

The Eleventh International Conference on
Numerical Methods and Applications

August 31 - September 04, 2026
Borovets, Bulgaria

NM&A'26

ABSTRACTS

PREFACE

ABOUT THE CONFERENCE

The Eleventh International Conference on “Numerical Methods and Applications” (NM&A’26) is organized by the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences. It will take place from August 31 to September 4, 2026, in Borovets, Bulgaria, and is dedicated to the memory of Prof. Raytcho Lazarov.

The conference continues the established NM&A series and provides a forum for the exchange of ideas among scientists who develop numerical methods and algorithms and researchers who apply them to challenging problems in science, engineering and technology. The scientific programme includes invited plenary lectures, presentations within four special sessions, and contributed talks. The official language of the conference is English.

The principal topics include numerical methods for differential and integral equations; approximation techniques in numerical analysis; numerical linear algebra; hierarchical and domain decomposition methods; parallel algorithms; Monte Carlo and Quasi-Monte Carlo methods; and applications in computational mechanics, physics, chemistry, biology and engineering.

LIST OF INVITED SPEAKERS:

- Yalchin Efendiev (Texas A&M University, USA)
- Oleg Iliev (Fraunhofer ITWM, Germany)
- Nedyu Popivanov (Bulgarian Academy of Sciences, Bulgaria)
- Petr Vabishchevich (Russian Academy of Sciences, Russia)
- Barbara Wohlmuth (Technical University of Munich, Germany)
- Ludmil Zikatanov (The Pennsylvania State University, USA)

LIST OF SPECIAL SESSIONS:

- **Numerical and Simulation-Based Methods for Decision Making under Uncertainty**
organized by Prof. DSc Stefka Fidanova (Institute of Information and Communication Technologies, Bulgarian Academy of Sciences) and Assoc. Prof. Dr. Velichka Traneva (Burgas State University “Prof. Dr. Assen Zlatarov”).
- **Numerical Methods for Engineering Innovation: From Digital Twins to Advanced Materials**
organized by Prof. Maria Datcheva, Prof. Ivan Georgiev and Prof. Roumen Iankov (Bulgarian Academy of Sciences).
- **Approximation Theory**
organized by Prof. Geno Nikolov and Prof. Rumen Uluchev (Sofia University “St. Kliment Ohridski”).

- **Monte Carlo and Quasi-Monte Carlo Methods**

organized by Prof. DSc Ivan Dimov and Prof. Emanouil Atanasov (Bulgarian Academy of Sciences).

ABOUT THIS BOOKLET

This booklet contains introductory conference information and a detailed table of contents, followed by the abstracts of the invited lectures, the special-session presentations and the contributed talks. The abstracts are grouped by session and arranged alphabetically by the family name of the first author. The complete alphabetical list of authors and participants, including affiliations, contact e-mail addresses available in the submitted files, and the page references of their abstracts is provided at the end of the booklet.

The refereed and presented full papers are planned for publication in a special volume of Springer's *Lecture Notes in Computer Science*.

CONFERENCE ORGANIZATION

Organized by

Institute of Information and Communication Technologies, Bulgarian Academy of Sciences.

In cooperation with

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences;

Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski";

Bulgarian Section of the Society for Industrial and Applied Mathematics (BGSIAM);

Center of Excellence in Informatics and Information and Communication Technologies.

Program Committee

Chairpersons: S. Margenov, G. Nikolov and N. Kolkovska.

Organizing Committee

Chairpersons: M. Datcheva and I. Georgiev.

Members: I. Bazhlekov, I. Christov, S.-M. Gurova, S. Harizanov, E. Lilkova and D. Slavchev.

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The organizers

August 2026

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Abstracts¹

¹Arranged by session and alphabetically within each session according to the family name of the first author.

Invited Lectures

Multiscale and Multicontinuum Methods

Efendiev Y.

Multiscale phenomena in heterogeneous media arise in a wide range of applications, including subsurface flow, porous media, composite materials, and reactive transport. A fundamental challenge is to develop coarse-scale models that are both computationally efficient and capable of capturing the essential physical mechanisms occurring across multiple spatial scales. Classical multiscale methods provide accurate numerical approximations of fine-scale solutions, while homogenization and multicontinuum approaches seek effective macroscopic descriptions. Bridging these two remains an important open problem.

In this talk, I will present recent developments in multiscale and multicontinuum modeling based on the Generalized Multiscale Finite Element Method (GMsFEM). The proposed framework establishes a direct connection between multiscale basis functions and multicontinuum representations, enabling the systematic derivation of physically meaningful macroscopic equations from multiscale discretizations. The approach naturally accommodates heterogeneous media with multiple interacting continua, varying numbers of continua across the computational domain, and complex multiscale features.

I will discuss the underlying mathematical ideas, the construction of continuum-dependent multiscale basis functions, and the resulting coarse-scale models. Applications to multiphase flow in heterogeneous porous media will be presented, illustrating how the framework captures interactions between mobile and trapped phases and leads to new effective macroscopic models. The talk will conclude with perspectives on extending these ideas to more general multiscale systems, including evolving continua, coupled multiphysics processes, and hierarchical multiscale modeling.

On Modeling and Simulation of some Heat and Mass Transfer Phase Changes Problems

Iliev O.

In 70s and 80s of the last century Raytcho Lazarov was leading in the Institute of Mathematics, BAS, a group on modeling and simulation of heat and mass transfer processes in the presence of phase change. The specific topic was solidification of metals and alloys, and the research and development was carried out as part of the collaboration between the Institute of Mathematics the Institute of Metal Science of BAS. In the first part of this talk some of the results obtained at that time under the leadership of Raytcho will be recalled.

Currently, convective drying is used by industry in the vast majority of battery electrode manufacturing processes. However, it is characterized by very high energy consumption and there are also limitations on the production speed. There is a demand for more efficient drying processes. Among the several technologies which are studied currently, the most promising and closest to the industrial standards is the near infrared radiation, NIR. There are a great number of experimental and numerical papers on convective drying, but NIR is still not widely studied. In this talk, we present an experimental and numerical study of electrode drying, including those with high-intensity NIR. We report several findings: (i) no vertical temperature gradient is observed in the carried experiments; (ii) NIR enables fast drying with good adhesion; (iii) no capillary limitations are observed in NIR drying of thin electrodes; (iv) presented comparison between the experimental and numerical results, shows that the model used correctly represents the experiment; (v) we elaborate on how NIR is heating the slurry volumetrically, in contrast to the surface heating in the convective drying.

Pohozhaev Identities and Applications

Popivanov N.

Beginning from the seminal Pohodzaev paper (1965), the Pohodzaev Identities, first developed for the Dirichlet problem for elliptic quasilinear equations, have been extended to study many cases for different PDE classes of equations, even for some fractional PDE's. The present talk I will focus on the extension of Pohodzaev approach in the last 25 years for its applications to some mixed elliptic-hyperbolic quasilinear equations. This study began from the series of results of Lupo-Payne, where using some symmetries in the linear homogeneous case, the dilation invariance law is strongly related to certain Pohodzaev type identities that give examples of critical exponent phenomena. Let us mention here the big difference with elliptic case where the work is with classical smooth solutions, for whom the situation is: in the case of supercritical power we have the nonexistence of nontrivial solutions in so called "starshaped domains", and in the opposite case of subcritical power there exist some nontrivial solutions. Now, for mixed type equations the statement of the problems in both cases are in some special functional weight classes of "generalized solutions". The reason is the singularity which usually naturally exists in the solution even in some classical domains. I will give some example when the generalized solution in the linear case has an exponential growth at only one point of singularity. The singularity does not propagate along the characteristic light cone. Some open problems will be formulated and discussed.

Keywords: Pohozhaev identities, critical exponent, supercritical cases, nonexistence of nontrivial solutions

Computational Homogenization of Flows in Porous Media With Memory

Vabishchevich P. N.

This study introduces a computational homogenization technique for modeling unsteady flows of an incompressible viscous fluid through periodic porous media with memory effects. On the macroscopic level, the flow is described by an integro-differential Darcy law whose tensorial memory kernel is obtained from unsteady cell problems. Our method determines the steady-state and transient components of the conductivity tensor by solving auxiliary boundary-value and spectral problems on the representative periodic cell. A key numerical step involves approximating the memory kernel with a Prony series (sum of exponentials), which reduces the nonlocal macroscopic problem to a local system of differential equations. We outline the spatial finite-element discretization and develop stable two-level time-stepping schemes. Finally, we demonstrate the proposed framework on a two-dimensional test problem, showcasing its effectiveness for unsteady filtration applications.

Keywords: unsteady flows in porous media, memory Darcy law, integro-differential equation, exponential sum approximation, two-level time discretization schemes

Hybrid PDE models for bio-medical applications

Wohlmuth B.

In this talk, we consider the mathematical modelling and numerical simulation of different bio-medical applications ranging from cerebral aneurysms to vascular tumor growth and drug response. We combine numerical schemes on different spatial scales and illustrate the mathematical and numerical challenges of the coupling of 0D-1D-3D models as well as of agent-based dynamics. Firstly, we consider an abstract framework for mixed dimensional approaches. While nonlinear hyperbolic 1D PDE models can effectively be used to describe the flow and transport in the vascular tree, homogenized 3D porous media models can be considered to simulate flow and transport in capillaries and tissue. We introduce a calibrated generic arterial network to generate inflow data for patient specific vasculature and tissue data sets. Secondly, we comment on the interaction of micro- and macro-scales effects. While agent-based simulation approaches can effectively model cell-cycle effects, the extensions to tissue-scale mechanical interactions is not straightforward. To overcome these limitations, agent based cell dynamics is coupled to a FEM based poro-elastic formulation of the surrounding tissue. This enables us to study the interplay between cellular processes and macroscopic mechanical forces, such as interstitial fluid flow and pressure-induced cell responses. Thirdly, we consider different aspects and mathematical challenges in case of

cerebral aneurysmen. From non-Newtonian 3D blood flow by Lattice Boltzmann methods in patient specific geometries to the endovascular coil embolization by an extended discrete elastic rod model taking into account bending, twisting and self-contact to the formation of clots by a system of reaction-advection-diffusion equations coupled to the Navier-Stokes system.

On Discretizations Using Quasi-Polynomial Spaces of Differential Forms

Zikatanov L.T., S. Wu

We consider extensions of the exponentially fitted finite element scheme for convection-diffusion equations of Xu and Zikatanov (1999); at some point Raytcho Lazarov asked whether such schemes extend to tensor valued coefficients. This resulted in the work of Lazarov and Zikatanov (2004), which gave the first relations between exponential fitting and the finite element exterior calculus. We extend this to quasi-polynomial spaces of differential forms with a positive weight and polynomial coefficients. We show that the unisolvent set of functionals for such spaces on a simplex in any spatial dimension is the same as the one used for the polynomial spaces. These results provide tools for studying exponentially fitted discretizations stable for general convection-diffusion problems in Hilbert differential complexes.

