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Mathematical modeling approaches for seasonal exacerbations of bacterial meningitis

Meltem Gölgeli

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The seasonal, periodic or momentary increase in the incidence of an infectious disease, corresponding to seasons or different time periods within the year, is an important process from a public health perspective and characterizes the dynamics of the spread of many infectious diseases. Mathematical modeling techniques are used to understand the multilayered structure of seasonal exacerbations of an infectious disease, and the tools of dynamical systems theory are used to analyze these models. In this talk, after an overview of some approaches in the literature on mathematical modeling of periodic exacerbations of infectious diseases, I will present a mathematical modeling approach for periodic exacerbations of bacterial meningitis and simulations of different scenarios for a possible bacterial meningitis outbreak.

Keywords: mathematical epidemiology, dynamical systems, stability

Data-driven modeling of complex materials

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Data-driven hyperelasticity holds significant promise for modeling the mechanical behavior of rubberlike materials and soft biological tissues. It offers a means to establish a direct connection between experimental data and the material's mechanical response, without the need for predefined analytical expressions for strain energy density functions or stress expressions. In this comprehensive study, we introduce a novel data-driven approach that encompasses four distinct kinematic strategies; (i) invariant-based formulation, (ii) modified invariant-based approach [1], (iii) principal stretch-based formulation, and (iv) dispersion-type anisotropic formulation to model the hyperelastic response of rubberlike materials, and soft biological tissues. The dispersion-type anisotropic formulation is constructed by leveraging the concept of the "generalized structure tensor," as established by Holzapfel et al. [2]. This formulation accounts for both in-plane and out-of-plane dispersion characteristics. To model hyperelastic behavior, we replace appropriate partial derivatives within the strain energy density functions with well-fitted B-spline interpolations where the control points are calibrated against experimental data obtained from uniaxial tension, triaxial shear, and (equi)biaxial tension deformations. The model calibration phase incorporates the normalization condition and the polyconvexity condition is enforced through the control points of the B-splines in order to ensure a stable constitutive response that allows unique solution in finite element analysis. The predictive capabilities of the proposed model are shown against Treloar, and Kawabata datasets; and linea alba, rectus sheath, aneurysmal abdominal aorta, and myocardium tissues. On the numerical side, we derive stress and moduli expressions necessary for finite element implementation. The performance of the model is demonstrated through representative boundary value problems. Overall, this work presents a powerful and versatile data-driven hyperelasticity framework that bridges the gap between experimental data and computational modeling, offering potential applications in diverse fields of material science and biomechanics.

Keywords: Data-driven model, hyperelasticity, rubber, biological tissue, finite element method

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Hopf bifurcations in a class of reaction-diffusion equations including two discrete time delays: An algorithm for determining Hopf bifurcation, and its applications

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We analyze Hopf bifurcation and its properties of a class of system of reaction-diffusion equations involving two discrete time delays. First, we discuss the existence of periodic solutions of this class under Neumann boundary conditions, and determine the required conditions on parameters of the system at which Hopf bifurcation arises near equilibrium point. Bifurcation analysis is carried out by choosing one of the delay parameter as a bifurcation parameter and fixing the other in its stability interval. Second, some properties of periodic solutions such as direction of Hopf bifurcation and stability of bifurcating periodic solution are studied through the normal form theory and the center manifold reduction for functional partial differential equations.
Moreover, an algorithm is developed in order to determine the existence of Hopf bifurcation (and its properties) of variety of system of reaction-diffusion equations that lie in the same class. The benefit of this algorithm is that it puts a very complex and long computations of existence of Hopf bifurcation for each equation in that class into a systematic schema. In other words, this algorithm consists of the conditions and formulae that are useful for completing the existence analysis of Hopf bifurcation by only using coefficients in the characteristic equation of the linearized system. Similarly, it is also useful for determining the direction analysis of the Hopf bifurcation merely by using the coefficients of the second degree Taylor polynomials of functions in the right hand side of the system. Finally, the existence of Hopf bifurcation for three different problems whose governing equations stay in that class is given by utilizing the algorithm derived, and thus the feasibility of the algorithm is presented.

Keywords: Hopf bifurcation, functional partial differential equations, reaction-diffusion system, delay differential equations, stability, periodic solutions, discrete time delays

Modeling and Inference Approaches for Biochemical Reaction Networks

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Biochemical processes are biochemical reaction networks (BRNs) of different species connected with multiple reactions. There are two fundamental approaches to modeling the dynamics of BRNs: deterministic and stochastic. According to the deterministic approach, BRNs are continuous-time continuous-state processes. Moreover, it uses Reaction Rate Equations (RREs), a set of Ordinary Differential Equations (ODEs), to model the state of the processes. By contrast, the stochastic approach assumes BRNs as continuous-time discrete-state Markov processes and utilizes the Random Time Change Model (RTCM) to model the system's state. Also, in the stochastic approach, the time evolution of the system's probability density function is represented by the Chemical Master Equation (CME). Diffusion approximation can be considered as a link between these two fundamental approaches, which assumes that BRNs continuous-time discrete-state processes whose state vector satisfies the Chemical Langevin Equation (CLE) and the probability density function satisfies the Fokker-Planck equation (FPE) [3].
It is well-known that the speed of reactions and the abundance of reactants in these processes cannot be classified into one category. To be more precise, BRNs have a multi-scale nature. Therefore, it is necessary to develop hybrid models combining different modeling approaches. In [2], we proposed a jump-diffusion approximation that couples the stochastic approach and diffusion approximation to model the dynamics of BRNs with multi-scale nature. The strategy of the model is to partition the reactions into fast and slow subgroups and model the fast group using diffusion approximation. At the same time, Markov chain representation is kept for slow groups. Therefore, we represent the system's state as a summation of the RTCM and the CLE. In [1], we showed that the time evolution of the joint probability density function of the jump-diffusion approximation is given by the hybrid master equation (HME), which involves terms from the CME and the FPE. Also, we constructed an algorithm to approximate its solution. We also presented a Bayesian inference method that combines the Monte Carlo Markov Chain (MCMC) methods and Sequential Monte Carlo (SMC) methods to estimate the unknown states/parameters of the BRNs modeled with jump-diffusion approximation. In this talk, based on the studies [1], [2], we give an overview of modeling approaches and the Bayesian estimation methods for the BRNs.

