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ABSTRACTS

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Abstracts[1]

[1] Arranged alphabetically according to the family name of the first author.

SUSHI for a Bingham Flow Model

Aboussi W., F. Benkhaldoun, A. Bradji

The main aim is to design a finite volume scheme for the following simple model of Bingham flow in cylinders

$$\rho u_t(x,t) - \mu\Delta u(x,t) - g\nabla\cdot\left(\frac{\nabla u}{|\nabla u|}\right)(x,t) = G(x,t), \quad (x,t)\in\Omega\times(0,T), \tag{1}$$

with initial and Dirichlet boundary conditions:

$$u(x,0) = u^0(x), \quad x\in\Omega \quad \text{and} \quad u(x,t) = 0, \quad (x,t)\in\partial\Omega\times(0,T). \tag{2}$$

As we can see that there is no sense to the previous equation when $\nabla u = 0$. A regularization problem can be given by

$$\rho\partial_t u_\varepsilon(x,t) - \mu\Delta u_\varepsilon(x,t) - g\nabla\cdot\left(\frac{\nabla u}{\sqrt{\varepsilon^2+|\nabla u|^2}}\right)(x,t) = C, \quad (x,t)\in\Omega\times(0,T) \tag{3}$$

where

$$u_\varepsilon(x,0) = u^0(x), \quad x\in\Omega \quad \text{and} \quad u_\varepsilon(x,t) = 0, \quad (x,t)\in\partial\Omega\times(0,T). \tag{4}$$

It is proved that the problem (1)–(2) can be written in the following variational inequation formulation: $u(t)\in H_0^1(\Omega)$, for *a.e.* $t\in(0,1)$, for all $v\in H_0^1(\Omega)$:

$$\rho\int_\Omega \partial_t u(x,t)(v(x)-u(x,t))dx + \mu\int_\Omega \nabla u(x,t)(\nabla v(x)-\nabla u(x,t))dx + g(j(v)-j(u)) \geq C\int_\Omega (v(x)-u(x,t))dx \tag{5}$$

with

$$u(0) = u^0 \quad \text{and} \quad j(v) = \int_\Omega |\nabla v|(x)dx. \tag{6}$$

In addition to this, the following error estimate, between the solution u_ε of (3)–(4) and the solution u of (5)–(6), holds

$$\|u_\varepsilon(t) - u_\varepsilon(t)\|_{L^2(\Omega)} \leq \sqrt{\frac{gm(\Omega)}{\mu\lambda_0}}\left(1-\exp\left(-\frac{2\mu\lambda_0}{\rho}t\right)\right)^{\frac{1}{2}}\sqrt{\varepsilon}. \tag{7}$$

To study the model (3)–(4) "rigorously" , we write it under the following general version of quasilinear parabolic equation, for $(x,t)\in\Omega\times(0,T)$

$$u_t(x,t) - \alpha\Delta u(x,t) - \nabla\cdot F(x,t,u(x,t),\nabla u(x,t)) = G(x,t,u(x,t),\nabla u(x,t)) \tag{8}$$

where Ω is an open bounded polyhedral subset in $\mathbb{R}^d$, with $d \in \mathbb{N}^\star = \mathbb{N} \setminus \{0\}$, $T > 0$, and

$$F(x,t,s,\theta) = \frac{g}{\rho\sqrt{\varepsilon^2 + |\theta|^2}}\theta,$$

We present an implicit finite volume scheme, using SUSHI (Scheme Using Stabilization and Hybrid Interfaces) for the gneralized equation (9) with initial and Dirichlet boundary conditions (2) and study its convergence.

Two–Stage Algorithm For Solving Vehicle Routing Problem with Time Windows

Alihodzic A., E. Tuba, M. Tuba

Many distribution problems in real-world applications can be expressed as vehicle routing problems with time windows (VRPTW). At these problems, it is well-known that determining the optimal number of vehicles and seeking the shortest distances produced with them present an NP-hard problem. The main objective of VRPTW is to minimize fleet size and assign a sequence of customers to each fleet truck, minimizing the overall distance such that all customers are served and the actual demand by each truck does not exceed its capacity. To address this problem, the efficient two-stage approach has been applied. In the first stage, our approach divides the fleet of customers into smaller clusters by using the K-means algorithm. In the second phase, the famous state-of-the-art CPLEX solver was applied to each cluster to find the shortest routes between customers and the smallest number of vehicles serving them. Also, in this phase, the size of obtained clusters is updated to assist the CPLEX solver in achieving the best performance. According to the results presented in the experimental analysis, it can be concluded that our approach can get sub-optimal solutions in real-time, which are very close to optimal ones.

Topological Dynamic Consistency of Numerical Methods for Dynamical Models in Biosciences

Anguelov R.

Qualitative analysis of dynamical systems modelling biological processes makes a valuable contribution to understanding these processes and elucidating relevant properties. These include, invariant sets (including equilibria) and their stability properties, existence of bifurcation thresholds, shape of trajectories, etc. Due to the high level of complexity of the biological system, the models often involve large number of parameters with unknown or only estimated values. In such setting, qualitative analysis tend to be more important

then high precision computations. Hence, the importance of numerical methods which accurately replicate the properties of the model. There are several attempts to capture in concepts like qualitative stability, dynamic consistency, structural stability under numerics. In this talk we present the concept of topological dynamic consistency of numerical methods which aligns the model and the method in such a way that all properties of the model which are of topological nature, like the mentioned above, are replicated. Further, we present some practical approaches of designing such methods. Let us remark that topological dynamic consistency cannot be derived through the standard tools of numerical analysis based on consistency, stability, order of approximation and convergence. The theory discussed in the talk is based on the structural stability of flows and maps.

Numerical Parameter Estimation in a Multiple Factor Model for Population Dynamics of Bee Colony

Atanasov A.Z., S.G. Georgiev, L.G. Vulkov

In the recent decades, the number of honeybee colonies suffers a steady decrease. This ubiquitous phenomenon is a worldwide and major problem. Honeybees not only produce honey and its derivative products, but also pollinate many kinds of plants. Actually, they are the main known pollinator on Earth. Thus, the decline in the number of colonies puts the ecological balance at severe risk. There are many attempts to stop and prevent the massive colony losses, which are known as Colony Collapse Disorder. Among the most powerful tools is the mathematical modelling. In this paper, we adopt a simple but robust model (W. Hong et al, 2022) which explains the population dynamics in a typical colony. Based on the system equalization principle, the authors seek the equilibrium points which describe a prolific development of the apiary. What is more, they outline the larval food consumption rate and the larval birth coefficient as the most sensitive and important parameters in the model. At the same time, they cannot be measured directly. In this study we propose a solution to the inverse problem of reconstructing the larval dynamics coefficients via discrete measurements of the level of food stores in the colony, which are feasibly observable in practice. Such an approach could help the professional beekeepers to diagnose and treat healthy problems of their apiaries.

Parameter Estimation Inspired by Temperature Measurements for a Chemotactic Model of Honeybee Thermoregulation

Atanasov A.Z., M.N. Koleva, L.G. Vulkov

Based on Keller-Segel model (R. Bastaansen et al., SIAM J. Appl. Math., 2020) and motivated from the laboratory experiments by temperature sensors embedded in the hive,

our effort is to develop a parameter estimation methodology for the thermoregulation process. The model is in the form of coupled reaction-diffusion-transport equations for the bee density $\rho \geq 0$ and the local temperature T. The first equation is the heat equation for T with reaction term $f(T)\rho$. Using real measured data, we first deal with reaction coefficient inverse problem (IP1) to reconstruct the density. Also, we solve the inverse problem (IP2) for simultaneous reconstruction of the bee density and initial temperature. Next, we solve numerically the strongly nonlinear convection-diffusion equation to recover again the density ρ. Our main goal, using the results of IP1 and IP2, is to study third inverse problem (IP3), based on the linearized convection-diffusion equation for estimation of three important parameters, that are difficult for observation.
Calibration algorithms are derived, based on minimization of least-square functionals. Their robustness and accuracy are tested against noisy synthetic data and available real data.