SPECIAL SESSION: Numerical and Simulation-Based Methods for Decision Making under Uncertainty

Simulation-Based Reinforcement Learning for Decision Making Under Uncertainty in Urban Traffic Signal Control

Boudjaoui Z.-E.

Urban traffic congestion remains a significant challenge in modern cities, resulting in increased travel times, fuel consumption, and environmental impacts. Conventional traffic signal control strategies are often based on fixedtime schedules and are unable to effectively adapt to dynamic and uncertain traffic conditions. To address this limitation, this work investigates the use of Reinforcement Learning (RL) for intelligent decision making in urban traffic signal control under uncertainty. The proposed approach relies on a simulation-based learning framework in which an RL agent interacts with a realistic traffic environment and learns optimal signal control policies through trial-and-error. The traffic network and vehicle movements are modeled and simulated using the Simulation of Urban Mobility (SUMO) platform, while the RL algorithms and the communication interface between the learning agent and the simulator are implemented in Python. The agent continuously observes the state of the traffic network, including queue lengths and vehicle waiting times, and dynamically adjusts traffic signal phases to improve traffic flow efficiency. The developed framework enables the evaluation of adaptive control strategies under varying traffic demands and uncertain operating conditions. Experimental results show that the reinforcement learning-based controller can reduce average waiting times, decrease queue lengths, and improve overall network performance when compared with traditional fixed-time signal control methods. The integration of SUMO and Python provides a flexible and scalable environment for the development and assessment of intelligent transportation solutions.

This research demonstrates the potential of simulation-based reinforcement learning as an effective tool for adaptive urban traffic management and supports the deployment of smart traffic control systems in future smart cities.

Keywords: Reinforcement Learning, Traffic Signal Control, SUMO, Python, Urban Traffic Management

Generalized Net for Evacuation of People with Mental Problems After Earthquake

Fidanova S., N. Bozakova, V. Ivanov

When a natural disaster occurs, such as an earthquake, flood, etc., there are vulnerable groups of people who cannot cope alone and need additional help. One such group is people with mental problems. This type of people are often disoriented and easily panic. Even if such a person is in good physical condition and able to evacuate the disaster site by himself, he needs additional care. In this research, we focus on the evacuation of people with mental problems after an earthquake. We propose a model of evacuation, based on Generalized Net (GN). The goal is to be able to play out a variety of scenarios and make the most appropriate decision given the specific situation. The purpose of the model is to support the local authorities for preliminary preparation and training of the staff who will provide assistance, as well as for a quick and adequate response after the occurrence of an earthquake. GN are very suitable for the description of inhomogeneous complex processes. With the help of GN, one can first describe the framework of the considered process, then replace each transition with a new network and thus add new details to the model. This makes it possible to describe a given process in depth and prevents important components from being omitted. Advance preparation can be crucial. When we have information about persons with mental problems, as well as information about the homes they live in and the likelihood of them getting injured and burned, local authorities and medical institutions can be prepared in advance and react adequately. Such type of models will lead to saving human lives and reducing casualties and disability.

Intuitionistic Fuzzy Pheromone ACO for Knitwear Production Scheduling

Fidanova S., J. Stanchov

The textile industry occupies a large share of the economy. One of its important sectors is the production of clothing. The production of knitted clothing is an important part of the textile industry. In order for production to be efficient, it must be well organized. Part of the overall organization is the distribution of the individual elements of a given garment for filling on the available machines. The goal is for the order to be completed in the minimum time. The aim of this development is to optimize the production of knitted garments. Optimization involves the allocation of jobs and materials to machines. For this purpose, we have applied two variants of the ant colony optimization method, traditional one and with intuitionistic fuzzy pheromone updating. We have made a comparison between the two variants of the algorithm.

Keywords: Combinatorial optimization, Ant colony optimization, Scheduling, Knitwear production

Acknowledgments: The work was partially supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018-C01, financed by the Research, Innovation and Digitalization for Smart Transformation Programme 2021-2027 and co-financed by the European Union.

Monte Carlo Search for Robust Global Portfolios: A Sharpe-CVaR Comparison

Gurova S.-M., T. Gurov, A. Kirilov

Portfolio optimization remains one of the most challenging applications of stochastic numerical methods due to the nonlinear relationship between expected return and financial risk. Monte Carlo techniques provide a flexible computational framework for exploring large feasible spaces of portfolio allocations without imposing restrictive assumptions on the optimization landscape. Their simplicity and robustness make them attractive for practical risk assessment and investment decision support.

In this work, a Monte Carlo optimization approach is employed to investigate portfolio selection under two widely used objective functions: maximization of the Sharpe ratio with a risk-free rate of 3% and minimization of the Conditional Value-at-Risk (CVaR) at the 5% confidence level. The study considers a diversified portfolio consisting of n global financial assets and examines three investment horizons (3, 5 and 10 years). Portfolio weights are generated using the Mersenne Twister pseudo-random number generator, while candidate portfolios N are simulated for each investment horizon. Expected return and portfolio risk are evaluated for every realization, and the optimal portfolio is selected according to the corresponding optimization criterion.

The numerical experiments demonstrate distinct characteristics of the two optimization objectives. The Sharpe-based optimization consistently produces higher expected returns at the expense of increased portfolio volatility, whereas the CVaR criterion generates more conservative allocations with improved downside risk protection. Among the investigated investment horizons, the five-year period provides the most favorable compromise between return and risk for both optimization criteria. The results also indicate that the obtained optimal solutions depend on the selected objective function, the historical observation window, and the stochastic nature of the Monte Carlo method.

Keywords: Monte Carlo simulation, Portfolio optimization, Sharpe ratio, Conditional Value-at-Risk

Acknowledgments: The work of the authors (S.-M. Gurova and A. Kirilov) was supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-

1.014-0018-C01, financed by the Research, Innovation and Digitalisation for Smart Transformation Programme 2021-2027 and co-financed by the European Union. The author's work (T. Gurov) was supported by the project "Digitalisation of the Economy in a Big Data Environment" BG16RFPR002-1.014-0013, funded by the European Regional Development Fund (ERDF) through the "Programme Research, Innovation and Digitalisation for Smart Transformation (PRIDST)".

Adaptive Portfolio Optimizations Based on Systematic Risk Assessment Using Stochastic Numerical Methods

Gurova S.-M., T. Gurov, A. Karaivanova

This work proposes an adaptive methodology for portfolio optimization, in which the choice of an optimization method is determined by a quantitative assessment of systematic market risk. For this purpose, the dominant eigenvalue of the correlation matrix of returns and its corresponding fraction of the explained variance (Fraction of Variance Explained, FVE) are examined as indicators of the strength of the general market factor and the level of systematic risk.

For a quick, approximate calculation of the largest eigenvalue of the correlation matrix, stochastic numerical methods such as the Almost Optimal Power Monte Carlo (AO PMC) and the Almost Optimal Power Quasi-Monte Carlo (AO PQMC) methods are used. In the described AO PMC algorithm, we use a Mersenne Twister (MT) pseudorandom number generator, whereas in AO PQMC we use a scrambled Sobol sequence. The FVE value serves as a criterion for choosing an appropriate portfolio optimization method. Depending on the values of systematic risk, i.e. FVE, adaptive optimization approaches are used, such as Mean-Variance optimization, Factor models, PCA-based optimization, and others.

Two numerical experiments were performed: (1) with monthly returns of 32 global assets for the period from January 2007 to March 2025, and (2) with monthly returns of 462 companies from the *S&P500* index for the period from 2015 until 2025. The results show that the proposed approach successfully identifies distinct market regimes using FVE and enables adaptive selection of the optimization method based on the current level of systematic risk.

Keywords: AO PMC and AO PQMC algorithms, correlation matrix, largest eigenvalue, system market risk, portfolio optimization

Acknowledgments: The work of the authors (S.-M. Gurova and A. Karaivanova) was supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018-C01, financed by the Research, Innovation and Digitalisation for Smart Transformation Programme 2021-2027 and co-financed by the European Union. The author's work (T. Gurov) was supported by the project "Digitalisation of the Economy in a Big

Data Environment” BG16RFPR002-1.014-0013, funded by the European Regional Development Fund (ERDF) through the ”Programme Research, Innovation and Digitalisation for Smart Transformation (PRIDST)”.

Intelligent Multi-Criteria Decision-Support Framework for Ecological Rehabilitation of the Aralkum Desert under Uncertainty

Khidirova C. M., K. K. Rakhimov, K. R. Nuritdinov

Ecological rehabilitation of the dried Aral Sea bed requires decisions under salinity, moisture deficit, aeolian erosion, sparse vegetation, and uncertain expert assessments. This paper proposes a method for ranking priority parcels for saxaul-based rehabilitation in the Aralkum Desert. The framework combines multimodal geospatial artificial intelligence with interval-valued intuitionistic fuzzy multi-criteria decision making. Sentinel-1 radar, Sentinel-2 optical data, ecological indices, topographic and meteorological variables, and parcel-neighbourhood information are fused by convolutional and transformer-based models. An uncertainty-aware layer estimates the reliability of each ecological indicator. For each parcel and criterion, evidence is represented by an interval-valued intuitionistic fuzzy number. Membership, non-membership, and hesitation represent suitability, unsuitability, and residual uncertainty. Hybrid objective-expert weights and a Choquet-type operator model criterion interactions. The originality lies in propagating predictive reliability into an interaction-aware fuzzy ranking model. Unlike crisp GIS overlays, it represents both hesitation and criterion dependence. A pilot experiment produces stable priorities under ecological, logistical, and uncertainty-averse scenarios, providing an interpretable numerical core for GIS-based rehabilitation planning.

Keywords: Aralkum, uncertainty, interval-valued intuitionistic fuzzy sets, multi-criteria decision making, ecological rehabilitation

Software System for Optimization of Metallic Nanostructures

Mikhov R., V. Myasnichenko, L. Kirilov, N. Sdobnyakov, S. Fidanova

The problem of optimizing the structure of nanoparticles and nanostructured materials is closely related to their stability, especially for nanoclusters containing only a few hundred atoms. This paper presents a software system for numerical optimization of metallic nanostructures using Monte Carlo methods. It implements algorithms previously developed by the authors [1]. The new system architecture is designed for high performance and flexibility, allowing the construction of complex experiment plans combining multiple

Monte Carlo algorithms and systematic variation of their parameters. The software runs on Linux and Windows operating systems, and is compatible with a wide range of existing software packages using the standard XYZ file format for atomic configurations. It has been used for modeling and optimization of various metallic and bimetallic nanostructures from 150 to 16,000 atoms, including nanoparticles, nanowires, nanofilms and nanocages.