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A parallel randomized Kaczmarz algorithm for the solution of sparse linear systems on distributed memory platforms

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One of the most challenging problems in science and engineering applications is the solution of linear systems of equations. There are several methods to handle the challenges such as computational cost and robustness, some examples include state-of-the-art parallel direct solvers, iterative methods with a parallel pre-conditioner or more recently introduced randomized techniques. Another challenge is that the equations derived from real-world applications are generally sparse, meaning that the coefficient matrix has many zero elements. A sequential randomized Kaczmarz and its shared memory implementations have been proposed in [1] and [2], respectively. In this work, we propose a new distributed memory parallel algorithm for sparse linear systems based on the randomized Kaczmarz method. In the proposed algorithm, the communication frequency and the way of handling the communication size are parameters that the user can choose and they affect the performance. We will present the performance results of the proposed algorithm on determined, under-determined, and over-determined realistic linear systems erived from real-world problems in different problem domains. We will compare the speed-ups of the proposed parallel randomized algorithm with different values of the communication frequencies, which is inversely proportional to the number of Randomized Kaczmarz iterations between communication operations. Another comparison will be the length of communication. Where there are several options: (i) Communicate the entire solution vector, (ii) communicate only the changes on the solution vector, (iii) communicate a predetermined number of changes. Finally, we will compare our results with other iterative solvers and discuss potential improvements for the proposed algorithm.

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Allee Effect in Continuous-Time and Discrete-Time Predator-Prey Systems with Leslie Type

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In this presentation, we will discuss the Allee effect in continuous-time predator-prey system with Leslie type and its discrete version. First, the stability analysis of continuous system will be given. Then, we will examine the bifurcations and chaotic behavior of the model. Next, the impact of Allee effect on the dynamics of both prey and predator populations will be discussed via numerical simulations. Second, discrete-time predator-prey system obtained by applying the forward Euler scheme to its continuous-time counterpart will be introduced. Afterwards, the conditions on parameters for stability and periodic solutions will be stated briefly. Finally, some numerical simulations will be shown to compare the Allee effect in maintaining the intricate balance between predator and prey populations and the importance of considering complex ecological interactions in order to accurately model and understand the population dynamics in continuous (overlapping) and discrete (non-overlapping) cases.

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Unit Cell Calculations Under Fully Characterized Stress States

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The available numerical methods for conducting finite element unit cell calculations under predefined stress states typically constrain the most general stress state to a single shear stress component superimposed on three normal stress components. This study represents an advancement in the field, expanding upon the current state of the art to enable the exploration of unit cell behavior under the most intricate stress states, encompassing three shear and three normal stress components [1]. The proposed methodology has been implemented within the commercial finite element software ABAQUS. Three-dimensional cubic unit cells, containing either a void or a particle at their center and subjected to various stress states, were analyzed. The results of these simulations demonstrate that the developed method offers both accuracy and computational efficiency. Moreover, simulations conducted on voided unit cells reveal that ductile failure demonstrates anisotropic behavior, with anisotropy becoming increasingly pronounced under the influence of shear loads.

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A Mathematical Model to Study the Fundamental Functions of Phagocytes and Inflammatory Cytokines Post-Myocardial Infarction

Mehtap Lafcı Büyükkahraman

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The heart has a limited capacity for regeneration and repair. Myocardial infarction (MI), which is characterized by continuing cell death and a proportionally diminished capacity of the heart to repair itself, is one of the major causes of morbidity and mortality worldwide. A mathematical model is presented to study the effects of phagocytes and inflammatory cytokines post-myocardial infarction. The model incorporates the interactions among macrophages, neutrophils, dead neutrophils, inflammatory cytokines, cardiomyocytes, and dead cardiomyocytes. The resulting system of nonlinear ordinary differential equations is studied analytically and numerically.

Mechanical Characterization of Lattice Materials via Additive Manufacturing and Digital Image Correlation Technique

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The advent of additive manufacturing has sparked a revolution in lattice material research, offering promising applications across diverse industries. However, assessing the mechanical properties of these intricate structures has posed a significant challenge. Ambiguities in plastic material testing standards and the financial hurdles tied to specialized testing equipment have hindered progress. This study presents a simplified, cost-effective methodology employing readily available tools and computational techniques. Our approach utilizes a Formlabs Form 3 Stereolithography (SLA) 3D printer with Formlabs Tough 1500 resin, coupled with the Instron-5944 2kN universal testing system[1]. We meticulously fabricated compression specimens adhering to ASTM standard D695-15[2], then produced hexagonal lattice configurations subjected to compression testing. Accurate displacement and strain measurements were achieved using digital image correlation (DIC) techniques, bolstered by open-source Ncorr software and the Point Track algorithm[3, 4]. One challenge in lattice experiments is creating a reliable speckle pattern on the lattice surface for precise DIC measurements, which we addressed using tattoo papers[5]. To validate our findings, we conducted finite element (FE) simulations of the compression experiments. These simulations closely matched our experimental results, highlighting the reliability of our methodology. In conclusion, our user-friendly approach simplifies lattice material characterization and deepens our understanding of their mechanical behavior. By integrating additive manufacturing, DIC techniques, and FE simulations, our methodology offers an accessible path for advancing lattice material research. It empowers researchers to explore these materials' mechanical properties without the financial constraints of expensive experimental setups, fostering progress in this field and expanding its industrial applications.

Keywords: Lattice Materials, Additive Manufacturing, Digital Image Correlation, Finite Element Method.

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An Investigation of Ion Transport Through the SARS-CoV-2 E Protein Ion Channels

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The E protein is one of the major structural proteins of RNA viruses. It is involved in replication, budding, and assembly. E proteins are known to form ion channels which slightly favor cation transport over anion. In the light of the ongoing pandemic, we compared SARS-CoV-1 and SARS-CoV-2 E protein ion channels in terms of their selectivity. The impact of the bath concentration and concentration gradients across the channel on the binding ratios of sodium and chloride ions have been also studied. Ion transport is described through the fourth-order Poisson–Nernst–Planck–Bikerman (4PNPBik) model which generalizes the traditional model by including ionic interactions between ions and their surrounding medium and non-ionic interactions between particles due to their finite size. The immersed boundary-lattice Boltzmann method (IB-LBM) is used for the solution of the system. The mathematical model has been validated by comparing analytical and experimental ion activity. Ion transport through SARS-CoV-2 E protein ion channel shows that cation selectivity is not as prominent as in E proteins of other RNA viruses. Furthermore, the chloride binding ratio increases as the concentration gradient increases. Additional analysis of the SARS-CoV-2 E protein suggested that as the bath concentration increases, the channel becomes increasingly more sodium selective. A potential gradient has a minimal effect on the binding ratio.

