 December			
8.50-9.00am	**S403**		
	Conference Update and Proceedings		
S403: Plenary Chair	**Vivien Challis**		
9.00-10:00am	Emilie Sauret (p.19) *A hybrid Lattice Boltzmann approach for simulating viscoelastic instabilities and elastic turbulence*		
	S409 Chairs: Simon Watt	S405 Pascal Buenzli	S307
10.00-10.20am	Kenneth Duru (p.33) *Towards energy-stable and conservative discontinuous Galerkin spectral element methods for Einstein's equations of general relativity in second order form*	Bishnu Lamichhane (p.25) *Efficient finite element methods for three-field formulations of elasticity and Reissner-Mindlin plate equations using biorthogonal systems*	
10.20-10:40am	Quoc Thong Le Gia (p.41) *Numerical solutions to an inverse problem of a non-linear Helmholtz equation*	Nathan March (p.38) *Multiscale computational homogenisation using spectral methods for additively manufactured metal part*	
10.40-11:00am	Ian H Sloan (p.30) *Removing the mask – reconstructing a scalar field on the sphere from a masked field*	Vivien Challis (p.48) *Understanding failure with computational finite fracture mechanics*	
11.00-11.30am	**Morning Tea**		
	S409 Chairs: Quoc Thong Le Gia	S405 Adrianne Jenner	S307
11.30-11.50am	Linda Stals (p.34) *A comparision of smoothing splines*	Qianqian Yang (p.40) *Continuous time random walk (CTRW) modelling framework in diffusion MRI*	
11.50-12:10pm	Stuart C. Hawkins (p.46) *An efficient coupled-FEM-BEM-based iterative method for the inverse medium problem in wave scattering*	Megan Farquhar (p.36) *Robust methods for mapping diffusion kurtosis*	
12.10-12.20pm	**S403**		
	Closing		

Plenary talks

Predictive Digital Twins: From Aerospace Engineering to Computational Oncology

Karen E Willcox (The University of Texas at Austin, USA)

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Digital twins represent the next frontier in the impact of computational science on grand challenges across science, technology and society. A digital twin is a computational model or set of coupled models that evolves over time to persistently represent the structure, behavior, and context of a unique physical system, process or biological entity. A digital twin is characterized by a dynamic two-way flow of information between the computational models and the physical system. A digital twin provides an integrated framework for calibration, data assimilation, planning, and optimal control. This talk will highlight the important roles of reduced-order modeling and uncertainty quantification in achieving robust, reliable digital twins at scale. The methodology will be illustrated for applications in aircraft structural digital twins and cancer patient digital twins.

Lattice Meets Lattice - Application of Lattice Cubature to Models in Lattice Gauge Theory

Frances Kuo (The University of New South Wales)

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Collaborators: Tobias Hartung (The Cyprus Institute), Karl Jansen (DESY Zeuthen), Ian Sloan (UNSW Sydney), Hernan Leovey (AXPO Trading & Sales), Dirk Nuyens (KU leuven)

In this joint venture between mathematicians and physicists, we develop efficient recursive strategies to tackle a class of high dimensional integrals having a special product structure with low order couplings, motivated by models in lattice gauge theory. A novel element of this work is the potential benefit in using a family of numerical integration methods called "lattice cubature rules". The group structure within lattice rules combined with the special structure in the physics integrands may allow efficient computations based on Fast Fourier Transforms. Applications to the quantum mechanical rotor and compact U(1) lattice gauge theory in two and three dimensions are considered.

Convergent evolving surface finite element algorithms for geometric evolution equations

Christian Lubich (University of Tuebingen, Germany)

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Collaborators: Balázs Kovács, Buyang Li

Geometric flows of closed surfaces are important in a variety of applications, ranging from the diffusion-driven motion of the surface of a crystal to models for biomembranes and tumor growth. Basic geometric flows are mean curvature flow (described by a spatially second-order evolution equation) and Willmore flow and the closely related surface diffusion flow (described by spatially fourth-order evolution equations). Devising provably convergent surface finite element algorithms for such geometric flows of closed two-dimensional surfaces has long remained an open problem, going back to pioneering work by Dziuk in 1988. Recently, Balázs Kovács, Buyang Li and I arrived at a solution to this problem for various geometric flows including those mentioned above. The proposed algorithms discretize nonlinear parabolic evolution equations for geometric quantities along the flow, in our cases for the normal vector and mean curvature, and use these evolving geometric quantities in the velocity law interpolated to the finite element space. This numerical approach admits a stability and convergence analysis with optimal rates of convergence for finite elements of polynomial degree at least two.

The Importance of Mathematics

Andy Wilkins (CSIRO)

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When I confess I'm a professional mathematician, I often receive incredulous stares. Most people see maths as a necessary evil when completing their tax returns, but pretty-much useless otherwise. In this lecture, I hope to demonstrate that mathematics is actually incredibly valuable, by presenting a cornucopia of mathematical applications that I have worked on. I will include every-day subjects such as washing machines, ball-point pens, doors, textiles, chickens and wine, as well as more specialised phenomena such as groundwater, structural optimisation, plasticity, energy storage and earth tides. While most of my examples contain university-level maths at their heart, this is a public lecture so I will not present endless opaque equations!

Perspectives on AI-powered brain microstructure imaging

Marco Palombo (Cardiff University, UK)

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Abstract: This talk presents recent advancements and exciting new perspectives on quantifying brain tissue structure at the cellular scale (the so-called microstructure) through diffusion-weighted MR imaging (dMRI) and spectroscopy (dMRS). I will showcase recent examples of how combining dMRI and dMRS measurements with computational modelling and machine learning offers unique capabilities to quantify the brain microstructure non-invasively. We discuss potential applications to several brain diseases and future directions of research.

Mathematical Modelling of Avascular Tumour Growth

Jennifer Flegg (The University of Melbourne)

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Cancer is a global health burden; around 1 in 2 people will be diagnosed with some form of cancer during their lifetime. Cancer biology is incredibly complicated, as illustrated by the difficulties surrounding its diagnosis and treatment. However, mathematics has the potential to mediate this complexity by abstracting the system using simplifying assumptions into a mathematical framework that can be analysed and/or solved numerically to gain biological insight.

In this talk, I'll introduce mathematical modelling of an important early stage of tumour growth – the avascular stage – where there is no blood supply to the tumour. I'll present several mathematical models that consider avascular tumours including growth in free suspension and growth in a surrounding gelatinous medium, a hydrogel, that mimics the properties of human tissues.

Likelihood-Free Bayesian Inference and Model Misspecification

Chris Drovandi (Queensland University of Technology)

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Likelihood-free (LFI) methods developed in computational statistics and machine learning are now widely adopted in many scientific disciplines for calibrating complex statistical models with intractable likelihood functions. These approaches are appealing, since the posterior distribution can be approximated with only the ability to simulate mock datasets from the model of interest. In this talk I will describe some LFI methods and discuss their performance under the commonly-encountered situation of model misspecification. I will also provide detail on how the methods can be extended to make them more robust to model misspecification.