Keywords: nanostructures, simulation, software systems, Monte Carlo methods, optimization

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Effects of Macroeconomic Data on Cash Flow Prediction in Consumer Credit Lending

Tomov D. N., A. Atanasov

Accurate cash flow prediction is essential for consumer credit portfolio management, supporting lending decisions, risk assessment, and portfolio optimization. Although macroeconomic information is widely used in credit risk analysis, its incremental contribution to loan-level cash flow prediction remains insufficiently explored. This study evaluates the contribution of macroeconomic variables to predictive cash flow modeling by comparing machine learning models developed with and without macroeconomic information. Four regression approaches of increasing complexity - Linear Regression, Decision Tree Regressor, Random Forest Regressor, and Extreme Gradient Boosting are evaluated using two datasets differing solely in the inclusion of macroeconomic variables. Model performance is assessed through predictive accuracy metrics, graphical analyses, and Cohen's f^2 effect size analysis to quantify the additional predictive value of macroeconomic information. The results demonstrate that incorporating macroeconomic variables improves predictive performance across all evaluated models and applicant cohorts. Nonlinear tree-based methods achieve larger improvements than Linear Regression, with the strongest gains observed for ensemble models. Effect size analysis reveals medium-to-large effects for several models in the Existing Applicant cohort, while improvements for New Applicants are smaller but remain measurable. These findings provide empirical evidence that macroeconomic information enhances consumer credit cash flow prediction, particularly when combined with nonlinear modeling approaches.

Keywords: cash flow prediction, consumer credit lending, macroeconomic variables

An Explainable AI Platform for Solving Circular Intuitionistic Fuzzy Transportation Problems Using the Zero Point Method

Traneva V., S. Tranev, P. Petrov, V. Todorov

Autonomous logistics and intelligent transportation systems increasingly require computational platforms capable of solving transportation optimization problems under uncertainty while providing transparent, reliable, and explainable decision support. Although numerous approaches have been proposed for intuitionistic fuzzy transportation problems, there is currently no integrated software environment supporting Circular Intuitionistic Fuzzy Transportation Problems (C-IFTPs) within a unified Explainable Artificial Intelligence (XAI) framework.

This paper presents an Explainable AI platform for modelling and solving Circular Intuitionistic Fuzzy Transportation Problems using the Circular Intuitionistic Fuzzy Zero Point Method (C-IFZPM). The developed software integrates indexed-matrix representation, Circular Intuitionistic Fuzzy transportation models, automatic data validation, optimization procedures, and explainable decision-support functionalities within a single computational environment. Transportation costs, supplies, and demands are represented by Circular Intuitionistic Fuzzy values, allowing uncertainty to be modelled through membership, non-membership, hesitation, and circular uncertainty.

The computational core of the platform is the Circular Intuitionistic Fuzzy Zero Point Method, which automatically constructs feasible transportation plans under uncertainty. The obtained solution is evaluated through a global Circular Intuitionistic Fuzzy transportation cost based on the proposed AGIO aggregation operator, providing optimistic, realistic, and pessimistic assessments of the transportation plan. The platform additionally generates indexed transportation matrices, graphical visualizations of transportation allocations, computational diagnostics, and publication-ready reports, thereby improving the transparency and interpretability of the optimization process. The originality of the proposed work lies in the integration of Circular Intuitionistic Fuzzy indexed matrices, the Circular Intuitionistic Fuzzy Zero Point Method, the AGIO aggregation framework, and Explainable Artificial Intelligence into a unified intelligent decision-support platform. Unlike existing approaches, the proposed system combines uncertainty modelling, optimization, visualization, and automatic interpretation of computational results within a single software environment.

A case study concerning emergency medical supply distribution from regional warehouses to hospitals demonstrates the applicability of the developed platform. The computational results show that the proposed Circular Intuitionistic Fuzzy Zero Point Method efficiently generates high-quality transportation plans while preserving the complete Circular Intuitionistic Fuzzy information throughout the optimization process. The platform provides an efficient, transparent, and extensible software environment for intelligent transportation planning under uncertainty.

Keywords: Circular intuitionistic fuzzy sets, Transportation problems, Zero Point Method, Explainable Artificial Intelligence, Decision-support systems; Indexed matrices, Intelligent logistics

Acknowledgements: Research was supported by the University-Wide Research Grant No. OUF-RD-15/2025 at BSU “Prof. Dr. Asen Zlatarov”, entitled “Extraction of Expert Knowledge through Innovative Analytical Methods”.

A Temporal Circular Intuitionistic Fuzzy Framework for Robust Robot Capacity Planning in Healthcare Systems

Traneva V., S. Ribagin, S. Tranev

Autonomous healthcare systems increasingly rely on robotic assistants whose required capacity must be determined under dynamically changing and uncertain operating conditions. Variations in patient demand, task duration, service efficiency, and expert assessments introduce uncertainty that reduces the effectiveness of conventional deterministic capacity planning approaches.

This paper proposes a Temporal Circular Intuitionistic Fuzzy (T-CIF) framework for robust robot capacity planning in healthcare systems. The methodology integrates Circular Intuitionistic Fuzzy Sets with temporal index matrices to represent dynamic uncertainty through membership, non-membership, hesitation, and circular uncertainty over successive decision periods. The temporal formulation enables the evolution of healthcare demand and robot workload to be incorporated directly into the capacity planning process.

The main contribution of the proposed framework is the integration of temporal Circular Intuitionistic Fuzzy modelling with computational decision-support techniques for uncertainty-aware robot capacity estimation. The developed numerical procedure generates capacity recommendations under optimistic, balanced, and pessimistic scenarios while preserving the temporal evolution of the healthcare system.

To investigate the stability of the obtained recommendations, a local sensitivity analysis is performed by systematically varying the principal model parameters, including healthcare demand, task duration, and expert evaluations. The influence of these factors on the recommended robot capacity is analysed, enabling the identification of the most uncertainty-sensitive parameters and providing an assessment of the robustness of the proposed planning methodology.

A numerical case study demonstrates the applicability of the proposed framework for determining the required number of autonomous healthcare robots under dynamically changing operational conditions. The results indicate that the Temporal Circular Intuitionistic Fuzzy framework provides reliable, transparent, and computationally efficient decision support while offering greater flexibility than conventional deterministic capacity planning methods.

Keywords: Temporal circular intuitionistic fuzzy sets, Healthcare robotics, Robot capacity planning, Temporal index matrices, Sensitivity analysis, Decision making under uncertainty

Acknowledgements: The research presented in this paper was supported by Project No. BG16RFPR002-1.014-0019-C01, “Establishment and Sustainable Development of a Centre of Competence in Mechatronics and Clean Technologies - MIRACle”.

An Indexed-Matrix Elliptic Intuitionistic Fuzzy Hungarian Algorithm for Assignment Problems under Uncertainty

Traneva V., S. Tranev

Assignment problems constitute a fundamental class of combinatorial optimization problems with numerous applications in logistics, cloud computing, intelligent scheduling, and decision-support systems. In modern artificial intelligence infrastructures, computational tasks must be dynamically assigned to heterogeneous GPU servers under uncertain processing times, resource availability, and expert assessments. Classical assignment algorithms rely on deterministic cost matrices and may therefore produce unreliable solutions in the presence of uncertainty.

This paper proposes an Indexed-Matrix Elliptic Intuitionistic Fuzzy Hungarian Algorithm (EIFHA) for solving assignment problems under uncertainty. The proposed approach extends the classical Hungarian algorithm by incorporating indexed Elliptic Intuitionistic Fuzzy cost matrices represented through Elliptic Intuitionistic Fuzzy Pairs. Each assignment cost simultaneously captures membership, non-membership, hesitation, and directional uncertainty, providing a richer mathematical representation of uncertain optimization information.

The main contribution of the proposed method is the development of an indexed-matrix Elliptic Intuitionistic Fuzzy extension of the Hungarian algorithm while preserving the computational structure and optimality properties of the classical procedure. All algorithmic stages, including row and column reductions, zero selection, assignment construction, and optimality verification, are reformulated within the Elliptic Intuitionistic Fuzzy framework. Consequently, the proposed methodology enables uncertainty-aware optimization without altering the fundamental principles of the Hungarian algorithm.

A numerical case study involving the assignment of artificial intelligence workloads to heterogeneous GPU computing nodes demonstrates the applicability and effectiveness of the proposed approach. The computational results indicate that EIFHA produces reliable assignment solutions while preserving uncertainty information throughout the optimization process. Compared with deterministic methods, the proposed algorithm provides richer decision-support information and improves the modelling of uncertainty in intelligent resource allocation problems.

Keywords: Assignment problems, Hungarian algorithm, Elliptic intuitionistic fuzzy sets, Indexed matrices, Cloud computing, Artificial intelligence

Acknowledgements: The work was supported by the Asen Zlatarov University under project Ref. No. NIH-528 titled "Advanced Intelligent Algorithms for Decision Making under Uncertainty", BSU "Prof. Dr. Asen Zlatarov".

Monte Carlo Stability Analysis for Multi-Agent Decision Making with Intuitionistic Fuzzy Evaluations

Traneva V., S. Tranev, V. Todorov

Decision making in multi-agent systems is frequently based on incomplete, subjective, or uncertain evaluations. Although deterministic ranking methods identify the preferred alternative under nominal conditions, they do not reveal whether this preference remains stable when the evaluations are perturbed. This paper presents an agent-based Monte Carlo framework for analysing the stability of decisions represented by intuitionistic fuzzy evaluations. Membership and non-membership degrees are subjected to bounded uniformly distributed perturbations, while only samples satisfying the intuitionistic fuzzy constraints are retained. For each admissible scenario, the alternatives are ranked using a score function, and empirical selection frequencies are computed at both the individual-agent and collective levels.

The proposed framework is illustrated using five agents, four alternatives, $N = 1000$ Monte Carlo simulation runs, and perturbation levels $\delta = 0.05$, $\delta = 0.10$, and $\delta = 0.15$. As the uncertainty level increases, the collective selection frequency of the nominally preferred alternative d_1 decreases from 0.612 to 0.484, whereas that of its principal competitor d_2 increases from 0.266 to 0.344. For one of the agents, d_2 becomes more frequently selected than d_1 at the highest perturbation level, revealing proximity to a decision boundary that is not apparent from the deterministic ranking alone.

The experimental results demonstrate that scenario-based selection frequencies provide an effective measure for identifying stable preferences, competing alternatives, and uncertainty-sensitive decisions in intuitionistic fuzzy multi-agent environments. Since the results depend on the adopted perturbation distribution, uncertainty magnitude, and constrained sampling procedure, the presented numerical study should be regarded as an illustrative validation of the proposed framework rather than as distribution-independent evidence of decision robustness.

Keywords: Monte Carlo simulation, Intuitionistic fuzzy sets, Multi-agent decision making, Stability analysis, Uncertainty quantification, Decision robustness

Acknowledgements: Research was supported by the University-Wide Research Grant No. OUF-RD-15/2025 at BSU “Prof. Dr. Asen Zlatarov”, entitled “Extraction of Expert Knowledge through Innovative Analytical Methods”.

Migration Patterns in Populations of Myopic Agents under Distance-Dependent Wage Uncertainty

Vassilev A.