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Multiphysics modeling of the high intensity focused ultrasound ablation of liver tumor

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High intensity focused ultrasound (HIFU) is very promising new technology, that has many therapeutic applications, among them are the treatment of cancer in different organs without major side effects. Focused ultrasound is completely non-invasive and currently many clinical trials are performed for cancer treatment in different organs. With the ultrasound beam being focused, thermal energy can be added primarily to a small region of tissues with little or no deposition at all on the surrounding tissues. However, during propagation through different organs the beam can be distorted, and healthy tissues can be damaged. Appropriate treatment planning is necessary in order to avoid side effects. Simulation of nonlinear wave propagation in three dimensional geometries is very time consuming process. Mathematical and computational model is constructed that includes nonlinear ultrasound propagation in heterogeneous tissues, takes into account the effect of blood flow on the thermal therapy and cavitation. For nonlinear wave propagation three-dimensional parallel solver on GPU has been developed. Simulations of HIFU tumor ablation in a patient specific liver geometry will be presented and it will be shown that the treatment time can be sufficiently reduced up to several minutes. The presented results will be validated by the in-vivo and ex-vivo experimental data.

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A new approach for boundary element formulation of viscoelasticity in time domain

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A novel non-iterative algorithmic formulation for generalized models of viscoelasticity under quasistatic conditions is proposed within the framework of the boundary element method (BEM). The proposed time-domain algorithm is constructed for a generic rheological model of linear viscoelasticity that can either be straightforwardly simplified to recover the basic Kelvin and Maxwell models or readily furthered towards the generalized models of viscoelasticity through serial or parallel extensions. The formulation exploits the hybrid semi-implicit update of strain-like internal variables, contrary to the existing rate formulations of viscoelasticity developed within BEM. The mesh-free Cartesian transformation method (CTM) and the radial point integration (RPIM) technique are utilized to overcome the indispensable domain integrals arising in the BEM formulation of inelasticity due to the internal variables.
The excellent performance of the proposed BEM formulation of viscoelasticity is demonstrated by means of boundary value problems (BVPs) with uniform and non-uniform strain fields, where quantitative comparisons are conducted with the analytical methods and finite element method (FEM), respectively. The results generated using the proposed BEM approach for creep and relaxation experiments in the uniform-strain BVPs indicate perfect agreement with the analytical results and the robustness of the semi-implicit integration scheme. Moreover, BVPs with non-uniform strain fields involving higher strain/stress evolution in the neighborhood of corners or edges under cyclic axial and shear loadings are also considered. The comparisons made with FEM based on global force displacement diagrams and local stress/strain variations along selected paths indicate excellent agreement.

Novel Formulation for Fast and Accurate Solutions of Electromagnetic Problems Involving Open and Closed Perfectly Conducting Surfaces

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In this study, we present a novel formulation for broadband, fast, accurate, and efficient solutions of electromagnetic problems involving open and closed perfectly conducting surfaces. The proposed formulation, called the hybrid potential-field formulation (HPFF), employs the recently developed combined potential-field formulation (CPFF) [1] on closed surfaces, and potential formulations (PFs) on open surfaces. By properly combining PFs with field formulations, the proposed formulation does not suffer from low-frequency (dense-discretization) breakdowns and internal-resonance problems, which are well-known issues of the surface-integral-equation formulations in the literature.

There are various formulations in the literature for the solutions of electromagnetic problems involving perfect electric conductors. The electric-field integral equation (EFIE), the magnetic-field integral equation (MFIE), and a combination of the two, namely, the combined-field integral equation (CFIE) are very well-known surface integral equations. The hybrid-field integral equation (HFIE) is also available by formulating closed surfaces with CFIE and open surfaces with EFIE [2]. However, these surface integral equations do not always produce well-conditioned matrix systems. For example, EFIE is known to suffer from both low-frequency breakdowns and internal-resonance problems. In addition, HFIE is prone to low-frequency breakdowns since it employs EFIE on open surfaces. For low-frequency (dense discretization) problems, recently developed PFs are very suitable. However, it was shown that PFs suffer from internal-resonance problems for closed surfaces [1].

The objective of this study is to develop a novel formulation unaffected by low-frequency breakdowns and internal-resonance problems so that it can produce accurate and efficient electromagnetic simulations in a broad range of frequencies. Our approach is to properly combine the recently developed CPFF with PFs, which are applied on closed and open surfaces, respectively. The proposed formulation's superior performance is shown on electromagnetic problems involving both canonical and complicated geometries. The problems are solved iteratively with the generalized minimal residual (GMRES) method, and the matrix-vector multiplications are efficiently calculated with a broadband implementation of the multilevel fast multipole algorithm. Hence, a truly broadband implementationis developed for electromagnetic problems involving open and closed conductors.

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Design and Simulations of Near-Zero-Index Transmission Systems

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Near-zero-index (NZI) materials belong to a category of metamaterials known for exhibiting relative permittivity and/or permeability values that approach zero. These materials hold great promise for various electromagnetic applications, including wave transformation, beam focusing, and tunneling, to name a few [1]. This study demonstrates that NZI structures with relatively simple geometries can serve as efficient waveguides, offering potential advantages over conventional metallic designs. Both homogenized and realized NZI structures involving dielectric unit cells are considered in the simulations. Specifically, dielectric cylindrical rod arrays having Dirac-like dispersion [1] are used to realize NZI structures.

To perform precise and efficient simulations of both homogenized and realized NZI structures, an in-house implementation of surface integral equations and the multilevel fast multipole algorithm (MLFMA) are used. The choice of surface integral equations is crucial for fast and accurate simulations of these NZI structures, given their distinctive electromagnetic characteristics. For the designs consisting of dielectric unit cells with ordinary material properties, the electric-magnetic current combined-field integral equation (JMCFIE) is used. However, for homogeneous NZI models, a mixed formulation is employed for fast and accurate simulations [2]. Furthermore, to overcome lowfrequency breakdowns stemming from near-zero constitutive parameters, the use of MLFMA with approximate diagonalization (AD-MLFMA) is proposed. This approach ensures stable and efficient simulations, even when dealing with extremely small permittivity and permeability values.

In this study, two distinct NZI designs capable of directing waves at a precise 90-degree angle are presented. It is shown that material properties and geometric modifications are crucial to obtain intended radiation characteristics. Specifically, with a careful material selection, such as $\epsilon_r = \mu_r = 5 \times 10^{-3}$, waves can be efficiently rotated by 90 degrees, with strong radiation observed at the output region of homogeneous NZI waveguides. In addition, we consider actual structures involving periodic arrangements of dielectric rods, while, as the rod material, we use copper-filled PLA with $\epsilon_r = 7.8 + i0.3$ and $\mu_r = 0.65 + i0.018$. After many trials, radii and center-to-center distances are set to 0.15λ and 0.65λ, respectively. As a result, it is observed that beam steerings and wave manipulations are possible and applicable with relatively simple NZI structures, demonstrating remarkable potential of them in practical applications.