A hybrid Lattice Boltzmann approach for simulating viscoelastic instabilities and elastic turbulence

Emilie Sauret **(**Queensland University of Technology)

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Viscoelastic fluids exhibit nonlinear properties, which offer a range of practical benefits. In absence of inertial effects, viscoelastic fluids generate an anisotropic elastic stress that transitions the flow to a chaotic regime, elastic turbulence (ET). With similar features as inertial turbulence (increased flow resistance, enhanced mixing, broadband spectrum), viscoelastic instabilities, specifically ET, have emerged as a solution to the long-encountered mixing challenges in microfluidics, as well as enhancing heat transfer in micro-cooling technologies.

Recently, lattice Boltzmann methods (LBM) have emerged as a viable numerical tool for studying viscoelastic fluids. However, the inability to preserve numerical stability, especially at high elastic effects have restricted previous LBM attempts from simulating viscoelastic instabilities.

Here, I will present a hybrid LBM model, capable of overcoming stability issues when simulating viscoelastic instabilities. First, the model is applied to simulate ET for which I will demonstrate that the global artificial diffusivity commonly used to enhance numerical stability can introduce unphysical artifacts, resulting in a loss of physical meaningfulness. Subsequently, I will present a new artificial diffusivity, which preserves stability while accurately retaining all features of ET. Finally, I will demonstrate the applicability of the model by exploring viscoelastic instabilities through different porous media.

Contributed talks

Approximating distribution functions in uncertainty quantification using quasi-Monte Carlo methods

Abi Srikumar * (UNSW)

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Collaborators: Alexander D. Gilbert, Frances Y. Kuo and Ian H. Sloan

As high-dimensional problems become increasingly prevalent in many applications, the effective evaluation of these problems within the limits of our current technology poses a great hurdle due to the exponential increase in computational cost as dimensionality increases. One class of strategies for evaluating such problems efficiently are quasi-Monte Carlo (QMC) methods. Recently the application of quasi-Monte Carlo methods to approximate expected values associated with solutions to elliptic partial differential equations with random coefficients in uncertainty quantification has been of great interest. In this talk, we look into extending this from the computation of expected values of functionals of the PDE solution to the approximation of distribution functions. This done by reformulating these functions as expectations of an indicator function. However due to the discontinuous nature of the indicator functions, we do not have an integrand that is conducive to obtaining the optimal rate of error convergence. We seek to alleviate this issue using preintegration, whereby we integrate out a single variable of the discontinuous function in order to obtain a function of one dimension less with a sufficient level of smoothness to apply QMC methods. Some theoretical results regarding the error bounds associated with such approximations and the results of numerical experiments will be presented.

Random Walks on Irregular Spatial Networks and their Advection-Diffusion-Reaction Continuum Limit

Adel Mehrpooya * (Queensland University of Technology)

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Collaborators: Dr. Pascal Buenzli, Dr. Vivien Challis

The osteocyte network is a living network of cells embedded in bone tissue that plays a significant role in the mechanical regulation of bone. When osteocytes are stimulated mechanically, they emit signaling molecules propagating throughout the osteocyte network to the bone surface, where they induce new bone formation or bone resorption. These processes adapt the bone structure to mechanical loads, and they enable the detection and repair of micro-damage which modifies the bone structure. It remains poorly understood how osteocyte network properties such as the spatial density of osteocytes and the number of connections between them influence how and when bone formation or bone resorption occur. In this work, we study the propagation of signaling molecules reacting and diffusing in spatial networks. We use random walk models, and discrete, compartmental models on irregular 1D networks with near and far connections, and jump probabilities that may be space dependent. The continuum limit of these models is an advection-diffusion-reaction equation where diffusivity and drift velocity explicitly depend on network structure such as node density and node connectivity. Numerical simulations of the discrete model, the stochastic model and the corresponding advection-diffusion-reaction equation match well when the number of nodes is large and when network properties are sufficiently regular. On more irregular networks with sharp changes or discontinuities in drift $u(x)$ and diffusion $D(x)$, the discrete model is a robust discretization method for the advection-diffusion-reaction equation. Our simulation results also indicate that connections with far nodes increase the noise in signaling. This increase occurs due to a concurrent increase in diffusivity.

What insight computational mathematical modelling brings to Multiple Sclerosis

Adrianne Jenner (Queensland University of Technology)

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Multiple Sclerosis (MS) is a disease of the central nervous system where the immune system attacks nerve coatings, resulting in eventual nerve axon death. There is a significant lack of mathematical modelling of MS and neuroimmunology. To investigate this problem, we developed a set of partial differential equations capturing cellular behaviours spatially. In this talk, we present how we applied a Finite Volume Method (FVM) discretization to numerically simulate this model. We also discuss our preliminary results of initialising the simulations with patient MRIs for disease densities. In presenting our work, we hope to gain more insight from the computational modelling community on other methods that could be used in our work.

Temperature field in fluids flowing through micro-channels in the slip regime

Amani Ahmed Otaif* (Curtin University)

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This work considers the heat transfer of an incompressible Newtonian fluid flowing through a circular micro-tube. The problem involves both fluid flow and heat transfer, and the interaction between the two processes. Exact solutions of the velocity field for the transient flow of fluids through microtubes have been developed in the literature. However, the associated temperature field in the microflow has not been investigated. A mathematical model is presented in this paper to investigate the heat transfer process and determine the temperature field in microflows in the slip regime. A computation scheme is developed using the finite difference method to solve the problem numerically. The influence of boundary slip on the temperature field is then investigated.

Mathematical modelling of the drying of fruits and vegetables

Anthony Vine * (Queensland University of Technology)
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Fruits and vegetables contain over 80% water making them highly perishable commodities. Removal of this water by way of convective drying has become the most common method of preserving fruits and vegetables, however, this is an energy intensive and time consuming process. Mathematical modelling is an ideal way to optimize the drying parameters in order to reduce the overall operational costs. Fruits are comprised of a complex structure of cells consisting of vacuoles, cytoplasm, membranes, cell wall, and gaseous pores. Water is found within the cell interstices, bound to the cell wall, and in the porous space between cells. The location of water within the cellular matrix determines its rate of transport. Accurate modelling of mass transport in food materials requires knowledge of how water transport properties depend on this material structure. In this work different mathematical models of drying are compared to identify the moisture migration mechanisms within each of the domains of the cellular matrix and the mass transfer rates between these domains. Experimental results for the convective drying of apples are used to analyse the accuracy of the simulated moisture content and temperature distributions computed by the various models.

Efficient finite element methods for three-field formulations of elasticity and Reissner-Mindlin plate equations using biorthogonal systems

Bishnu Lamichhane (University of Newcastle)
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We present efficient finite element methods for nearly incompressible elasticity and Reissner-Mindlin plate equations using biorthogonal systems. While a standard finite element method using low order polynomial interpolations do not converge uniformly for these problems, we formulate three-field formulations and then apply finite element approaches based on biorthogonal systems to obtain a uniformly converging scheme. We will also present some numerical examples to demonstrate the performance of our approach.

