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Peruvian Conference on Scientific Computing

October 3 - 6, 2022
Universidad Nacional de San Antonio Abad del Cusco
Cusco - Perú

Topics of Interest

- Modelling, Simulation & Optimisation
- Computational Fluid Dynamics
- Subsurface Flows
- Mathematical Epidemiology
- Climate and Environmental Topics
- Finite Elements

Invited Speakers

- Roland Becker (Univ. Pau, France)
- Erik Burman (UCL - London, UK)
- Omar Ghattas (Univ. of Texas at Austin, USA)
- Roxana Lopez-Cruz (UNMSM, Lima, Perú)
- Insa Neuweiler (Univ. of Hannover, Germany)
- Olga Vasilieva (Univ. del Valle, Colombia)

Contents

CHAPTER 1

Welcome

We welcome everybody to the

Peruvian Conference on Scientific Computing
October 3 - 6, 2022, Cusco, Peru

The objective of this conference is to bring together Peruvian and international researchers working in the area of Scientific Computing, in particular in the fields Modeling, Simulation and Optimization with Differential Equations. A focus will lie on topics that are of particular interest for researchers in South America, such as Subsurface Flows, Mathematical Epidemiology or Climate and Environmental topics. The scientific part will be complemented by an attractive social program. Specific topics of interest are: Modeling, Simulation and Optimisation Computational Fluid Dynamics Subsurface Flows Mathematical Epidemiology Climate and Environmental Topics Finite Elements.

The location of the Conference is

Paraninfo Universitario of the Universidad Nacional de San Antonio Abad del Cusco, Peru Plaza de Armas, Cusco

Beautifully located within the Andean Mountains, Cusco is the ancient capital of the Inca empire and offers plenty of touristic sights, ruins and stunning sceneries.

Our six invited speakers are:

- Roland Becker (Univ. Pau, France)
- Erik Burman (UCL - London, UK)
- Omar Ghattas (Univ. of Texas at Austin, USA)
- Roxana Lopez-Cruz (UNMSM - Lima, Peru)
- Insa Neuweiler (Univ. of Hannover, Germany)
- Olga Vasilieva (Universidad del Valle, Colombia)

Along, we could **gather** 38 **contributed talks and** 25 **posters**.

All information can be found on

`https://www.pec3.org/events/cusco2022/`

The conference is part of the DAAD project "Peruvian Competence Center for Scientific Computing" (PeC3), which runs from 2019-2022.

PeC3 is a network of universities and scientists from Peru and Germany with the goal to foster research and education in scientific computing, applied and computational mathematics. The idea of PeC3 started in 2014 and was consolidated in the subsequent years with several summer and winter schools on numerical methods for partial differential equations at different universities in Peru and South America. Applied mathematics and scientific computing with a focus on modeling, simulation and optimization are becoming more relevant and growing in importance worldwide. The numerical simulation and optimization are - in addition to the experiment - increasingly established in many scientific applications. This development has been accelerated in recent decades by the availability of high-performance computers and the associated basic mathematical research.

We look very much forward to meeting all participants and wish everybody an enjoyable and stimulating conference.

The Scientific Committee:

- P. Bastian (Heidelberg University, Germany)
- P. Benner (MPI Magdeburg, Germany)
- M. Braack (CAU Kiel, Germany)
- S. Frei (Univ. of Konstanz, Germany)
- S. May (Univ. of Uppsala, Sweden)
- I. Neitzel (Univ. Bonn, Germany)
- T. Richter (OVGU Magdeburg, Germany)
- O. Rubio Mercedes (UNT Trujillo, Peru)
- D. Rueda Castillo (UNALM - Lima, Peru)
- S. Sager (OVGU Magdeburg, Germany)
- K. Schratz (Sorbonne Univ., France)
- T. Wick (Univ. of Hannover, Germany)

CHAPTER 2

Time table

Sunday	02.10.2022
18:00-20:00	Registration (details t.b.a.)

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Monday	03.10.2022		
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10:20-10:50	Coffee Break		
10:50-11:10	Kaya Local problems for stabilizing the convection-diffusion-reaction equation		
11:10-11:30	Merino A Semi-smooth Newton Method for Regularized Lq–quasinorm Sparse Optimal Control Problems		
11:30-11:50	Steinbach Principal Geodesic Analysis in Director-Based Dynamics of Hybrid Mechanical Systems		
11:50-12:10	Konzen QRDOM with FEM for anisotropic transport problems		
12:10-12:30	Schieweck Pressure post-processing for the continuous Galerkin-Petrov space-time discretization of the nonstationary Stokes problem		
12:30-14:00	Lunch Break		
	Plenary Talk		
14:00-14:50	Becker Adaptive finite element methods for parameter estimation problems		
14:50-15:10	Bustinza An a posteriori error estimator for an incompressible elasticity problem with mixed boundary conditions		
15:10-15:30	Delacruz-Araujo Aggregation of active superparamagnetic colloidal particles in strong magnetic field using Brownian dynamics simulation.		
15:30-16:00	Coffee Break		
16:00-16:20	Cruzado-Sánchez Systematization of quaternion approach as a singularity-free model to track orientation dynamics of rigid bodies: Application to simulation of colloids composed by anisotropic particles.	16:00-16:20	Kinnewig Simulation of optical components by solving the time-harmonic Maxwell equations with adaptive finite elements
16:20-16:40	Pérez-Marcos A microstructural and magneto-mechanical study of a magnetic colloid suspension of interacting magnetic particles in the presence of an external magnetic field using Brownian dynamics simulations	16:20-16:40	Wittum Doubly enriched finite volume spaces for the DNS of fluid-particle interaction
16:40-17:00	Castro-Merino Obtaining Master Curves in Extremely Bidisperse Magnetorheological Fluids Using MATLAB	16:40-17:00	Valdés Improving the computational performance of the IRKA method
17:00-17:20	Menacho-Abanto Shifted-dipole magnetic fluids: effect of the dipolar shift on the arrested chain growth and their microstructure	17:00-17:20	Aguilar An Overview on Conjugate Gradient methods for Optimization, Extensions and Applications
17:20-17:40	Rubio-Briceño Assembly of colloidal magnetic Janus particles in an external uniform magnetic field	17:20-17:40	Garloff High Relative Accuracy Computing with Matrices Appearing in Computer Aided Geometric Design

Tuesday	04.10.2022		
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09:20-09:40	Bürger A degenerating convection-diffusion system modelling froth flotation with drainage		
09:40-10:00	Zegarra Vasquez Large-scale simulation of single-phase flow in 3D fractured porous media using a mixed hybrid FEM		
10:00-10:30	Coffee Break		
10:30-10:50	Johansen Embedded Boundaries with Higher Order Accuracy for Geophysical Applications	10:30-10:50	Soszynska Multirate Adaptive Time-stepping Schemes for Coupled Systems of PDEs
10:50-11:10	Leal Richards model for simulations of water infiltration in agricultural soil using DuMux	10:50-11:10	Dominguez Modelling ACL in PEMWEs using a multiscale method
11:10-11:30	Lifonzo Salcedo Application of finite element method coupled with artificial neural network for simulating seepage in earth dams	11:10-11:30	Rodriguez Patarroyo Numerical solution of the equations of motion of magnetic nanoparticles used in biomedicine in the bloodstream, using Brownian molecular dynamics.
11:30-11:50	Gutierrez-Pachas Complementarity problems and applications	11:30-11:50	Shen Efficient positivity/bound preserving schemes for complex nonlinear systems
11:50-12:10	Neyra Salvador A glimpse at variational inequalities and the obstacle-type problem	11:50-12:10	Tello Real-Time Contactless Breathing Monitoring System Using Radar with Web Server

12.10-14.30	Lunch Break and Poster Session
	Barturen Statistical analysis to estimate the spatial variation in sediment fluxes in a limited data context. Case of study: Peruvian western Andes
	Huayna An approach to calculate a preconditioned basis separator in an interior point method
	Aparicio Problema mixto en 1D para la ecuación de Poisson con condiciones de contorno Neumann puro
	Avalos Duality theory of Convex Analysis: An application to the complete electrode model
	Gordillo-Suarez Modelo estadístico para la abundancia del estadio de huevos de la Diaphorina Citri
	Carranza Analysis of third order linear analytic differential equations with a regular singularity: Bessel and other classical equations
	Ferrer Análisis de la realidad del fútbol de menores en Lima-Perú
	Arce Aplicación de modelos matemáticos para estimar la estabilidad del nivel del agua en un sistema de dos tanques en serie con variaciones en la demanda del servicio
	Pantoja Regiones de Voronoi para optimizar geoespacialmente los puntos de recarga para vehículos eléctricos, una propuesta para Bogotá D.C.(Colombia)
	Laos Virtualization of scientific software based on Arch Linux in GitPod
	Salazar Small Satellites as platforms for Engineering Education
	Castillo Vehicular traffic noise and the performance estudents's and teachers's University César Vallejo-Trujillo-Perú
	Oruro Morphodynamics neuroscience. A computational approach to dendritogenesis of pyramidal cells in the developing olfactory cortex
	Rincón-Cardozo Modelo matematico de la tubercolosis asociada a factores socioeconomicos en la ciudad de Cali, Colombia
	Konzen ANN application to one-dimensional inverse transport problems
	Patarroyo Inferential model from machine learning based on health data mental Colombia compared to the world level
	Navarro Exploring parameter spaces in Holomorphic Dynamics
	Romero Mathematical model of a predator-prey food chain: plankton-anchovy
	Morales Simulation of fluid dynamics and CO 2 gas exchange in the alveolar sacs of the human lung
	Horna Stochastic dynamics for the primitive equation in two dimensions
	Rojas Diferential equations applied to viral diseases
	Ubaldo Remote sensing air quality analysis of Peru based on PM2.5 values
	Risco Effect of microstructure on the magnetization of a suspension of magnetic Janus particles
	Ancajima Existence of weak solution for a non-linear parabolic problem with fractional derivates
	Paredes The inexact Restoration Method applied to the Minimization problems with orthogonality constraints
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15:30-17:30	Trip to Sacsayhuaman

Wednesday	**05.10.2022**
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09:20-09:40	Cardona-Salgado Dengue control by releasing sterile male mosquitos
09:40-10:00	Campo Modeling the Wolbachia imperfect maternal transmission in Aedes aegypti mosquitoes
10:00-10:30	Coffee Break
10:30-10:50	Ramírez Bernate Implementation of control strategies in spatial dynamics using sterile insect techniques
10:50-11:10	Rubio Simulation of the behaviour of covid-19 with the stochastic SIR model: case of Perú
11:10-11:30	Mehlmann The influence of solver tolerances on large scale coupled climate simulations
11:30-11:50	Campos Velho Data assimilation by TPU for Ocean Circulation Model
11:50-12:10	Menkovski Scientific computing with deep generative models
12:10-14:00	Lunch Break
	Plenary Talk
14:00-14:50	Lopez-Cruz Implications of the delayed feedback effect on the stability of a SIR epidemic model
14:50-15:10	Minakowski A priori and a posteriori error estimates for the Deep Ritz method applied to the Laplace and Stokes problem
15:10-15:30	Prudhomme On the approximation of the wave equation operator using deep learning
15:30-16:00	Coffee Break
16:00-17:00	Closing and Discussion

Thursday	**06.10.2022**
08:00-18:00	Excursion

CHAPTER 3

Key Lectures

Adaptive finite element methods for parameter estimation problems

Roland Becker [1]

We consider adaptive finite element methods for optimisation problems with constraints defined by an elliptic PDE. First, we review the standard framework for proving convergence and rate optimality based on reduction of the error estimator. Then we discuss the generalisation to goal-oriented error estimation, which can be seen as a first step towards parameter estimation. Of special interest will be the case of finite-dimensional parameters, which frequently occurs in practice. We also discuss the question of error estimation with the respect to the parameters, which is interesting, since in many situations the parameter error can be expected to be of higher order than the error in the state (or co-state) variable. Finally we discuss algorithms for the minimisation of smooth convex functions on finite-element subspaces, giving the possibility to analyse the interplay between iterative solution and mesh refinement.