Richardson Extrapolation and Its Variants

Bayleyegn T., I. Faragó, Á. Havasi, Z. Zlatev

Richardson extrapolation is a sequence acceleration method, which has long been used to enhance the accuracy of time integration methods for solving differential equations. Its classical version is based on a suitable linear combination of numerical solutions obtained by the same numerical method with two different discretization parameters. We present the principle of Richardson extrapolation, and introduce two possible generalizations of this method called repeated Richardson extrapolation (RRE) and multiple Richardson extrapolation (MRE). We investigate how the application of these schemes changes the absolute stability regions of certain underlying numerical methods, including explicit and implicit Runge-Kutta methods, an issue that is important when stiff systems of ordinary differential equations are to be solved numerically. The convergence of the new methods obtained by combinig certain Runge-Kutta methods with these generalized Richardson extrapolation procedures are also analysed and illustrated with numerical experiments.

Cnvergence Analysis of a Finite Volume Scheme for a Distributed Order Diffusion Equation

Benkhaldoun F., A. Bradji

In this work, we are interested with the following type of fractional order diffusion equations (called distributed order diffusion equations):

$$D_t^{\omega} u(x,t) - \Delta u(x,t) = f(x,t), \qquad (x,t) \in \Omega \times (0,T), \tag{9}$$

where Ω is an open bounded connected subset of $\mathbb{R}^d$ ($d \in \mathbb{N}^\star$), $T > 0$, and f is a given function. Here D_t^ω is the distributed order diffusion operator

$$D_t^\omega u(t) = \int_0^1 \omega(\alpha) \partial_t^\alpha u(t) d\alpha, \tag{10}$$

where ∂_t^α is the Caputo derivative defined by:

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u_s(s) ds \tag{11}$$

and ω is a given function defined on $(0,1)$ and satisfying the following three assumptions:

- ω is assumed to be at least continuous, for the sake of simplicity.
- $\omega(\alpha) \geq 0$.
- $\int_0^1 \omega(\alpha) d\alpha = c_0 > 0$.

Initial condition is given by:

$$u(x,0) = u^0(x), \qquad x \in \Omega, \tag{12}$$

where u^0 is a given function defined on Ω.
For the sake of simplicity, we consider the homogeneous Dirichlet boundary conditions:

$$u(x,t) = 0, \qquad (x,t) \in \partial\Omega \times (0,T). \tag{13}$$

This work is an extension of some of our previous works which dealt with finite volume methods for time fractional diffusion equations in which the fractional Caputo derivatives are only given by (11).
We first design an implicit finite volume scheme for (9)–(13) and then prove its well-posedness and convergence.

SUSHI for a Time Fractional Diffusion Equation with Delay

Benkhaldoun F., A. Bradji

SUSHI (Scheme Using Stabilization and Hybrid Interfaces) is a finite volume method developed at the first time to approximate heterogeneous and anisotropic diffusion problems. It has been applied later to approximate several types of partial differential equations. One of the main features of SUSHI is that a consistent and stable Discrete Gradient is developed on general finite volume meshes in which the control volumes can only be assumed to be polyhedral (the boundary of each control volume is a finite union of subsets of hyperplanes).

In this work, we are interested with SUSHI applied to Time Fractional Diffusion Equations with a Delay. We establish a SUSHI scheme along with a convergence analysis.

Optimal Learning of Solutions of PDEs

Binev P., A. Bonito, R. DeVore, G. Petrova

This paper studies the problem of learning an unknown function f from given data about f. The learning problem is to give an approximation $\hat{f}$ to f that predicts the values of f away from the data. There are numerous settings for this learning problem depending on (i) what additional information we have about f (known as a model class assumption), (ii) how we measure the accuracy of how well $\hat{f}$ predicts f, (iii) what is known about the data and data sites, (iv) whether the data observations are polluted by noise. Although the settings for the results are very general, the featured model assumption is that f is a solution of a (parametric) PDE and belongs to a compact manifold of the possible solutions or to a unit ball of a Banach space that contains this manifold.
A mathematical description of the optimal performance possible (the smallest possible error of recovery) is known in the presence of a model class assumption. Under standard model class assumptions, it is shown in this paper that a near optimal $\hat{f}$ can be found by solving a certain discrete over-parameterized optimization problem with a penalty term. Here, near optimal means that the error is bounded by a fixed constant times the optimal error. This explains the advantage of over-parameterization which is commonly used in modern machine learning. The main results of this paper prove that over-parameterized learning with an appropriate loss function gives a near optimal approximation $\hat{f}$ of the function f from which the data is collected. Quantitative bounds are given for how much over-parameterization needs to be employed and how the penalization needs to be scaled in order to guarantee a near optimal recovery of f. An extension of these results to the case where the data is polluted by additive deterministic noise is also given.

On the Numerical Simulation of Epidemiological Outbreak Data Involving Uncertainties in the Rate Parameters

Borisov M., S. Markov

Statistical data collected from observing epidemiological outbreaks of various diseases often have specific wave-like forms, thereby the data themselves contain statistical errors. A number of epidemiological mathematical models formulated in terms of ODEs (or reaction networks) offer solutions that have the potential to simulate well the observed wave-like statistical data. These solutions are usually smooth functions of time presented as mathematical (algebraic) expressions involving so-called rate parameters. We briefly denote such expressions outbreak functions and consider these functions as functions of two variables: time and rate. Moreover, we assume that the rate variable may accept interval values, so that the outbreak functions turn into so-called interval functions. Our idea in this

work is to numerically simulate epidemiological outbreak data with statistical uncertainties using interval outbreak functions. To offer a precise definition of the term numerical simulation in such a setting, we begin with basic outbreak functions generated by simple epidemiological models such as the SI and SIR models (reaction networks). The latter models generate exponential solutions, so the total mathematical problem mostly relies on exponential regression using interval input data.

Analysis of Effective Properties of Poroelastic Composites with Surface Effects Depending on Boundary Conditions in Homogenization Problems

Chebakov M.I., M. Datcheva, A.V. Nasedkin, A.A. Nasedkina

The paper considers the homogenization problems for two-component poroelastic composites with a random structure of nanosized inclusions. The nanoscale nature of the inclusions was taken into account according to the generalized Gurtin-Murdoch theory by specifying surface elastic and porous stresses at the interface boundaries, the scale factor of which was related to the size of the inclusions.

The formulation of homogenization problems was based on the theory of effective moduli, considering Hill's energy relations. The problems of static poroelasticity were solved in accordance with the Biot and filtration models. A feature of this investigation was the comparison of solutions of four types of homogenization problems with different boundary conditions. Namely, linear essential boundary conditions for displacements or constant natural boundary conditions for stress vectors were taken as mechanical boundary conditions. Similarly, linear boundary conditions for the pore pressure or constant boundary conditions for the normal components of the filtration rate were taken as pore conditions. Combinations of one of the two mechanical and pore boundary conditions yielded four types of homogenization problems.

Modeling of representative volumes and solving problems of determining the effective material moduli were carried out in the ANSYS finite element package. Representative volumes were built in the form of a cubic grid of hexahedral finite elements with poroelastic properties of materials of one of the two phases and with a random arrangement of elements of the second phase. To take into account interface effects, the interfaces were covered with shell elements with options for membrane stresses. When solving problems of poroelasticity, the well-known porothermoelastic analogy between the problems of poroelasticity and thermoelasticity was used, which allows solving problems of poroelasticity as the corresponding problems of thermoelasticity with elastic and thermal properties. After solving the thermoelastic problems, the averaged stresses and heat fluxes were calculated for bulk and shell thermoelastic finite elements. Finally, the effective properties were determined by the corresponding formulas of the homogenization method and the inverse transition to poroelastic problems.

The results of computational experiments made it possible to study the effective moduli depending on the boundary conditions, on the percentage of inclusions, their characteristic nanosizes, and areas of interface boundaries.

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Numerical Solution of Systems Involving Fractional Powers of SPD Matrices Based on Vabishchevich Approach

Duan B., R. Lazarov, J. Pasciak

We develop and study an algorithm for approximately solving the linear algebraic system $\mathcal{A}_h^\alpha u_h = f_h$, $0 < \alpha < 1$, where $u_h, f_h \in \mathcal{R}^d$. The finite dimensional operator $\mathcal{A}_h$ (represented by a matrix) is symmetric and positive definite and is obtained from an approximation scheme for a second order elliptic problems, e.g., finite element/difference scheme or spectral or spectral element methods. We assume that the corresponding mass and stiffness matrices are sparse and the linear system $(\mathcal{A}_h + c)u_h = f_h$, can be solved efficiently for any $c \geq 0$. Due to P. Vabishchevich, the solution of this problem is reduced to the solution of an initial value problem of a certain pseudo-parabolic operator equation. We propose a stable and exponentially convergent time stepping scheme based on Padé approximation of the pseudo-parabolic problem. The rigorous analysis shows that the asymptotic cost of the proposed scheme is solving $\mathcal{O}(\log_2 d)$ sparse systems. The presented numerical tests demonstrate the efficiency of the proposed scheme and confirm the theoretical findings.