Laminar flow through rectangular channels with walls of different permeabilities: a contraction mapping approach

David Bee Olmedo * (UNSW)

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Collaborators: Mareike Dressler and Christopher C. Tisdell

An example of laminar flow through porous media involves a rectangular channel with a pair of parallel walls through which fluid is injected in or extracted out. Although this type of problem dates back to the 20th century and draws upon perturbation techniques as a partial method of solution, a firm mathematical foundation regarding qualitative and quantitative properties of solutions is yet to be fully developed. For example, we still do not know: if these types of problems are well-posed; where the precise solution lies; if and how approximations converge to the solution; and what the estimates on approximation errors are. In this talk, our strategy involves developing insight via new and interesting connections between the boundary value problem arising from modelling of the laminar flow and the theory of fixed points of operators.

Evaluation of maceral interface quality in 3D micro-CT images of metallurgical coke

David Ronald Jenkins (University of Newcastle, NSW)

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Collaborators: Ai Wang

Metallurgical coke is a crucial component in the production of steel worldwide. It is a porous composite material, created by conversion of metallurgical coal in a coke oven. A key property of metallurgical coke is its strength, and there is evidence that poor interface quality between the two key components (called macerals) of coke can have deleterious effect on coke strength. Here we create small samples of coke mixing macerals of various types of coal and image them using high resolution 3D micro-CT, with pixel size around 8 micron. We use a Gabor filter, combined with morphology techniques to isolate the different components in the samples. We then develop a measure, called excess porosity to quantify the quality of the interfaces between macerals. This measure enables us to highlight problem interactions between macerals.

Stable and accurate method for simulating the Anisotropic Diffusion in toroidally confined magnetic fields

Dean Muir* (Australian National University)

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Collaborators: Kenneth Duru, Matthew Hole, Stuart Hudson

In magnetic toroidal confinement fusion, transport of particles or temperature happens primarily along magnetic field lines, with the ratio of diffusion parallel and perpendicular to the field lines sometimes exceeding the order of 10^8. A simple way of modelling transport is though solutions to the anisotropic diffusion equation, however the ratio of diffusion coefficients can prove a challenge for numerical solvers. In this presentation we will discuss a novel approach to solving the anisotropic diffusion equation in a periodic slab using summation by parts finite difference methods. The diffusion parallel to the magnetic field lines is computed by interpolation and then addition to the perpendicular diffusion by a parallel penalty term. The method is efficient, provably energy stable and asymptotic-preserving. We will present numerical experiments verifying the numerical accuracy and stability of the method.

Adaptive dual-grid mapping method for solving the advection-diffusion-reaction equation in a heterogeneous medium

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Collaborators: Elliot Carr, Ian Turner

Substantial research conducted by the wider scientific community is focussed on the development of models describing heat and mass transport phenomena. Often, the associated PDE models are highly complex and not amenable to analytical solution methods. This is especially evident for models describing processes in heterogeneous media, where the computational cost of numerical simulation is high due to the prohibitive number of nodes required to capture the heterogeneous structure. In this talk, I will outline an adaptive dual-grid mapping method for accurately computing solutions to the heterogeneous advection-diffusion-reaction equation on coupled coarse and fine-scale grids. Using a spatial discretisation of the governing equations on a fine-scale grid, a novel mapping is developed, allowing solutions to be accurately computed on a coarse-scale grid, and then accurately reconstructed on the fine-scale grid.

A scalable two-point correlation and lineal path function computation method.

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Collaborators: Dr Bishnu Lamichhane

Coke is a solid carbon fuel used in a blast furnace along with iron ore to manufacture iron. Iron is a necessary raw material for steel production, and this blast furnace route accounts for approx 70% of steel production globally. Coke microstructure is highly variable and consists of features at a wide range of length scales. Understanding coke microstructure is crucial to producing more efficient coke that meets the requirements of future steel-making technologies. We present a scalable, histogram-free parallel method to efficiently compute the angularly resolved two-point correlation and lineal path functions for large 3D coke microstructure images.

Adaptive batch strategy using a leverage score based initialisation for calculating the minimum volume covering ellipsoid

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The minimum volume covering ellipsoid (MVCE) problem arises in many applied and theoretical areas. Statistical applications include the closely related D-optimal design problem, as well as outlier detection and clustering. Containing ellipsoids are used in control theory, to efficiently analyse dynamical systems subjected to perturbations. MVCEs are also used in computational geometry and computer graphics, in particular, for collision detection. We present a new initialisation of an adaptive batch strategy to compute the $(1+\epsilon)$-approximate MVCE for a set of n points in R^d. We focus on moderately sized datasets (up to $d = 100$, $n = 1\,000\,000$). The adaptive batch strategy works in an optimisation-deletion-adaptation cycle: we solve the MVCE problem using a smaller number of points, we delete points from consideration that are guaranteed to not lie on the boundary of the MVCE, and then carefully select a new batch of points. We propose a new initialisation, which involves selecting the points corresponding to the s highest leverage scores. We show using numerical examples that this new initialisation tends to improve computation time as well as reduce the total number of cycles, as compared with initialising with the first s points.

Resilience of Multigrid Method in Parallel Adaptive Mesh Refinment

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Collaborators: Linda Stals, QuanLing Deng

As marching towards the era of exascale computation, execution faults have been observed more than ever from supercomputing facilities. In our study, we particularly focus on recovering loss of approximation due to occurred faults during the runtime of multigrid methods - arguably one of the fastest linear system solvers. Our multigrid method is defined and implemented in adaptively refined meshes. Unlike the similar problem proposed in structured meshes where the convergence for local fault recovery was well-behaved, we observed convergence deterioration in our setting. In this talk, we borrow the ideas from multigrid convergence theory to demonstrate the cause of convergence deterioration and show that it's possible to resort the convergence with extra mesh modification.

Multi-component lattice Boltzmann for large density and viscosity ratio fluids

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The lattice Boltzmann (LB) method is a computationally efficient numerical technique used to model the (simultaneous) flow of one or more (immiscible) fluids. One of the most popular LB methods for multi-component flows is the pseudo-potential model, based on attractive or repulsive intra-molecular interactions between the different fluid components which leads to phase separation of the components. This pseudo-potential model can compute immiscible flows of fluids with comparable density and viscosities but becomes unstable or inaccurate for more practical fluid pairs with large density and viscosity differences (such as water and air or oil and gas). In this work we seek to understand the underlying mathematical reasons for this loss of numerical stability in fluids with large differences in their material properties (such as viscosity) through a detailed Chapman-Enskog analysis. An important necessary condition for numerical stability is found. We then consider modifications of the pseudo-potential method, based on this necessary condition, to achieve greater stability. The new method is applied to fluid pairs with high viscosity and density ratios and validated against analytical and independent (experimental or numerical) results. Subsequently, we proceed to apply the method to some realistic scenarios such as displacement of oil from a porous medium.