This work studies the patterns of migration emerging in populations of economic agents that relocate spatially in search of better remuneration. The model combines myopic individual decision-making with an aggregate conservation-law description of the evolving population density. Agents face uncertainty about the precise wage levels in different locations, which is formalized as a probability distribution over the wage level for a particular location. From the standpoint of an individual agent more distant locations are characterized by distributions with higher variance, reflecting an increase in uncertainty as a function of distance. Agents estimate the spatial profile of wages and migrate towards the location offering the highest estimated wage. Migration decisions are made myopically, i.e. through a sequence of static optimization problems where agents decide on current consumption, saving and job search/relocation effort. This micro-level behaviour induces a velocity field over the space of locations and assets, which in turn determines the evolution of the aggregate population density. The resulting migration patterns are studied numerically under alternative assumptions about the probability distribution representing uncertainty about the wage level and the loss function used to construct wage estimates.

Keywords: migration patterns, myopic agents, wage uncertainty, numerical simulation

SPECIAL SESSION: Numerical Methods for Engineering Innovation: From Digital Twins to Advanced Materials

Once More about the Starting Point in Contour Normalization

Dimov D. T.

The normalization of 2D contours – by translation, scale, rotation and the starting point shift (SPS), etc. is often used in the processing of 2D figures given by the silhouette, most often in binary images (binarized, halftone and/or color, etc.), 2D point clouds, contours of 2D slices of 3D point clouds, slices of 3D surfaces, etc. Interestingly, a starting point is always selected (assigned) in the contour. Its position globally and/or locally (relative to the contour), together with other characteristic normalization parameters, depends on the method of obtaining the contour, for example, when comparing contours, which is a basic processing in contour informatics.

The natural representation of 2D contours as a sequence of points in the complex plane leads to the convenience of direct application of 1D Fourier transforms, i.e. to the so-called Fourier descriptors for contours. Most of the known linear transformations of 2D contours have analogues in the Fourier frequency space, but many operations, e.g. exact comparison of contours, are performed more simply in the object plane than in the frequency (Fourier) one, i.e. when a normalization by the starting point is mandatory.

In [1] we described a basic scheme for normalization of 2D contours. Later, the scheme was cited in [2] for the case of contours of discontinuous (broken) 2D shapes, namely: "It is also possible to define invariant Fourier descriptors that still keep the phase information, as already observed by Dimov and Laskov [1]". The relatively high and uniform citations of [2] (over 45 in total in the years so far) gives us reason to publish our extension – an exact formula for SPS, now.

In the normalization by SPS, our Eq.19 in [1] adds a deviation in the rotation of the contour. However, the deviation can be compensated by successive corrections according to Definition 2 to Eq.19 in [1]. If the deviation is not small enough, an additional normalization by rotation is required, after which – an additional normalization by SPS and so on, several ($\sim 1-3$) iterations, because the procedure is monotonically (and quite quickly) convergent. [1] gives an estimate of the error and the minimum number of iterations to reach the required pair of normalizations, by SPS and by rotation.²

In the present report, we present an exact one-act formula for independent normalization under SPS and prove it by a limit transition to an infinite number of iterations via Eq.19, [1]. The exact formula obtained was kindly provided to the authors of [2] for their purposes in [2] and has remained unpublished until now. In the current report, we further describe our motivation, comparative discussion, and experiments.

keywords: Normalization of 2D Contours, Starting Point Normalization, Fourier Descriptors

²The SPS procedure of [1] is indeed inconvenient, but at the time of submission of the article it seemed an acceptable compromise given the limitations of the publication size.

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UAV Rapid Prototyping Methodology

Georgiev G., D. Zafirov

The rapid development of unmanned aviation systems as dual-use products has necessitated the modernization of their development process in order to accelerate it. The methodology proposed in the article allows this process to be drastically shortened to a few weeks. It is an iterative cycle, including the following stages: Basic requirements and mission definition; Conceptual sizing and design; Generative 3D design; Simulation of digital twins; Computational fluid dynamics; Finite element analysis; Flight dynamics simulation; Rapid prototyping; Testing with hardware in the loop; Tests in a controlled environment to determine the level of technological readiness. The working version of the proposed methodology has been tested in the development of unmanned aviation systems as JoWi 1, JoWi 2, Discovery Copter and VTOL Aircraft. The final form of this methodology will be used in future developments.

keywords: UAS, CFD, AFEA, 3D prototyping, digital twins, simulations, TRL

3D Documentation of Architectural Plans: A Multimodal Approach for the "All Saints" Church in Ochusha, Bulgaria

Georgiev P., G. Evtimov, D. Mihaylova, I. Georgiev

Digitalization of structures has become a standard and the first to be applied in the study of buildings. Most of the tools rely on laser or digital images to create a point cloud and a 3D model. However, it is difficult to have an accurate digital twin of the inside and outside of a structure with only one method. The current study presents a multimodal methodology for the complete digitalization of a building. It combines aerial photogrammetry, terrestrial laser scanning, and 360-degree photography. A geodetic grid is applied to the combined model to scale and position it. The results from the survey are utilized to create an architectural plan with sub-centimetric resolution. The object of study is the "All Saints" church in the village of Ochusha near the town of Kostenets, Bulgaria. It is a typical late-Revival-period Orthodox temple of great significance to the local community [1]. The digital survey and subsequent models have greatly helped in

future conservation and restoration works in the church. It has assured the preservation of the structure for future generations at least as a digital twin.

Keywords: Laser Scanning, UAV Photogrammetry, 360 Photography, Digital Twins, Revival Period

Acknowledgments: The research presented in this paper was done within the CLaDA-BG, the Bulgarian national research infrastructure for resources and technologies for linguistic, cultural and historical heritage, integrated within CLARIN EU and DARIAH EU, funded by the Ministry of Education and Science of the Republic of Bulgaria. (support for the Bulgarian National Roadmap for Research Infrastructure). The authors would also like to thank the Bulgarian National Science Fund for funding the research under the project "An integral approach in creating digital twins of archeological immovable monuments using innovative technologies", Contract KP-06-H82/1 - 06.12.2024. Last but not least, we would like to express our sincere gratitude to Prof. Georgi Tomov for bringing to light this temple from the Revival period and for his staunch support throughout the project.

Asymptotic Behavior of Electrorheological Fluid Flow in Thin Domains with Tresca Friction

Mourad D.

This article investigates the steady flow of an incompressible non-Newtonian fluid in a thin three-dimensional domain. The fluid viscosity is governed by a variable power-law model, while external body forces act throughout the domain. On a portion of the boundary, the wall friction is modeled by the Tresca law. The resulting mathematical formulation leads to a system of nonlinear variational inequalities. The main objective is to analyze the asymptotic behavior of the solution as the thickness of the domain tends to zero. By applying a suitable change of variables, we rigorously derive the corresponding limit problem while preserving the intrinsic nonlinearity of the flow. This asymptotic analysis leads to a generalized Reynolds-type equation describing the effective behavior of the fluid in the thin-film regime.

Keywords: Non-Newtonian fluid, Reynolds equation, Variational formulation, Tresca law.

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Exploring Statistical and Machine Learning Approaches to Photovoltaic Energy Yield Forecasting

Naskinova I., F. Sapundzhi, M. Lazarova, M. Kolev, S. Georgiev, V. Todorov

Forecasts of monthly photovoltaic output inform revenue planning and operational scheduling for small installations, yet the choice of model is often made on how closely a candidate reproduces the data used to estimate it, and the range of approaches examined in any single study tends to be narrow. This exploratory study extends our earlier analysis [1,2] of a grid-connected rooftop plant in South-Western Bulgaria, drawing on an extended record of 151 consecutive months from 2012 to 2024, with total output of 522.8 MWh and the corresponded metered revenue. Rather than advancing a single preferred specification, we survey how a broad set of methods behaves when each is asked to forecast periods it has not seen, using rolling-origin evaluation at horizons of one to four months. The comparison includes seasonal naive and exponential smoothing benchmarks, regularized regression, nearest neighbors, random forests, gradient boosting, Gaussian processes and recurrent networks, assessed for point accuracy and for the calibration of their predictive intervals. We further examine how far four zero-production months, plausibly reflecting metering interruption, and normalization against reanalysis irradiance affect the picture that emerges. Preliminary results suggest that the annual cycle dominates: a non-seasonal specification performs no better than a seasonal naive forecast out-of-sample, while seasonally aware statistical and learning methods reduce the error considerably, with simple exponential smoothing remaining competitive throughout. The analysis is based on a single photovoltaic installation and results should be considered indicative and are offered as a basis for wider testing.

Keywords: photovoltaic energy yield, time series forecasting; machine learning, rolling-origin validation, probabilistic forecasting; performance degradation

Earlier studies extended by this work

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Parametric Finite Element Analysis of Tooth–Cement–Restoration Systems

Raykovska M., N. Nikolova, A. Gusiyska,
I. Georgiev, R. Iankov, M. Datcheva

This study evaluates the mechanical behavior of the tooth–cement–restoration system using finite element analysis (FEA). The investigation encompasses four geometric models (Z1, Z2, Z3, and

Z4), where the primary tooth geometry remains constant while four different inlay/filling geometries are evaluated. An intermediary bonding cement layer is explicitly integrated into each model.

A detailed geometric and corresponding finite element model of the three-component system was developed. A boundary value problem under static loading was defined, applying an identical combination of normal force ($F_n = 600$ N) and tangential force ($F_t = 150$ N) across all cases.

A series of boundary value simulations were performed, taking into account the mechanical material properties (Young's modulus and Poisson's ratio) for dental tissues (Enamel: $E = 84,100$ MPa, $\nu = 0.33$; Dentin: $E = 18,600$ MPa, $\nu = 0.32$), restorative inlay materials (Composite I1, IPS E.max CAD Li-Si I2, Nanoceramic resin I3, and Hybrid-ceramic I4), and bonding cements (Resin-modified glass-ionomer C1: $E = 12,163$ MPa, $\nu = 0.30$; Dual-cure resin C2: $E = 8,300$ MPa, $\nu = 0.24$).

The simulations yielded total deformation fields, equivalent (von Mises) stress distributions, and identified critical peak stress concentration zones within both the restorative materials and the cement layer. Analysis of these results enables a comprehensive evaluation of the biomechanical performance of each configuration to determine the optimal approach for tooth structure restoration.

Keywords: Finite Element Method, stress-strain state, dental inlay, bonding cement, biomechanics, von Mises stress

Acknowledgements: This work was supported by the Bulgarian National Science Fund under Grant No. KP-06-N83/8. The authors gratefully acknowledge the access to the micro-CT equipment and software for CT data analysis provided through Project BG16RFPR002-1.014-0018-C01 "Centre of Excellence in Informatics and ICT" and to the ANSYS software provided through Project BG16RFPR002-1.014-0006 "National Centre of Mechatronics and Clean Technologies", financed by the Science and Education for Smart Growth Operational Program and co-financed by the European Union through the European Structural and Investment funds.