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Optimizations of Nanoantenna Arrays for Improved Power Enhancement

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Nanoantennas are devices that became popular in the past century and are widely used nowadays. Some of the important usages of them include but are not limited to bio-sensing and detecting, information processing, imaging and focusing, nano-links for energy transfer, and energy harvesting [1]. Their working principles come from the materials they are being made of, which are called plasmonic materials and can be exemplified as gold, silver, and copper. These materials have the capability of creating strongly enhanced fields when enlightened by electromagnetic waves at optical frequencies. At an optimal frequency called the resonance frequency of a nanoantenna, the electric field intensity reaches its peak. The resonance frequency of a nanoantenna depends on the shape and material as well as the environment. In order to investigate the effects of different parameters listed above, we use an in-house implementation of the multilevel fast multipole algorithm (MLFMA) [2], which is a powerful method that has been developed for solving large electromagnetic problems faster and more accurately. We also use the modified combined-tangential formulation (MCTF), which provides stable solutions of plasmonic problems with broad ranges of negative permittivity values. The fast and efficient simulation environment facilitates the examination of peculiar properties of nanoantennas and optimizations of them.

One of the commonly used shapes for nanoantennas is bowtie. In this study, we investigate how an array made by these optimized bowties operates, and in which arrangement it gives an optimal power enhancement. First, we make some parametric analyses on the frequency and materials, where a bowtie unit cell is examined to reach relatively high power enhancement values in the intended optical frequency regimes. Specifically, we obtained strongly enhanced fields with a silver nanoantenna at 450 THz. Then, we focus on nanoantenna arrays, e.g., 3×3 arrays, and optimizations on vertical and horizontal distances between nanoantennas. In order to obtain the best results considering power enhancements, we employ genetic algorithms (GAs). Genetic algorithm is a stochastic optimizer, which means that it produces and uses random variables for optimization. Inspiring the natural selection, GA provides optimized results, which corresponds to the best distributions of nanoantennas for power enhancement.

As a result, thanks to the efficient simulation environment and GAs, we achieve a prototype of silver nanoantena arrays with optimized spatial distributions. With positive outcomes, fabrications of them can commence. It should also be noted that this study is expected to have a guiding influence on future studies about plasmonic structures.

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A Kind of Asymmetric and Nonlinear Matrix and Its Algebraic Properties

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In this presentation, we present a new analogue of the Filbert and Lilbert matrices whose indices have different asymmetric and nonlinear rules according to their row numbers. Explicit formula are derived for the LU-decompositions, their inverses and the inverse of the main matrix as well as its determinant. To prove the claimed results we use backward induction method. The asymmetric variants of the Filbert and Lilbert matrices are obtained from our results for a particular q value.

Keywords: Filbert matrix, Lilbert matrix, q-analogue, LU-decomposition, inverse matrix, determinant

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Placement of the Multiple Magnetic Sources for the MHD Flow via Optimal Control

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In this contribution, the optimal control of the fully developed, steady, laminar, unidirectional flow of an incompressible electrically conducting fluid is considered in a rectangular duct [1]. Thin wires carrying electric current are used as magnetic sources to generate the magnetic field and placed along, below and/or above the channel. The aim of the control is to determine the optimal placement of magnetic sources by using the axis coordinates of the sources as control variables to derive the fluid into the desired velocity and induced magnetic field. The control formulations are given for multiple number of magnetic sources via adjoint method admitting control constraints. Also, directionally aligned layouts are used to reduce the number of unknown control parameters when four sources are placed. A gradient based optimization algorithm with bound supports on the controls, L-BFGS-B is used within the discretize-then-optimize framework. Direct solutions of the MHD equations are obtained using the finite element method with quadratic elements.

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Genetic Algorithm Optimizations on Digital Electric Currents for Equivalent Scattering Properties

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In this research endeavor, our primary objective is to obtain scattering properties of an arbitrary and relatively complicated structure with surface currents defined on a regular surface enclosing the structure. In comparison with the standard equivalence algorithms, in this study, only electric currents are used on equivalent surfaces. Furthermore, these electric currents are defined in such a way that magnitudes of them are bounded and represented by different numbers of bits. The proposed strategy enables definition of digital currents on smooth and simple surfaces to represent enclosed complex geometries. Particularly, one-bit optimizations allow us to obtain equivalent scattering characteristics. Accordingly, it becomes possible to simplify electromagnetic simulations of complicated structures, where electromagnetic characteristics are represented by radiation of equivalent digital surface currents. For example, digital currents on canonical surfaces can be used in subsequent electromagnetic simulations, which may require less time and computational resources compared to standard simulation approaches.

In this study, in order to find equivalent currents, we use genetic algorithms (GAs). Specifically, we employ GAs to optimize digital currents on simple surfaces so that we can obtain equivalent scattering characteristics of complicated structures. Even though there are slight differences between the optimized and actual scattering characteristics, the similarity of the results has been remarkable in initial trials.

In the electromagnetic simulations, we use the multilevel fast multipole algorithm (MLFMA) [1]. MLFMA performs matrix-vector multiplications with O(N logN) complexity, significantly reducing simulation time and memory requirements. In addition, as an iterative solver, we use GMRES, which is known to work well in solutions of matrix equations obtained by surface integral equations. On the other hand, it should be emphasized that digitalization of currents via equivalent surfaces does not depend on the type of the solver or acceleration algorithm.

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Design and Investigation of Electromagnetic Responses of Near-Zero-Index Metamaterials Involving Dielectric Rods with Variable Cross Sections

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Near-zero-index (NZI) structures are a class of metamaterials that can be used in various electromagnetic applications, such as beam focusing, cloaking, and tunneling, to name a few [1]–[3]. These structures, which effectively demonstrate refractive index values that are close to zero, can be obtained by properly arranging unit cells, such as dielectric rods. The use of dielectric rod arrays for their metamaterial properties is widely known in the literature. However, in most of the studies, the dielectric rods are assumed to have perfect geometric shapes, such as cylinders [4] with a predefined and fixed cross section. In this study, we consider NZI structures that are constructed by using dielectric rods with varying cross sections and employ this variability for the purpose of designing new devices.