The Effect of Immune Cells as a Treatment for Cancer Using an Agent-based Model

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Collaborators: Hasitha N Weerasinghe, Pamela M Burrage, Dan V Nicolau Jr., Kevin Burrage

Agent-based modelling can be applied to understand intra-tumoural communication in the tumour microenvironment (TME). This study investigates the importance of immune cell activities in the TME by introducing immune cells into the TME as a treatment. We develop a two-dimensional discrete agent-based model to study the impact of tumour microenvironmental factors on cancer progression and invasion. Initially, the domain is a healthy tissue that consists of healthy cells and extracellular matrix (ECM) proteins. A random healthy cell mutates, and the daughter cell turns into a tumour cell. Due to the uncontrolled growth of tumour cells, the domain becomes crowded with tumour cells. We introduce immune cells into the system at the diagnosed time of the disease by considering three strategies. In strategy one, we merely insert immune cells once after diagnosing the tumour. In strategy two, we insert immune cells into the system after the tumour is diagnosed and also repeat inserting immune cells at specific time frequencies. Under strategy three, we insert immune cells into the system after the tumour is diagnosed and repeat inserting immune cells if the percentage of immune cells drops below a specified threshold. We study the impact of immune cells on tumour progression and invasion according to the mass of the tumour at the diagnosed time. Results of the study show the importance of identifying a tumour in its early stages and applying immune cells using a certain strategy.

Removing the mask – reconstructing a scalar field on the sphere from a masked field

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The paper analyses a spectral approach to the recovery of a scalar field, given only information about a masked version of the field together with precise information about the (smooth) mask. The theory is developed for a general mask, and later specialised to the case of an axially symmetric mask. Numerical experiments are given for the case of an axial mask motivated by the cosmic microwave background, assuming that the underlying field is a Gaussian random field with an artificial angular power spectrum of moderate degree ($\ell \leq 100$). The recovery is highly satisfactory in the absence of noise, even in the presence of noise of moderate magnitude.

A polytopal discrete de Rham scheme for the Yang—Mills equations

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Collaborators: Jerome Droniou, Todd Oliynyk

The Yang–Mills equations come from a type of gauge theory in physics, where the symmetries of the Lagrangian are captured by a particular choice of a non-abelian Lie group. In the case of $U(1)$, the non-linear terms deriving from the Lie bracket on the associated Lie algebra vanish, and the system simplifies to Maxwell's equations. In the standard electromagnetism problem, the constraints cannot be imposed; they are instead satisfied through the evolution of initial data that meets certain requirements. There exists many numerical methods for Maxwell's equations that reproduce this feature by relying on a discrete version of certain properties of the de Rham sequence, allowing the replication of the continuous proof. In the Yang—Mills equations, the non-linear terms appearing in both the constraint and evolution become problematic for these discretisation techniques, and further adaptations must be made to reconstruct the preservation of the constraint. We present a constraint preserving discretisation of the Yang–Mills equations based on the discrete de Rham sequence (DDR), along with energy estimates and 3D numerical results.

Electrohydrodynamic control of viscous fingering during fluid displacement

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Collaborators: Zhongzheng Wang and Emilie Sauret

Interfacial instabilities are a common phenomenon for multicomponent fluid flows, which can be beneficial or detrimental depending on the practical applications. Therefore, different strategies have been deployed to manipulate this instability. In this study, the active control of the interfacial instability of viscous fingering realized by taking advantage of electrohydrodynamics is demonstrated numerically. Based on the coupled solution of the governing equations of the electric field and fluid flow, a numerical model is developed. Specifically, the pseudopotential LB model, also known as Shan-Chen (SC) model, is employed to simulate the multicomponent fluid system due to its popularity and simplicity. Moreover, the governing equations for the electric field are solved by finite difference method (FDM). Then, the obtained electric force is incorporated into the SC model through a source term. The coupled LB-FD model for electrohydrodynamics is validated using the droplet deformation benchmark, which agrees well with the analytical solution. Initial simulations are carried out for investigating the interfacial development of viscous fingering in the presence of an electric field using the validated model. The results show that a horizontal electric field suppresses the viscous fingering, while a vertical electric field aggravates it.

A physics-informed deep learning-based meshfree method for hydrodynamics modelling

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Collaborators: Emilie Sauret, Yuantong Gu

We introduce the general neural particle method (gNPM), a meshfree method for hydrodynamics modelling based on physics-informed deep learning (PGDL) technique [1, 2]. In the gNPM, artificial neural networks (ANNs) are used to predict fluid field variables in terms of pressure and velocity. Furthermore, the explicit and implicit Runge-Kutta (RK) methods are applied to cope with temporal integration. It is worth noting that the neural networks in the gNPM is trained through the physics laws in the fluid mechanics and the corresponding boundary conditions. The spatial differential terms in the governing equations are analytically obtained through automatic differentiation rather than relying on the surrounding nodes or particles. Therefore, the proposed gNPM can cope with the unevenly distributed particles and achieve high accuracy, while the traditional meshfree method can produce severe failure. Finally, several hydrodynamics benchmark problems are conducted to demonstrate the performance of the proposed gNPM. [1] J. Bai, Y. Zhou, Y. Ma, H. Jeong, H. Zhan, C. Rathnayaka, E. Sauret, Y. Gu, A general Neural Particle Method for hydrodynamics modeling, Computer Methods in Applied Mechanics and Engineering, 393 (2022). [2] H. Wessels, C. Weißenfels, P. Wriggers, The neural particle method – An updated Lagrangian physics informed neural network for computational fluid dynamics, Computer Methods in Applied Mechanics and Engineering, 368 (2020).

Dynamic equations on time scales and some foundational biological models

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Collaborators: Christopher C. Tisdell

Dynamic equations on time scales is a mathematical framework that is designed to enable mathematicians to model and understand phenomena that display both discrete and continuous characteristics. Researchers have utilized the field of time scales to better understand several distinctive hybrid population models. However, in the race to publish and push out these results, some foundational and rudimentary linear models are yet to be fully explored. As the field tends to more unique and complex species interactions, the absence of simple linear results makes it difficult for students looking to study this area of mathematics. Especially for undergraduate or Honours students, having such results explicitly provided in their basic form is necessary from a pedagogical perspective as only having advanced and complex models can be intimidating and off-putting. In this talk, we formulate the general linear population models of two-species interaction on time scales and also challenge the popular periodic cicada population model on time scales and offer some more realistic assumptions and adjustments.

Optimal Hessian Recovery Using a Biorthogonal System with an Application to Adaptive Refinements

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In this talk, we present a method of recovering the Hessian from a linear finite element approach to achieve a higher rate of convergence. This method uses an L^2-based projection as well as boundary modification to achieve and improve the convergence rate. The projection uses a biorthogonal system to make the computation more numerically efficient. We present numerical examples to illustrate the efficiency and optimality of our approach on different meshes. The performance of our approach on adaptively refined meshes is briefly explored.

Towards energy-stable and conservative discontinuous Galerkin spectral element methods for Einstein's equations of general relativity in second order form

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Collaborators: Siyang Wang and Kenny Wiratama

Numerical methods for solving the Einstein's equations of general relativity are often derived for the first order systems, by first rewriting the underlying system of second order partial differential equations (PDE) as a system of first order hyperbolic PDEs. The reduction to first order system has the potential to introduce some numerical and computational inefficiencies, as well as numerical stability issues. There are several benefits for solving the equations in second order form. However, it appears to be more difficult to guarantee numerical stability for the naturally second order systems than for first order reductions of them. In this presentation we take a first, but an important, step towards designing of provably stable and high-accurate discontinuous Galerkin spectral element methods for the Einstein's equations of general relativity in second order form.