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Stabilised finite element methods for ill-posed problems with conditional stability

Erik Burman [1]

In this talk we will discuss some recent advances in the use of stabilised finite element methods for ill-posed elliptic problems. Such problems appear in a variety of inverse problems and are notoriously difficult to solve numerically. We will consider the special case of unique continuation where the boundary conditions are unknown, but measurements of the solution are available in some subset of the bulk domain. For this problem we present a theory reminiscent of Lax equivalence theorem where we combine consistency, numerical stability and the physical stability of the problem to obtain error bounds. The influence of data perturbations and solution regularity on the bounds will be discussed. Different finite element methods such continuous Galerkin or a hybridised discontinuous Galerkin method enter the framework and we will illustrate the theory with some numerical examples. If time allows we will also discuss the application of the theory to more complex problems, such as the linearised Navier-Stokes' equations or control problems subject to the wave equation.

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Implications of the delayed Feedback effect on the stability of a SIR epidemic model

Roxana López-Cruz [1]

A basic mathematical model in epidemiology is the SIR (Susceptible–Infected–Removed) model, which is commonly used to characterize and study the dynamics of the spread of some infectious diseases. In humans, the time scale of a disease can be short and not necessarily fatal, but in some animals (for example, insects) this same short time scale can make the disease fatal if we take into account their life expectancy. In this work, we will see how a positive feedback effect (decrease of the susceptible population at small densities) in a SIR model can cause a qualitative characterization of the dynamics defined by the original SIR model.
Finally, we will also show with numerical simulations how a delay in the feedback effect causes very interesting qualitative changes of the system with epidemiological significance.

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Geometric Deep Neural Network Surrogates for Bayesian Inverse Problems

Omar Ghattas [1]

Bayesian inverse problems (BIPs) governed by large-scale complex models (such as PDEs) in high parameter dimensions are often intractable. Efficient evaluation of the parameter-to-observable (p2o) map, which involves solution of the forward model, is key to making BIPs tractable. Surrogate approximations of p2o maps have the potential to greatly accelerate BIPs, provided the p2o map can be trained using modest numbers of model solves. Unfortunately, constructing such surrogates presents significant challenges when the parameter dimension is high and the forward model is expensive.

Deep neural networks (DNNs) have emerged as leading contenders for overcoming these challenges. We demonstrate that black box application of DNNs for problems with infinite dimensional parameter fields leads to poor results, particularly when training data are limited due to the expense of the model. However, by constructing a network architecture that is adapted to the geometry of the p2o map as revealed through adjoint PDEs, one can construct a dimension-independent "reduced basis" DNN surrogate with superior generalization properties using only limited training data. We employ this reduced basis DNN surrogate to make tractable the solution of Bayesian optimal experimental design problems, in particular for finding sensor locations that maximize the expected information gain. Application to inverse wave scattering is presented.

This work is joint with Tom O'Leary-Roseberry, Keyi Wu, and Peng Chen.

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Multi-rate mass-transfer models for flow and transport in heterogeneous porous media

Insa Neuweiler [1]

Many environmental engineering problems involve flow and transport processes in the subsurface. Estimating, for example, travel times of contaminants requires predicting flow and transport with numerical models. The heterogeneous structure of the subsurface is one of the big challenges for such model predictions. An example for highly heterogeneous subsurface structure is fractured rock. The length scales to be resolved in a numerical model can go down to several millimeters, while length scales of interest are often in the range of tens of meters. The requires also capturing processes on a variety of time scales. Apart from the numerical challenges, the details of the structure are usually not known, so that the model geometry is highly uncertain.

As direct numerical modeling is often not feasible, upscaled models are used instead. In case of highly heterogeneous media, upscaled models could be based on a multi-rate mass-transfer approach. The connected, highly permeably domain is conceptualized as one fast continuum, while the poorly permeably domain is conceptualized as another, slow continuum. In a double porosity model, the transport is only described explicitly in the fast continuum, while the slow continuum is described as a storage or, equivalently, trapping site. The mass transfer between these continua is described by a model. Typically, single rate transfer models, or, as a superposition of different single rate transfer models, multi-rate mass-transfer models, are used. The models need to capture the dynamics of the mass exchange. The influence of the geometry of the continua and their hydraulic properties is captured by the parameters of the rate terms. To have predictive models, it is thus crucial to relate the model parameters to the transport processes and to the properties and geometry of the medium.

The concept and parametrization of a multi-rate mass-transfer approach for two-phase flow in fractured media will be outlined and demonstrated for the case that fluid flow in the matrix is dominated by capillary forces. Also, first results towards a multi-rate mass-transfer approach for advective solute transport process in highly heterogeneous media will be shown.

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Male-biased releases of *Wolbachia*-carrying mosquitoes for dengue control

Olga Vasilieva [1]

During the last decade, *Wolbachia*-based biological control has come forward as an ecologically friendly and potentially cost-effective method for the prevention and control of dengue and other arboviral infections. The World Mosquito Program[2] promotes and encourages this type of control by performing field releases in numerous dengue-affected areas around the globe.

The principal vector species, such as *Aedes aegypti* females, lose their vectorial competence and become less capable of transmitting the virus to humans if deliberately infected with *Wolbachia* symbiotic bacterium.

The main objective of Wolbachia-based biocontrol is to replace wild vectors (fully capable of transmitting arboviral infections) with Wolbachia-carrying insects bearing a reduced transmission capacity. This final goal, known as population replacement, can be achieved by performing a single inundative or multiple inoculative releases of mosquitoes transinfected with Wolbachia during artificial mass-rearing.

In this presentation, we study the effect of Wolbachia-based biocontrol on dengue transmission while considering two types of releases: sex-unbiased and male-biased. On the one hand, sex-unbiased releases are cheaper, for they do not require the sex-separation of eggs [1]. On the other hand, male-biased releases reduce the number of female mosquitoes in the target locality and thus the number of bites per human host. Here, it is worth mentioning that Wolbachia-carrying females bite people and are still capable of transmitting the virus even though their vectorial capacity is limited.

Using the sex-structured population dynamics model describing the evolution of wild and Wolbachia-carrying mosquitoes [2], we propose an SEIR-SEI-type epidemiological framework for dengue transmission. This framework is then employed for performing an epidemiological assessment of Wolbachia-based control to prevent dengue morbidity. To give a realistic example, we simulate this type of preventive control applied to Cali, a sizeable Colombian city commonly recognized as a hyperendemic area regarding dengue morbidity.

Acknowledgments. This research is supported by the National Fund for Science, Technology, and Innovation (Autonomous Heritage Fund *Francisco José de Caldas*) by way of the Research Program No. 1106-852-69523, Contract: CT FP 80740-439-2020 (Colombian Ministry of Science, Technology,

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[2]WMP, https://www.worldmosquitoprogram.org/

and Innovation – Minciencias). The credit for this work goes to all members of the Research Program.

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CHAPTER 4

Talks

Shifted-dipole magnetic fluids: effect of the dipolar shift on the arrested chain growth and their microstructure

Jose F. Menacho-Abanto [1] Ubaldo M. Córdova-Figueroa [2]
Ronal A. Delacruz-Araujo [3]

In this work, the three-dimensional self-assembly of a dilute suspension of magnetic Janus particles with a magnetic dipole laterally displaced from their center was studied using Brownian dynamics simulations. Microstructure and aggregation properties were determined from the temporal evolution of the positions and orientations of the particles. The average size of clusters, the nucleation and growth process, the population distribution, and the effective radius of clusters were evaluated for a diluted suspension (1% volume fraction) for different values of the dipolar shift (s) – which adopts values in the range 0≤s≤1 when dimensionless using the radius of the particle. When the value of the dipolar shift is small (s ⟶ 0), chain and ring-shaped structures are formed which are typically observed in particles with a centered dipole (s = 0). At intermediate dipolar shifts (0.2 ≤ s ≤0.3), aggregates are formed mainly in the form of vesicles that in some cases coexist with rings and micelles. Finally, for s≥0.3, the formation of spherical micelles is observed that progressively decrease in size as s increases until reaching aggregates of 2 or 3 particles. For intermediate and high dipolar displacements, the system saturates to a small cluster size (few particles per aggregate) very suitable for magnetic suspension design with high stability. This study shows that new magnetic fluids can be designed by controlling the dipole displacement of their component particles to influence their microstructure and therefore their macroscopic properties, for use in potential applications.

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Male-biased releases of *Wolbachia*-carrying mosquitoes for dengue control

Hans Aguilar [1]

This work aims to identify the current state of the art of the latest research related to Conjugate Gradient (CG) methods for unconstrained optimization through a systematic literature review according to the methodology proposed by Kitchenham and Charter, to answer the following research questions: Q1: In what research areas are the conjugate gradient method used? Q2: Can Dai-Yuan conjugate gradient algorithm be effectively applied in portfolio selection? Q3: Have conjugate gradient methods been used to develop large-scale numerical results? Q4: What conjugate gradient methods have been used to minimize quasiconvex or nonconvex functions? We obtain useful results to extend the applications of the CG methods, develop efficient algorithms, and continue studying theoretical convergence results.

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Aggregation of active superparamagnetic colloidal particles in strong magnetic field using Brownian dynamics simulation.