We introduce two new types of dielectric rods, specifically, those with concave and convex shapes. Considering different cross-sectional shapes, we investigate the effect of height of the rods on the electromagnetic characteristics of NZI metamaterials, as the height can significantly alter scattering and radiation patterns. We show that, by reshaping the rods in various ratios in terms of convex and concave shapes, the electromagnetic properties of NZI structures can be manipulated. Specifically, electromagnetic responses of the considered NZI structures depend on both cross sections, i.e., concave or convex, and height values. The obtained results illustrate not only dependence but also the high sensitivity of electromagnetic responses on the cross sections of dielectric rods. Consequently, our preliminary findings demonstrate the feasibility of using the designed structures as compact and sensitive sensors.

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A Hadamard Variational Formula for a Laplace-Steklov EVP: Derivation and Applications

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We focus on a Laplace-Steklov eigenvalue problem, and aim at deriving an associated first order Hadamard-type variational formula. The eigenproblem is a novel one that is characterized by the spectral parameter appearing both in the differential equation and boundary conditions. The primary objective is to analyse the effects of boundary variations on the spectrum of the associated operator under some assumptions. We consider a number of applications of this Hadamard variational formula which are based on some variations of the unit disc. We obtain the corresponding rates of change of the eigenvalues as the boundary of the problem domain deforms. We illustrate these results by means of various numerical examples obtained using a standard finite element method.

The variable sum exdeg index

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Many topological indices have been introduced and studied on different graphs. These studies have been done on deterministic structures and graphs with the lowest and highest values of these indices have been determined. On the other hand, the probabilistic study of these indices has received less attention due to the complexity of the calculations. Also, the probabilistic study is always accompanied by various restrictions during the investigation. One of these indices that has been studied less even in deterministic structures is the variable sum exdeg index. This index firstly introduced by Vukicević to predict some physicochemical properties of chemical compounds. Let G be a (finite, simple, and connected) graph with vertex set $V(G)$ and and edge set $E(G)$. The variable sum exdeg index of G is defined as

$$S_a(G) = \sum_{uv \in E(G)} (a^{d(u)} + a^{d(v)}) = \sum_{v \in V(G)} d(v) a^{d(v)},$$

where $a \in (0, 1) \cup (1,\infty)$, and $d(v)$ is the degree of a vertex $v \in V(G)$. Through a recurrence equation, we determine the expectation and the variance of this index in random tree structures for domain $a \in (0, 1)$. Also, we show some convergence in probability related to this index. As the main result and through the martingale central limit theorem, the asymptotic normality of this index is given.

Design and Simulation of Electromagnetic Beam Splitters Based on Near-Zero-Index Metamaterials

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Near-zero-index (NZI) materials have received a lot of interest in recent years because of their unique ability to alter electromagnetic waves. These materials possess effective refractive indices close to zero, resulting in extraordinary wave phenomena. Thanks to these features, they can be used in diverse applications, such as wave transformation, beam focusing, and invisibility cloaking, to name a few [1]. Near-zero refractive index values can be achieved by simultaneously decreasing relative permittivity and permeability, leading to epsilon-mu-near-zero (EMNZ) materials, which are used in this study. EMNZ materials can be realized by periodically arranged dielectric rods [1].

Due to the extremely small constitutive parameters of NZI structures, their simulations are quite challenging. Therefore, we use an efficient simulation environment based on novel surface formulations and the multilevel fast multipole algorithm (MLFMA) [2]-[4]. In addition, we use a low-frequency form of MLFMA [3]. The proper use of surface formulations and MLFMA enables us to reach potential designs that can be realized by periodically arranging unit cells. We note that NZI shells as beam generators [5], which have central cavities, with inner excitations have been examined in detail. In this novel study, NZI structures are externally excited by using directive sources, such as complex source point beams (CSPBs). We aim to receive incoming waves and split them in intended directions via the designed NZI structures.

In this study, our aim is to obtain transmitter-receiver (transceiver) devices with relatively compact geometries. To achieve this homogeneous models are initially designed. Then, successful homogeneous NZI designs in terms of power density distributions are realized by dielectric rod grids.

In conclusion, we present design and simulation of electromagnetic beam splitters that are based on NZI materials. The initial results demonstrate that re-directing beams may be achieved by using relatively compact geometries. However, receiving incoming fields efficiently with small amounts of reflections appears to be a major challenge for NZI beam splitters. Research is ongoing to improve the designs by minimizing reflections via optimizations.

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Calibration-Based Polynomial-Fit Non-Uniformity Correction on Thermal Imaging Systems

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Infrared Focal Plane Arrays (IRFPAs) are used in many areas today as they provide the imaging ability to electro-optical systems. However, the raw images acquired from IRFPAs are usually not useful forthwith since there exist several undesired effects. Non-uniformity (NU) is one of these undesired effects which is caused by several factors such as the cosine-fourth-power effect, photo-detectors on IRFPA being nonidentical, fixed-pattern noise, etc. To eliminate NU and obtain a clearer image, an appropriate non-uniformity correction (NUC) procedure must be applied to the raw image. There are fundamentally two different types of NUC methods that are scene-based and calibration-based. Calibration-based methods rely on adjusting the responsivity of each photo-detector on IRFPA by calibrating the photo-detector response with the help of a uniform radiation source, while scenebased methods rely on correcting the image based on scenery by adjusting NUC parameters in run time with the help of neural-network algorithms, Kalman filter, etc. In this study, a calibrationbased Polynomial-Fit NUC (PFNUC) method is presented and compared to a 2-point NUC (2PNUC) method that is currently used in a serial production thermal imaging system. 2PNUC is one of the most common NUC methods used in thermal imaging systems, where the response of the IRFPA is calibrated based on the raw images taken from a blackbody (BB) at two different temperatures. A gain factor and an offset value are calculated for each photo-detector by using digital signal levels (well-fill level) of the raw image. Ultimately, a gain and an offset table (NUC tables) are formed and applied to the raw image. In serial production systems, each system is usually calibrated at constant BB temperatures. However, this is not appropriate since there may be a considerable amount of variance in the average responsivity of IRFPAs used in systems that may be caused by a couple of reasons such as the different optical transmissions in optics due to imperfection in optical coatings, primitive methods during focus and alignment of the optics, slightly different gain factors on the read-out circuits of the IRFPAs, etc. Given that, when 2PNUC is performed at constant BB temperatures, it leads to both systems being calibrated at different well-fill levels and having different residual NU (RNU) over their dynamic range, which is quite an unwanted characteristic from systems of the same production line. RNU is a measure of how non-uniform is the response of the IRFPA when a uniform radiation source is present in its field of view and an evaluation metric for the NUC method. Despite the average responsivity variance in IRFPAs, the well-fill curve characteristics are quite similar, so it is possible to perform a polynomial fitting. Given that a PFNUC method is proposed and the responses of IRFPAs are calibrated based on a third-order polynomial-fit estimation in which the well-fill levels of each photo-detector are fitted to the median values of IRFPA at four different raw BB images over the dynamic range. By doing so, the coefficients of the fitted polynomial are calculated and the PFNUC tables are formed. A third order PFNUC covers the polynomial characteristics of photo-detectors' responsivities on IRFPA greatly and it decreases the total RNU by around 50% on average.