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Numerical Solution of a Nonlinear One-Dimensional Heat-Transfer Model for Thin Metallic Components Produced by Additive Manufacturing

Stoynov M., I. Faragó, S. Filipov

Thermal analysis plays a fundamental role in metal additive manufacturing, where the temperature evolution during the printing process directly influences cooling rates, thermal gradients, residual stresses, microstructure, and ultimately the quality of the manufactured component. Although the physical process is inherently three-dimensional, reduced one-dimensional models provide an efficient and computationally inexpensive alternative for slender metallic components, enabling rapid simulation, parameter studies, and process optimization while preserving the dominant heat-transfer mechanisms. The incorporation of temperature-dependent material properties is particularly important because the large temperature variations occurring during metal deposition lead to strongly nonlinear thermal behavior.

This work considers a nonlinear one-dimensional transient heat-transfer model describing axial heat conduction in a thin metallic component subjected to a prescribed heat flux at one end and distributed convective and radiative heat losses along its lateral surface. The governing equation includes temperature-dependent thermal conductivity, resulting in a nonlinear initial-boundary value problem representative of a broad class of reduced thermal models arising in additive manufacturing.

The proposed numerical solution combines implicit Euler time discretization with a second-order finite difference approximation in space. At each time level, the resulting nonlinear algebraic system is solved by Newton's method, providing a unified framework for treating the nonlinear conductivity and nonlinear surface heat losses. Numerical experiments will investigate the convergence, computational efficiency, and robustness of the method, together with the influence of temperature-dependent thermal conductivity and surface cooling on the predicted temperature evolution. The proposed methodology provides an efficient numerical tool for nonlinear one-dimensional heat-transfer models and contributes to the computational analysis of thermal processes in metal additive manufacturing.

Keywords: Nonlinear heat conduction, finite difference method; Newton's method, implicit Euler method, additive manufacturing

Explicit Analysis of the Interaction Between a Plane Pulse Propagating in a Viscoelastic Matrix and a Rigid Elastic Cylindrical Inclusion

Zhelyazov T.

The contribution presents an analytical procedure aimed at the analysis of the interaction between a plane pulse propagating in a viscoelastic matrix and a scatterer – a rigid (with respect to the matrix) elastic inclusion of cylindrical cross-section. The solution for the plane pulse is constructed from the solution for a harmonic wave in cylindrical representation in terms of potentials. Using the potentials, various quantities of interest, such as stresses or displacements, are calculated. Subsequently, after a Fourier transform and integration over frequencies from minus to plus infinity in the complex plane, the results for a P-pulse are obtained. The above approach is compared with an alternative one that uses a Laplace integral transform. The algorithm accounts for the boundary conditions at the interface between the matrix and the inclusion. Furthermore,

the effect on the rigidity ratio 'matrix rigidity'/'inclusion rigidity' is studied.

Keywords: nonstationary wave process, scatterer, reflected wave

SPECIAL SESSION: Approximation Theory

On The Regularity of Certain Three-Row Almost Hermitian Incidence Matrices

Konstantinova B., G. Nikolov

We prove that certain three-row almost Hermitian incidence matrices are regular, that is, the associated Birkhoff interpolation problem with algebraic polynomials possesses a unique solution. Our proof is based on investigation of certain quadratic forms of specific Jacobi polynomials and their derivatives.

Keywords: Birkhoff interpolation problem, almost Hermitian matrices, Jacobi polynomials, inequalities for real root polynomials.

Analysis of an Algorithm for High Precision Calculation of the Zeta Function

Naidenov N.

We study an algorithm intended for multivalue calculating of $\zeta(z)$ at $\{s + 2k\}_{k=0}^K$ with precision of N decimal digits. The core of the algorithm is an infinite recurrence formula for $\zeta(s)$, see [1] or [2]. This formula is not the fastest converging in its class, but our choice is motivated by the calculation of other special functions, as well as the possibility of deeper analysis.

The algorithm contains a management of the precision, which has to increase with k . We introduce the *precision factors* $\{P_k\}_{k=0}^{n_2}$ representing the increase in accuracy requirements ($P_k = P_k(s, N) \geq 1$ and $n_2 \geq K$ is the number of the last calculated zeta value).

It turns out that, in its basic form, the algorithm still allows a small loss of true decimal digits $L = \lg(|err_0(s, N)|10^N)$. We also consider a modified variant of the algorithm depending on a parameter $q_N \geq 1$, which has to be chosen such that $|err_k(s, N, q_N)| \leq 1/(P_k 10^N)$, $k = 0, \dots, n_2$. We describe the algorithm and the new results of both theoretical and numerical research of the quantities $L = L(s, N)$ and $\bar{q}_N(s, N)$ - the least q_N with the above property.

Keywords: zeta function, recurrence relation, high precision computation

Acknowledgments: The author was supported by the Bulgarian National Research Fund under Contract KP-06-N62/4.

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Quadrature and Cubature Formulae: Monotonicity, Definiteness and a Posteriori Error Estimates

Nikolov G.

The usual way for construction of quadrature formulae makes use of interpolation by algebraic or trigonometric polynomials. Appropriate choice of the interpolation nodes provides quadrature formulae of the highest algebraic/trigonometric degree of precision (Gauss-type quadratures). More generally, Gauss-type quadratures are those that have minimal number of nodes and ensure exact evaluation of a definite integral for integrands from a given finite dimensional space. An alternative to the highest (Gaussian) degree of precision approach is the concept of optimality: quadrature formulae are designed to possess minimal error bound in certain classes of functions. In the Sobolev classes of periodic functions both concepts lead to the same solution: quadrature formulae with equidistant nodes. In the non-periodic Sobolev classes, though the existence and uniqueness of the optimal quadrature formulae are known, the optimal quadratures are unknown in general.

In my talk I will focus on Gauss-type quadratures associated with spaces of spline functions with equispaced knots. Such quadrature formulae are known to be asymptotically optimal in the non-periodic Sobolev classes. Explicit construction of Gauss-type quadrature formulae for spaces of low-degree splines will be given. Properties like monotonicity, definiteness and a posteriori error estimates for integrands from some cones of generalized convex functions will be discussed. These properties will be shown to hold for some modifications of the product trapezoidal cubature formulae.

Keywords: Peano kernel representation, Sobolev classes of functions, spline functions, blending cubature formulae.

Acknowledgements: This research was supported by the Bulgarian National Research Fund under Contract KP-06-N62/4.

Error Estimation of Gaussian Quadrature Formulae for Jacobi Weight Functions and Some of Their Modifications

Pejčev A., D. Jandrlić, M. Spalević, S. Spalević, R. Orive, L. Mihić

For analytic functions in a neighborhood of the real interval $[-1, 1]$, we study the remainder terms of Gauss quadrature rules with respect to Jacobi weight functions $\omega(x) = (1-x)^\alpha(1+x)^\beta$ and some of their modifications, namely

$$\omega_1(x) = \frac{(1-x)^\alpha(1+x)^\beta}{(v-x)}, \quad \omega_2(x) = (v-x)(1-x)^\alpha(1+x)^\beta,$$

where $\alpha, \beta > 1$, $v \in \mathbb{R}$, and $|v| > 1$. Quadrature formulas concerned with these kinds of weight functions have been considered recently by D. Lj. Djukić et al.

Keywords: Gaussian quadratures, polynomials, weight function, kernel, maximum, modulus

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Recent Progress on Smoothest Interpolation

Tenev A., R. Uluchev

In general, the problem on the smoothest interpolation was stated by Allan Pinkus (1988) as follows: given real data $y_0, y_1, \dots, y_{N+1}$ find knots $a \leq x_0 < x_1 < \dots < x_{N+1} \leq b$ and an interpolant f from the Sobolev space $W_p^r[a, b]$ for which both infima are attained:

$$\inf_{a \leq x_0 < x_1 < \dots < x_{N+1} \leq b} \inf_{f \in W_p^r[a, b]} \{ \|f^{(r)}\|_p : f(x_j) = y_j, j = 0, 1, \dots, N+1 \}.$$

In 2018, V. Ivanova and R. Uluchev studied a variant of the above extremal problem for the case $p = 2$ and $r = 3$, involving additional zero boundary conditions on the derivatives. However, the existence part was not completely solved.

Here we fill this gap and provide a result regarding the existence of optimal knots and the smoothest interpolant for this particular case.

A new numerical algorithm for solving the extremal problem in the general case is proposed. Finally, we discuss a few open problems related to the topic.

Keywords: interpolation, splines

SPECIAL SESSION: Monte Carlo and Quasi-Monte Carlo Methods

GPU-Based Optimization of Low-Correlation Point Sequences for High-Dimensional Problems

Atanasov E.

Low-discrepancy sequences are widely used for the numerical estimation of multidimensional integrals, solving integral equations and in other quasi-Monte Carlo simulation algorithms, with applications in physics, chemistry, finance. For high-dimensional problems the theoretical approaches often have limited applicability as there is substantial gap between observed performance of these methods and the worst-case estimates that have been proven. In many cases such out-performance has been attributed to the low effective dimensionality of the underlying problems. That is why we designed a new class of point sequences, which are numerically optimised with the primary objective to obtain uniform 2D projections and low correlations between coordinates. These sequences have a relatively small number of points but a substantial number of dimensions, which is a typical situation in mathematical finance and in other areas where the constructive dimensionality of the problem is high but function evaluations are expensive. In this work we present our methodology, our algorithmic and computational considerations for making the optimisation problem feasible for solving on GPU-enabled high-performance computing systems. We also study the quality of distribution of the obtained sequences as well as their performance on various numerical integration tasks, comparing them with standard Monte Carlo sampling and classical Sobol and Halton sequences.

Keywords: high-performance computing, low-discrepancy sequences

Acknowledgments: The work was partially supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018, financed by the Research, Innovation and Digitalization for Smart Transformation Programme 2021-2027 and co-financed by the European Union. The research that led to these results was carried out using an infrastructure purchased under the National Roadmap for RI, financially coordinated by the MES of the Republic of Bulgaria (grant No D01-98/26.06.2025).

Scrambled Quasi- Monte Carlo Sensitivity Analysis of the UNI-DEM Air Pollution Model

Ostromsky Tz., V. Todorov, M. Lazarova, F. Sapundzhi, V. Traneva

Global sensitivity analysis of large-scale atmospheric models requires the repeated approximation of multidimensional integrals and becomes particularly challenging when first-order, total-order,

or interaction sensitivity indices are very small. In such cases, the corresponding variance contributions may be several orders of magnitude below the total model variance, leading to substantial loss of accuracy for conventional Monte Carlo estimators. This study investigates randomized quasi-Monte Carlo methods for the accurate estimation of variance-based Sobol’ sensitivity indices. The numerical comparison includes conventional random uniform sampling, classical Sobol’ and Halton low-discrepancy sequences, and scrambled variants of both sequences. Their performance is evaluated in terms of the relative errors obtained when estimating the model mean, total variance, first-order indices, total-order indices, and selected second-order interaction effects for increasing sample sizes.

The computational framework is applied to the Unified Danish Eulerian Model (UNI-DEM), a large-scale atmospheric chemistry and transport model. The analysis examines the sensitivity of atmospheric pollutant concentrations to variations in anthropogenic emissions and selected chemical reaction rates. The numerical experiments include both influential parameters and parameters associated with very small sensitivity indices, which are especially difficult to estimate reliably.