Ronal A. Delacruz-Araujo [1] Luis Y. Rivera-Rivera [2]
Ubaldo M. Córdova-Figueroa [3]

Active colloids are promising candidates for developing reconfigurable materials due to their potential assemble into tunable structures dictated by the relative competition between particle-particle interactions (e.g. magnetic) and the propulsive strength of the particles. In this work, we perform Brownian dynamics simulations of a dilute suspension of active superparamagnetic colloids under a strong magnetic field and analyze their aggregation and fragmentation process in light of these competing mechanisms. Different mean cluster size of chain-like structures are observed depending on the Péclet number (Pe)–the ratio between self-propulsion and Brownian forces–and the nondimensional magnetic interaction strength–the ratio between the magnetic dipole-dipole and Brownian forces. When the Pe is less than the magnetic interaction strength an enhanced aggregation rate is observed in the nucleation process, followed by a power-law behavior for the growth process with exponents in the range typically observed for passive magnetic particles. At intermediate ratio between Pe and the magnetic interaction strength enhanced aggregation rate is also observed in the nucleation process while in the growth process the system reaches a steady state mean chain size. In this regime, the tipycal power law behavior of passive system is broken. Finally, no aggregation occurs at high ratio between Pe and the magnetic interaction strength . This study shows that a self-propulsion force can serve as an actuator in applications where an accurate control over the colloidal structures and rate of aggregation is required.

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Implementation of control strategies in spatial dynamics using sterile insect techniques

Carmen A. Ramírez [1]

We propose the extension of an entomological model structured by sex that was studied in [1], which served as the basis for the design of control strategies based on the release of sterile male mosquitoes (*Aedes spp*) with the aim of eliminating the population of wild vectors in some target locality. The authors in [1] analyzed the population dynamics of the mosquito over time, in which they considered different types of periodic impulsive control strategies in different situations (open-loop control, closed-loop control, and mixed control), providing sufficient conditions to reach the elimination. Our proposal involves the study of spatial dynamics, adding to the same model the terms referring to the dispersion of the mosquito to subsequently make comparisons. Unlike the temporal model, the spatial model allows selecting specific points of the domain to make releases, as well as varying the dispersion coefficient in different parts of the domain, allowing heterogeneity to be given to the space, which greatly influences the results obtained.

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Assembly of colloidal magnetic Janus particles in an external uniform magnetic field

Juan P. Rubio-Briceño [1] Ubaldo M. Córdova-Figueroa [2]
Ronal A. Delacruz-Araujo [3]

The assembly of colloidal magnetic Janus particles with the laterally displaced dipole (or shifted, s) in the presence of an external uniform magnetic field in a Newtonian fluid in a three-dimensional system using Brownian dynamics simulation will be studied. The parameters that are evaluated dynamically are the average size of the clusters and the nucleation and growth process, for different values of the dipole displacement, which is the relationship between the distance of the dipole and the radius of the particle, and different values of α that is the relationship between the magnetic torque by the external field and with the Brownian torque. The structures that are obtained for α values of 1, and dipolar displacement of 0.1 are in the form of a gel; and for dipolar displacement between 0.2 and 0.3 micelles and rings are obtained; and with a value of 0.4 and 0.5 doublets, triplets and quadruplets are obtained. For values of α=3-10, with shifted between 0.1 and 0.25, wires, double chains and rings are obtained; and for shifted values of 0.3 and 0.5, staggered chains, micelles, quintuplets, quadruplets and triplets are obtained, being more compact when increasing the dipole distance. For values of α=20-100, with shifted between 0.1 and 0.25, double chains and wires are obtained; for shifted values from 0.3 to 0.5, double chains, staggered chains are obtained. These results help a better understanding of the dynamics of Janus particles and help in the creation of new materials.

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A degenerating convection-diffusion system modelling froth flotation with drainage

Raimund Bürger[1] Stefan Diehl[2] Mari Carmen Martí[3]
Yolanda Vásquez[4]

Froth flotation is a common unit operation used in mineral processing [6, 7]. It serves to separate valuable mineral particles from worthless gangue particles in finely ground ores. The valuable mineral particles are hydrophobic and attach to bubbles of air injected into the pulp. This creates bubble-particle aggregates that rise to the top of the flotation column where they accumulate to a froth or foam layer that is removed through a launder for further processing. At the same time, the hydrophilic gangue particles settle and are removed continuously. The drainage of liquid due to capillarity is essential for the formation of a stable froth layer. This effect is included into a previously formulated hyperbolic system of partial differential equations that models the volume fractions of floating aggregates and settling hydrophilic solids [1, 2]. The construction of desired steady-state solutions with a froth layer is detailed and feasibility conditions on the feed volume fractions and the volumetric flows of feed, underflow and wash water are visualized in so-called operating charts [3, 4]. A monotone numerical scheme is derived and employed to simulate the dynamic behaviour of a flotation column. It is also proven that, under a suitable Courant-Friedrichs-Lewy (CFL) condition, the approximate volume fractions are bounded between zero and one when the initial data are. The presentation summarizes research detailed in [5].

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An a posteriori error estimator for an incompressible elasticity problem with mixed boundary conditions

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In this talk, we propose an augmented finite element formulation for an incompressible elasticity problem. We consider mixed boundary conditions: null displacement on some part of the boundary (Dirichlet), and a given traction on the other part (Neumann). First, we assume the situation where the traction on Neumann boundary is also zero. By introducing the stress as an additional unknown, we derive an augmented variational formulation for the stress and the displacement, at continuous and discrete levels. We prove that the scheme is well-posed, stable and convergent. After that, we deduce an a posteriori error estimator, which is reliable and efficient. As a by product, we are able to extend and adapt the described procedure to the case where the traction on Neumann boundary is given and is non null. Finally, we show some numerical tests, that are in agreement with our theoretical results.

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Modeling the Wolbachia imperfect maternal transmission in Aedes aegypti mosquitoes

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Aedes aegypti is the vector that presents the greatest risk of transmitting arboviruses causing diseases such as dengue, Zika, yellow fever, and chikungunya. It is a domestic mosquito that reproduces in articial or natural containers that store water, and this mosquito species is widely distributed in the American continent. Wolbachia-based biocontrol has recently emerged as a potential method for preventing and controlling of dengue and other vector-borne diseases. When deliberately infected with Wolbachia, major vector species, such as Aedes aegypti females, become less capable of getting viral infections and transmitting the virus to human hosts.With the purpose of establishing optimal strategies for the release of eggs and/or mosquitoes adults inoculated with the Wolbachia bacterium, in this work we study the eect of the Imperfect maternal transmission and cytoplasmic ncompatibility, in the dynamics of Interaction of the two populations of the vector: with and without Wolbachia. to visualize and anticipate the pros and cons of biological control based on Wolbachia estimating its potential to reduce dengue transmission. The model is centered on the mosquito population only.

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Obtaining Master Curves in Extremely Bidisperse Magnetorheological Fluids Using MATLAB

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Magnetorheological fluids (MRFs) are smart materials with controllable mechanical properties, which are of interest for the fabrication of high-performance viscous dampers to design antiseismic buildings. To improve the stability of the MRFs and their magnetorheological effect, extremely bidisperse MRFs (Bi-MRFs) were synthesized using ferrofluids as solvent. Despite the advantages of Bi-MRFs compared to their monodisperse counterpart, the underlying mechanisms that determine its magneto-mechanical properties are still not fully understood. Because damping applications require the use of optimal properties of Bi-MRFs, it is important to obtain the master curves of these stimuli-responsive suspensions. The optimum values of relevant parameters, such as external magnetic field, particle concentration, and particle size ratio can be obtained from these master curves. Recent studies have demonstrated that the quadratic and sub-quadratic regions, observed for the field-dependent yield stress, can be mathematically modeled in one equation using the hyperbolic tangent and error functions. To the best of our knowledge, no other functions have been used to obtain master curves in Bi-MRFs. However, a great variety of well-studied functions can be used for this purpose. In this work, we present a detailed comparison of six functions to obtain master curves in Bi- MRFs. A MATLAB code was developed to automatically obtain the master curves and to compare the different functions that can be used in these magnetic systems. Our results demonstrated that the power law function was one of the best to obtain the master curve for Bi-MRFs, which opens the possibility of using additional functions to obtain master curves for these smart fluids that could be used in antiseismic damper applications.

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Modelling ACL in PEMWEs using a multi-scale method

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Use of renewable and green sources of energy is nowadays a necessary goal to achieve. Hydrogen fuel cells become every day a more suitable choice for this purpose. Producing Hydrogen in safe and efficient ways is a desirable goal. One way to produce it is a Proton Exchange Membrane Water Electrolyser (PEMWE).

This kind of devices usually exhibit rapid corrosion on the anode side under work conditions causing decreasing or lacking performance [1]. Having better understanding of this yet non fully known process will help to develop sustainable solutions for PEMWEs that aim to mitigate the mentioned corrosion effect. That is why mathematical modelling and numerical simulation approaches will be suitable scientific tools describing the processes better [3, 6, 4, 5].

In this work we present a multiscale method [2] that splits the problem into two sub-problems: the fast and slow process. The fast will simulate the micro-kinetic process that models the interactions between the particles inside the ACL and also the transport of Hydrogen and Oxygen throw the PEMWE. On the other hand, the slow process will simulate the degradation of the reactive component of the ACL made of Iridium material. Experimental simulation results will be presented in which this method allows to reduce the computation of 500 hours of simulation from days to minutes.

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High Relative Accuracy Computing with Matrices Appearing in Computer Aided Geometric Design

Jürgen Garloff [1] Mohammad Adm [2] Fatima Rasheed [3]

The development of algorithms for computing eigenvalues, eigenvectors, singular values, the inverse matrix, and related quantities with high relative accuracy has found increasing interest, see the survey article [2]. Here we mean by that an algorithm can be performed with *high relative accuracy* that the relative distance of the computed solution from the exact solution is bounded by a constant times the unit roundoff, provided that the initial data are exact. The main source of the loss of relative accuracy is the cancelation of significant digits when floating point numbers of equal signs and approximate magnitude are subtracted.

In Computer Aided Geometric Design (CAGD), many problems involve totally nonnegative matrices, i.e., matrices having all their minors nonnegative, see, e.g., [3]. We present the condensed form of the so-called Cauchon Algorithm [1] and reformulate the computations in such a way that they can be performed without any subtraction of numbers of equal sign. This provides the basis for an algorithm needing $O(n^3)$ arithmetic operations for the computation of all the eigenvalues of an n-by-n nonsingular totally nonnegative matrix with guaranteed high relative accuracy, independently of the condition number of the matrix. We compare our approach with the one by P. Koev [1] which relies on the bidiagonal factorization of a nonsingular totally nonnegative matrix.