Keywords: Thermal Imaging Systems, Infrared Focal Plane Array, Non-Uniformity Correction, Sensor Characterization, Serial Production Systems

Data-Driven Model Discovery and Control: Parallel Computation-Based Testing and Analysis

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Dynamic Mode Decomposition with Control (DMDc), a data-driven model discovery technique together with integral action based Model Predictive Control (MPC) was tested for a single operating point of the aircraft, and its real-time applicability was explained in studies [1]-[2]. Now in this paper, these studies have been expanded and the DMDc-MPC framework is tested under many different operating conditions.
To comprehensively evaluate the DMDc-MPC technique's adaptability and performance, a series of tests are conducted under a variety of conditions. Parallel computation is employed to facilitate rapid and scalable testing, enabling the quick analysis of the DMDc-MPC framework behavior. The elapsed times resulting from parallel calculation are compared with serial calculation.
This research contributes to the advancement of control strategies for highly maneuverable aircraft, shedding light on the potential of the DMDc-MPC technique in addressing the unique challenges posed by these aircraft. The findings serve as a foundation for further research and development in the field of autonomous and agile flight control.

Keywords: DMDc-MPC, Highly Maneuverable Aircraft, Parallel Computation, Flight Control, Model Predictive Control, Adaptability, Autonomous Systems

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New finite differences for solving equations of the modified Helmholtz type

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Finite difference methods (FDMs) are widely used in the solutions of many linear and non-linear ordinary and partial differential equations. In this study, a new finite difference method has been developed to solve boundary value problems governed by a differential equation in the form of a modified Helmholtz equation. The new FDM is derived from the conventional FDM by reducing the truncation error in the finite difference formulas used for the approximation of the derivative terms, [1, 2]. Because it does not involve truncation error, the new FDM is considered a numerically precise approach. The derivative-type boundary conditions are also approximated by using the same concept. Although the linear systems generated by the new and conventional FDMs have identical structures, the new FDM solves the governing continuous problem without the need for a fine mesh and produces more accurate results. The application problem has been selected from the area of magnetohydrodynamics, which is an appealing and comprehensive research field in fluid dynamics, in order to establish and verify the FDM codes and to carry out a quantitative comparison of the new and conventional finite difference approaches.

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Mitigating noise-related object detection problems in JWST MIRI images by FFT-based methods

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Various methods developed to disentangle source signals in images from noise signals. Several noise profiles are well-defined and can be extracted from the image comparatively easily. Others can be more random, and worse still, they can compound the noise in images together which further jeopardizes reaching the actual signal from the source.

Fourier transformation and related techniques project the digital numbers in the images into the spectral domain and facilitate the removal of periodic noises. The level-3 data from the Middle Infrared Imaging (MIRI) instrument of the James-Webb Space Telescope (JWST) also suffers from many types of noises, including pattern-like periodic ones. This situation is even more pronounced when the brightness value (again digital numbers) read from the detector is low. In other words, MIRI images of darker regions of the space have visible periodic noise as vertical and horizontal strips. As a result, masking of faint objects and spurious false positives by these prevent reaching 100 % potential of this critical data source.

This study first utilizes Fast Fourier Transformation (FFT) and relevant techniques to separate source signals and noise from benchmark image data with varying types and intensities of sources. Then, it will show the results of applying this post-processing to the MIRI images on the standard celestial object detection algorithms, e.g., aperture photometry. All codes will be in Python and provided right after the presentation, and the data was downloaded from the Mikulski Archive for Space Telescopes, MAST of Space Telescope Science Institute.

Multi-Criteria Decision Making with Various Fuzzy Sets

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Multi-Criteria Decision Making (MCDM) is a fundamental framework for tackling complex decision problems characterized by multiple conflicting criteria. Fuzzy sets, introduced by Zadeh in the 1960s, have significantly enriched MCDM (1) by providing a means to model and manage uncertainty and imprecision. This abstract provides a comprehensive overview of various fuzzy set types, including Type-1 (2), Type-2 (3), Intuitionistic (4), and Q-Rung fuzzy sets (5), within the context of MCDM. These fuzzy sets offer a flexible approach for representing and reasoning with vague and ambiguous information.
The abstract explores the fundamental characteristics, and integration methodologies of these fuzzy sets. Decision-makers across diverse domains benefit from these fuzzy sets by gaining the ability to make informed choices while considering various criteria and sources of uncertainty.

Keywords: Multi-Criteria Decision Making, Fuzzy Sets, Type-1 Fuzzy Sets, Type-2 Fuzzy Sets, Intuitionistic Fuzzy Sets, Q-Rung Fuzzy Sets, Uncertainty Modeling, Decision Support, MCDM Applications.

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Forecasting the Evolutionary Pathways of the SARS-CoV-2 Spike Protein via the Calculation of Mutability Landscapes

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Viruses, known as infectious agents, cause diseases and deaths in humans. Although vaccines and drugs have been developed to prevent these effects, through mutations in the genetics of viruses, the virus acquires features such as escaping the immune system and binding better to the host cell, thus becoming resistant to the treatments offered. The global COVID-19 pandemic has highlighted the need for rapid, reliable, and efficient tracking and forecasting of the changes in genetic material as new SARS-CoV-2 variants arise. Developing appropriate drugs and vaccines for the new genetic content of the virus is costly and takes a long time. For this reason, it is of great importance to be able to predict the mutations that may occur in the genetics of SARS-CoV-2 and the effects of these mutations before they occur and take the necessary precautions. Here we studied the evolution process of SARS-CoV-2 and predicted the key mutations that may occur in the future. To this end, first, the gene sequences of the spike region are obtained from GISAID database, and then the sequences are aligned with various multiple alignment methods (Clustal Omega, MAFFT, TCoffee, etc.). Then these alignments are used to calculate the mutability scores for each amino acid using scoring functions (Karlin, Sander, Valder, etc.). By examining the correlation between the scores obtained, regions that are protected and prone to change have been obtained. Future mutations have been predicted by examining using the calculated mutability scores and the experimental mutation rate ($8x10^{-4}$ mutation/nucleotide/year) obtained, using random walk method.