The results show that quasi-Monte Carlo methods generally achieve substantially lower relative errors than conventional random sampling. Scrambling further improves the accuracy and robustness of the low-discrepancy sequences for many first-order and total-order indices. At a sample size of approximately 65500, the scrambled methods reduce the relative errors for several sensitivity measures by multiple orders of magnitude compared with conventional Monte Carlo sampling. Scrambled Sobol’ sampling performs particularly well for a broad range of first-order and total-order indices, whereas scrambled Halton sampling provides highly accurate estimates for several small-valued indices. The classical Sobol’ sequence nevertheless remains competitive and produces the most accurate results for some dominant parameters and interaction effects. Thus, no single sequence uniformly dominates for all estimated quantities, and extremely small sensitivity indices remain difficult to approximate at moderate sample sizes. The results also show that no single sequence uniformly dominates for every estimated quantity and that extremely small indices remain difficult to approximate accurately at moderate sample sizes. Nevertheless, scrambling substantially improves the robustness of low-discrepancy sampling for many first-order and total-order indices. Overall, scrambled quasi-Monte Carlo methods provide an efficient and reliable framework for global sensitivity analysis of complex atmospheric chemistry models, particularly when the objective is to identify weak but potentially important parameter effects.

To summarize, the results demonstrate that scrambled quasi-Monte Carlo methods provide an efficient and reliable framework for global sensitivity analysis of complex atmospheric models. Although developed for large-scale atmospheric chemistry simulations, such sensitivity analysis, based on randomized quasi-Monte Carlo techniques have considerably broader applicability. Similar methodologies can be employed in the creation of digital twins of various large natural objects and archaeological monuments to quantify the influence of measurement uncertainties, sensor calibration parameters, point-cloud registration accuracy, and data-fusion strategies on the quality of reconstructed three-dimensional models.

CONTRIBUTED TALKS

Some Applications of Partial Differential Equations in Medical Image Processing

Bazlyankov G., T. Ivanov

One of the key challenges in modern medicine lies in the extraction of data from medical images and its interpretation. We concentrate on magnetic resonance imaging (MRI) with special focus on brain scans of patients with multiple sclerosis [1].

In the wake of many machine learning-based algorithms for medical image processing, we present some more descriptive PDE models which aim to tackle problems such as brain extraction, lesion segmentation, and prediction of the future development of the disease. The novel results include simulations of future lesions in patients with multiple sclerosis based on a model of the cellular dynamics of the disease. We also present the numerical methods used to approximately solve the PDE systems.

Keywords: medical images, multiple sclerosis, partial differential equations, numerical methods

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On a New Gradient Scheme for a Distributed Order Diffusion Wave Equation

Benkhaldoun F., A. Bradji

Dedicated to the memory of Prof. Raytcho Lazarov

We consider a new numerical scheme approximating a distributed order diffusion wave equation. The distributed order operator is defined via an integral of the usual fractional Caputo derivative. We apply the GDM (Gradient Discretization Method) [3], developed recently, to a Distributed Order Diffusion Wave Equation. The distributed order operator of a function u , denoted by $\mathbb{D}_t^\alpha u$, is defined via an integral, over $\alpha \in (1, 2)$, of the usual fractional Caputo derivative of order α , denoted by $\partial_t^\alpha u$, of u multiplied by a weight function. This means that the order of differentiation distributes over the range $(1, 2)$. GDM is a general framework of discretization and analysis of several conforming and non-conforming numerical methods applied to partial differential equations. GDM encompasses, for instance, conforming and non-conforming finite

element and mixed finite element methods and SUSHI [4]. We first establish a new fully discrete scheme in which the discretization in space is performed using GDM whereas the discretization of $\mathbb{D}_t^\alpha u$ is given by an approximation of the integral, over the $(1, 2)$, using the known Mid-Point rule, and the approximation of $\partial_t^\alpha u$, is performed using the known L_1 -formula on the uniform temporal mesh combined with a Crank-Nicolson type method. We prove a new $L_\infty(H^1)$ -error estimate thanks to a well-developed discrete a priori estimate. This work is a continuation of some of our previous works dealt with SUSHI and GDM for time fractional diffusion wave equations with fixed fractional order, and of [1], which dealt with a SUSHI for a distributed order diffusion equation (whose order is belongs to $(0, 1)$).

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Deriving Formulas for Mean Angular Momentum and Kinetic Energy of the Brownian Motion of Particles

Buša J., V. Lisý, J. Tóthová

The chaotic motion a charged Brownian particle in a static external magnetic field is described by the generalized Langevin equations, taking into account memory effects. Using the solutions for displacement and velocity in Laplace space, we obtained analytical formulas for the mean angular momentum and kinetic energy of BP for Ornstein-Uhlenbeck thermal noise.

This report describes the partial fraction decomposition of the solutions Laplace transforms, and the calculation of the corresponding integrals.

Keywords: Brownian particle in magnetic field, Langevin equations, mean angular momentum; mean kinetic energy

Acknowledgments: This work was supported by the Scientific Grant Agency of the Slovak Republic through grant VEGA 1/0197/26. All high precision and analytic Maple calculations were performed using the JINR MLIT Licence Management System.

Post-processing and Evaluation of NEX-GDDP-CMIP6 Precipitation Data for Hydrological Modelling in Bulgaria

Chervenkov H., K. Slavov

High-resolution climate estimations are essential for decision-making and the development of effective adaptation and mitigation policies. Global climate models (GCMs) remain physically consistent tools for quantifying past, present, and future climate, but they often exhibit biases and provide suboptimal resolution. Impact models are widely used to assess the climate change effects, yet they require high-resolution, unbiased input data. Persistent biases can compromise the reliability, necessitating the use of correction methods for post-processing climate model outputs prior to impact studies. The abundance of GCM estimations and downscaling methods complicates the construction of downscaled and bias corrected subsets of GCMs. Bulgaria demonstrates significant climatic and hydrological diversity. This study aims to post-process and evaluate precipitation outputs from 25 GCMs within the NEX-GDDP-CMIP6 project, providing hydrological community with consistent and reliable data. The methodology centers on quantile delta mapping, which is applied within a consistent framework to assess its performance relative to the ERA5-Land reference for 1981–2010. Multiple evaluation metrics are employed, with emphasis on probability density function-based statistics, to propose a practical approach for selecting a representative subset of NEXGDDP- CMIP6 models.

Keywords: Precipitation Data, NEX-GDDP-CMIP6, ERA5-Land, Quantile Delta Mapping, Perkins Skill Score

A Linear Method for Stereo Extrinsic Calibration via a Translation-Free Pairwise-Difference Formulation

Filipov S. M., N. Ilieva, V. Metodiev

We consider the problem of estimating the relative pose between two calibrated cameras from image observations of common targets when the distances from each camera to the targets are also available. Such range information may be obtained independently, for example through positioning systems or auxiliary sensors, and provides additional geometric constraints beyond image measurements alone. In contrast, classical stereo calibration and bundle-adjustment methods typically rely only on image correspondences and lead to nonlinear optimization problems. In this work, we exploit the availability of distance measurements to reformulate the problem in a linear framework. Image observations are first converted into unit bearing vectors and combined

with the known distances to reconstruct the target coordinates in the local reference frames of the two cameras. We then introduce a translation-free pairwise-difference formulation, in which the translation is eliminated by subtracting pairs of target equations. By temporarily treating the entries of the rotation matrix as independent variables, we obtain a linear matrix equation for the rotation, which is solved in the least squares sense. The resulting matrix is subsequently projected onto the rotation group via polar decomposition, and the translation vector is recovered by averaging. The method requires four or more targets. In the absence of noise, the system is consistent and the exact solution is recovered. For noisy data, the formulation yields a well-posed linear least squares problem. Owing to this linear structure, the approach avoids the initialization sensitivity and convergence difficulties commonly encountered in nonlinear optimization-based methods. A series of numerical experiments is proposed to assess accuracy, stability, and conditioning under varying levels of image and range noise, different target configurations, and long-distance scenarios, and to compare the method with bundle adjustment and classical rigid-registration techniques.

Keywords: stereo extrinsic calibration; pose estimation, linear least squares; range measurements, pairwise differences

Extreme Computer Arithmetic with Reals - the Exact and the Permissibly Approximate: A Research of the Extreme

Genoff J.

The simple sad truth that real numerical values in general have infinite range and/or infinite accuracy makes the efforts to represent them and operate on them in the contemporary binary von Neumann computer, which is finite in any aspect, almost a chimera. Various ideas have been in development for decades and each one struggles for the optimal compromise amidst the triangle of: representation size (a.k.a. precision), operations execution time (a.k.a. performance), and numerical accuracy and/or range. These computation methods can be categorized in: true exact ones that give truly exact numeric results, at the cost of an explosive precision growth and performance degradation; and approximate ones that deliver an inexact, but so called verified numeric results, with an opportunity of controlled precision and performance.

This paper presents a thorough research of the exact real arithmetic methods that are distinguished by their well-established and widely adopted in practice software implementations. The aim is to recap the issues amidst the above triad, and to propose a solution to achieve true exact computation results by dynamically selecting the most appropriate specific method of values representation and respective operations. The choice is strictly based on information theoretic considerations that are expressed in a desire to preserve the numbers' precision size. Besides, the study extends to models that are not so much exact, but are widely adopted for the so called "verified" computing: interval arithmetic numbers and ball arithmetic numbers.

Experimental investigation of these solutions is presented, with specific results from long-term tiny-time-step simulations of chaotic systems.

Keywords: exact real arithmetic, approximate real arithmetic

The Product BURA Method for Super-Diffusion

Harizanov S., D. Slavchev, N. Kosturski

The talk is devoted to the application of the product BURA method for solving FDM discretizations of fractional elliptic operators of power $\alpha \in (1, 2)$. Such problems give rise to linear systems of the type $\mathbb{A}^\alpha u = f$, where the matrix $\mathbb{A} \in \mathbb{R}^{n \times n}$ is the finite difference discretization of an elliptic operator $\mathcal{A}$ on a regular grid with step $h = 1/(n+1)$, thus it is symmetric positive definite and sparse. In practice, to control the discretization error in the computations, one needs to consider fine meshes with $h \sim \mathcal{O}(10^{-4})$, where the direct derivation of the exact solution is computationally impossible. Applying the classical BURA method leads to violation of the discrete maximum principle, respectively to meaningless from a physical point of view approximations of $\mathbf{u}$.