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Embedded Boundaries with Higher Order Accuracy for Geophysical Applications

Hans Johansen [1] Nate Overton-Katz [2]

We present several higher-order finite volume discretizations for geophysics simulations, and demonstrate how they provide computational and accuracy advantages over typical lower-order methods. Higher-order mapped multi-block grid methods with adaptive mesh refinement can provide a very accurate approach for modestly complex geometries, without having to use fully unstructured mesh methods. For extremely complex geometries, embedded boundary "cut cell" methods use regular stencil calculations in interior regions and special geometry-based interpolation near boundaries to achieve higher-order accuracy and stability with small cut cells. There are even situations where using both approaches - smooth mappings with embedded boundaries - can have advantages. We'll present a survey of a few applications for each case, and discuss our progress on implementing these techniques in an HPC / GPU context.

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Local problems for stabilizing the convection-diffusion-reaction equation

Utku Kaya [1] Malte Braack [2]

For convection-dominated problems, the Galerkin finite element method's straightforward application gives rise to spurious approximations. Here, as a remedy, we introduce a two-level method, where the solution space is a group space that consists of continuous and discontinuous parts. The formulation of interest is consistent, stable, and provides control over the streamline derivative. Additionally, we propose an iterative solution scheme which facilitates computation of the solutions in a cost-inexpensive manner. Numerical experiments based on well-known examples validate theoretical findings.

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Sebastian Kinnewig [1] Thomas Wick [2]

Optical components are of great research interest, as they have many promising applications, for example in quantum computing or in medicine. As it is very challenging to design complex optical components, numerical simulations are necessary to support the design process of such optical devices. To simulate the behavior of the electro-magnetic field inside of waveguides and other optical components, we use the time-harmonic Maxwell equations. Because of their ill-posed nature, suitable numerical solvers need to be developed [1]. In this talk, we present a combination of adaptive mesh refinement along with domain decomposition methods for realizing such numerical simulations. To this end, we develop numerical algorithms and implement (and debug) them in the open source finite element software deal.II (differential equations analysis library). Furthermore, we consider some practical applications that arise in our research excellence cluster PhoenixD, and compare the simulation results with measurement results.

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QRDOM with FEM for anisotropic transport problems

Pedro H.A. Konzen [1] Leonardo F. Guidi [2] Thomas Richter [3]

It is consider the numerical simulation of one group neutron transport problems in anisotropic media in rectangular domains. Such problems can be modeled by an integral-differential equation, and one of the most widely used techniques to solve it is known as the Discrete Ordinates Method (DOM). It consists in approximating the integral term by using an appropriate quadrature set, which leads to a system of partial differential equations. It is well known that the DOM approximation may produce unrealistic oscillatory solutions known as the ray effects. As an alternative, it is presented the Quasi-Random Discrete Ordinates Method (QRDOM), which preserves the main characteristics of the DOM, but it has the advantage of providing approximate solutions with mitigated ray effects. Its central idea is to explore a quasi-Monte Carlo integration within the classical source iteration technique. Through the discussion of benchmark problems, we present the advantages and disadvantages of the application of the QRDOM with finite element discretization. As well, we point its potential further applications to more complex particle transport problems.

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Richards model for simulations of water infiltration in agricultural soil using DuMu$^{\mathrm{x}}$

John J. Leal Gomez [1] Guillermo A. Martínez Girón [2]
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The objective is to simulate water infiltration phenomena based on the Richards model [1], in agricultural soils using specific parameters such as soil type, density, porosity, matric potential, and moisture holding capacity, among others. The simulation was performed using DuMu^x [2], a C++ framework for porous media applications. Nowadays, these matters are crucial for agriculture due to the concern for efficient use and saving of water [3], since large quantities of water are wasted annually for crops, and it is necessary to contrast the results of the simulations with the quantities currently used with traditional irrigation methods.

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A microstructural and magneto-mechanical study of a magnetic colloidal suspension of interacting magnetic particles in the presence of an external magnetic field using Brownian dynamics simulations

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Magnetic colloidal suspensions are of great interest due to the potential applications in different areas such as biomedicine and engineering (e.g., cancer treatment, anti-seismic devices). These applications demand a crucial understanding of their magnetic properties under external conditions (e.g., magnetic fields). The present work then studies the microstructural and magneto-mechanical properties of a suspension of identical ferromagnetic spherical colloidal particles inmersed in a viscous Newtonian fluid under a uniform magnetic field. Properties such as mean cluster size, effective radius, nucleation-growth factor, magnetization, and magnetic susceptibility are studied in terms of the particle volume fraction ϕ, the Langevin parameter α, and the dipolar coupling parameter λ. Here, α and λ are dimensionless quantities that measure the competence of the magnetic torque and the strength of the dipole-dipole interaction, respectively, with the fluid thermal fluctuations. The aforementioned magnetic properties are calculated by examining the spatial-orientational-temporal evolution of the magnetic particles, which are obtained using a well-known computation method called Brownian dynamics (BD) simulations. Simulations are carried out for magnetic colloidal suspensions comprised of 500 particles, values of ϕ ranging from 0.0001 to 0.01, α from 0 to 100 and λ from 0 to 100. The preliminary results show that, for a constant value of ϕ, the mean cluster size growths with λ at high values of α. And, for high values of λ, the mean cluster size does not change for any α value. It is also found that the magnetization curve as a function of α increases with λ. For $\lambda = 0$, our magnetization curve is in complete agreement with the Langevin function that characterizes the magnetization

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of a very dilute suspension of non-interacting magnetic particles. Finally, values of the effective radius qualitatively exhibit the formation of rigid chains in the suspensions at high values of α and λ.

The influence of solver tolerances on large scale coupled climate simulations

Carolin Mehlmann [1]

Subject of the talk is the influence of numerical tolerances as well the development of a new Newton solver for a specific problem in climate science, the Snowball Earth hypothesis: 630-750 million years ago the Earth might have been in deep freeze with completely ice-covered oceans. Climate simulations that investigate the Snowball Earth hypothesis typically approximate the nonlinear sea ice processes with only a few solver iterations due to the high numerical costs. The influence of this inaccuracy as well as the development of fast and robust solving methods are current research questions. We show that the underlying coupled set of equations that describes the sea ice dynamics in climate models can be formulated as an energy minimization problem. Based on the theoretical analysis we derive a new Newton method that leads to faster and more robust Newton convergence than currently used methods. In the context of the Snowball Earth hypothesis, we demonstrate that the numerical tolerances are more important for the resulting climate dynamics than usual tuning param- eters. These are alarming results, since the numerical accuracy of nonlinear sea ice processes have never been considered to be important for past, present, or future climate projections.

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Scientific computing with deep generative models

Vlado Menkovski [1]

Machine Learning(ML) has been taking a more prominent role in supporting scientific computing, offering significant improvements in computational complexity. In these settings, first principles simulators are used to produce ground truth data from which a target variable(s) is computed. Then ML is used to model the dependency of the simulation parameters on the target variable. For example, in a front tracking fluid simulation of a bubble of gas in a liquid, a first principle simulator can produce the evolution of the surface of the bubble over time. From this data, the variable of interest such as the surface area of the bubble can be calculated as a factor in the gas absorption in the liquid. To scale this method to a large number of system configurations, an ML model can be used to predict the surface area directly from the simulation parameters such as the volume of the bubbles, the viscosity of the liquid, and so on. While such an approach usually provides significant improvements in computational complexity, it also presents a number of limitations. The ML model is typically a 'black box' and hard to interpret. The model's generalization capabilities are usually limited to parameter ranges present in the training data. It is usually challenging to incorporate domain knowledge in such models as symmetries or conserved properties. Advances in ML, particularly deep generative models have created opportunities to use ML to directly simulate the observations rather than model the relationships to target variables. In this talk, we aim to argue the advantages of developing such data-driven simulators to significantly scale up first principle simulators, while being able to incorporate domain knowledge and the existing data analysis pipelines. We will present recent work using deep generative models in a number of fields ranging from fluid dynamics, nuclear fusion, and computational biology in order to demonstrate the advantages of these models and the challenges that we have faced in adopting ML models for simulation.

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A Semi-smooth Newton Method for Regularized L^q–quasinorm Sparse Optimal Control Problems

Pedro Merino [1]

A semi-smooth Newton method (SSN) in the spirit of [2] is derived for a class of nonconvex optimal control problems governed by linear elliptic partial differential equations with control and state constraints. The nonconvex term considered in the cost functional arises from a Huber–type regularization of the L^q–quasinorm ($q \in (0, 1)$) introduced in [1]. The state-constrained case is deduced using a Laurentiev approximation. The proposed SSN solves the optimality system of the regularized problem resulting from the application of *difference–of–convex functions* programming tools.

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A priori and a posteriori error estimates for the Deep Ritz method applied to the Laplace and Stokes problem

Piotr Minakowski [1] Thomas Richter [2]

We analyze neural network solutions to partial differential equations obtained with Physics Informed Neural Networks. In particular, we apply tools of classical finite element error analysis to obtain conclusions about the error of the Deep Ritz method applied to the Laplace and the Stokes equations. Further, we develop an a posteriori error estimator for neural network approximations of partial differential equations. The proposed approach is based on the dual weighted residual estimator. It is destined to serve as a stopping criterion that guarantees the accuracy of the solution independently of the design of the neural network training. The result is equipped with computational examples for Laplace and Stokes problems.

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Complementarity problems and applications

Daniel Alexis Gutierrez-Pachas [1] Sandro Rodriguez Mazorche [2]

Developing efficient numerical strategies to model complex systems is helpful, providing tools to solve problems with high computational costs. This presentation introduces a concise and practical numerical approach to solving complementarity problems and illustrates the theory with numerical examples.

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Numerical solution of the equations of motion of magnetic nanoparticles used in biomedicine in the bloodstream, using Brownian molecular dynamics.

Diego Julian Rodriguez Patarroyo [1] John Jairo Leal Gómez [2]
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This article shows the results of the implementation of molecular dynamics methods, and Brownian molecular dynamics to determine the trajectory of the magnetic nanoparticles used in the Magnet Targering Delievering (MTD) technique. The increase in computational capacity in the last three decades, has allowed the implementation and development of new techniques for modeling systems of the order of nanometers among the most recent are the group of techniques framed under the label of first principles. In particular Monte Carlo, molecular dynamics and cellular automata. The development of models specified in these techniques will allow to reduce the costs of the experimental tests, as well as minimize the impact of the invivo tests. Considerable variations were observed when introducing different interactions into the model. When taking into account the collisions between the magnetic NPs and the erythrocytes, distorted trajectories are observed, but on average the effect of the external magnetic field allows the efficiency to increase due to the addressing produced.