An Energy Stable Discontinuous Galerkin Spectral Element Method for the Linearized Serre Equations

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Collaborators: Kenneth Duru, Stephen Roberts, Christopher Zoppou

In this talk, we consider the Serre equations, which are nonlinear dispersive wave equations that describe the motion of free surface water waves. In one spatial dimension, we derive well-posed boundary conditions for the linearized Serre equations. A provably stable and conservative discontinuous Galerkin spectral element method is proposed for the initial boundary value problem, with simple upwind numerical fluxes. We derive discrete energy estimates for the numerical approximation and prove a priori error estimates in the energy norm. Detailed numerical examples are provided to verify the theoretical analysis and show convergence of numerical errors.

A comparision of smoothing splines

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In a number of previous CTAC conferences we have presented the development of a discrete thin-plate spline solver. We have recently made substantial progress with a fast iterative solver and adaptive finite element methods. However, when presenting out work we are inevitably compared with other, more widely known, smoothing techniques. In this talk I will give some results comparing the discrete thin-plate spline solver to techniques such as the thin-plate spline and Gaussian basis functions as well as compact basis functions such as the Buhmann and Wendland basis functions. One aspect that has a big impact on the results are the smoothing parameters. I will present some of the available techniques for determining those parameters.

Simplified models of diffusive transport in radially-symmetric media

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Collaborators: Elliot Carr, Matthew Simpson

Simple reduced-order mathematical models are commonly proposed in applications such as drug delivery and food drying to approximate PDE models describing the spatial and temporal dynamics of diffusive heat and mass transport. Such reduced-order models are appealing as they bypass solving the PDE model, while also allowing for a simplified analysis and interpretation of results. Recently, a moment-matching approach was proposed and used to develop a simple single-term exponential model for the temporal evolution of the spatial-average of the diffusion equation in homogeneous radially-symmetric geometries. In this talk, I show how this approach can be extended to two-term exponential models that significantly improve on the accuracy of the single-term exponential model, in comparisons with the continuum spatial-average and stochastic simulations.

Computing expected moments of the Rényi parking problem on the circle

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A. Rényi [Magyar Tud. Akad. Mat. Kutató Int. Közl. 3 (1-2), 1958, pp. 109-127] discussed a one-dimensional random parking problem. Random parking can be seen to be a point process where the samples are the set of locations of the parked cars. Rényi derived an integral equation for the expected size of the samples. Here we consider the circular parking problem. We derive integral equations for the expected first and second moments of the samples. We then use spectral methods to obtain highly accurate approximations of these expected moments in addition to the expected size of the samples. We provide error bounds and validation by computational experiments.

Normally-distributed compositional data: a review of computational methods

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Compositional data, which is data consisting of fractions or probabilities, is common in many fields including ecology, economics, physical science and political science. If these data would otherwise be normally distributed, their spread can be conveniently represented by a multivariate normal distribution truncated to the non-negative space under a unit simplex. For calculations on truncated distributions, it is often useful to obtain rapid estimates of their integral, mean and covariance; these quantities characterising the truncated distribution will generally possess different values to the corresponding non-truncated distribution. In this talk, I will review the currently available computational methods which can estimate all of these quantities for compositional data that would otherwise be normally-distributed.

Robust methods for mapping diffusion kurtosis

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Collaborators: Qianqian Yang, Viktor Vegh

Diffusion weighted magnetic resonance imaging (DW-MRI) captures the random movement of water molecules in biological tissues. Many modern imaging studies, particularly in neuroimaging, have focussed on collecting and extracting information from this data. A range of mathematical models are routinely applied to infer tissue microstructure. Diffusion kurtosis imaging models have been applied to quantify the non-Gaussian diffusion of water molecules. We present a fast and robust method of computing kurtosis via the sub-diffusion mathematical framework. We evaluate our method through a combination of simulations and the Connectome 1.0 human brain data. Our results show that fitting the sub-diffusion model to multiple diffusion time data greatly improves the quality of estimation. Suggestions about the optimal acquisition protocols are made. Our findings suggest that robust estimates of mean kurtosis can be achieved within clinically feasible acquisition times.

Fractional Diffusion Model Generalised by the Distributed-order Operator Involving Variable Diffusion Coefficients

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Collaborators: Fawang Liu, Ian W. Turner, Vo V. Anh

The diffusion process plays a crucial role in various fields, such as fluid dynamics, microorganisms, heat conduction, food processing and medical imaging. Since molecular diffusion usually takes place in complex materials and disordered media, there still exist many challenges to describing the diffusion process in the real world. Fractional calculus is a powerful tool for modelling complex physical processes due to its non-local property. This research generalised a fractional diffusion model by using the distributed-order fractional operator in time and the Riesz fractional derivative in space. Moreover, variable diffusion coefficients are introduced to better capture the diffusion complexity. The two-dimensional fractional diffusion model is discretised by the finite element method in space. The approximation of the distributed-order operator is implemented by the L2-1_σ formula. Numerical examples are provided to verify the effectiveness of the proposed numerical methods. This generalised fractional dynamic model may offer more insights into characterising diffusion behaviours in complex and disordered media.

Numerical analysis of stochastic Stefan problem using the gradient discretization method

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Collaborators: Jerome Droniou, Kim Ngan Le

The gradient discretization method (GDM) - a generic framework encompassing many classical numerical methods - is studied for a general stochastic Stefan problem with multiplicative noise. The convergence of gradient scheme solutions is proved by compactness method using discrete functional analysis tools and Skorohod theorem. The martingale representation theorem is then used to show the existence of the weak martingale solution. The generic convergence results established in the GDM framework are applicable to a range of different numerical methods, including for example mass-lumped finite elements, but also some finite volume methods, mimetic methods, lowest-order virtual element methods, etc. The theoretical results are illustrated by numerical tests using mass-lumped conforming $_{|1}$ finite elements method.

Multiscale computational homogenisation using spectral methods for additively manufactured metal part

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Collaborators: Dayalan Gunasegeram (CSIRO), Indrajeet Katti (RMIT), Samuel McNeil (CSIRO)

Metal additive manufacturing is a technique that allows for the layer-by-layer construction of bespoke metal parts with complex geometries through the melting of metal alloy powder or wire via a heat source. These parts find mission-critical applications in industries such as medical, aerospace, automotive and defence. The mechanical properties of these parts are dependent upon the local microstructure and are of critical importance in determining their suitability for their intended purpose. These mechanical properties can be calculated using computational homogenisation, which uses the solution of boundary value problems on a representative section of the microstructure. In additive manufacturing, these microstructures can vary at multiple scales, with the smallest heterogeneities occurring at the nanometre scale and the largest representative sections of the microstructure comprising hundreds of micrometres. As the mesh required to consider these small-scale heterogeneities is computationally intractable, we discuss a three-scale methodology using computational homogenisation techniques to link between the nanometre scale and micrometre scale and, again, between the micrometre scale and millimetre scale. We use spectral methods to improve the computational efficiency of our multiscale methodology compared to standard numerical techniques and discuss the computational advantages of our methodology.