Ant Algorithm for GPS Surveying Problem with Fuzzy Pheromone Updating

Fidanova S., K. Atanassov

GPS system has important part of our life. We use it everyday for navi- gation, but it has other important use too. The GPS navigation is used by vessels, aircraft and vehicles for safety passage. Other use is geodetic survey. GPS gives more precise coordinates comparing with traditional methods. Scientific use of GPS includes measurement of crystal deformation, moni- toring of earthquake processes, volcano eruption process, ruffing, mountain building. These applications needs very precise measurement. GPS satellites transmit signals to Earth. A receive on the Earth detect them and convert to useful measurement. Thus the location of the receiver can be computed. The GPS surveying problem search for the best order of the sessions. It is difficult optimization problem which needs huge amount of computational resources, therefore is impractical to apply traditional numer-

ical methods. On this problem we apply Ant Colony Optimization (ACO) algorithm, which is a methaheuristic method. We propose ACO with two variants intuitionistic fuzzy pheromone updating. The proposed algorithm is tested on 8 test problems with dimension from 38 to 432 sessions. The variants of our algorithm is compared with traditional ACO algorithm. GPS surveying is ordered problem. The order of the session in the solution is important. The similar fuzzy pheromone updating we apply on Multidimensional Knapsack Problem (MKP). MKP is unordered problem. The order of the elements of the solution is not important. We compared differences of algorithm performance and quality of achieved solution, when the idea for fuzzy pheromone is applied on so different class of problems.

Mathematical Modelling of Nonlinear Heat Conduction with Relaxing Boundary Conditions

Filipov S.M., I. Faragó, A. Avdzhieva

This paper considers one dimensional unsteady heat condition in a media with temperature dependent thermal conductivity. When the thermal conductivity depends on the temperature, the corresponding heat conduction equation is nonlinear. The equation is considered on a finite space interval. At one or both boundaries a relaxing boundary condition is applied. The relaxing boundary condition is a time dependent condition that approaches continuously, as time increases, a certain time independent condition. Such behavior at the boundaries arises naturally in some physical systems. As an example, we provide a simple physical model that can give rise to either Dirichlet or convective relaxing boundary condition. Due to the dependence of the thermal conductivity on the temperature, the convective condition is nonlinear. For the solution of the heat equation, we propose a new numerical approach whereby, contrary to the traditional approach, the equation is first discretized in time. We use implicit time discretization, which provides for unconditional stability of the method, unlike the explicit time discretization whereby the method is only conditionally stable. The arising sequence of ordinary differential equations, together with the boundary conditions, constitutes a sequence of nonlinear two-point boundary value problems (TPBVPs). If an initial condition is given, we can solve the first nonlinear TPBVP and get an approximation of the temperature at the first time level. Using the obtained solution, we can solve the next TPBVP and get an approximation of the temperature at the next time and so on. For the solution of the nonlinear TPBVPs, we apply the finite difference method. The nonlinear algebraic systems arising from the finite difference discretization are solved numerically using the Newton's iterative method. A number of example problems are solved demonstrating the efficiency of the proposed method.

Covering a Set of Points with a Minimum Number of Equal Circles via Simulated Annealing

Filipov S.M., F.N. Tomova

This work considers the following problem. Given n points in the plane, what is the minimum number of circles of radius r needed to cover all n points? A point is covered if it lies inside at least one circle. Covering all points with minimum number of circles can be viewed as a constrained optimization problem. Indeed, the number of circles needs to be minimized under the constraint that all points are covered. In this form the problem is hard to tackle since one cannot use the great number of powerful unconstrained optimization techniques available. This work proposes a way of converting the original problem to an unconstrained optimization problem by introducing an objective function, called energy, in such a way that if a configuration of circles minimizes the energy, then it necessarily covers all points and does this with a minimum number of circles. Thus, the original problem is reduced to finding a configuration of circles that minimizes the energy. To solve this problem, we propose a variant of the simulated annealing technique. Starting at some high temperature, the following Monte Carlo simulation is performed. Consecutive attempts are made to move a randomly chosen circle to a randomly chosen position. At each several attempts to move a circle, an attempt to either remove a randomly chosen circle or add a circle to a random position is made. The moves are accepted or rejected according to the standard rule of acceptance in simulated annealing. After a certain number of attempts the temperature is reduced according to some cooling schedule and the procedure is repeated until the temperature has become low enough. The slower the cooling of the system and the lower the final temperature is, the higher the probability that the final configuration of circles reached by the simulation is a configuration with minimum energy. The proposed Monte Carlo simulation is tested on several systems demonstrating the suitability of the method for finding configurations with minimum energy, hence solving the original problem of covering all n points with a minimum number of circles.

Random Sequences in Vehicle Routing Problem

Gülşen M.E., O. Yayla

The purpose of this study is to both combine a clustering approach with Monte Carlo Simulation method for solving the Capacitated Vehicle Routing Problem (CVRP) and to compare the performance effects of the random number generators on Monte Carlo Simulation. Firstly, to investigate the clustering technique, combination of two heuristic methods – Nearest Neighbor Insertion (NNI) and Clarke and Wright's Savings (CWS) – has been merged with a clustering step made with of random projection based clustering. Random projection trees used mostly to reduce the dimensionality on big data applications.

We have tried to employ this approach for gathering sub problems from CVRP instances and combine the results of the sub problems to present a solution. Two types of experiments conducted in order to understand first if the clustering approach is useful for solving CVRP instances and second is to compare the effects of random number generators on Monte Carlo Simulations for solving CVRP instances. For the first part, the experiments made on five different types of CVRP instance sets for the purpose of avoiding dependence between instance sets and the method. For the second part, the experiments prepared based on the random number generator types and their variants on three different instance sets and on twenty different instances. The random number generators used in this study gathered from on respect to two perspective, our first aim was to compare the mostly known and used RNGs on simulation based studies which are Linear Congruential Generator (LCG) and its shift variant, Multiple Recursive Generator (MRG) and its shift variant and the others chosen concerning the improvements in the random number generator algorithms which are Mersenne Twister Pseudo Random Generator (MT) and Permuted Congruential Generator (PCG). The results of experiments suggested the random projection clustering combination with NNI and CWS algorithms can increase the cost performance of the algorithms and the second part of the experiments had showed that the PCG and MT pseudo random generators can generate better results than the other random number generators.

Three-Dimensional Supervised Image Processing

Harizanov S., I. Georgiev

In this talk we present an efficient numerical algorithm for segmentation and feature extraction of high-resolution images. Our main practical motivation is generation of volume 3D models through micro-CT and their postprocessing. The algorithm is based on Graph-Laplacian 2-phase segmentation via discrete volume-constrained quadratic optimization. Its computational efficiency relies on a reformulation of the cost function via applying a convenient change of basis in $\mathbb{R}^n$, for which the cost function is almost fully split element-wise. Furthermore, we perform implicit computation of the action of the dense M-matrix $Q^{-1/2}$ on $\mathbb{R}^n$, based on (k, k) best uniform rational approximation (BURA) of $\sqrt{t}$, $t \in [0, 1]$. The approximate solution inherits most of the important properties of the exact solution, in particular non-negativity, while tightly controlling the ℓ_2 relative error. The conducted numerical experiments confirm both the reliability and the efficiency of the proposed machinery. In addition, the proposed reformulation allows for cheap inclusion of additional linear terms in the functional, which can be interpreted as a "hybrid" segmentation process with data fidelity term based on the outputs of more than one classical segmentation algorithms.

The reported results are partially supported by the Bulgarian National Science Fund under grant BNSF-DN11/9 from 15.12.2017.