The proposed alternative is to apply the product BURA method, where the power α is split into powers $\{\alpha_i\}_{i=1}^l$, such that $\alpha_i \in (0, 1]$, and $\alpha = \sum_{i=1}^l \alpha_i$. Then, sequentially, we apply the BURA method for each α_i . Each application is properly rescaled in order for the smoothest component of $\mathbf{u}$ to be exactly computed. In such a setup, it is theoretically hard to derive a robust error estimation. However, we provide numerical arguments that the order of the value of the relative error $\|\mathbf{u} - \mathbf{u}_{BURA}\|_2 / \|f\|_2$ is unaffected by h , thus one can start with a very coarse grid of $h \sim \mathcal{O}(10^{-1})$, where $\mathbf{u}$ can be explicitly computed and conclude how the expected error will behave on fine meshes. The theoretical aspects of the proposed methodology will be discussed, as well.

Keywords: fractional diffusion, BURA, error analysis

Acknowledgments: The work is supported by the BNSF under grant No. KP-06-N72/2.

Computing Periodic Orbits for the Chaotic Three-Body Problem

Hristov I., R. Hristova

The classical Newtonian three-body problem with zero angular momentum and equal masses is considered. Numerical searches for collisionless periodic orbits for two well-known types of initial conditions – the free-fall and the Eulerian half-twist initial conditions, are conducted. The searches are based on Newton's method, with initial approximations obtained using the grid-search method.

In the chaotic regions of the search domains, we have a strong sensitivity of the solutions to the initial conditions, which is expressed in an exponential deviation of neighboring trajectories. Due to this sensitivity and the inevitable introduction of rounding and truncation errors in the numerical methods, we have an exponential error growth. In this case the standard ODE solvers using double precision floating-point arithmetic generally do not allow accurate solutions to be computed. In order to overcome this problem and to follow the trajectories accurately over long enough time intervals, we use the high-order and high-precision Taylor series method. However, accurate tracking of trajectories is not sufficient for the ultimate success of Newton's method,

because the exponential deviation of neighboring trajectories continues to prevent the obtaining of good initial approximations through the grid-search method. In this report, we show that for Newton's method to be efficient, the symmetries of the periodic orbits associated with the specific initial conditions must be exploited.

Keywords: three-body problem, periodic orbits, Newton's method

Projection of Cold Thermal Sensation for RCP4.5 Scenario over Bulgaria

Ivanov V., G. Gadzhev, I. Georgieva

The hot and cold thermal stress may cause a number of health effects for human beings. The studies for different periods, continents and regions use two basic sources of data - observations and model simulations. Any of them have its own advantages and disadvantages. Our study is focused on Bulgaria, located in the Balkan Peninsula. That region is part of the more broadly one named Mediterranean. Different findings based on different future projections and models, suggest that the Mediterranean would be one of several regions in the world under influence of the relatively high temperature increasing, leading to many consequences as droughts and heat-related diseases. Our focus is on the cold conditions for RCP4.5 scenario in Bulgaria, as that topic is less investigated as a whole. The results are based on model simulations with regional climate model RegCM4. The results show that the cold cases are relatively more than the ones without thermal stress, and generally that difference increases with the topography height. The most notable differences are at night hours.

Keywords: UTCI, RegCM4, RCP, Comfort, Southeastern Europe

Complex Surface Patterning During Heteroepitaxial Nitride Growth: A Continuum Approach to Modelling Vicinal Instabilities

Ivanov V., V. Tonchev

Regular step-flow growth (SFG) on vicinal crystal surfaces allows for precise morphology control during semiconductor device manufacturing. Regular SFG, however, can be disrupted by two main nonlinear instabilities: step bunching and step meandering, where growth loses regularity in the flow-normal and tangential directions, respectively. Many theoretical studies and modelling approaches exist for these instabilities in the homoepitaxial case, but the heteroepitaxial case remains largely unaddressed despite its technological importance for group-III nitride growth. In this study, we propose a new minimal model of step bunching and step meandering in heteroepitaxial systems, based on a nonlinear coupled system of PDEs. To reach realistic system scales, we provide a highly efficient numerical implementation using GPGPU computing for an implicit finite difference scheme, coupled with an efficient GMRES implementation based on automatic differentiation (autodiff).

Further, we investigate the model structure in detail. The model is an L^2 -gradient flow of a Ginzburg-Landau-type energy functional with a Lennard-Jones-type (LJ) interaction potential. We first enumerate and classify all critical points of the LJ potential and hence determine the stability of the corresponding ODE system. Then, further identifying the PDE model as a generalized vectorial Allen-Cahn system, we apply recent developments in slow-manifold theory to prove that meanders are metastable structures, composed of domains corresponding to energetically degenerate global minimizers of the LJ potential connected by thin interfaces moving exponentially slowly. Thus, any further coarsening of the meanders, once formed, is not observable in numerical simulations.

Computational Identification of Several Sources in a Time-Fractional Diffusion Equation

Koleva M., L. G. Vulkov

Many heat and mass transfer processes are described by inverse problems for classical and fractional parabolic equations. We consider a problem of determining several time-dependent sources in a time-fractional diffusion equation from measurements of the solution at interior points. The inverse problem is first reformulated as a loaded time-fractional diffusion equation for the unknown function. To approximate the Caputo time-fractional derivative, we employ the L1 method, which leads to a loaded implicit difference scheme for the approximation of the differential problem. We then propose a parametric representation of the discrete solution, which is obtained by solving an auxiliary linear algebraic system. Numerical results are presented for various choices of the parameters. The computed maximum temporal errors at different times and for several measurement locations demonstrate the efficiency of the proposed approach.

Keywords: time-fractional diffusion, inverse problem, source identification, interior point measurement, finite difference scheme

GPU Accelerated Non-Overlapping BURA Domain Decomposition Preconditioning

Kosturski N., S. Margenov, Y. Vutov

This work studies the performance of a GPU accelerated non-overlapping domain decomposition (DD) preconditioner for finite element method (FEM) discretization of the Poisson equation. The ParMETIS library is used to partition the mesh into sub-domains Ω_i , $i = 1, 2, \dots, p$, with interface γ . For the preconditioning of the obtained linear system, a block factorization of the matrix A is used, where the blocks correspond to the degrees of freedom internal to Ω_i and those on γ . The inverse of the Schur complement, corresponding to the unknowns on γ , is approximated using the best uniform rational approximation (BURA) of order k of $\Lambda^{-1/2}$, where Λ is the discretization of the Laplace-Beltrami operator on the interface γ . The inverses of the blocks

corresponding to the unknowns internal to Ω_i can be computed without any communication, which makes them well suited for GPU acceleration. Numerical experiments are presented to demonstrate the applicability, accuracy, and parallel performance of the proposed GPU accelerated approach.

Keywords: BURA, FEM, Domain Decomposition

Adaptive Schemes for Hyperbolic Systems of Conservation Laws

Kurganov A.

I will present new adaptive schemes for the one- and two-dimensional hyperbolic systems of conservation laws. Our schemes are based on an adaption strategy recently introduced in [1]. We use a smoothness indicator to automatically detect “rough” parts of the computed solution and within the “rough” areas, we detect neighborhoods of linearly degenerate contact discontinuities, in which we employ the second-order finite-volume low-dissipation central-upwind scheme with an overcompressive limiter, which helps to sharply resolve contact discontinuities. In the rest of the “rough” areas, we switch to the dissipative Minmod2 limiter, which is sufficiently sharp to accurately resolve genuinely nonlinear shock waves. Finally, in smooth parts, we replace the limited second-order scheme with a quasi-linear high-order (either fifth, seventh, or ninth order in space and third order in time) finite-difference scheme, recently proposed in [2, 3]. I will demonstrate the advantage of the resulting adaptive schemes on a number of challenging numerical examples for both one- and two-dimensional Euler equations of gas dynamics.

Keywords: adaptive schemes, low-dissipation central-upwind numerical fluxes, smoothness indicators, overcompressive and dissipative limiters, quasi-linear fifth-order finite-difference scheme

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A Multilevel Finite-Basis Physics-Informed Neural Network Method for Two-Dimensional Time-Dependent Single-Temperature Radiation Diffusion Equations

Li X., B. Liu, C. Yan

Two-dimensional single-temperature radiation diffusion equations are challenging due to strong nonlinearity, variable or discontinuous diffusion coefficients, and long-time transient behavior. We introduce a multilevel finite-basis physics-informed neural network (FBPINN) method that combines overlapping domain decomposition, local neural subnetworks, and partition-of-unity window functions to construct a globally smooth mesh-free approximation. A hard-constraint ansatz is used to impose initial and boundary conditions analytically, while a causality-aware time-scheduling strategy improves stability for time-dependent simulations. Numerical experiments show that the proposed method achieves higher accuracy and better robustness than standard PINNs, and captures sharp interfacial features effectively, suggesting that multilevel FBPINNs are a promising scientific machine learning framework for two-dimensional radiation diffusion problems.

Keywords: FBPINN, radiation diffusion equations, neural network, multilevel methods

Maximum Principles for Parabolic Spectral Fractional Diffusion - Reaction Problems

Margenov S., S. Harizanov

The maximum principle is a fundamental qualitative property of partial differential equations, and preserving it at the discrete level is often essential for the reliability of numerical simulations. This talk addresses the analysis and efficient numerical solution of multidimensional fractional diffusion–reaction problems, with particular emphasis on monotonicity and discrete maximum principles. The fractional diffusion operator is defined spectrally with fractional exponent $\alpha \in (0, 1/2)$. Spatial discretization is performed using finite difference and finite element methods with mass lumping. Owing to the nonlocal nature of fractional operators, the resulting matrices A^α are dense, making computational efficiency a key challenge. To address this, we employ best uniform rational approximation (BURA) and uniform rational approximation (URA) to efficiently solve the associated linear systems. We note that, in the finite element setting, the matrix A^α is generally not a Stieltjes matrix, even when the mesh contains no obtuse triangles. Nevertheless, we prove unconditional monotonicity of the elliptic part of the discrete operator, whereas such a property generally does not extend to the time-dependent problem. We also point out a perhaps counterintuitive feature of fractional diffusion: matrix - vector multiplication with A^α may be computationally more expensive than solving linear systems involving A^α .

Keywords: maximum principle; non-negativity preserving; fractional diffusion; rational approximation

A Second Order Operator Splitting Scheme For The Navier-Stokes Equations

Moravski A.

Efficiently solving the Navier-Stokes equations has proven to be immensely important in modern engineering and physics. In recent years, advancements have been made utilising the finite element method to solve the system under complex geometries and to better take advantage of modern hardware. A traditional approach to the equations that lends itself to a FEM implementation is Chorin's method, which is founded upon a split in the differential operator. Our goal in this paper was to advance this idea by adapting a second order split proposed in an earlier work by Codina in the context of the FEM and investigate its accuracy and efficacy. To this end, we developed an implementation in the Mathematica language and ran numerical experiments on the 2D DFG benchmark. Our numerical results demonstrated a marked increase in efficacy between the standard Chorin method and the second order method, due to the latter's more relaxed time step requirements. We also computed a numerical estimate of the order of convergence for the proposed second order method. This estimate fell short of the expected second order, but it was still a significant improvement over Chorin's method. These results serve as a proof of concept for the method and pointers towards directions for further testing and improvement.