Simulation of surfactant-laden drops impacting on a flat surface: effect of Marangoni's stresses

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Collaborators: Ravindra Pethiyagoda, Arvind Kumar, Timothy J. Moroney, Philip Taylor, Justin J.

Abstract: Crop protection products are extensively used by farmers for weed and pest control in order to maximise crop yields. Unfortunately, the application of these products is often accompanied by undesirable effects on the environment and human health, which means that it is crucial to find solution to reduce the sprayed quantity. One way to decrease the amount of sprayed products is to optimise the quantity of liquid which remains on plants. When sprayed drops impact the plant surface, they can either adhere, bounce-off or shatter. The outcome results from the complex interaction between the liquid, gas and solid phases. Many commercial products increase the chance of adhesion by adding surfactant, which lowers the surface tension. The impact of pure Newtonian drops on simple surfaces has been extensively studied. But the impact of surfactant-laden drops still needs to be better understood. Surfactant dynamically affects the liquid surface tension, which leads to Marangoni's stresses. During our research, we created an extension of OpenFOAM to simulate the impact of surfactant-laden drops on flat surfaces by solving the Navier-Stoke and sorption equations with the coupled Volume-of-fluid/level-set approach. The simulations show that i) Marangoni's stresses tend to reduce the maximum spreading and ii) the Marangoni's stresses are stronger for high-speed impact.

Constructing Virtual Representations of Laminated Timber Products

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Collaborators: Professor Ian Turner, Dr Steven Psaltis, Dr Maryam Shirmohammadi (DAF)

The complex structure of timber has traditionally been difficult to model as it is a highly heterogeneous material. In structural timber species, such as Radiata Pine, the density can vary by up to a factor of four times within the span of a few millimetres over the growth rings. Numerical simulation methods are becoming more prevalent as a method of predicting moisture migration, stress and strain distributions, and fungal/rot intrusion in timber. A computational mesh that captures heterogeneities present within structural timbers is required. In this work, a low-cost algorithmic method is developed that utilises image analysis techniques and spectral segmentation to produce a three-dimensional computational mesh of a laminated timber product. Starting with a photograph or a scan of the end grain of a timber board, an image mask is produced by employing thresholding and image smoothing techniques. This mask highlights the darker, latewood sections of the board providing a binary image of the growth ring locations. The growth rings are then identified using a spectral clustering algorithm, which performs exceptionally well on the three test images (quartersawn, plainsawn and back sawn boards). Lastly using the light intensity data of the image, the density of the board can be associated with each mesh element. Meshes of multiple timber boards can then be combined to produce the final mesh of a laminated timber product.

A comprehensive approach and solution techniques for operating theatre scheduling

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Collaborators: Paul Corry

Operating theatre scheduling is widely accepted as being an extremely important driver of hospital capacity, efficiency, and output. Despite the vast amount of published theoretical work on operating room management, only a very small percentage of this work has been implemented in an operational setting. Nothing has been found that incorporates all the factors within one study such that it is scalable and generic enough to be implemented in any hospital. The aim of this paper is to provide a novel comprehensive scheduling approach and to provide solution techniques which are fast and produce near if not optimal solutions. The desired outcome is to bridge the gap between research and the real world by demonstrating that the scheduling tool may be implemented in a large South-East Queensland hospital. Over 300 million major procedures are performed worldwide annually (Dobson (2020). If this new scheduling approach can increase patient throughput by just 3%, then that translates to 9 million additional procedures and an associated reduction in patient waiting times, using existing resources. Likewise, given that healthcare is a $10 trillion industry, even a 1% reduction of costs would have a profound impact. It is also intended that the study will identify future research opportunities to optimise staff levels, equipment, and instrument tray inventory.

Continuous time random walk (CTRW) modelling framework in diffusion MRI

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Collaborators: Viktor Vegh, David C. Reutens

Diffusion magnetic resonance imaging (MRI), which measures the random motion of water molecules in biological tissues, has become a pillar of modern neuroimaging. One major challenge in the field of diffusion MRI is that the measurement is at millimetre scale while the tissue microstructure, providing key insight into diagnosis and treatment of central nervous system diseases and disorders, is at microscale. Many models have been proposed to link millimetre measurements with microscale tissue properties. In this talk, we focus on the continuous time random walk modelling framework, which considers the diffusion of water molecules as an anomalous (Non-Gaussian) transport process and infers microstructure information through different anomalous diffusion parameters. We also show that CTRW modelling framework is able to unify several established non-Gaussian models, including the prevalent diffusional kurtosis imaging (DKI) model. This link between the DKI and sub-diffusion (a special case of CTRW) models led to a new robust and accurate technique for generating maps of kurtosis and diffusivity using the sub-diffusion parameters. Superior tissue contrast is achieved in kurtosis maps based on the sub-diffusion model. Overall, our results suggest that anomalous diffusion models under the CTRW framework play an important role in mapping tissue microstructure and deriving tissue specific micro-parameters.

Multi-scale modelling of Arctic sea ice floes

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Collaborators: Nan Chen (UW-Madison) and Sam Stechmann (UW-Madison)

In this talk, I will start with some quick facts about Arctic sea ice floes and then give a quick review of the evolution of sea ice models. The first models are Eulerian continuum models that describe the sea ice floes as viscous-plastics (Hilber 1979). Lagrangian particle models have been developed recently, showing improved model performance, especially in ice-marginal zones where sea ice is fragmented. The most successful one is the discrete element method (DEM). It characterises the physical quantities of each sea ice floe along its trajectory under the Lagrangian coordinates. The major challenges are 1) model coupling in different frames of reference (Lagrangian for sea ice while Eulerian for the ocean and atmosphere dynamics); 2) the heavy computational cost when the number of the floes is large; and 3) inaccurate floe parameterisation when the floe distribution has multiscale features. I will present a superfloe parameterisation to reduce the computational cost and a superparameterisation to capture the multiscale features. The superfloe parameterisation algorithm generates a small number of superfloes that effectively approximate a considerable number of the floes. The parameterisation scheme satisfies several important physics constraints that guarantee similar short-term dynamical behaviour while maintaining long-range uncertainties, especially the non-Gaussian statistical features, of the full system. In addition, the superfloe parameterisation facilitates noise inflation in data assimilation that recovers the unobserved ocean field underneath the sea ice. To capture the multiscale features, we follow the derivation of the Boltzmann equation for particles and superparameterise the sea ice floes as continuity equations governing the statistical moments of mass density and linear and angular velocities. This leads to a particle-continuum coupled model. The continuum part captures the large scales and the particle part captures the small scales. The particle model is localised and fully parallelised for computation efficiency. I will present several numerical experiments to demonstrate the success of the proposed schemes. This is joint work with Nan Chen (UW-Madison) and Sam Stechmann (UW-Madison).

Numerical solutions to an inverse problem of a non-linear Helmholtz equation

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Collaborators: Hrushikesh Mhaskar (Claremont Graduate University)

In this work, we construct numerical solutions to an inverse problem of a nonlinear Helmholtz equation defined in a spherical shell region between two concentric spheres centred at the origin. Assuming that the values of the forward problem are known at sufficiently many points, we would like to determine the form of the non-linear term on the right-hand side of the equation via its Chebyshev coefficients.