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On the approximation of the wave equation operator using deep learning

Ziad Aldirany [1] Marc Laforest [2] Régis Cottereau [3]
Serge Prudhomme [4]

Deep operator networks (DeepONets) have demonstrated the capability of approximating nonlinear operators for initial- and boundary-value problems. One attractive feature of DeepONets is their versatility since they do not rely on prior knowledge about the solution structure of a problem and can thus be directly applied to a large class of problems. However, convergence in identifying the parameters of the networks may sometimes be slow. In order to improve on DeepONets for approximating the wave equation, we introduce the Green operator networks (GreenONets), which use the representation of the exact solution to the homogeneous wave equation in term of the Green's function. A comparison between the GreenONets and the DeepONets is shown on a series of numerical experiments for homogeneous and heterogeneous medias.

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Simulation of the behaviour of covid-19 with the stochastic SIR model: case of Perú

Obidio Rubio [1]

We described the behaviour of the covid 19 in Perú, using the nonlinear Galerkin method on the stochastic-sensible-infected recovered- stochastic (SIRS) model [1]

following the techniques of [2] of discretization for stochastic differential equations we establish on ensemble of trajectories with data showed in [3]

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Application of finite element method coupled with artificial neural network for simulating seepage in earth dams

Cesar Lifonzo [1]

In this research work, a metaheuristic model has been developed using artificial neural networks coupled with the finite element method to carry out the analysis and dynamic simulations of the seepage phenomenon in earthen dams and similar structures, taking into account a heterogeneous and anisotropic soil. The ANN metaheuristic model consists of a multilayer network with a sigmoidal activation function trained using the backpropagation algorithm with an optimal architecture of 2 neurons in the input layer, 93 in the hidden layer, and one output. The coupled model comprises mathematical modeling, numerical analysis and computational simulation of seepage through the Cuchoquesera dam, Ayacucho-Peru. For the training and validation of the model, historical data from the piezometers from 2002 to 2021 recorded in the Cuchoquesera dam were used. The water levels calculated by the developed model have been satisfactorily compared with the real data measured by the piezometers. Finally, for the numerical simulation, a computer code in Python has been implemented for the analysis and simulation of the seepage in the Cuchoquesera Dam.

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Dengue control by releasing sterile male mosquitoes

Daiver Cardona-Salgado [1] Olga Vasilieva [2]

Dengue is a global problem, and its spread follows global climate change. The Sterile Insect Technique (SIT) has gained visibility as a vector control option. This technique includes mass-rearing of Aedes aegypti in the lab, their separation by gender, elimination of females, and sterilization of males by ionizing radiation. Further, sterilized male insects are released in a targeted locality to reduce the wild mosquito population.

We propose an epidemiological model as a baseline to determine the constant number of sterilized male mosquitoes to be released daily. The primary goal is to reduce the effective reproductive number of the disease below one. Also, we explore the relationship between the cost of intervention expressed through the total number of released sterile insects and the lab capacity for their mass-rearing.

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A glimpse at variational inequalities and the obstacle-type problem

Cristhian Neyra Salvador [1]

The theory of variational inequalities was born in 1959 due to the Signorini problem, which covered physical issues. Currently, it is a powerful tool in applied mathematics, physics, engineering, chemistry, and biology. The results obtained in this theory have developed branches of pure mathematics. This work begins with the study of variational inequalities in finite and infinite dimensional spaces and a brief extension to operators. Then the formulation of the obstacle-type problem and its importance is presented. Its respective analysis of existence and uniqueness of solution and some properties of regularity is made.

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Systematization of quaternion approach as a singularity-free model to track orientation dynamics of rigid bodies: Application to simulation of colloids composed by anisotropic particles.

Luis E. Cruzado-Sánchez [1] Obidio E. Rubio Mercedes [2]
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The tracking over time of rigid bodies is a practice that is carried out either as an input for the study in different fields of research and engineering or to be applied directly to follow both the position and the orientation of the bodies. As for position tracking, there is no major inconvenience than following the position of the barycenter of the rigid body in question, but where exists difficulty is in being able to determine the orientation at each instant. The usual method for dealing with this problem is the Euler angles method. But, in this method there are orientations in which the method fails since zeros appear as denominators within the operations, these orientations are known as singularities. To avoid this problem, a method called rotations using quaternions is usually chosen, which manages to solve the problem of singularities, however, the little knowledge it has about quaternions means that their use is avoided. This work systematizes the use of quaternions in rigid body rotation dynamics. To achieve this objective, we started with the fundamentals of linear algebra, Euler-based rigid body dynamics, and quaternion properties. We obtained a systematic development of how quaternions are used in rigid body rotations. Moreover, the equations of motion for the translation and rotation of rigid bodies, all these without the loss of physical visualization and without the appearance of any singularity. This will allow the study of physical phenomena in which the Euler angles method is not usable. The development of a computational code to track the translational and rotational dynamics of anisotropic nanoparticles is in progress, which will allow us to address the design of new multifunctional materials.

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Pressure post-processing for the continuous Galerkin-Petrov space-time discretization of the nonstationary Stokes problem

Friedhelm Schieweck [1] Markus Bause [2] Gunar Matthies [3]

As a variational method in space and time we study the continuous Galerkin-Petrov discretization (cGP(k)-method) for the numerical solution of the nonstationary Stokes problem. Here, the fully discrete solution $(u_{\tau h}(t), p_{\tau h}(t))$ on each time interval is a polynomial in time of order k with values in a finite element product space $V_h \times Q_h$ where (V_h, Q_h) is an arbitrary inf-sup stable pair of finite element spaces with approximation order r for the velocity in the H^1-norm and for the pressure in the L^2-norm. The test functions in the variational method are, on each time interval, polynomials in time of order $k-1$ with values in $V_h \times Q_h$. The global continuity of the velocity trajectory $u_{\tau h}(t)$ is realized within a time marching process by a local initial condition at $t = t_{n-1}$ on each new time interval $I_n = (t_{n-1}, t_n]$. However, we do not require an initial condition for the pressure on each time interval. This leads on the one hand to a globally discontinuous pressure trajectory and on the other hand to a non-unique pressure solution of the variational problem. From the set of pressure solutions we determine a suitable solution by means of post-processing which guarantees a pressure approximation that is, with respect to time, superconvergent of order τ^{k+2}, for $k \geq 2$, and optimal of order τ^2, for $k = 1$, where τ denotes the time step size.

Similarly, we can compute in a very inexpensive way by means of a simple post-processing step a lifted post-processed solution $(\tilde{u}_{\tau h}(t), \tilde{p}_{\tau h}(t))$ such that the velocity $\tilde{u}_{\tau h}(t)$ is globally C^1-continuous in time and a polynomial of order $k+1$ on each time interval and $\tilde{p}_{\tau h}(t)$ is globally continuous in time and a polynomial of order $k+1$ on each time interval. For this approximation $(\tilde{u}_{\tau h}(t), \tilde{p}_{\tau h}(t))$, we can prove an optimal estimate for the velocity error in $L^2(L^2)$ of the order $\tau^{k+2} + h^{r+1}$, where h denotes the space mesh size and r the polynomial degree for the velocity approximation in V_h. Moreover, we prove an optimal $L^2(L^2)$ estimate for the pressure error of the order $\tau^{k+2} + h^r$, where the polynomial degree for the pressure approximation in Q_h is $r-1$

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due to the inf-sup condition.

Key ingredients of the analysis are a special higher order interpolate of the exact solution in time, a mixed Ritz-projection in space and the proof of superconvergence of the error in the time derivative for the velocity in the points of the k-point Gaussian quadrature formula on the local time interval.

Efficient positivity/bound preserving schemes for complex nonlinear systems

Jie Shen [1]

Solutions for a large class of partial differential equations (PDEs) arising from sciences and engineering applications are required to be positive to be positive or within a specified bound. It is of critical importance that their numerical approximations preserve the positivity/bound at the discrete level, as violation of the positivity/bound preserving may render the discrete problems ill posed.

I will present several efficient and accurate approaches: (i) through reformulation as Wasserstein gradient flows; (ii) through a suitable functional transform; and (iii) through a Lagrange multiplier. These approaches have different advantages, are all relatively easy to implement and can be combined with most spatial discretization.

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Multirate Adaptive Time-stepping Schemes for Coupled Systems of PDEs

Martyna Soszynska [1] Thomas Richter [2]

We study time discretization schemes for coupled systems of partial differential equations. We assume that the subproblems are defined over spatially distinct domains with a common interface, where the coupling is enforced. Each of the physical problems can be governed by a different type of equations (either parabolic or hyperbolic) and therefore can exhibit different dynamics. Fluid-structure interactions are one type of important application problems that fall into this framework. Here however, we will consider linear problems only.

Our aim is to develop time discretization schemes allowing for different time-step sizes in each of the domains without violating the coupling conditions. We are able to achieve it by formulating the problems within the space-time framework. Although the formulation is monolithic, we solve the systems sequentially relying on a partitioned approach. We further develop an a posteriori error estimator based on the dual weighted residual method. This estimator is then used as an adaptivity criterion [?]. To justify this method, we show stability estimates.

Principal Geodesic Analysis in Director-Based Dynamics of Hybrid Mechanical Systems

Cristian Gebhardt [3] Jenny Schubert [4] Marc Steinbach [5]

In this talk, we present new computational realizations of principal geodesic analysis for the unit sphere S^2 and the special orthogonal group SO(3). In particular, we address the construction of long-time smooth lifts across branches of the respective logarithm maps. To this end, we pay special attention to certain critical numerical aspects such as singularities and their

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consequences on the numerical precision. Moreover, we apply principal geodesic analysis to investigate the behavior of several mechanical systems that are very rich in dynamics. The examples chosen are computationally modeled by employing a director-based formulation for rigid and flexible mechanical systems. Finally, we test our numerical machinery with the examples.

Real-Time Contactless Breathing Monitoring System Using Radar with Web Server

Alcides Bernardo Tello [1] Yonel Chocano Figueroa [2]
Anderson Daniel Torres Bernardo [3] Jose Angel Falcon Riva Aguero [4]

As an innovative monitoring system, methods for non-contact human vital signs detection have been on the rise recently. Although different technologies use different principles, the chief purpose is physical health assessment. Nevertheless, in practice, the position and angle of an individual are not always in an ideal condition for the current vital signs monitoring programs to obtain reliable information. Therefore, this study proposed a method of automatic gain of low-frequency signals used to track the monitoring signals of the human signs dynamically. This study also designed a web system that processes and stores millimetre-wave radar technology data to detect the patient's heartbeat and breathing rate with a touch-free approach. Additionally, this system proved to be helpful for non-sensory perception and information gathering in daily life. Afterwards, the algorithm that monitors the vital signs analyses the breathing pattern and heart rate and variations after the human signs enter a static state. The reference design was a customised respiratory and heart rate signal extraction based on the STM32F401 chip and 24G Doppler radar sensor. Our method has successfully detected apnea events to alert the patient. Ultimately, the contactless method is particularly suitable for the pandemic as it is the best way to prevent the transmission of infectious illnesses; furthermore, it provides a steady stream of data to be stored in the server for further use and analysis.