A Database of High Precision Trivial Choreographies for the Planar Three-Body Problem

Hristov I., R. Hristova, I. Puzynin, T. Puzynina, Z. Sharipov, Z. Tukhliev

A choreography is a periodic orbit in which the three bodies move along one and the same trajectory with a time delay of $T/3$, where T is the period of the solution. A choreography is called trivial if it is a topological power of the famous figure-eight orbit. In this work we use a modified Newton's method based on the Continuous analog of Newton's method and high precision arithmetic for a specialized numerical search for new trivial choreographies. As a result of the search we computed a high precision database of such orbits. All found solutions are given with 150 correct decimal digits.

Evaluation of the Effective Material Properties of Media with Voids Based on Numerical Homogenization and Microstructure Testing Data

Iankov R., I. Georgiev, E. Kolosiva, M. Chebakov, M. Datcheva

This work is devoted to a 3D hybrid numerical-experimental homogenization strategy for determination of elastic characteristics of materials with closed voids. The performed homogenization procedure employs micro-computed tomography (uCT) and instrumented indentation testing data (IIT). Based on the uCT data a 3D geometrical model of a cubic representative elementary volume (RVE) is created assuming periodic microstructure of the material with closed voids. Creating the RVE respects the following principle of equivalence: the porosity assigned to the RVE is the same as the porosity calculated based on the uCT images. Next, this geometrical model is used to generate the respective finite element model where, for simplicity, the voids are considered to have a spherical form. The numerical homogenization technique includes proper periodic boundary conditions with unit force applied in normal and shear directions. The employed constitutive model for the solid phase is the linear elastic model whose parameters are determined based on IIT data. It is performed a validation and verification study using simplified geometries for the RVE and under different assumptions for modelling the voids.

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Numerical Analysis of Contact Interaction of Parabolic Stamp with Poroelastic Functionally Graded Layer Taking into Account Surface Stresses

Iankov R., A.V. Nasedkin, A.A. Nasedkina

In this paper, we consider the problem of the contact of a non-deformable parabolic indenter with a poroelastic layer with material properties that are functionally gradient in thickness. For the poroelastic material of the layer, the Biot model was adopted, and the surface stresses were taken into account according to the Gurtin-Murdoch theory with a scale factor related to the size of the contact zone.

The formulated problems were solved numerically in the ANSYS finite element package for further comparison of the results with experimental data on the indentation of poroelastic materials. Special user programs were developed in the APDL ANSYS macro language, which allow solving the problems under consideration with various input geometric and physical data.

For the convenience of using surface elements with suitable properties in ANSYS, a porothermoelastic analogy was used, taking into account which, instead of problems of poroelasticity, the corresponding thermoelastic problems with planar and surface elements were solved. According to the methodology for solving contact problems, when constructing a mesh of finite elements, the partition was thickened near the contact zone. To ensure the stability of numerical calculations for a nanoscale contact, a transition to a dimensionless formulation was preliminarily carried out. Further, to consider surface stresses, shell elements with membrane stress options were additionally determined on the layer surface. Based on the constructed finite element models, as a result of the numerical solution of contact problems for various functional laws of change in the material properties of the layer and surface moduli, contact stress distributions, contact area sizes, stress intensities and pore pressure were analyzed.

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Finite Element Analysis of Wave Propagation in Viscoelastic Media

Ivanov R., S. Pshenichnov, M. Datcheva

The methodology for explicit wave propagation analysis in viscoelastic media by the commercial software package ABAQUS is described. For the material model, the relation between kernel parameters in dimensionless time used in theoretical solutions, and the Prony series expansion used in the numerical simulation of viscoelasticity in the time domain is explained. Two models were developed: (a) a single layer fixed at its base and having infinite length in the other two directions, and (b) a cross section of an infinitely long cylinder fixed at its internal circumference. For the first model, the P-wave propagation was studied by applying a triangular or smoothed-step normal stress pulse on its surface. For the second model, the P-wave propagation was studied by applying a smoothed-step normal stress pulse on the external surface, and also the S-wave propagation was studied by applying a smoothed-step shear stress pulse on the external surface. Variations of the viscoelastic material behavior were considered by different parameters of the relaxation kernels. For the layer problem, a singular relaxation kernel was considered as well. In order to demonstrate the performance of the method, the numerical solutions are compared to available theoretical solutions obtained by the second author. An excellent match was achieved for the wave propagation velocities, the shape and magnitude of the stress spikes, and the apparent damping of wave motion for all cases where regular relaxation kernels were applied, the results being practically identical. For the singular kernel however, the numerical solution resembles the analytical one only in an average sense; that is, the area of the peak regions is practically identical, and so is the apparent damping of both the analytical and the numerical solution.

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VNS for Community Detection on Undirected Graphs

Jovanović D., T. Davidović, D. Urošević, T. Jakšić Krüger, D. Ramljak

We propose a variable neighborhood search (VNS) metaheuristic to address the community detection problem on undirected graphs. Graphs are used to mathematically model various types of networks, such as transportation networks, biological networks, electric power networks, social networks, etc. The community in the network refers to the subset of nodes with relatively close internal connections and relatively sparse external connections.

The members of a community should have greater similarity, but with obvious differences among members from different communities. The community detection problem assumes partitioning graph into communities, and is one of long standing and challenging optimization tasks. Community detection can help people to gain insight into the networks structural organization, and grasp the relations between network nodes. Due to its complexity, community detection problems are usually treated by metaheuristic methods and our VNS approach is not an exception. We implemented several variants of VNS, with an aim to evaluate the effectiveness of different algorithmic components such as: initial solution generation, shaking and local search procedures. The experimental analysis is conducted on the benchmark set from the literature, using modularity as the score for measuring quality of solutions. The conducted experimental evaluation shows that preliminary results of our best performing VNS variant are competitive in comparison to the state-of-the-art methods from the literature.

A Finite Element Method for Reconstruction of Time-dependent Convection Coefficient and Source in Magnetohydrodynamics System

Kandilarov J.D., L.G. Vulkov

A finite element Galerkin method is employed for the estimation of unknown time-dependent convection coefficient and source in 1-D magnetohydrodynamics flow system. In this inverse problem two integral observations are posed. The Galerkin procedure is analyzed and optimal error estimates are derived. Nonclassical formulation of the inverse problem is derived. Numerical algorithms solving the arising system of two loaded parabolic equations are proposed. Numerical experiments illustrate the efficiency of the algorithms.

Epsilon Subdifferential Method and Integrability

Konstantinov M., N. Zlateva

We develop a novel variant of the epsilon subdifferential method and use it to give a new proof of Moreau-Rockafellar theorem that a proper, lower semicontinuous and convex function on a finite dimensional space is determined up to a constant by its subdifferential.

Echo State Network for Features Extraction and Segmentation of Tomography Images

Koprinkova-Hristova P., I. Georgiev, S. Nikolova, D. Toneva

In present work we apply a recently developed Echo state network (ESN) approach for features extractions from gray scale images aimed at their segmentation. The key idea is to exploit intrinsically tuned ESN reservoir for generation of multiple features from the intensity value of each pixel of the original image. Next kmeans clustering is applied to divide image into several segments (clusters) based on newly extracted features.
The gray images data are a collection of computer tomography slices of bones. After their segmentation a 3-dimensional reconstruction of the tested objects were generated. Our results demonstrated that increased number of clusters in combination with increased number of extracted features per pixel reveal new details in the gray scale images. The obtained results are a good basis for further development of hierarchical (deep) approach for gray images segmentation combining ESN and clustering approaches.
The reported results are partially supported by the Bulgarian National Science Fund under grant BNSF-DN11/9 from 15.12.2017.

2D Asymptotic Models for Transversely Inhomogeneous Elastic Plates

Kaplunov J.

3D equations in isotropic elasticity for a transversely inhomogeneous layer are subject to asymptotic analysis over low-frequency domain, see J. Kaplunov, B. Erbas and N. Ege, "Asymptotic derivation of 2D dynamic equations of motion for transversely inhomogeneous elastic plates", Int J Eng Sci 178(2022), 103723, and also references therein. The leading and first order approximations are derived. Apparently for the first time, the constant coefficients in the associated 2D plate equations are expressed through explicit formulae involving single and repeated integrals across the thickness. Comparisons with previous adhoc considerations on the subject are presented, along with examples of numerical implementation.