Robust discretisations for poromechanics formulations using total pressure

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Collaborators: Kent-Andre Mardal, Mirolsav Kuchta, Martin Hornkjøl

I will discuss discretisations for a fluid-poroelasticity interaction model. A five-field finite element scheme solves for Stokes velocity-pressure and Biot displacement-total pressure-fluid pressure. One of the distinctive features of the formulation is that its stability is established robustly in all material parameters. We propose robust preconditioners for this perturbed saddle-point problem using operators in weighted fractional spaces at the interface. The performance is corroborated by several test cases with applications into brain tissue.

Modelling droplet dynamics without resolving interfaces using smoothed particle hydrodynamics

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Collaborators: TJ Moroney; IW Turner; R Pethiyagoda; SW McCue

Understanding the dynamics of droplets on rough surfaces is crucial to the improvement of agrochemical formulations and spray technologies. Models of droplet-canopy interactions could lead to more efficient application of agrochemicals to crops and therefore lower water usage and runoff. Models of droplets on substrates usually require a boundary condition at the contact line (the curve where the gas, liquid, and solid phases meet) that specifies the angle the droplet makes with the substrate. This contact angle is determined experimentally on a flat surface for a particular fluid-substrate pair. Adapting these models to rough surfaces is challenging as the contact angle may not be constant around the contact line. We propose in this work a different approach in which surface tension and the contact angle are not explicitly prescribed. Rather, they are consequences of inter-particle forces that mimic cohesion and adhesion – the actual physical phenomena that give rise to surface tension and the contact angle. We use an adapted smoothed particle hydrodynamics (SPH) scheme, including pairwise forces between the mesoscopic "particles" of fluid. This does not require a local boundary condition at the contact line, instead using static particles to represent the substrate. We show good qualitative results of droplets settling on rough surfaces and discuss the direction of future work, with a focus on parameter fitting for the introduced inter-particle forces.

Summation by Parts Analysis with Finite Volume: Linearized Shallow Water Wave Equation with

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Collaborators: Kenneth Duru, Stephen Roberts, Christopher Zoppou

In this presentation, we will discuss well posed and energy stable boundary conditions for the linearized shallow water wave equation. We derived a finite volume method encapsulated in the summation by parts (SBP) framework. This facilitates the development of provably energy stable numerical implementations of well posed boundary conditions using penalties. We will present the proof of numerical stability by deriving discrete energy estimates analogous to the continuous energy estimates. This is demonstrated for a non-trivial transmissive boundary condition for the shallow water wave equation.

Numerical analysis of the axisymmetric lattice Boltzmann method for steady and oscillatory flows in periodic geometries

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Collaborators: A/Prof. Peter Johnston and Dr Barbara Johnston

When compared to more typical computational fluid dynamics (CFD) techniques, the lattice Boltzmann method (LBM) is relatively new and unexplored. In recent years, axisymmetric LBM formulations, which can simulate flow in rotationally symmetric 3D geometries, have been published. The goal of this talk is to verify a novel axisymmetric LBM implementation using numerical criteria. Firstly, Hagen–Poiseuille and Womersley flow are considered within a straight tube where analytic solutions are available. Here we establish sufficient accuracy of the approximated flow and study the effects of changing simulation parameters (e.g. Reynolds number, Womersley number) and spatial/temporal parameters (e.g. relaxation time, mesh nodes, time steps). Next, steady and oscillatory flows within a periodically-varying, longitudinally asymmetric geometry are considered. Analytic solutions are not available in this case; however, the validity of the axisymmetric LBM for curved boundaries is ensured through convergence and mesh independence studies. Guaranteeing reasonable flow field determination for this shape is relevant to a larger problem where particulate suspension is pumped back and forth through a membrane of axisymmetric micropores - sometimes producing particle transport when there is no net flow of the carrier fluid.

A structure-preserving approach to simulating Hamiltonian systems with dissipation

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Collaborators: David Pfefferlé (UWA), Matthew Hole (ANU), Michael Kraus (IPP, Germany)

Hamiltonian systems occur naturally in many physical problems, including those in plasma physics. The behaviour of charged particles in electromagnetic fields, which consistently influence each other, can be modelled through the Vlasov-Maxwell equations — a 6D time-dependent system of hyperbolic partial differential equations. The Hamiltonian structure of this problem has recently been exploited in the design of numerical solvers, as it provides one way to ensure the numerical preservation of invariants (or first integrals) associated with the problem. Unfortunately, introducing dissipation into such systems (most often through global integral operators) can spoil the conservation properties of these methods. In this talk, we present the metriplectic approach, which is a formalism for producing structure-preserving methods for Hamiltonian systems with dissipation. It works to reproduce the dissipative terms through using an entropy-like quantity and metric bracket that are constructed to be compatible with the Hamiltonian structure, and this can be carried into the numerical discretisation of the problem as well. The talk will present an introduction to this topic, illustrated through examples.

A sequential method for efficiently parameterising ecosystem models

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Collaborators: Prof Chris Drovandi and Dr Matthew Adams

Ensemble ecosystem models are valuable decision-making tools for understanding the effects of conservation actions and human impacts on threatened species. Models parameterised with dynamic systems constraints - stable coexistence of species - help us understand ecosystems with limited data availability. However existing methods are computationally inefficient, preventing larger networks from being studied. Using Bayesian approaches, we build on the current methods to overcome this technical obstacle. Compared with the existing method, we find that using a sequential Monte Carlo approach yields similar parameter inferences and model predictions while being significantly faster. Consequently, we can study larger and more realistic networks, improving ecosystem modelling capabilities.

Ship wake analysis using machine learning

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Collaborators: Professor Timothy Moroney, Doctor Ravindra Pethiyagoda, Professor Scott McCue

Ship wake analysis is a complex problem. A promising way to analyse ship wakes is to measure surface heights at a single point over time, and process this signal using time-frequency analysis. The wake signal is found to encode a large amount of data about the source of the disturbance, such as the speed of the ship and its distance from the sensor. However, to date the amount of information that can be analytically extracted from this signal is still limited. For example, [Torsvik et al] derived two formulae to calculate the speed of the ship and its distance from the sensor, but the average error from their experiment was as big as 17%. Motivated by the link between short-time discrete Fourier transforms and convolutional layers, we utilise the powerful technology of convolutional neural networks to analyse the signals. For this, we require a large database of signals on which to train. Here we investigate using mathematical models based on linear water wave theory to generate suitable synthetic data. Early results suggest that this machine learning approach can indeed identify more subtle features carried by these synthetic signals. Future work will extend this approach to more sophisticated mathematical models, and validate on real data.

Chaotic flow in competitive exothermic-endothermic reaction systems

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We study the effects of two-dimensional chaotic advection on a chemical system characterised by competitive exothermic and endothermic reactions. In previous studies, in which advective flow and reaction processes were assumed to dominate weak diffusive effects, two distinct behaviours were observed in the system. The first, when the stirring is fast and the reaction is slow. In this case, flame quenching occurs. In contrast, when the stirring is slow and the reaction is fast, local temperature perturbations lead to a stationary flame with a complex filament structure. When the diffusion process is more influential, as for example in many microfluidic contexts, a third type of behaviour is possible, in which an expanding swirling travelling wave develops. We explore the diffusion-dominated behaviour in more detail.