Keywords: Navier-Stokes, Finite Element Method, Operator Splitting

Digital Brain Twins Trained via EEGs

Nedelcheva S., G. Rusev, P. Koprinkova-Hristova, N. Bocheva

The paper presents results from training of 3-dimensional spike timing neural network (3D-SNN) models of test subjects brains. For the training aim EEG recordings from the brain surface were collected during performance of a visual perception experiment were collected. The stimuli consist of 1735 randomly oriented Gabor elements positioned on a regular hexagonal grid [1]. Considering that the brain areas have structural connectivity based mainly on the distances between them, in our previous work [1] we investigated the possibility of using EEG recordings to reconstruct the mutual influence of deeper brain areas during conscious visual perception. In current study we use EEG recordings from 30 test subjects to train their digital brain twins. Then we feed into the trained 3D-SNN models the visual stimuli they perceive during experiment and recorded the overall brain regions activity provoked by it. Comparison was made with the recorded real EEG activity.

Keywords: EEG signal, spike timing neural network, STDP rule, visual perception

Acknowledgments: The work is partially supported by the Bulgarian Science Fund under the project "Modelling post-perceptual stages of cognitive processing and conscious representations of visual information" No KP-06-N52/6 from 12.11.2021. All calculations were performed on the

supercomputer HEMUS at the Centre of Excellence in Informatics and ICT, financed by the OP SESG and co-financed by the EU through the ESIF.

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ERP Topography Maps for Brain Analysis

Nedelcheva S., G. Rusev, P. Koprinkova-Hristova, N. Bocheva

The paper presents results from event related potential (ERP) topography analysis of the brain activity obtained from the EEG recordings from the test subjects performing a visual perception experiment. The stimuli consist of 1735 randomly oriented Gabor elements positioned on a regular hexagonal grid [1]. They mimic spiral dot motion. In some of the stimuli the direction of motion remain the same while for the others it changes from clockwise to counter-clockwise and vice versa. The test subject has to discover this change that is considered as the event to be detected by its brain. The topography maps of 30 test subjects were designed using MNE software. They aim to discover mutual correlations between brain surface areas during visual perception of motion as well as of the way visual signal propagates through the brain cortex.

Keywords: EEG signal, ERP, visual perception, brain topography

Acknowledgments: The work is partially supported by the Bulgarian Science Fund under the project "Modelling post-perceptual stages of cognitive processing and conscious representations of visual information" No KP-06-N52/6 from 12.11.2021.

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SCAnet: Structure-Based Prediction of Protein–Protein Binding Free Energies with a 3D Convolutional Neural Network

Petkov P., E. Lilkova, N. Ilieva, L. Litov

Accurate prediction of protein–protein binding free energy remains a major challenge in computational structural biology, particularly when experimental affinity data are limited. Here, we present SCAnet (Scanning Convolutional Affinity Network), a structure-based three-dimensional convolutional neural network designed to provide physically meaningful estimates of absolute binding free energies while maintaining a deliberately simple architecture. Protein complexes are represented on a three-dimensional spatial grid using residue-level physicochemical encoding, and complementary structural features are extracted through parallel max- and average-pooling pathways. The model was developed and optimized using experimentally characterized complexes from the PROXiMATE database. Several architectures were systematically evaluated, including the incorporation of pH as an additional input parameter. The applicability of SCAnet was examined in two SARS-CoV-2-related case studies. First, the network was used to predict the binding free energies of Spike receptor-binding motif variants carrying the N501Y and E484K mutations to the human ACE2 receptor. The predictions were compared with experimental measurements and theoretical estimates and reproduced the main mutation-induced trends in binding affinity despite the substantial variability of the available experimental data. Second, SCAnet was applied to complexes of the viral helicase NSP13 with NSP8-derived peptides and related interaction partners, enabling quantitative comparison of alternative binding modes and helping to identify NSP8-derived fragments with favourable NSP13-binding properties.

These results suggest that a relatively simple structure-based neural network can provide physically meaningful estimates of protein–protein and protein–peptide binding free energies and can serve as a practical tool for comparing molecular interactions in biologically relevant protein systems.

Keywords: protein-protein interactions; binding free energy; CNN; SARS-CoV-2-related case studies

Acknowledgments: This research was partially funded by the Bulgarian National Science Fund under grants KP-06-N72/3/2023 and KP-06-COST-20/2023, and also supported by the Centre of Excellence in Informatics and ICT under the Grant No BG16RFPR002-1.014-0018-C01, financed by the Research, Innovation and Digitalization for Smart Transformation Programme 2021-2027 and co financed by the European Union. We acknowledge stimulating discussions within the COST Action CA21169 “Information, Coding, and Biological Function: The Dynamics of Life (DYNALIFE).

Computational Modeling of Nonlinear Relationships Using Polynomial and Ensemble Methods

Popstoilov M., F. Sapundzhi, M. Lazarova, S. Georgiev

The approximation of nonlinear relationships between computational descriptors and biological activity is one of the key problems in computational biology. In this paper we provide a comparison of several methods that can be used to model the nonlinear relationship between biological activity and two docking-derived descriptors. The comparison includes a third-degree polynomial approximation estimated by the least-square method and four different data-driven regression approaches: k -nearest neighbors, gradient boosting, random forest and highly randomized tree. The hyperparameter optimization is performed using grid search, while the data-driven models are evaluated through ten-fold cross-validation with the sum of squared errors (SSE), coefficient of determination (R2), and root mean squared error (RMSE) metrics. The numerical results show that ensemble methods perform better than k -nearest neighbors and that gradient boosting provides the best results: $R^2 = 0.999$, $RMSE = 0.487$. The obtained results are compared with polynomial response surface to assess the ability of data-driven methods to approximate the complex non-linear dependencies without imposing a fixed global function form. The main contribution is a unified comparison of parametric, neighborhood-based, and ensemble approximation methods according to the same criteria. The proposed approach can be applied to other nonlinear modeling problems involving computational descriptors and experimental observations.

Keywords: computational modeling, nonlinear approximation, numerical regression, ensemble methods, structure-activity relationship

On the Application of Implicit Euler Scheme with Adaptive Time Stepping for a Fractional-in-Space Diffusion Model of RFA Ablation

Slavchev D., S. Margenov

We investigate the application of an adaptive-in-time implicit Euler scheme for Radio Frequency Ablation (RFA) of liver tumors modelled with Fractional Laplace operator. Radio Frequency Ablation is an important type of minimally invasive treatment to solid tumors in kidneys, liver or lungs. Irreversible cellular damage and coagulative necrosis is induced on the tumor cells, while damage to healthy tissues is minimized. We use a model for RFA of hepatic tumors based on a fractional bioheat Pennes equation $\rho c \partial T_0 / \partial t = k_\alpha (-\Delta)^\alpha T_0 + \mathbf{J} \cdot \mathbf{E}$, $\alpha \in (1, 1.5)$ where ρ is density, c – specific heat capacity, T_0 – temperature above $T_b = 37^\circ C$, α – fractional power of the Laplace operator $-\Delta$, $\mathbf{J} \cdot \mathbf{E}$ – Ohmic heating and $k_\alpha = \ell^{2(\alpha-1)}$ is the fractional thermal conductivity in the superdiffusive regime with ℓ being specific length characterizing the capillary network. After discretization with FEM in space and implicit Euler in time the problem is reduced to solving series of dense linear system of algebraic equations. With constant time step τ and m steps the overall computational complexity is $O(N^3) + mO(N^2)$.

In this work we investigate the use of an adaptive explicit-implicit Euler scheme in order to achieve better computational efficiency. The explicit-implicit scheme uses one time step of the explicit Euler method (with computation complexity of $O(N^2)$) to obtain a solution and then based on the estimated error of the explicit solution determines the time step for the implicit method. This allows for solving the problem with fewer time steps. We analyze the solution times and determine the parameters in which the proposed method is efficient.

Keywords: adaptive explicit-implicit Euler, fractional Laplacian, fractional in space Pennes bio-heat equation

Acknowledgments: The work of the authors was supported by the Centre of Excellence in Informatics and ICT under Grant No. BG16RFPR002-1.014-0018-C01, financed by the Research, Innovation, and Digitalization for Smart Transformation Programme 2021–2027 and co-financed by the European Union. The authors also acknowledge support from the Bulgarian National Science Fund under Grant No. KP-06-N72/2.

Gauss-type Quadrature Rules with Fixed Weights Associated with Prescribed Nodes

Tomanović J.

Among interpolatory quadrature rules with m prescribed and n free nodes, the maximum algebraic degree of exactness is $2n - 1 + m$, and it is achieved by the Christoffel quadrature rule. Its construction requires the computation of the n free nodes and all $m + n$ weights. However, if the integrand vanishes at all prescribed nodes, the corresponding m weights need not be computed. In this case, the quadrature rule involves only the n free nodes, while preserving the algebraic degree of exactness $2n - 1 + m$.

In general, the integrand does not vanish at all prescribed nodes. To overcome this limitation, we propose a decomposition of the integrand into two parts. The first part can be integrated exactly and therefore introduces no quadrature error. Moreover, the integral of the first part is represented by a finite sum involving fixed weights associated with the prescribed nodes, eliminating the need to recompute these weights when the number of free nodes changes.

The second part vanishes at all prescribed nodes, enabling the construction of a quadrature rule with only n free nodes that is exact for all polynomials of degree at most $2n - 1 + m$ having the m prescribed nodes as zeros. The resulting quadrature, whose construction is based on the Gauss quadrature rule for a suitably modified weight function, inherits the key properties of Gauss quadrature: all its nodes are pairwise distinct and lie in the interior of the integration interval, all its weights are positive, and the rule converges. The theoretical results are supported by several numerical examples.

Keywords: Gauss quadrature, Christoffel quadrature, prescribed nodes, fixed weights, modified weight function

Semi-Implicit Finite Difference Schemes for Nonlinear Advection-Adsorption PDEs: Robustness Analysis Across Diverse Isotherm Models and Operating Conditions

Zarcheva M., K. Kostova, T. Ivanov

In the present work, we consider the numerical solution of a nonlinear advection–adsorption PDE system. Adsorption is an important physicochemical process with numerous applications. While there are many studies on the subject, most focus on specific operating scenarios, motivating the development of robust numerical methods applicable across a wide range of conditions.

To this end, we consider the problem of a fixed-bed adsorption with a linear driving force model and construct both a semi-implicit first-order upwind scheme and a semi-implicit Lax–Wendroff-type finite difference scheme to approximate the PDE system. We investigate their performance under various operating conditions by computing the corresponding breakthrough curves for a variety of adsorbates with distinct chemical and adsorption properties. Furthermore, we assess the robustness of the schemes across diverse adsorption isotherm models and perform a sensitivity analysis on key model parameters, including porosity, density, filter dimensions, and fluid velocity. We validate the numerical results by estimating the convergence order using the Runge–Richardson method with three nested meshes. Finally, we compare the numerical solutions with experimental breakthrough data available in the literature to confirm the accuracy of the proposed methods.

Keywords: Advection, Adsorption, Nonlinear PDEs, Finite Difference Methods

Part C

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