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Controlling the Molecular Structure and Electrical Conductivity of DNA via Photoswitch Molecules

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The ever-increasing size of digital data requires novel storage techniques and materials that provide data storage densities surpassing today's semiconductors. It is also important to write, read and store at a low cost and in an energy efficient manner. Biomolecules such as DNA and RNA, which are the fundamental building blocks for genetic information, are considered as a solution to this problem. Over the last two decades, it has been shown that the electrical conduction of DNA can be controlled by sequence, environmental factors and doping with different molecules. Uncovering the mechanisms of these effects is important to create DNA based circuits with desired properties. It is also known that light-sensitive molecules such as azobenzene, butadiene and stilbene change their structure (cis/trans) when excited by light of different wavelengths, and such molecules are called photoswitch molecules. Here, we investigated whether the conductivity of DNA can be controlled with the help of photoswitch molecules using atomistic and quantum mechanical methods.

In this presentation, we first discuss the results of the molecular dynamic trajectories and the effect of the attached photoswitch molecules on the selected DNA sequences. Then we used clustering algorithms to find the most representative molecular conformation for further analysis. Finally, the electrical conductivities of the bare DNA and the azobenzene (cis and trans) attached DNA were calculated using DFT and Green Function based transport calculations. We demonstrated that, the photoswitch molecules can be used to tune the conductivity of DNA.

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Investigating the Charge Transport Properties of Nucleic Acid Analogues with Density Functional Theory

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In terrestrial organisms, DNA carries genetic information and plays roles in protein synthesis and evolution through mutations. Besides its importance in life, DNA is also a significant building block for nanotechnology applications, especially for molecular electronics with their self-assembly ability and tunable electronic conductivity. Even though they can act as transistors, rectifiers etc. with their electronic characteristics, integration of DNA to electronic devices have some difficulties within currently available technologies due to its unstable behavior in high temperatures (above ~70 oC). By using nucleic acid analogues, which have similar properties with DNA but have more structural stability in higher temperatures, we may overcome this limitation. Here, we showed that nucleic acid analogues can create different charge transport pathways by using molecular dynamics and DFT (Gaussian 09, B3LYP/6-31G(d,p)) calculations. First of all, the necessary force field parameters for the analogues are generated by using antechamber based on bsc1 and gaff force fields, and partial charges are calculated with DFT (Gaussian 09, B3LYP/6-31G(d,p)) for unknown parts of the nucleic acids. After the MD simulations, we classified the conformations with clustering algorithms among 50,000 different molecular structures. We select the representative conformation of each different cluster to see the effect of different conformations on the overall charge transport properties of the molecule. Our research shows that different conformations of the same molecule and the density of states in the electrode coupled region of the DNA affect the charge transport properties. We showed that modifying DNA with the analogues can decrease the conductance up to 10 times.

Keywords: DNA, RNA, Nucleic Acid Analogues, Electrical Conductivity, Molecular Dynamics, Density Functional Theory

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Homogenization of nanocomposites with agglomerating particles using embedded element method

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Composite materials are used in different industries due to their superior and tunable properties. On the other hand, analytical approaches and tests are challenging and insufficient in the computation of their mechanical properties. Therefore, precise and efficient procedures should be used to calculate their homogenized effective properties.

The aim of this study is to create a framework to compute the effective mechanical properties of nanocomposites efficiently and precisely. A crucial point to consider while calculating the effective properties is the effect of agglomeration. The agglomeration generally negatively affects the mechanical properties of nanocomposites.

While achieving the objective, various methods are employed, and scripts are developed to ease the computational process. The preprocessing effort and the computational cost are decreased using representative volume elements and employing the embedded element method. Numerous studies have been conducted to prove the efficiency and reliability of the methods. After proving that the aforementioned approaches give compatible results after convergence studies, the outcomes of the studies are presented.

Agglomerations are formed as larger spheres inside the matrix. Close particles vanish, and agglomeration is placed instead of selected particles. The mechanical properties of the agglomeration are assigned using the inverse rule of mixture. The effect of the agglomerations is observed by comparing the homogenized elastic properties of cases with and without agglomerations using the computational homogenization method. Also, a study is conducted showing the relation between the particle size and agglomeration effect on mechanical properties. Ultimately, the results are compared with the literature, and similar trends in the degradation of elastic properties are observed.

Topology Optimizations of Dielectric Slabs Using Machine Learning and Genetic Algorithms

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In electromagnetic applications, optimizations are crucial to reach high-performance designs in terms of electromagnetic features on demand, including but not limited to absorbers, antennas, metamaterials, frequency-selective surfaces, optical and photonic devices, and solar cells. Among many optimization methods, heuristic ones, e.g., genetic algorithms (GAs), are usually used to reach optimal devices since objective functions of optimization problems are easy to define, even consisting of multi-objective ones, in heuristic algorithms. Recently, we have shown various electromagnetic design applications [1] using a combination of GAs and the multilevel fast multipole algorithm (MLFMA). However, due to the nature of heuristic algorithms, optimizations require large numbers of generations, i.e., they may require too much time to reach optimal structures. In addition, such algorithms may provide poor results in multi-objective cases.

In this study, we present an effective optimization technique that requires small numbers of generations for topology optimizations of three-dimensional dielectric slabs to be employed in electromagnetic applications, such as absorption, reflection, scattering, and transmission. The optimization method involves an effective combination of self-directed machine learning [2], GAs, and the MLFMA. A neural network is integrated with MLFMA solutions to be substituted as the optimization objective. As generations progress, in order to obtain a highly accurate network in accordance with the optimization objective, the network's training data is improved by new MLFMA solutions based on the network's prediction of the optimal design (self-directed), which is obtained by using GAs. Considering dielectric slabs, we perform consecutive, as well as simultaneous, shaping of top and bottom surfaces. In order to carry out free deformations to reach optimal designs that can be fabricated via 3D printers, a multi-grid approach with Bezier surfaces [3] is employed. In order to perform multi-grid optimizations, grid sizes that contain control points to define Bezier surfaces are systematically changed during optimization generations. This way, grids become finer as generations progress, allowing crucial fine-tuning operations in the last stages of optimizations.

We present rigorous optimizations, which show that slabs with desired electromagnetic properties can be obtained via the presented method. Initial numerical results demonstrate the success of the developed optimization method compared to the traditional GAs in terms of the number of generations, particularly considering the total times required to reach solutions, and the success of final designs considering objective functions.