Simulation Investigations of Pyramidal Cells Layer Effect on Conscious Visual Perception

Koprinkova-Hristova P., S. Nedelcheva

The aim of our research is to develop a brain-inspired spike timing neural network model of conscious visual perception accounting for latest theory of consciousness.
Among variety of opinions where the neural correlates of consciousness might be the dendrite theory was a recently developed one. It states that the conscious perception has strong dependence on the connectivity between sensory signals' relay (thalamus) and brain cortex areas responsible for signals' processing and perception. The theory says that it is mediated via neural pyramidal cells. These neurons have complicated morphological structure including a sophisticated dendrite three that is able to connect/disconnect the thalamus from the sensory cortex areas.
In present research we upgraded our spike timing neural network model of visual information perception including a layer of pyramidal neurons between the thalamus and the primary visual cortex. The model was implemented in latest version of NEST simulator using the neuron compartment model allowing for design of user defined dendrite structure. Our design is based on the literature information about pyramidal neurons dendrite structure and their influence on the thalamo-cortical connectivity.
We conducted simulation experiments exploring variety of pyramidal neurons parameters in an attempt to mimic their influence on the conscious visual perception as it was reported in the literature.

Non-Overlapping Domain Decomposition Methods of Optimal Computational Complexity

Kosturski N., S. Margenov, Y. Vutov

Schwartz's original method was proposed in 1869, which considered the Poisson equation with Dirichlet boundary conditions in a domain consisting of a circle and an overlapping square. Nowadays this approach provides powerful tools for efficient parallel solution of large-scale systems of algebraic equations arising from the discretization of partial differential equations. Two kinds of preconditioners are constructed in this way: overlapping and non-overlapping domain decomposition (DD).
We consider the second order elliptic equation $-\mathcal{A}u = f$ in $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, equipped with appropriate boundary conditions on $\Gamma = \partial\Omega$. Assume that the finite element method is applied for numerical solution of the problem using linear elements on a quasi-uniform triangulation $\mathcal{T}_h$, thus obtaining the linear system $A\mathbf{u} = \mathbf{f}$. We now assume that $\{\Omega_i\}_{i=1}^m$

is a non-overlapping partitioning of Ω with interface $\gamma \subset \mathbb{R}^{d-1}$. The stiffness matrix A is written in the form

$$A = \begin{pmatrix} A_D & A_{D\gamma} \\ A_{\gamma D} & A_\gamma \end{pmatrix} = \begin{pmatrix} A_D & \\ A_{\gamma D} & S \end{pmatrix} \begin{pmatrix} I & A_D^{-1} A_{D\gamma} \\ & I \end{pmatrix},$$

$A_D = Diag\,(A_1, A_2, \cdots, A_m)$, the blocks A_i correspond to the subdomains Ω_i, $i = 1, 2, \cdots, m$, A_γ - to the interface, and S is the Schur complement. Then following new non-overlapping DD preconditioner $C_{DD,k}^{BURA}$ is analyzed

$$A = \begin{pmatrix} A_D & \\ A_{\gamma D} & \sigma C_{1/2,k}^{BURA}(\Lambda) \end{pmatrix} \begin{pmatrix} I & A_D^{-1} A_{D\gamma} \\ & I \end{pmatrix}.$$

Here $C_{1/2,k}^{BURA}(\Lambda)$ is the best uniform rational approximation of degree k of $\Lambda^{1/2}$, Λ is the discrete Laplacian corresponding to $\mathcal{T}_h \cap \gamma$, $\sigma > 0$ is a scaling parameter. The BURA based non-overlapping DD preconditioner has optimal computational complexity. Key to the theory is the spectral equivalence between the energy norm associated with the Steklov-Poincaré operator on γ and the corresponding Sobolev norm of index 1/2. Estimates are independent of the geometry of γ. The theoretical results are illustrated by numerical experiments.

On the Decision Making Under Uncertainty

Krastanov M.I., B.K. Stefanov

The aspect of decision making under uncertainty has received an increasing interest in the recent years in the context of dynamical games. We study a discrete dynamical game on infinite-time horizon. This game is widely used in modeling optimal control problems in the presence of unknown but bounded disturbances. The main results provide necessary and sufficient conditions of Pontryagin's maximum principle type for a pair of strategies to determine a *Nash equilibrium*. The presented example illustrates the possible engineering applications.

Blocking the Immunosuppressing Action of the ORF6 Protein of the SARS-CoV-2 Virus: Computational Assays

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

Orf6 is one of several accessory proteins, that the SARS-CoV-2 virus expresses, which are generally considered to not be essential and are not required for the *in vitro* viral

replication. However, they appear to be responsible for the pathogenicity of the virus and for regulation of the host immune response. Among the nine accessory proteins of the SAR-CoV-2 virus, the Orf6 is considered to be the most important and has been shown to contribute significantly to the COVID-19 lung pathology and disease outcome. This makes the inhibition of its activity in the host cells a promising approach for reducing the pathogenic effects of the virus on the body.
The SARS-CoV-2 Orf6 function is to block the type-I interferon signalling in the cells, which is the primary driver of an antiviral state in non-immune cells. To accomplish that, the protein binds the Rae1-Nup98 complex, a dynamic component of the nuclear pore complex that is responsible for thaffiing mRNA in and out of the cell nucleus.
Orf6 is a relatively small (61 amino acid residues) protein that is membrane-bound. It also has a very flexible C-terminal tail, that contains several acidic amino acid residues. This part of the protein is considered to be responsible for the interaction with the Rae1-Nup98 complex.
Here, we report our computational studies on the structure of the SARS-CoV-2 Orf6 protein and its interaction with the Rae1-Nup98 complex. We also probe a possible inhibition of this interaction by either a full-lenght hIFNγ or a peptide, encompassing the C-terminal tails of this cytokine. We demonstrate that binding of the C-terminal domain of the SARS-CoV-2 Orf6 to either hIFNγ C-terminal peptides or the full-length cytokine molecule, has the potential to inhibit the interaction of the pathogenic protein with the Rae1-Nup98 complex.

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Why Do We Sleep? – Multi-Physics Problems Related to Brain Clearance

Mardal K.–A.

Recent theories suggest that a fundamental reason for sleep is simply clearance of metabolic waste produced during the activities of the day. In this talk we will present multi-physics problems and numerical schemes that target these applications. In particular, we will be lead from basic applications of neuroscience into multi-physics problems involving Stokes, Biot and fractional solvers at the brain-fluid interface.

An Inequality for Polynomials on the Standard Simplex

Milev L., N. Naidenov

Let

$$\Delta := \{(x, y) \in \mathbb{R}^2 : x \geq 0,\ y \geq 0,\ x + y \leq 1\}$$

be the standard simplex in $\mathbb{R}^2$ and $\partial\Delta$ be the boundary of Δ. We use the notations $\|f\|_\Delta$ and $\|f\|_{\partial\Delta}$ for the uniform norm of a continuous function f on Δ and $\partial\Delta$, respectively. Denote by π_n the set of all real algebraic polynomials of two variables and of total degree not exceeding n. Let $B_\Delta := \{p \in \pi_2 : \|p\|_\Delta \leq 1\}$ and $B_{\partial\Delta} := \{p \in \pi_2 : \|p\|_{\partial\Delta} \leq 1\}$.
Recently we described the set of all extreme points of B_Δ. Recall that a point p of a convex set B in a linear space is *extreme* if the equality $p = \lambda p_1 + (1 - \lambda)p_2$, for some $p_1, p_2 \in B$ and $\lambda \in (0, 1)$, implies $p_1 = p_2 = p$.
In the present paper we give a full description of the strictly definite extreme points of $B_{\partial\Delta}$.
As an application we prove the following sharp inequality:

$$\|p\|_\Delta \leq \frac{5}{3} \|p\|_{\partial\Delta}, \quad \text{for every } p \in \pi_2.$$

We hope that the above inequality can be useful in studying numerical problems related with estimates for uniform norms of polynomials and splines.

A Theoretical Analysis on the Bound Violation Probability in Differential Evolution Algorithm

Mitran M.–A.