Self-similarity and Fractalisation in Interfacial Hydrodynamics

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Collaborators: Dr. Michael Dallaston, Prof. Scott McCue.

Thin film equations are classes of nonlinear partial differential equations, which are applied in industrial and scientific modelling to describe the dynamics of viscous liquid flow on solid surfaces. Our work investigates the self-similar dewetting behaviour of thin film models, particularly for the case of Marangoni-driven rupture, where iterated patterns form and create an intriguing hierarchical structure. This phenomenon leads us to search for an unstable periodic orbit in a rescaled similarity space. In this talk we will discuss computational techniques used to explore this problem, such as non-uniform finite differences, moving mesh and the use of Newton's method to iterate to unstable invariant solutions.

An efficient coupled-FEM-BEM-based iterative method for the inverse medium problem in wave scattering

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Collaborators: Linda Stals, Sherwin Bagheri

We present a computational method for reconstructing the refractive index of an unknown medium with embedded metal inclusions using far-field wave scattering data. Our numerical scheme is based on a thin plate spline ansatz for the refractive index, which can be efficiently constructed and evaluated even for complex multiply-connected domains. Our method is based on the Levenburg-Marquardt iteration, and the Jacobian is shown to satisfy an inhomogeneous wave scattering problem using a novel hybrid surface-volume integral equation that generalises the Lippman-Schwinger equation. Numerical experiments, using an extension of the coupled FEM-BEM method for the inhomogeneous wave scattering problems, demonstrate the effectiveness of our method by reconstructing several challenging scatterers.

DIRT: Tensorised Rosenblatt Transport for High-Dimensional Stochastic Computation

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Collaborators: Sergey Dolgov; Rob Scheichl

Characterising intractable high-dimensional random variables is one of the fundamental challenges in stochastic computation. It has broad applications in statistical physics, machine learning, uncertainty quantification, econometrics, and beyond. The recent surge of transport maps offers a mathematical foundation and new insights for tackling this challenge. In this talk, we will present a functional tensor-train (TT) based order-preserving construction of inverse Rosenblatt transport in high dimensions. It characterises intractable random variables via couplings with tractable reference random variables. By integrating our TT-based approach into a nested approximation framework inspired by deep neural networks, we are able to significantly expand its capability to random variables with complicated nonlinear interactions and concentrated density functions. We demonstrate the efficacy of the resulting deep inverse Rosenblatt transport (DIRT) on a range of applications in statistical learning and uncertainty quantification, including parameter estimation for dynamical systems, PDE-constrained inverse problems, and Bayesian filtering.

Accurate and efficient multiscale simulation of a heterogeneous elastic beam via computation on small sparse patches

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Collaborators: Thien Tran-Duc, J.E. Bunder, and Yannis Kevrekidis

Modern 'smart' materials have complex microscale structure, often with unknown macroscale closure. We are developing the Equation-Free Patch Scheme to efficiently and accurately simulate over large scales through computations on only small well-separated patches of the microscale system. Here the microscale system is a beam of random heterogeneous elasticity. The continuing challenge is to compute the given physics on just the microscale patches, and couple the patches across unsimulated macroscale space, in order to establish efficiency, accuracy, consistency, and stability on the macroscale. Dynamical systems theory supports the scheme. Anybody can attack cognate problems via our Matlab/Octave Toolbox [github.com/uoa1184615/EquationFreeGit]. This research program is to develop a systematic approach, both computationally and analytically proven, to model and compute accurately macroscale system levels of general complex physical and engineering systems.

Understanding failure with computational finite fracture mechanics

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Collaborators: Zachary Wegert, Joseph Grotowski, Anthony Roberts

How do we predict the stress at which a perforated plate will fail? While the question is simple, classical approaches are contradictory and don't match experimental data. In this talk I'll discuss our approach to this problem using a more recent paradigm called finite fracture mechanics. Finite fracture mechanics predicts the load at which a sample will fail as the solution of a minimisation problem. We solve this minimisation problem computationally to predict the failure strength of perforated plates with holes of different shapes and sizes. Our computational study elucidates the competition between strength and toughness in determining failure within the finite fracture mechanics paradigm. I will also share our progress validating the computational results with experimental data.

Empirical investigation for the fractional Black-Scholes models with S&P 500 index options

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Collaborators: Fawang Liu

This work focuses on exploring the underlying meanings of fractional order α of the fractional Black-Scholes (BS) models by employing the S&P 500 index options. First, we present finite difference methods and employ a modified hybrid Nelder-Mead simplex search and particle swarm optimization (MH-NMSS-PSO) algorithm to estimate the parameters of the fractional BS models. Second, we examine European call and put options under extreme stock market conditions such as the Covid-19 recession and the 2008 global financial crisis.

The unstructured finite element method for the magnetohydrodynamic flow and heat transfer on a two-dimensional irregular convex domain

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In this paper, we consider the magnetohydrodynamic (MHD) flow and heat transfer of the classical Newtonian fluid in an irregular straight channel. A spatial fractional operator is introduced to modify the classical Fourier's law of thermal conduction, and we obtain the space fractional coupled model. With the help of the unstructured mesh finite element method, the coupled model is solved numerically. Finally, a numerical example is proposed to verify the stability and the efficiency of the numerical method.

Resolving the dynamic properties of PCL by coarse grain simulations

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Collaborators: Zhuoqun Zheng; Chengkai Li; Haifei Zhan; Liangzhi Kou; Yuantong Gu

Polycaprolactone (PCL) is a degradable biomaterial, extensively used as ink in 3D printing. The full atomic simulation of PCL can be expensive to describe some structural features in the experiment, such as large molecular weight, crystallinity, and phase aggregation. Coarse grain simulations can reduce computation costs by mapping several atoms into a bead. In this research, PCL-customized potentials are developed via the bottom-up approach on different CG levels. The structural distribution can be reproduced accurately using the iterative Boltzmann inversion. The potentials and the thermostat are modified to resolve some dynamic properties. With these modifications, the dynamic properties, such as heat capacity, diffusion, Young's modulus, and viscosity, can be reproduced accurately. These modification methods can be useful to establish the multiphysics coarse grain model and help to investigate the physical phenomena in the PCL printing process in the future.

Optimal PML parameters for efficient numerical simulation of waves in unbounded domain

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Collaborators: Kenneth Duru

The PML is a perfectly non-reflecting layer that simulates efficient absorption of waves. However in practice, once the layer is truncated and discretised, the PML is no longer a completely non-reflecting medium. This arises due to numerical reflection errors introduced by approximation, and the finite layer width, which means that the residual outgoing waves will be reflected from the outer boundary and travel back through the layer and corrupt the solution. Therefore, the PML parameters must be tuned and optimised in order to enable optimal performance of the PML in numerical wave solvers. In this presentation we discuss how to derive optimal PML parameters for the acoustic wave equation. Using a multi-block strategy, we will present a numerical implementation of the PML that completely eliminates the PML errors. Numerical experiments will be presented to verify the analysis.

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