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Improving the computational performance of the IRKA method

Matías Valdés[1] Ernesto Dufrechou[2] Pablo Ezzatti[3]
Jens Saak[4]

We consider the Iterative Rational Krylov Algorithm (IRKA) [1] for Model Order Reduction of a Linear Time Invariant system. This is an iterative algorithm, that starts with an initial Reduced Order Model (ROM), represented by a set of r shifts, and refines these shifts until the set converges to an optimal ROM. Each step of this procedure implies, as its most demanding operation from a computational point of view, the solution of a sequence of r pairs of shifted linear systems: $(A - \sigma_i E)\, x = b$ and $(A - \sigma_i E)^T\, y = c$.

We first evaluate a baseline implementation of the IRKA, which solves each pair of shifted linear systems by BiCG, preconditioned with ILU. Our study shows that the most important bottleneck in this procedure is the preconditioner computation.

Considering the experimental results, we move from the original implementation, where the preconditioner is computed for each step of the IRKA and for each shift, to a new variant that leverages an adaptive strategy.

The performance of the proposed method is compared with the baseline implementation, showing a significant reduction in the execution time, while maintaining the convergence of IRKA to the same reduced model.

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Large-scale simulation of single-phase flow in 3D fractured porous media using a mixed hybrid FEM

Michel Kern[1] Géraldine Pichot[1] Martin Vohralík[1] Daniel Zegarra Vasquez[1] [2]

In the underground, fractures are discontinuities in the medium in the form of narrow zones. Fractures are very numerous and present at all scales, with very heterogeneous sizes and permeabilities. The permeability of the neighboring rock matrix is generally about two orders of magnitude lower than that of fractures. This is why fractures are preferential channels for flow, therefore making fractures play a vital role in a large number of industrial and environmental applications.

One commonly used geometrical representation of fractured porous media is the discrete fracture matrix model (DFM) in which fractures are represented as manifolds of codimension 1. The model for single-phase flow in DFMs is described in [1], where Darcy's law in the fractures includes an additional source term that takes into account the coupling with the rock matrix. Because of the growing geometric complexity in large fracture networks, test cases recently proposed in the literature are mainly 2D, or 3D but with a limited number of fractures, about 50 [2].

In this talk we present `nef-flow-fpm`, our mixed hybrid finite element method solver, inspired by [3], for the steady-state flow problem in 3D DFMs. Meshing the fracture network is carried out thanks to a specialized surface mesh generator (`MODFRAC` [4]). The surface mesh is then used as input for the volume mesh generator (`GHS3D` [5]). The black-box solvers integrated in `nef-flow-fpm` are both direct solvers [6, 7] and iterative solvers [8]. After validating `nef-flow-fpm` with the test cases presented in [2], we propose larger test cases up to 23 430 fractures, generated with a genetic algorithm [9], in order to assess the performance of the integrated solvers. As expected, direct solvers suffer from large memory consumption, while iterative solvers need a large number of iterations. Thus, we underline the challenges and the necessity of developing a dedicated, robust and efficient linear solver for even larger networks, for instance ~ 1.1 million fractures [10].

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Data assimilation by TPU for Ocean Circulation Model

Marcelo P. Ramos [1] Luiz A. Vieira Dias [2]
Haroldo F. de Campos Velho *

This talk deals with data assimilation (DA). DA is a mathematical procedure ap- plied to compute a differential equation system's initial condition (*analysis*). The procedure combines, in the best way, data from observations and a previous prediction (*background*) for calculating the analysis for the next forecasting cycle. There are several methods to implement DA. We have employed a neural network approach to reduce the Kalman filter's computational effort [2]. In this presentation, preliminary results will be shown implementing the neural network technique for DA on the TPU – TTensor Processing Unit. Synthetic measurements are used for evaluating the neural network performances for a 2D ocean circulation model by using shallow water equations [1].

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Doubly enriched finite volume spaces for the DNS of fluid-particle interaction

Jonas Simon [1] Susanne Höllbacher [2] Gabriel Wittum [3]

We present double enriched finite volume spaces for the simulation of free particles in a fluid. This involves forces beeing exchanged between the particles and the fluid at the interface. In an earlier work we derived a monotithic scheme which includes the interaction forces into the Navier-Stokes equations by direct coupling. In multiphase flows oscillations and spurious velocities are a common issue. The surface force term yields a jump in the pressure and therefore the oscillations are usually resolved by extending the spaces on cut elements in order to resolve the discontinuity. For the construction of the enriched spaces proposed in this paper we exploit the Petrov-Galerkin formulation of the vertex-centered finite volume method (PG-FVM). From the perspective of the finite volume scheme we argue that wrong discrete normal directions at the interface are the origin of the oscillations. The new perspective of normal vectors suggests to look at gradients rather than values of the enriching shape functions. The crucial parameter of the enrichement functions therefore is the gradient of the shape functions and especially the one of the test space. The distinguishing feature of our construction therefore is an enrichment that is based on the choice of shape functions with consistent gradients. These derivations finally yield a fitted scheme for the immersed interface. We further propose a strategy ensuring a well-conditioned system independent of the location of the interface. Numerical tests were conducted using the PG-FVM. We demonstrate that the enriched spaces are able to eliminate the oscillations.

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CHAPTER 5

Poster

Existence of weak solution for a non-linear parabolic problem with fractional derivates

Raúl A. Sanchez Ancajima [1] Luis J. Caucha Morales [2]

The main objective of this work is to demostrate the existence and unique of weak solution for a nonlinear parabolic problem with fractional derivatives for the spatial and temporal variables on a one-dimensional domain. Using the Nehari Manifold method and its relationship with the Fibering Maps, the existence of a weak solution for the stationary case was demostrated. Finally, using the Arzela-Ascoli Theorem and Banach's Fixed Point Theorem, the existence and uniqueness of a weak solution for the non-linear parabolic problem were shown.

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Aplicación de modelos matemáticos para estimar la estabilidad del nivel del agua en un sistema de dos tanques en serie con variaciones en la demanda del servicio

Nilthon Arce [1]

En este trabajo de investigación se desarrolló un sistema de dos tanques en serie. En este sistema, el agua fluye del primer tanque al segundo. Hubo variaciones de apertura en la válvula de entrada, manteniendo fijo la apertura de la válvula de salida. Usando ecuaciones diferenciales, la matriz jacobiana y autovalores, fue posible analizar la estabilidad de los puntos de equilibrio del sistema. Para estimar en tiempo real los niveles de los tanques, se implementó el modelo no lineal y lineal. Ambos modelos identificaron los puntos de equilibrio del sistema, esto aseguró la demanda del servicio. Se aplicó un proceso de simulación para evaluar el comportamiento de los modelos en el tiempo, estos obtuvieron resultados similares. Esta simulación se realizó utilizando la herramienta Simulink de Matlab. El análisis de resultados sugirió el uso del modelo lineal para implementar el sistema de control, ya que sus composiciones de funciones de transferencia son menos complejas y más eficientes de implementar.
Palabras clave: Dos tanques en serie, puntos de equilibrio, estabilidad, sistemas de control.

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Duality theory of Convex Analysis: An application to the complete electrode model

Josué Daniel Díaz Avalos [1]

The duality theory of convex analysis is a general and versatile framework for problems in applied mathematics that can be written as optimization problems. Roughly speaking, the goal is to formulate a "dual" problem from the original one and explore the relations between these. As a result, properties that have physical interpretations and practical applications arise. In this work, the duality theory is applied to the complete electrode model, which is possibly the best for Electrical Impedance Tomography (EIT). Then, a posteriori error estimates are obtained and used to assess approximate solutions. The finite element method is employed in our numerical tests.

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Statistical analysis to estimate the spatial variation in sediment fluxes in a limited data context. Case of study: Peruvian western Andes

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The tropical Andes has been less studied in terms of sediment yield processes in comparison to other major mountain ranges in the world. Small to medium-sized rivers such as the ones flowing towards the Pacific Ocean have been relegated. They highlighted the link between sediment yield, anthropogenic and natural factors, e.g. climate, topography, river runoff, lithology and vegetation cover. In this study, we identified the spatial patterns of specific sediment yield along the western slopes of the Peruvian Andes between 3° and 13° S latitude for 21 catchments over a 30-yr period. We collected and analysed data from 22 environmental factors to elucidate their importance on spatially varying sediment yield. Given the scarcity of data on sediment yield, we included an uncertainty assessment based on bootstrapping approaches as to get a better grasp on the potential range of specific sediment yields in the study region. The river discharge time series was complete by downscaling gridded daily discharge data. Using statistical techniques including Spearman correlation rank, univariate and multivariate regression analyses, we were able to determine the importance of the 22 environmental variables on the specific sediment yield. Our results shown that the specific sediment yield varies strongly along the Peruvian western Andes. We reported higher-than-average specific sediment yields for the central part ($6° - 11°$ S) with values higher than 2000 t km-2 yr-1 and low and uniform yields of under 500 t km-2 yr-1 in the southern part (11° - 14.5° S). About 55% of the observed variance can be explained by river discharge (Q90) and river steepness index (ks50). By adding an anthropogenic variable based on land cover, the explained variance in SSY increases up to 63%. Our study therefore provides important new insights in the ongoing scientific debate on sediment yield variability in the western Andes.

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Modelo matematico de la tubercolosis asociada a factores socioeconomicos en la ciudad de Cali, Colombia

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Según la Organización Mundial de la Salud (OMS) es alarmante el aumento de la tuberculosis (TB), enfermedad infecciosa trasmitida por el bacilo denominado Mycobacterium tuberculosis, que afecta frecuentemente a los seres humanos y en los últimos años tras la pandemia se ha propagado con gran velocidad, la OMS afirma que en el año 2020 fallecieron 1,5 millones de personas por tuberculosis. En Colombia los escenarios ambientales, sociales y económicos sumados a estilos de vida desfavorables influyen y favorecen las condiciones ideales para la propagación de la TB en la comunidad por tal motivo para el desarrollo de esta investigación se construyó un modelo basado en compartimentos que busca relacionar dichos factores con la tasa de transmisión de la enfermedad, con el fin de observar la dinámica de transmisión en el municipio de Cali, este modelo considera cuatro grupos poblacionales que corresponden a susceptibles, latentes, infectados y tratados.