This study is focused on Differential Evolution (DE) algorithm, a populationbased metaheuristic that is one of the most effective search methods for solving continuous optimization problems. Using a population of candidate solutions, the search is performed in a stochastic manner, relying on four basic steps: initialization, mutation, crossover and selection. The optimization problem addressed in this study is aiming to find the minimum of a function $f : [a, b]^D \to R, a, b \in R$. The mutation operator involved in DE might lead to infeasible candidate solutions, i.e. one or all of their components exceed the lower or upper bounds. A component x_i of a candidate solution is infeasible if $x_i \notin [a, b]$, with $i = \overline{1, D}$ and it becomes the subject of a repairing or substitution strategy. The practical relevance of this study is given by the fact that in many real-world problems the design variables are limited to physical ranges and since values exceeding the bounds cannot be used to compute the objective function they must be dismissed or repaired. The repairing strategy considered in this work is a stochastic variant of the projection to bounds strategy,

known as exponential confined. This study involves the standard DE/rand/1 mutation operator that consists of choosing three random individuals from the population of candidate solutions and adding to the first of them (noted here as x_R, the reference point) a scaled difference between the two others: $y_i = x_R + F \cdot (x_{r_2} - x_{r_3})$. Let X_R, X_{r_2}, X_{r_3} , Y denote the continuous random variables which take the values x_R, x_{r_2}, x_{r_3} respectively y during the evolutionary process. The main contributions of this paper are: (i) deriving the probability density function (pdf) of points generated by the mutation operator combined with the correction strategy (six cases are considered in the theoretical analysis, depending whether the points belong to the subpopulation corresponding to feasible mutants or the subpopulation corresponding to mutants whose components were corrected); (ii) obtaining the bound violation probability as an analytical expression depending on the reference point; (iii) formulating hypotheses regarding the impact of the reference point on the bound violation probability. The paper is structured in two main parts. The first one aims to determine the pdf of the random variable describing the values obtained using the mutation operator in conjunction with the correction strategy. In the second part, the previously computed pdf is used in order to determine the probability of generating infeasible components within the individuals generated by the mutation operator. This study aims to provide theoretical grounding for empirical observed behaviour and for the design of strategies to correct the out of bounds configurations.

Simulation and Experimental Verification of Ultrasonic Wave Propagation in Imperfect Concrete Structures using XFEM

Nguyen–Tuan L., M. Müller, H.–M. Ludwig, T. Lahmer

Ultrasonic based crack detection using analog analysis is widely used in the detection of damages and imperfection in the structures. However, when the damage is complex and experimental data is limited, the reconstructed damages will not be accurate. Model based inverse analysis emerges as an alternative method for such 'ill-posed problem', where the full waveform recorded is inverse-analysed in order to reconstruct the imperfection in the structure. The method requires an accurate numerical model allowing us to reproduce natural behaviour of the real structure. In this paper, we introduce an Extended Finite Element Method (XFEM) to simulate the wave propagation in imperfect concrete structure. The XFEM allows simulating a small discontinuity in the structure and the change of this discontinuity without re-meshing the whole structure. Therefore, the simulated structure is kept consistent while the structural discontinuity changes. For validation of the model, ultrasonic experiments are also carried out in the lab. Simultaneously, we improve the model with XFEM mass lumping technique and viscous boundary conditions in order to simulate the behaviour of the structure as accurate as in experiments. The simulations and experiments with and without cracks are presented, and the results are analysed in terms of time-of-flight, wavelength, and spectrum. With the help of a modelling of the waveforms,

structural changes may be identified more precisely, and the usage and life-time of concrete structures can be optimized.

New Bounds for the Extreme Zeroes of Classical Orthogonal Polynomials

Nikolov G.

The zeros of classical orthogonal polynomials have been a topic of inten- sive investigation. There are many reasons for this interest, such as the nice electrostatic interpretation of the zeros of the Jacobi, Laguerre and Hermite polynomials, their important role as nodes of Gaussian quadrature formulae, as well as the key role these zeros play in some extremal problems.
Derivation of sharp upper and lower bounds for the extreme zeros is of particular interest. We apply a simple approach to obtain new bounds for the extreme zeros of the classical orthogonal polynomials. Typically, comparison of the different estimates does not single out "best bounds" as these estimates depend on two or three parameters. Although our bounds are given in terms of simple expressions which facilitate their manipulation, we show that they are competitive with the best known bounds obtained recently.

Sensitivity Analysis of an Air Pollution Model with Using Innovative Monte Carlo Methods in Calculating Multidimensional Integrals

Ostromsky Tz., V. Todorov, I. Dimov, R. Georgieva

By definition sensitivity analysis is a procedure for studying how sensitive is the output of some mathematical model to the uncertainties of the input data. A large-scale mathematical model, describing remote transport of air pollutants, the Unified Danish Eulerian Model (UNI-DEM), is used in this particular sensitivity study. This model was developed at the Danish National Environmental Research Institute and scientists from the IICT - BAS in Bulgaria contributed significantly to its improvement and parallel implementation. It was chosen as one of the most advanced large-scale mathematical models that appropriately describe the atmosperic physical and chemical processes in full. Sensitivity analysis is most often deduced by variance-based methods. Sobol variance-based approach for has been applied to compute the corresponding global sensitivity measures, which leads to multidimensional integrals. An inovative stochastic approaches for calculation of these multidimensional integrals are analyzed and discussed.

A large number of numerical experiments must be carried out in order to collect the necessary data for such comprehensive sensitivity study. A special modification (SA-DEM) of the model was created for this purpose. One of the largest supercomputers in Europe and the most powerful in Bulgaria, the petascale EuroHPC supercomputer Discoverer is used to perform efficiently this huge amount of computations.
The obtained results can be used for evaluating the reliability of the model output results and to identify the input parameters that should be measured more precisely in order to improve the accuracy of some results of higher priority.

Graph Representation of Antibody Complexity

Pashov A., Sh. Pashova, P. Petrov

We have shown that the global analysis of the antibody diversity can be a source of biomarkers in cancer and autoimmunity. The antibody repertoire is studied in two alternative approaches repertoire sequencing (RepSeq) and functional analysis (igome) using arrays of diverse structures (e.g., peptides or glycans) as targets. The igome technique uses high throughput probing of the repertoire with a phage display random peptide library followed by next generation sequencing. It yields approximately 10^6 different sequences, each a target for at least one antibody in the repertoire. Each sequence represents a peptide ligand imitating actual antibody epitope so they are called mimotopes.
The global properties of RepSeq genetic data have been successfully studied using graphs based on the Levenshtein distance as a metric and a suitable cut off to establish similarity. We used a similar approach to summarize igome data with longest common subsequence as a metric. In addition, we extracted a graph from antibody binding data of samples from the blood of 21 patients probed with 4200 peptides from naturally occurring protein sequences. The binding profiles for each peptide were compared using F test and similar profiles were connected to represent plausible cross-reactivity.
Interestingly, all the three graph representations of the antibody complexity yielded small world type of networks evolving through random attachment as demonstrated by exponential degree distribution and inverse dependence of clustering coefficient on degree. This common property is in agreement with existing hypotheses of positive selection of antibodies. Negative selection of the repertoire as a mechanism to avoid autoimmunity is well documented but the existence also of a positive selection step has been a contentious hypothesis. Furthermore, both the igome graph and the reactivity graph yielded additional novel information interpretable in biological terms, e.g. in autoimmune diseases the IgM repertoire showed depletion of particular B cell clones, probably caused by the overexpressed pathogenic autoantibodies selecting the emerging IgM repertoire; IgM antibodies showed sex dependent reactivity which correlated with the recognition of different tumor antigens in brain tumors; etc.
Thus, representing the relation between the antibodies as a graph is a useful omics tool for

the study of the properties of the antibody repertoire on a global level providing biological insight to processes which were hard to study with traditional biological approaches.

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Machine Learning For Monitoring of Complex Detector Systems

Pavlov B., L. Litov, P. Petkov, N. Ilieva

The increasing complexity of modern Nuclear and Particle Physics experiments and the huge amount of collected data leads to practical problems related to the monitoring of the experimental setups and the data quality certification. This problem is even more pressing for the large-scale experiments at the Large Hadron Collider (LHC) at CERN. The LHC experiments collect data for years in harsh but also varying conditions. Monitoring the detector systems and experimental data certification is a key task to ensure obtaining reliable physical results.

Aiming at the development of customised ML tools for data certification for this specific use case we report the results of a *proof-of-concept study* on a setup of 1056 individual detector modules, roughly equivalent to the detector systems of the on-going experiments at CERN. The sample data – accelerator instantaneous luminosity, detectors counting rates and currents – was generated through a specially developed Monte Carlo protocol, encompassing three steps. First, the instantaneous luminosity and the global parameters are simulated using their proper time constants within several hundred synthetic runs to emulate a one-year data acquisition. Next, the individual response of each chamber is simulated independently. This step is run on a cluster and the scaling is linear. Finally, a data synchronization tool is used to prepare the data for the ML step.