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Topology Optimization using Lattice Materials with Isotropy Condition

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Lattice materials have a lot of advantages such as lightness, stiffness, vibration damping, and heat insulation. Nowadays the use of lattice materials has begun to become widespread in many different areas since the designs which are generated by lattice materials can be manufactured with additive manufacturing technologies. When the design is performed by lattice materials proper densities of lattice cells in a part are determined by doing density mapping with homogenization-based topology optimization. However, the mechanical behaviors of most of the lattice materials which change by direction as with composite materials are not isotropic. For the Solid Isotropic Material with Penalization (SIMP) method, which is used commonly in topology optimization for density mapping in commercial software due to its simplicity, some problems appear in the use of lattice materials, since homogenized properties, which are not isotropic, generate different stress and displacement in different direction.
The method of isotropy conditioned density mapping (ICDM) is proposed to solve the problem within the scope of this thesis. Lattice cells, which are modeled by strut elements that ensure isotropy condition of homogenized elastic properties at whole density values, are determined with this proposed model. Since these lattice cells ensure isotropy conditions, the SIMP method can be used in topology optimization. The density range, which can be used in topology optimization, is determined to be produced with additive manufacturing. To show the effectiveness of the proposed method, three-dimensional examples used in the literature have been designed. The results of the optimized design which is generated by the proposed ICDM model are compared with the results in the literature to demonstrate its effectiveness. It was shown that macroscopic distributions of lattice cells can be obtainable with topology optimization with the SIMP method available in commercial software when the lattice configurations, which ensure isotropy condition, are determined with this proposed method.

Keywords: Lattice materials, Homogenization, Isotropy, Topology optimization, Additive manufacturing.

The Utility of Docking Programs for the Characterization of Peptide Protein Interactions

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Characterized by headache, fever, dyspnea, and even acute respiration distress syndrome and multiple organ failure, COVID-19 is a disease caused by SARS-CoV-2. This virus enters the host cell via its Spike Glycoprotein, interacting with host cell transmembrane protein ACE2 (angiotensin II converting enzyme). Therefore, to develop drugs against this disease, Spike Glycoprotein of SARS-CoV-2 and its specific interactions with ACE2 has a great importance. Due to their unique specialties such as being flexible, biocompatible, and target-specific, peptides are perfect candidate for rational drug design. Therefore, peptide-based drug design against COVID-19 by targeting to block Spike-ACE2 interaction is thought to be one of the best strategies on preventing the entry of the virus. Here we studied the efficacy of various molecular docking programs (i. e., Autodock Vina, HADDOCK, HPEPDOCK etc.) in terms of their ability to identify the binding site, binding conformation, and binding affinity. To this end, we conducted two benchmarking studies to dock known small molecules and peptides onto proteins. In the first one, we chose neuraminidase protein as the receptor protein and commercial drugs such as Oseltamivir, Laninamivir, Zanamivir and Peramivir as ligands. These drugs are used against H1N1 influenza virus, and their binding characteristics are well studied. In the second one, we use the same set of programs to dock peptides onto Spike Glycoprotein. These peptides have been obtained from ACE2 protein, which takes place in the Spike-ACE2 interaction site. Here, we discuss the results of the benchmarking studies and the efficacy of molecular docking programs for further design of peptide-based drugs against COVID-19.

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Phase-Field Regularized Cohesive Modeling of Hydraulic Fracture

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Hydraulic fracturing is a drilling method that facilitates the extraction of underground energy resources such as hydrocarbons and geothermal energy through the injection of high-pressure fluid into low-permeable reservoirs. Over the last decade, the hydraulic fracturing of porous reservoirs has gained much attention due to the drastically increased demand for underground energy resources. Besides the fieldwork and experimental studies, the theoretical and numerical modeling of hydraulic fracture using crack modeling has also become an active area of research. To model the crack onset and propagation in hydraulically fracked media, the phase-field method is one of the most prevalent fracture modeling approaches. Despite its advantages, the crack opening displacement calculation using the phase-field method remains arduous due to the crack-smearing nature of the phase-field method. On the other hand, the crack opening displacement is required to model fluid flow in the crack of hydraulic fracturing. In this study, we propose a novel and efficient crack-opening displacement calculation method incorporated into a multiphase model for the hydraulic fracturing of porous media using the phase-field model. To this end, the behavior of porous media is modeled within the framework of poroelasticity, while the phase-field method accounts for the cohesive fracture in a saturated porous medium created by the pressurized injection fluid. The fluid flow in the crack is modeled using the Darcy-Poiseulle flow and a novel crack-opening displacement method. The modeling capacity of the proposed approach is demonstrated through representative numerical examples that include comparative studies with the existing crack-opening calculation procedures.

Keywords: Phase-field method, Crack opening displacement, Hydraulic fracturing.

Numerical Simulation of Low-Velocity Impact on [05/903]s CFRP Beam Considering Accurate Experimental Conditions

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Composite materials are extensively employed in aerospace, renewable energy, and transportation industries due to their exceptional strength-to-weight ratios. However, their weak interfacial characteristics make them vulnerable to out-of-plane loadings, including lowvelocity impact (LVI) events, which can result in internal failures like matrix cracking and delamination. While experiments can determine the failure behaviour and resistance of composites to LVI, there is a growing interest in replacing a significant portion of experimental efforts with physically accurate numerical simulations. To validate these simulations and their associated damage models, direct observation of the dynamic evolution of damage becomes important. In a recent experimental study by Bozkurt and Coker [1], [05/903]s CFRP beam specimens subjected to transverse impact loadings were analysed with full-field digital image correlation method, and in-situ progression of matrix cracking followed by dynamic progression of delamination were captured. In this study, we constructed the finite element (FE) model of the LVI experiments presented in [1]. Our objectives are to reproduce the observed damage accurately and to investigate its dynamic progression beyond the limitations of experimental observations. The numerical model is constructed in the commercial FE package ABAQUS/Explicit and incorporates the following features. For modeling ply damage, we employed a three-dimensional continuum damage mechanics approach, utilizing the LaRC05 damage initiation criterion implemented through a user-defined subroutine (VUMAT) with an explicit integration scheme. To simulate delamination damage, we employed the cohesive zone method and inserted built-in cohesive elements at the 0°/90° interfaces. To replicate the experimental boundaries, we proposed a heuristic approach for modeling boundary conditions (BCs) by assembling spring elements at the corresponding boundary nodes. The stiffness of these springs was determined based on minimizing the differences between the full-field displacements and strains obtained from both the experiment and simulation. The numerical simulations showed good agreement with the experimental results in terms of failure load, sequence, and initiation location. The influence of experimental boundaries on the dynamic damage characteristics is illuminated by utilizing the proposed BCs approach. By comparing the numerical findings with the experiments, we gained further insights into the damage growth in composite beams under LVI loading.

Keywords: Polymer-matrix composites, Low-velocity impact, Finite element method.

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