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Analysis of third order linear analytic differential equations with a regular singularity: Bessel and other classical equations

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We study third order linear differential equations with analytic coefficients under the viewpoint of explicitly constructing solutions and studying their convergence. We consider both homogeneous and non-homogeneous cases. In the homogeneous case with a regular singular point we address some untouched aspects of the classical theory like the complete description of the space of solutions. For this we identify the influence of resonances. We also study the convergence of formal solutions and a concrete way of constructing a third solution from two given solutions. These techniques apply, via classical order reduction and variation of parameters, to a complete description of the solutions of an analytic non-homogeneous equation with a regular singularity in terms of the given coefficients. We also propose models of order three for the classical differential equations like Airy, Chebychev, Laguerre, Lagrange and Hermite. We obtain explicit solutions to these models enforcing the properties they share with their order two counterparts. The final part contains some computer generated graphs of the solutions of these models. We believe our results are constructive and concrete making them useful in applied sciences and engineering.

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Dora Elizabeth Castillo León [1]

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Acoustics is a branch of physics that deals with studying sound, another form of energy in direct relation to the human habitat. On the one hand, the noise pollution suffered by the man of our time, makes the care of sound and noise management, which is nothing more than an unpleasant sound in general, requires a serious study at the time of designing or redistributing environments within a building, as well as adopt certain environmental policies of the environment. In the case of fluid media, in the case of air, what can begin to be studied are the levels of sound intensity. In the case of fluid media, in the case of air, what can begin to be studied are the levels of sound intensity. When speaking of the amplitude as a parameter of sound, it is said that it is directly related to the intensity of the acoustic oscillation. I is defined as the given distance from the source of the disturbance, as the power per unit area, at that distance. The unit of intensity is then:

$$AcousticIntensity = \frac{Watt}{cm^2}$$

A intensity of the sound source can be defined as the (sound) energy per unit of time and per unit area:

$$I = \frac{Potencia}{superficie}(\frac{Watt}{cm^2})$$

The lowest intensity perceived by the human ear is

$$I_0 = 10^{-16}\frac{Potencia}{superficie}(\frac{W}{cm^2})$$

The relationship between the scale in decibels and the intensity of sound is established by the formula:

$$d\beta = 10\log(\frac{I}{I_0})$$

In the decibel scale range for the human ear, which extends from 0 to 120 $d\beta$, 3 significant values can be characterized:

- 0 $d\beta$ dB Minimum threshold value

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- 80 $d\beta$ dB dangerous sound value
- 120 $d\beta$ dB Maximum value that causes hearing impairment

Above this last value, the sensation of sound begins to turn into pain and the destruction of the auditory apparatus occurs in a short time. But also sounds of high intensity level if received for long periods inevitably lead to deafness. In terms of traffic in large cities near universities, this noise generates discomfort among teachers and students, reflecting on academic performance and other mental health problems. [4].

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Remote sensing air quality analysis of Peru based on PM2.5 values

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Lima is in the top 5 cities in South America with the lowest air quality based on PM2.5 measurements. Air quality measurement remains a challenge in Peru due to two main reasons. First, no integrated measurement network is deployed in the country, where the capital city (Lima) represents 38 % of the total ground measurement stations. Second, most of the measurement stations from the National Meteorology and Hydrology Service (SENAMHI) exhibit temporal gaps caused by inactivity or malfunctioning. These problems motivate us to use remote sensing to overcome them. This work uses satellite data to evaluate the air quality index (AQI). First, we obtained the aerosol optical depth from two sources: i) VIIRS (6 km of spatial resolution) and ii) VIIRS (750 m of spatial resolution). Then, we evaluated the PM2.5 values using the AOD-PM relationship. Finally, we compared the standard EPA-AQI with our temporal analysis results from Dec-2021 to Jan-2022.

Our satellite data results of PM2.5 in Lima (in $\mu g m^{-3}$) show a minimum value of 9.33, an average of 29.91, and a maximum value of 79.23. Our ground estimation analysis of PM2.5 in Lima based on SENAMHI data shows a minimum value of 7.3, an average of 21.77, and a maximum value of 56.07. These results represent an *moderate* AQI classification (according to EPA) and are similar to the 2021 World Air Quality Report value ($\approx$ 29 AQI). Based on satellite data, Peru's national PM2.5 results exhibit a minimum value of 9.1, an average of 29.90, and a maximum value of 155.8. Our results show that: i) Lima has a lower AQI than the average national value in Peru, and ii) there is a growing trend of PM2.5 in Lima, which need to be validated with the ground measurements.

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Análisis de la realidad del fútbol de menores en Lima-Perú

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A través de este trabajo se propone otorgar evidencia científica sobre la realidad del futbol masculino de menores, después de la etapa clasificatoria para el mundial Catar 2022. Mediante el modelamiento computacional, usando la metodología propuesta en [1, 2, 3]; donde se emplearán diferentes parámetros para definir sus modelos y utilizando la última tecnología disponible.

Es por esto que, proponemos una contribución científica, que pueda ser el punto de partida para el desarrollo y potenciación del talento deportivo juvenil masculino para el fútbol, **enfocado hacia el alto rendimiento de este deporte en el Perú**.

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Problema mixto en 1D para la ecuación de Poisson con condiciones de contorno Neumann puro

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En este trabajo abordaremos el fundamento teórico y la descripci'on del método mixto de elementos finitos el cual nos da la posibilidad de anadir variables adicionales, en particular, utilizar dos espacios para aproximar dos variables diferentes. Finalmente utilizaremos este método para hallar una aproximación de la solución de la ecuacion de Poisson 1D con condiciones de contorno Neumann puro y mostraremos los resultados de la implementación elaborada utilizando el lenguaje de programación Python.

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The purpose of this work is to establish the stochastic flow, following associated with the primitive equations in two dimensions with the presence of multiplicative white noise in the force similar in [4]. A reformulation of the model is presented as a random dynamical system establishing its asymptotic dynamics. For this purpose, we use the theory of random dynamical systems[1,2], to determine the existence of a random attractor [4].

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An approach to calculate a preconditioned basis separator in an interior point method

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This work analyzes the Mehrotraís predictor-corrector method to solve linear programming problems. The central point of the process is the resolution of an increased standard system, which provides Newtonís direction. The drawback found here is that this system is ill-conditioned when several iterations and when it is close to the optimum point. For this reason, we proceeded to precondition said system using Suñagua's approach. This technique uses the essential and non-basic components of the system through the partial pivot strategy to solve the system using iterative methods, such as the method of conjugated gradients. In addition, this work includes various numerical experiments that demonstrate the efficiency of our proposal compared to other interior point algorithms explored in the literature.

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ANN application to one-dimensional inverse transport problems

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Source inverse particle transport problems has many important applications in energy generation, health, manufacturing and others. The main idea is to estimate one or more properties of the particle source from selected measurements of the particle intensity/density. In nuclear energy generation, this could mean to determine the source from outside the power plant kernel. In health, it can help to identify and localize tumor cells from non-invasive measurements. In manufacturing, it can be applied to online quality control from indirect measurements. In this work, we assume the particle transport problem is modeled by the linear transport Boltzmann equation stated in an one-dimensional domain. The inverse problem is described as a regression problem where an Artificial Neural Network (ANN) is trained as the regression model. Following an supervised strategy, a multilayer perceptron network is calibrated from a training set. The training samples are selected solutions of the direct transport problem from different sources. Validation of the ANN is also performed by applying selected solutions of the direct problem. Two different test cases are presented. One is the source location problem, which consist in estimating the location of a given source from scalar flux measurements in the border of the domain. The second, is the source determination, where the goal is the determination of a parameter of a given class of sources, also from scalar fluxes measurements on the border. In both test cases, we have found very good determination coefficients R^2=0.999 (training and validation), which indicates the availability of the proposed methodology to the solution of inverse particle transport problems.

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Virtualization of scientific software based on Arch Linux in GitPod

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We developed an open source repository hosted on GitHub to use scientific software based on the Arch Linux distribution, with an up-to-date software ecosystem that includes DUNE python bindings, DuMu^x, FEniCS, deal.II, Gmsh, preCICE adapters, among others. Unlike other projects such as BioArchLinux [?] or Arch Linux for education [?], we include some tutorials on GitHub Classroom to allow the practice to any newcomer. Automated deployed and available for free use allowing virtualization inside GitPod [?].

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Simulation of fluid dynamics and CO_2 gas exchange in the alveolar sacs of the human lung

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The dynamics of gas transport in the alveolar sacs is generated by respiration mechanisms, and so is the gas distribution and gases exchange with the cardiovascular system. The analysis was made with a mathematical model using the Galerkin method and existence and uniqueness of weak solutions in the Arbitrary Lagrangian-Eulerian (ALE) coordinates was proven. Numerical simulations were made with finite element methods on a moving domain using the Local projection Stabilization (LPS) for pressure stabilization. The estimations showed that the energy dissipation for the fluid is a consequence of the moving domain and the fluid properties. In conclusion, energy dissipation for the gas concentration was produced whe n the domain deformation is greater than a constant depending on the coefficients of solubility and diffusion of the gas.

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Exploring parameter spaces in Holomorphic Dynamics

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In this work, we explore the Mandelbrot sets and Julia sets associated with families of rational maps. We show how simulations using programming languages for these fractals are essential to establish some conjectures related to some topological properties of the connection locus of a Blaschke model.

This poster is dedicated to exploring some dynamical aspects of a family of Blaschke products as a function of a complex parameter, with a single critical point (cubic type) on the circle, a critical value (the parameter), and two superatractors fixed at zero and infinity. The variation of the critical value determines, in the dynamic plane, the connectivity of the Julia sets and in the parameter plane, the existence of escape components, that is, parameters for which the critical point escapes by iteration to zero or infinity. Furthermore, we define the locus of no escape for the Blaschke family [4], where numerical experiments suggest the presence of baby Mandelbrot sets.

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Morphodynamics neuroscience. A computational approach to dendritogenesis of pyramidal cells in the developing olfactory cortex

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We recently showed that pyramidal cells in the rat anterior piriform cortex (aPC) undergo dramatic changes to their intrinsic electrophysiological properties between the first and second postnatal week ([1]). Another group has shown that those cells undergo dendritic morphological changes during the same age period ([1]). Still, no study to date has thoroughly characterized dynamical changes in the dendritic morphology of aPC pyramidal(Pyr) cells that may underlie the functional development of this neuronal population. We addressed this knowledge gap with a computational approach modeling the dynamic changes in the morphological maturation of Pyr cells dendrites during the first postnatal week. We modeled the dendritic growth as an agent-based model using three diffusion models (MAP, tubulin, and calcium) and mathematical equations for developing neurons ([2],[3]). We use experimental data from Moreno et al. to fit dendritic growth's timing and spatial distribution. We first simulate a dendritic growth adjusted to postnatal day (P) 1 based on experimental data of Moreno. Next, we simulated a group of neurons mimicking the development of dendritic growth from P1 to P8 (phase 1) and P8 to P14 (phase 2). In both phases, neurons were adjusted or not adjusted to the experimental data. Our results show that in both phases, the number of dendritic branches in the group of not adjusted neurons surpasses the experimental reference number of 52 when it reaches 1800 μm length. From the simulation, we found that neurons of phase 1 have a lower rate of branching and elongation than neurons of phase 2. Contrary to what can be inferred for dynamic changes in the morphological maturation of Pyr cells dendrites from Moreno's experimental data, our model shows a higher branching ramification in phase 2 neurons. It is possible that other factors we are not considering here, such as sensory input, could have affected the dendritic maturation morphology in phase 2, thus reducing ramification branching during this development phase. Finding these factors and their

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mechanisms could help understand dendrites' morphological maturational changes.