Two different ML tools were implemented and tested. The first one correlates simulated detector rate with the accelerator luminosity, using linear regression. The second one, computationally more challenging, uses Horovod and TensorFlow to allow for the simultaneous use of GPUs on several nodes. A built-in autoencoder predicts the detector current. The difference between the predicted by the tool current and the "measured" one is used to spot possible inconsistencies in the detector operation. Both tools were ported and executed on CINECA's supercomputer Marconi100 and a good scaling was achieved.

We report the performance of both tools in terms of speedup with respect to the execution on one node. The performance of the autoencoder ML tool is analyzed using Horovod timeline file and some possible bottlenecks are discussed.

Acknowledgements. Computational resources for this study were provided at the supercomputer Marconi100 within the PRACE-6IP Project under Horison 2020 Program, Grant 823767.

Demanded Scale for Modern Numerical Optimisation

Penev K.

Modern online services facilitate many aspects of the human life such as goods and food shopping and delivery. The number of requested services is growing fast and at the same time can be seen growth of unattended constraints, unforeseen limitations and accidental events which affect the quality and feasibility of the service. Efficient management of online delivery requires optimisation at appropriate scale. This article discusses examples of online delivery services, which require optimization, points out advantages, and limitations, highlights their scale and the role of numerical methods for reducing the cost and time for delivery. Initial investigation illustrates algorithms capabilities to resolve such tasks and discusses current issues. Experimental results on high dimensional tests and consideration of further work conclude the article.

In Silico Studies on the Peptide–Membrane–Interaction Energetics

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

The complexity of biomolecular systems and interactions renders them challenging and expensive for detailed experimental examinations. Computational modelling and *in silico* experiments, providing reliable information about measurable macroscopic quantities based on synthetic microscopic data, substantially reduce the time and resources needed for these examinations. The physical property that governs the behaviour of molecular systems and the processes within them is the free energy. However, it is notoriously difficult to estimate reliably and accurately the free energy of biomolecular systems using standard molecular-dynamics (MD) simulations. This requires the application of advanced enhanced sampling techniques when estimation of the energetics of a biomolecular process is necessary.
Membrane-active peptides are promising biological molecules with possible applications in the treatment of various infection diseases. Within this class of small biological molecules, antimicrobial peptides (AMPs) attract the greatest research interest due to their broad-spectrum activity against a wide variety of pathogens and their potential application as a therapeutic alternative in the case of multi-drug resistant bacterial strains. AMPs exert their action by interacting with target cellular membranes, whereas they either insert into or penetrate the lipid bilayer. However, this interaction poses a number of challenges to standard atomistic simulations, due to slow relaxation times of the lipid bilayer, conformational changes in the peptides upon interaction with the membrane, peptide self-assembly, and pore formation, requiring prohibitively long simulation times.
Here we report the application of different enhanced sampling methods, including metadynamics and umbrella sampling, to the estimation of the free energy of interaction between

AMPs within peptide nanoclusters, as well as AMPs and model bacterial membranes.

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Construction of Reduced Basis Approximations of the Solutions to a Non–Linear Eco–Evolutionary Model

Rashkov P.

Reduced basis methods find application in approximating the numerical solutions to parametrised partial differential equations obtained via a high-fidelity discretisation (typically Galerkin method) by solutions to associated problems of lower dimension. The method's advantage originates from the property that the manifold containing the high-fidelity solutions for different parameter values in the finite element space could sometimes be approximated by linear combinations of basis elements of a subspace of lower dimension, as well as on the affine dependence of the considered problem on the free parameter.
We apply this method to construct a reduced basis approximation for the solutions to a non-linear eco-evolutionary model describing growth, spread and competition of two interacting populations – chemo-sensitive and chemo-resistant cancer cells during chemotherapy. The free parameter in the model represents the rate of therapy-induced loss of chemo-sensitive cells, and takes values in a compact set.
The approach for the reduced basis construction follows an offline-online stage decomposition. During the offline stage, solutions of the Galerkin problem for carefully chosen values of the parameter are orthonormalised to form the basis. In this stage we use two alternative paths: a) a proper orthogonal decomposition (POD) and b) a POD-greedy algorithm employing an a-posteriori estimator for the approximation error between the high-fidelity solution and the reduceced basis approximate solution.
The performance of the two approaches for the offline stage is illustrated via two examples implemented in the finite element library `FreeFem++`.

Epidemiological Models for Vector-Borne Diseases with Multiple Variants

Rashkov P., B.W. Kooi

Dengue fever is a vector-borne disease affecting millions of people in South America, parts of Africa and South Asia. Its epidemiology is characterised by cocirculating multiple variants of the pathogen, the dengue virus. Mathematical modelling of dengue faces the challenges of finding a balance between accurate description of the disease dynamics, the different scales of modelling, and the associated levels of complexity which allow for establishing tractable causal relationships. One approach in dengue modelling has been to use host-only models that include the vector dynamics implicitly, based on a quasi-steady state approximation in order to reduce complexity. However, these models are not directly suited for studies of intervention measures such as pest control or personal protection via repellents, which may influence the mosquito dynamics in a nonlinear fashion.
We discuss some issues which emerge repeatedly in the mathematical models of dengue: differences in structure (host-only vs. host-vector models) and the effect on dynamic behaviour, the theoretical rationale that allows complexity reduction via time-scale separation, and ecological effects due to seasonal changes in the vector population. Numerical bifurcation analysis is used to compare the bifurcation structure of a host-vector model of dengue with 2 variants and reinfection to that of previous host-only models.

Protein Structure Alignment and RMSD Calculations

Sapundzhi F., M. Popstoilov, M. Lazarova

The algorithms for protein structure alignment between two backbone chains play important roles in many applications areas including bioinformatics, computational biology, structure prediction and others. The problem of finding the optimal global alignment between two protein structures in R3 has been shown to be NP-hard. The local alignments can be represented as a graph. When we group mutually consistent local alignments it is equivalent to finding cliques in graph which is NP-complete problem. In the current study we present a toll that calculates the root mean square distance (RMSD) between aligned structures. As the implementation language the object-oriented programming language C sharp has been chosen.

Tensor Product Approach to Solving Chemical Master Equation for Epidemiological Modelling

Savostyanov D.

Epidemiological modelling is crucial to inform healthcare policies and to support decision making for disease prevention and control. The recent outbreak of COVID-19 pandemic raised a significant scientific and public debate regarding the quality of the mathematical models used to predict the effect of the pandemics and to choose an appropriate response strategy. One of the first epidemiological models, proposed by Kermack and McKendrick in 1927, assumes that each member of the population, be it a susceptible, infected, or recovered person, has the same chance of getting in contact with other members. The state of the system is then described by the fractions of susceptible, infected and recovered compartment of population, and the dynamics of epidemic is modelled by three nonlinear ordinary differential equations. This model captures well the main ways in which epidemic can develop, and can be easily solved by classical numerical methods for ODEs, which explains its popularity in academic curriculum and popular science. However, compartmental models substitute true population sizes, which are non-negative integer numbers, with real-valued proxies. This introduces modelling errors especially for small populations, and makes it impossible to answer certain questions, for example, when the epidemic ends, as the exponentially decaying real valued solution technically never becomes zero.
A stochastic (probabilistic) model of epidemic attempts to describe it mathematically more accurately by focusing on the probabilities to find the system in a state with a particular number of susceptible, infected and recovered people at a certain moment of time. This leads to linear ordinary differential equations for the probability density function. This system of these ODEs, known as a master equation, or forward Kolmogorov equation, can be difficult to solve due to its large size. We attempt to solve the chemical master equation accurately using the recently proposed algorithms based on low–rank tensor product decompositions, and compare the results with the state-of-the-art approaches to this problem.