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Regiones de Voronoi para optimizar geoespacialmente los puntos de recarga para vehículos eléctricos, una propuesta para Bogotá D.C.(Colombia)

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La estimación de los puntos de recraga para VE requiere utilizar técnicas de análisis de tipo estadístico (estadísticas descriptivas, modelos de regresión lineal y logística, análisis de componentes principales), la geoestadísticas (Interpolación kriging, modelos de variograma) y machine learning (k-medias, árboles de decisión), sin olvidar la importancia que cumplen todas las herramientas con el apoyo de las matemáticas. Una primera aproximación se presenta mediante el estudio de los diagramas de Voronoi que en combinación con la estadística y geoestadística se convierten en una buena estrategía para la estimacación de puntos de recarga para VE. Los diagramas de Voronoi, en principio constituyen una especie de mosaico, cuya propiedad fundamental consiste en la división del lugar geométrico por medio de puntos y la asignación a cada uno de ellos, de la región que se encuentre más cerca de ese punto que de cualquier otro, es así, como los diagramas de Voronoi permiten resolver computacionalmente tiempos razonables en un camino posible para que un automovil se desplace en medio de un entorno dinámico hacia el punto de recarga más cercano de su ubicación, [2],[1], [3].

En la actualidad, la forma fácil de construir regiones de Voronoi con Python es usando el paquete Geovoronoi, con información de centros comercial, centros educativos, densidad poblacional. La información se graba primero como un dataframe, luego como un geodataframe, para ser convertidos en puntos en un sistema de coordenadas de referencia(CRS), luego se hallan los polígonos correspondientes a la población de interés, que permite crear las regiones de Voronoi y obtener finalmente las regiones delimitadas cada una con un punto que se considera el más cercno para la región con respecto a sus puntos vecinos, [4], [5]

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The Inexact Restoration Method applied to the Minimization problems with orthogonality constraints

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In this work, we present and study the non monotone algorithm inexact restoration to solve minimization problems with orthogonality constraints, which combines the Inexact Restoration Method of Fischer and Friedlander [5] and the nonmonotone criteria of Zhang and Hager [3]. We develop the theoretical tools to characterize the subspace tangent of the feasible set, which allows us to describe the proposed algorithm. We show, under certain hypothesis, the good definition of the Algorithm as well as the global convergence to viable points of the problem. The inexact restoration method is an iterative method that consists of two phases: viability and optimality. In this work, the feasibility phase will be obtained in an exact way by using the Cayley transformation. Therefore, the sequence of restored points belong to the viable set. In the optimality phase, the descent directions can be obtained in two ways: projected spectral gradient or the minimization of the Lagrangian, both on the tangent subspace. To solve this minimization we use the conjugate gradient method [4]. The computational implementation of the proposed algorithm is performed on MATLAB and is compared with the Wen et al method [6] and the Conjugated Gradient method from ManOpt library for different test problems in the literature.

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Inferential model from machine learning based on health data mental Colombia compared to the world level

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Scientific advances since its inception have been an advantage for the community and all branches of study, especially artificial intelligence (AI) has contributed significantly in recent years with its various potentialities, one of its uses is the creation of networks neuronal through Machine Learning. Therefore, the main objective of this article is to carry out a bibliographic review of several to determine the state of the art of the use of Machine Learning applied to mental health, a database search was carried out where 80 articles were preselected, of which 41 articles were chosen according to the inclusion criteria, resulting in that mental illnesses such as depression, suicidal thoughts and anguish, top the lists of investigated mental illnesses, likewise in most articles they did not specify the population, also, It was defined that the most used method are vector machines, neural networks and decision trees conclusions. It was concluded that Colombia has lagged behind the research in the field, therefore, more studies of mental health with data analysis are needed to diagnose and prevent mental problems.

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Effect of microstructure on the magnetization of a suspension of magnetic Janus particles

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In this work, the three-dimensional self-assembly of a dilute suspension of magnetic Janus particles with a magnetic dipole laterally displaced from their center was studied using Brownian dynamics simulations. Microstructure and aggregation properties were determined from the temporal evolution of the positions and orientations of the particles. The average size of clusters, the nucleation and growth process, the population distribution, and the effective radius of clusters were evaluated for a diluted suspension (1% volume fraction) for different values of the dipolar shift (s) – which adopts values in the range $0 \leq s \leq 1$ when dimensionless using the radius of the particle. When the value of the dipolar shift is small ($s \longrightarrow 0$), chain and ring-shaped structures are formed which are typically observed in particles with a centered dipole ($s = 0$). At intermediate dipolar shifts ($0.2 \leq s \leq 0.3$), aggregates are formed mainly in the form of vesicles that in some cases coexist with rings and micelles. Finally, for $s \geq 0.3$, the formation of spherical micelles is observed that progressively decrease in size as s increases until reaching aggregates of 2 or 3 particles. For intermediate and high dipolar displacements, the system saturates to a small cluster size (few particles per aggregate) very suitable for magnetic suspension design with high stability. This study shows that new magnetic fluids can be designed by controlling the dipole displacement of their component particles to influence their microstructure and therefore their macroscopic properties, for use in potential applications.

Differential equations applied to viral diseases

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In this report, a first order nonlinear ordinary differential equation problem is addressed in viral diseases, for which the model of a Bernoulli-type equation

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is used, this equation is logistic, its function and logistic curve are obtained, also qualitative theory is applied in order to verify the data obtained are correct. Mathematical models applied in other areas and their solution are presented.

Keywords: Initial value problems, existence, uniqueness, continuous dependence and continuation of solutions to ordinary differential equations; Modeling and interdisciplinarity (aspects of mathematics education); Explicit solutions, first integrals of ordinary differential equations

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Mathematical model of a predator-prey food chain: plankton-anchovy

Neisser Pino Romero [1]

In the present work, a mathematical model is built that represents the dynamics that exist between phytoplankton (F), zooplankton (Z) and anchovy (A) from the model of Samares and Anal. This food chain occurs in the Peruvian maritime area where there is a three-link ecosystem, in addition to the fact that the food chain is a main axis in the ecological balance within the sea. The behavior of the populations (maritime species) will be studied where the stability of the model (Routh-Hurwitz criterion) in the long term will be determined, where it will be analyzed with the Dulac-Bendixon criterion to evaluate the existence of closed periodic orbits. And the respective computational simulations to complement the study and interpret the situations that affect the maritime ecosystem.

$$\begin{cases} \frac{dF}{dt} = rF\left(1-\frac{F}{K}\right) - \frac{\alpha_1 F\cdot Z}{k_1+F} - \frac{\alpha_2 F\cdot A}{k_2+F} - \mu_1 F \quad , \quad F(0)=F_o \geq 0 \\ \frac{dZ}{dt} = \frac{\beta_1 F\cdot Z}{k_1+F} - \frac{\alpha_3 Z\cdot A}{k_3+Z} - \mu_2 Z \quad , \quad Z(0)=Z_o \geq 0 \\ \frac{dA}{dt} = \frac{\beta_2 F\cdot A}{k_2+F} + \frac{\beta_3 Z\cdot A}{k_3+Z} - \mu_3 A \quad , \quad A(0)=A_o \geq 0 \\ r, K, k_1, k_2, k_3, \alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \mu_1, \mu_2, \mu_3 > 0 \\ \alpha_1 > \beta_1 \ , \ \alpha_2 > \beta_2 \ , \ \alpha_3 > \beta_3 \end{cases}$$

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Small Satellites as platforms for Engineering Education

Aldo André Díaz-Salazar [1]

Satellite Engineering is being leveraged by the recent use of small satellites, called CubeSATs. A CubeSAT is a square satellite of 10cm3 of size equipped with an on-board computer and sensors for collecting environmental measurements and even satellite images. Due to its reduced cost, small educational satellites are excellent platforms for instructors and scholars involved in STEAM (Science, Technology, Engineering, Arts and Mathematics) skills training. Applications where the CubeSAT technology has proved to be advantageous are in Meteorology, Agriculture, Communications and Remote Sensing, as demonstrated recently, for instance, by the European Space Agency (ESA). The aim of this talk would be to discuss two CubeSAT applications currently being developed at the Federal University of Goias (UFG, Brazil). The first is a study of the South Atlantic Anomaly (SAA) in Earth's magnetosphere. By using tri-axial magnetometers, the aim of this mission is to estimate the intensity of the magnetic field and localization of SAA using a novel simultaneous localization and mapping (SLAM) approach. The second is a study of the Araguaia river located in Brazil from aeroespace using remote sensing technology. In this case, it is used a camera to monitor the status of preservation of this natural resource by analyzing images in order to infer deforestation and potencial areas of desertification. Both works take part in the Brazilian Satellite Olympiad (OBSAT), currently at stage 3 out of 5, and would potentially end up with an orbital launch.

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Modelo estadístico para la abundancia del estadio de huevos de la Diaphorina Citri

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Diaphorina citri es el insecto asociado con la transmisión de la bacteria Candidatus Liberibacter asiaticus (CLas) agente causal de la enfermedad huanglongbing (HLB), que afecta los sistemas productivos de cítricos. El objetivo de este trabajo fue determinar la dinámica poblacional de D. citri sobre especies del género Citrus en Sevilla - Zona bananera (Magdalena). El estudio se realizó mediante monitoreos quincenales de octubre de 2019 a octubre de 2020 en un lote de 16 variedades de cítricos injertados sobre los portainjertos CPB 4475 y Sunky X English del centro de investigación de la región Caribe de AGROSAVIA, se recolectaron brotes vegetativos en los que se contabilizaron los estados inmaduros de D. citri. El seguimiento de los adultos se realizó mediante su captura en trampas adhesivas de color amarillo. Para el análisis de los datos se utilizó el modelo Binomial Negativo Cero Inflado (ZINB) con las funciones de enlace log y logística, se realizó el ajuste del número de huevos en función de variables climáticas, para los cual se realizó una selección de variable, a partir del Análisis de Componentes Principales (ACPACP).

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