On the Application of a Hierarchical Semi-Separable Compression Solver for Parabolic Fractional Diffusion Problems with Varying Time Steps

Slavchev D., S. Margenov

Anomalous diffusion describes many physical, biological, economic, etc. processes and phenomena that have non-local nature. It is modeled with the Fractional Laplace operator (hence the name fractional diffusion). In this work we use the Integral deffinition of the

Fractional Laplacian with the Riesz potential in order to model the problem in space and discretize it with the Finite Element Method. For the discretization in time we apply an implicit Euler scheme with varying time step. This leads to solving a series of systems of linear algebraic equations with dense matrices. Solving such problems numerically is a computationally expensive task. The model problem that we are studying introduces sudden changes in the right hand side and the time steps are suitably smaller around such points. When the step changes the factorization of the matrix must be recomputed, since it depends on the size of the time step. When using block LU factorization solvers this forces the computation of the factorization from scratch. This process has computational complexity of $O(n^3)$. When applying Hierarchical Semi-Separable (HSS) compression, however, we need to compress the matrix only once (computational complexity of $O(rn^2)$) and use ULV-like factoriza- tion (computational complexity $O(r^2n)$) when the step changes. Here r is the maximum off-diagonal rank, found during the compression process. For problems with suitable structure $r \ll n$. When the time step doesn't change we only need to solve with the factorized matrix: Computational complexity of $O(n^2)$ for block LU based solvers and $O(nr)$ for the HSS based solver. In this work we study the performance, parallel efficiency and accuracy of an HSS solver from the STRUctured Matrices PACKage and compare it to a block LU based solver from Intel®'s Math Kernel Library. We present numerical experiments obtained on the AVITOHOL supercomputer that show the advantages of using the HSS compression based solver for this problem.

An Optimized Stochastic Method Based on $\Lambda\Pi_\tau$ Sobol Quasirandom Sequences for the Fredholm Integral Equation

Todorov V., I. Dimov, R. Georgieva, Tz. Ostromsky

In this paper we propose and analyse an optimized advanced biased stochastic methods for solving a class of integral equations- the second kind Fredholm integral equations. We study and compare innovative possible approaches to compute linear functionals of the integral under consideration: biased Monte Carlo method based on evaluation of truncated Liouville-Neumann series and transformation of this problem into the problem of computing a finite number of integrals. Advanced Monte Carlo algorithms for numerical integration based on modified Sobol sequence have been applied for computing linear functionals. In our investigation five biased Monte Carlo algorithms for numerical integration have been applied namely-Crude Monte Carlo method based on a high quality SIMD-oriented Mersenne Twister pseudorandom number generator; QuasiMonte Carlo based on $\Lambda\Pi_\tau$ Sobol quasirandom sequences; a stratified symmetrised MC algorithm MCA-MSS-2-S; a randomized Quasi-Monte Carlo algorithm MCA-MSS-1 based on a special procedure of shaking $\Lambda\Pi_\tau$ Sobol quasirandom points with a convergence rate $O\left(N^{-\frac{1}{2}-\frac{1}{d}}\right)$; and a randomized Quasi-Monte Carlo algorithm MCA-MSS-2 with a convergence rate $O\left(N^{-\frac{1}{2}-\frac{2}{d}}\right)$,

where d is the dimension of the problem under consideration. We have shown that the procedure of balancing of both stochastic and systematic errors is very important for the quality of the biased algorithms. MCA-MSS-2-S is an optimization over the algorithms MCA-MSS-1 and MCA-MSS-2 and gives the smallest relative stochastic error and the shortest computational time for a fixed number of steps in Liouville-Neumann series in comparison with MCA-MSS-1 and MCA-MSS-2, but serious restrictions about the choice of sample size exist for its implementation. The developed reliable approaches for solving integral equations will be important in different areas of applied mathematics, physics, and engineering.

Intuitionistic Fuzzy Knapsack Problem trough the Index Matrices Prism

Traneva V., P. Petrov, S. Tranev

Knapsack problem is a NP-hard combinatorial optimization problem that used in the business models. In this problem, a set of items are given with profits and weights. The objective of the problem is to select a subset of items so that the total profit of selling them is maximized without exceeding the capacity of the knapsack.
Contemporary pandemic environment with galloping inflation predetermines uncertainty in the parameters of this problem. Intuitionistic fuzzy logic, which is an extension of fuzzy logic, is a flexible tool for dealing with ambiguity. In this work, an intuitionistic fuzzy knapsack problem is defined with intuitionistic fuzzy values of weights and profits of items as well as the knapsack capacity. Here, an index-matrix approach is proposed for its optimal solution by extending the classical dynamic optimization algorithm and intuitionistic fuzzy propositional logic. In the algorithm, three scenarios are proposed to the decision maker for the final choice – pessimistic, optimistic and average. A software implementation to represent the proposed intuitionistic fuzzy algorithm is also developed and its effectiveness is demonstrated on an example.
The originality of the paper comes from the proposed intuitionistic fuzzy approach to the knapsack problem and its software implementation. The index matrix prism for solution of intuitionistic fuzzy knapsack problem can be applied to problems with imprecise parameters and can be extended in order to obtain the optimal solution for other types of n-dimensional knapsack problems by using n-dimensional index matrices for storage and analysis of data.

Numerical Solutions of the Boussinesq Equation with Nonlinear Restoring Force

Vucheva V., V.M. Vassilev, N. Kolkovska

In the present work, we consider the Boussinesq equation with non-linear restoring force. Equations of this type model the transverse or longitudinal vibration of an elastic rod subject to a constant tangential follower force and laying on a nonlinear elastic foundation due to which a cubic term appears in addition to the linear term corresponding to the purely Winkler foundation. The dynamical behavior of such mechanical systems is not well-studied in the current literature. In this work, we give a one-parameter family of exact solitary wave-like solutions (solitons) of the regarded non-linear equation in explicit analytic form.
We propose and study finite difference schemes to solve the considered problem. The nonlinear terms are approximated in two different ways. Both schemes have second order of approximation in space and time steps. The extensive numerical experiments show second order of convergence for single solitary wave and the interaction between two solitary waves.

Simulation of the Mechanical Wave Propagation in a Viscoelastic Media with and without Rigid Inclusion

Zhelyazov T., S. Pshenichnov

The contribution focuses on the numerical simulation of wave propagation in an array of solid inclusions regularly distributed in a viscoelastic matrix. Waves are provoked by a transient load. The study aims to compare the wave propagation in the viscoelastic continuum with and without the presence of solid inclusions. To this end, the stress and the displacement evolutions (in the time domain) are monitored at specified locations at the boundaries of the defined continuum. The case study contributes to a better understanding of the phenomena related to the reflection and diffraction of the mechanical waves by the solid inclusions. The modeled set-up often referred to in the literature as a phononic crystal, will possibly shed light on numerous practical applications. Among others, these are high sound adsorption and strategies for defect locations.

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A Posteriori Error Estimates in Finite Element Method by Preconditioning

Zikatanov L.T.

We present a framework that relates preconditioning with a posteriori error estimates in finite element methods. In particular, we use standard tools in subspace correction methods to obtain reliable and efficient error estimators. As a simple example, we recover the classical residual error estimators for the second order elliptic equations as well as present some new estimators for systems of PDEs. This is a joint work with Yuwen Li (Penn State).

Performance of Advanced Air Pollution Studies by Using a Digital Twin

Zlatev Z., I. Dimov, K. Georgiev

It is worthwhile to digitalize completely the complex processes related to the investigation of different air pollution phenomena in the European countries. One of the most important and most challenging of these phenomena is the treatment of some very complex problems arising in the study of the influence of the climatic changes on some potentially dangerous pollution levels, which can have damaging effects on some groups of human beings (first and foremost, on people suffering from asthmatic deceases). In order to resolve successfully this task, it is necessary to be able to handle efficiently each of the following four basic tasks (and several auxiliary tasks too):
(a) to prepare and then to use many times a large number of huge input files (containing first and foremost meteorological data, emission data and geographical data), which can be needed and must be applied in a long series of interesting studies with many scenarios,
(b) to develop appropriate mathematical models, which describe adequately the studied physical and chemical phenomena by large non-linear systems of partial differential equations,
(c) to apply reliable, very accurate and sufficiently fast numerical methods and to use these methods efficiently together with the appropriate input files when the enormous tasks are to be handled on different high speed parallel computer architectures
and
(d) to make the calculated output results easily understandable (also for non-specialists) by using appropriate sets of visualization and even animation techniques.
The preparation of such very complicated digital devices and their successful application in the investigation of some potentially dangerous pollution levels in different parts of Europe and Bulgaria over a long time-period consisting of sixteen consecutive years will be discussed in this talk.