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FOREWORD

Over the past two decades, computational science and engineering (CSE) has become an increasingly important part of research in academia, industry, and laboratories. Mathematics-based advanced computing is now a prevalent means of discovery and innovation in essentially all areas of science, engineering, technology, and society, and the CSE community is at the core of this transformation. The purpose of this workshop is to bring together researchers and scientists from a diversity of sub-disciplines from the fields of computational mathematics and engineering in Turkey and to create a stimulating atmosphere where researchers can meet and hear about each other’s work, hold discussions, exchange of ideas and experiences and hopefully initiate future collaborations.

We would like to thanks to all the participants with special emphasis to those who will enhance the quality of this workshop with their contributed talks.

Scientific Advisory Committee:

- Serdar Göktepe, Department of Civil Engineering, METU
- Bülent Karasözen, Institute of Applied Mathematics, METU
- Münevver Tezer, Department of Mathematics, METU
- Ömür Uğur, Institute of Applied Mathematics, METU
- Hamdullah Yücel, Institute of Applied Mathematics, METU

Organizing Committee:

- Pelin Çiloğlu, Institute of Applied Mathematics, METU
- Eda Oktay, Institute of Applied Mathematics, METU
- Ömür Uğur, Institute of Applied Mathematics, METU
- M. Alp Üreten, Institute of Applied Mathematics, METU
- Süleyman Yıldız, Institute of Applied Mathematics, METU
- Hamdullah Yücel, Institute of Applied Mathematics, METU
PROGRAMME

Saturday, 20 October 2018

08:30 - 09:15  Registration
09:15 - 09:30  Welcoming Remarks
09:30 - 10:50 Contributed Talks (Chair: Hamdullah Yücel)
10:50 - 11:10 Break
11:10 - 12:30 Contributed Talks (Chair: Hamdullah Yücel)
12:30 - 13:30 Lunch
13:30 - 14:50 Contributed Talks (Chair: Ömür Uğur)
14:50 - 15:10 Break
15:10 - 16:50 Contributed Talks (Chair: Murat Uzunca)
17:30 - Dinner at Çadır Kebap

Sunday, 21 October 2018

09:30 - 10:50 Contributed Talks (Chair: Murat Manguoğlu)
10:50 - 11:10 Break
11:10 - 12:30 Contributed Talks (Chair: Serdar Göktepe)
12:30 - 13:30 Lunch
13:30 - 15:10 Contributed Talks (Chair: Özgür Ergül)
15:10 - 15:30 Break
15:30 - 16:30 Panel Discussion (in Turkish)

Format of the Contributed Talks:

- The order of the speakers will be determined through random choice, by drawing names out of a hat. Speakers cannot request a specific time to talk.
- Each speaker should introduce himself or herself, the title and topic, and is expected to leave sufficient time, within the allocated time-slot, for discussion. Speakers have to prepare a talk that can be trimmed to various lengths (from seconds to 20 minutes). For a smooth meeting, the time table will be strictly enforced.
- As there exist limited slots for presentations, the accepted talks will be announced after the scientific evaluation.

Panel Discussion (in Turkish):

Mathematics-based advanced computing is now a prevalent means of discovery and innovation in essentially all areas of science, engineering, technology, and society, and the CSE community is at the core of this transformation. The aim of this panel is to discuss

Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey
• graduate education in computational science and engineering,
• how we can improve collaborations between mathematicians and engineers.
ABSTRACTS
In this study, a fast and efficient optimization environment is proposed for the design of arrays of nanoparticles with plasmonic properties, which can be utilized as crucial devices in the state–of–the–art nano-optical systems. This kind of arrays are already among the major instruments of THz and optical applications like optical power transmission, bio–sensing, light–beam steering, and optical coupling, thanks to their strong interactions with electromagnetic waves and ability to manipulate waves in subwavelength scales. In this study, we particularly focus on designing arrays of nanoparticles for two major purposes. The first is to gain active control on the radiation and scattering characteristics for beam steering applications [1], while the second is to obtain full transmission along bended nanowire systems [2]. Finding optimal array configurations for such type plasmonic problems requires extremely many computational simulations based on different parameters. Moreover, plasmonic properties of nanostructures result in significant numerical difficulties in their full-wave solutions. In this study, a novel mechanism has been developed for rigorous designs of nanoparticle arrays by combining genetic algorithms and a solver module based on surface integral equations and MLFMA. An electromagnetic problem can be defined as unknown electric and magnetic current densities induced on the plasmonic nanostructures that are located in a host medium under the excitation of external sources. For solutions, 3D surface models of metallic nanostructures are discretized by using triangular meshes, while the unknown surface current densities are represented as weighted sums of basis functions. Plasmonic properties of metals are included in these equations by using the frequency–dependent complex permittivity values depending on the material. Among different formulations known in the literature, MCTF is used as the main formulation since it is known to provide more accurate results for plasmonic objects in comparison to other formulations [3]. Dense matrix equations representing the discretized MCTF are solved with iterative Krylov–subspace algorithms and these solutions are accelerated by performing matrix vector multiplications with MLFMA. This solver module is integrated with an in–house implementation of genetic algorithms to find optimal configurations of nanoparticles for desired electromagnetic responses. Optimization trials are further accelerated by performing simultaneous simulations on multiple cores. The optimization mechanism provides interesting designs for nanoparticle arrays that demonstrate unprecedented levels of efficiency in target applications.

Bibliography

The Solution of MHD Duct Flow Inverse Problem using the DRBEM

Cemre Aydin¹, Munevver Tezer-Sezgin²

¹ Department of Mathematics, METU, Ankara, Turkey
² Department of Mathematics, METU, Ankara, Turkey

The Magnetohydrodynamic (MHD) flow in a rectangular duct where one part of its boundary allows both the varying conductivity and the slipping velocity is formulated as a direct and boundary inverse problem. The inverse formulation of the problem is constructed with underspecified and over-specified boundary conditions for the induced magnetic field and the velocity on opposite parts of the duct walls. The aim is to recompute both the conductivity constant in the induced current, and the slip length of the velocity on the underspecified wall. The convection-diffusion type MHD coupled equations for the direct and inverse formulations are discretized and solved as a whole by using the dual reciprocity boundary element method (DRBEM). The DRBEM provides both the velocity and induced magnetic field and their normal derivatives to be used as overspecified boundary conditions for the construction of inverse problem. In this study, two regularization techniques, namely as the Tikhonov regularization [1] and the well-posed iterations [2], are used for the ill-conditioned system of linear equations resulted from the discretization of the inverse problem. Slip velocity and induced magnetic field behaviours are examined for Hartmann number values in the range $Ha \leq 50$. Discretizing only the boundary of the problem region and providing both the unknowns and their normal derivatives on the underspecified wall are the main advantages of the DRBEM [3] for boundary inverse MHD flow duct problem so that the conductivity constant and the slip length between them can be recovered.

Bibliography

Fundamental Axisymmetric MHD Creeping Flows Produced by a Circular Ring Located Near a Plane Solid Slip Wall

Selçuk Han Aydin¹, Antoine Sellier²

¹ Department of Mathematics, Karadeniz Technical University, Trabzon, Turkey
shaydin@ktu.edu.tr

² LadHyX, Ecole Polytechnique, Paris, France
sellier@ladhyx.polytechnique.fr

This work determines two fundamental axisymmetric MHD viscous flows produced by distributing point forces on a circular ring immersed in a conducting Newtonian liquid, with uniform viscosity $\mu$ and conductivity $\sigma > 0$, bounded by a plane solid slip wall. Each flow has no swirl and satisfies a Navier slip condition, with slip length $\lambda \geq 0$, on the wall which is normal to the uniform magnetic field $B$ prevailing in the liquid. In addition, the circular ring plane is parallel with the wall while the ring-wall gap is $z_0 > 0$ and the ring radius is $r_0$. One flow is obtained by putting on the ring point unit forces parallel with $B$ while the second flow is induced by a radial distribution of unit forces on the ring. Both velocity and pressure fields for these flows are analytically obtained and the resulting flow patterns are numerically investigated versus $r_0, z_0, \lambda$ and the so-called Hartmann layer thickness $d$. 

Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey
Discontinuous Galerkin Methods for Unsteady Convection Diffusion Equation with Random Coefficients

Pelin Çiloğlu¹, Hamdullah Yücel²

¹ Institute of Applied Mathematics, METU, Ankara, Turkey  pciloglu@metu.edu.tr
² Institute of Applied Mathematics, METU, Ankara, Turkey  yucelh@metu.edu.tr

Partial differential equations (PDEs) with random input data is one of the most powerful tools to model oil and gas production as well as groundwater pollution control. However, the information available on the input data is very limited, which causes high level of uncertainty in approximating the solution to these problems. To identify the random coefficients, the well-known technique Karhunen Loève (K–L) expansion has some limitations. K–L expansion approach leads to extremely high dimensional systems with Kronecker product structure and only preserves two-point statistics, i.e., mean and covariance. To address the limitations of the standard K–L expansion, we propose Kernel Principal Component Analysis (PCA).

In this talk, we investigate the numerical solution of unsteady convection diffusion equation with random input data by using stochastic Galerkin method. Since the local mass conservation play a crucial role in reservoir simulation and transport problem, we used discontinuous Galerkin method for the spatial discretization. On the other hand the dG(0) is performed for the temporal discretization. We provide some numerical results to illustrate the efficiency of the proposed approach.

Bibliography

A Numerical Study of Second Order Time Stepping Methods for the Boussinesq Equations

Medine Demir¹, Aytekin Çibik², Songül Kaya Merdan³

¹Middle East Technical University, ²Gazi University, ³Middle East Technical University

dmedine@metu.edu.tr, abayram@gazi.edu.tr, smerdan@metu.edu.tr

The Boussinesq approximation is a way to solve nonisothermal flow such as natural convection problems, without having to solve for the full compressible formulation of the Navier-Stokes equations. Natural convection is related with an increasing number of fields including oceanography, meteorology and geophysical context [1, 2, 4]. Moreover, because of its presence both in nature and engineering applications, it has highly taken attention from academic societies. The accurate and efficient numerical solution of these flows are known to be the core of many applications.

In this context, we aimed to study a new, efficient and accurate numerical scheme for a family of second order time stepping methods for the Boussinesq system, by extending an earlier study of [3] for the Navier-Stokes equations (NSE) based on the pioneering work for [5, 6]. The main idea of this study is to incorporate linearizations and stabilization terms such that the discrete curvature solutions in velocity, temperature and pressure are proportional to this combination. The method requires the solution of only one linear system per time step. We prove unconditional stability of the method and also derive a priori error bound. The derived theoretical results are supported by several numerical experiments which prove the efficiency and the accuracy of the method.

Bibliography


Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey
Parameter Control for Fluid Flow and Heat Transfer with Variable Viscosity Under the External Magnetic Field

Cansu Evcin\textsuperscript{1,4}, Ömür Uğur\textsuperscript{2}, Münnevver Tezer-Sezgin\textsuperscript{3}

\textsuperscript{1} Institute of Applied Mathematics, METU, cbilgir@metu.edu.tr
\textsuperscript{2} Institute of Applied Mathematics, METU, ougur@metu.edu.tr
\textsuperscript{3} Department of Mathematics, METU, munt@metu.edu.tr
\textsuperscript{4} Department of Mathematics, NKU

Optimal control solution of the laminar, fully developed, steady electrically conducting fluid flow with the heat transfer is considered under the effect of an external uniform magnetic field. Either the fluid is Newtonian with a temperature dependent viscosity, where the Hall effect is also taken into consideration, or the fluid is non-Newtonian, which is modeled by a power law model with a flow dependent viscosity. The viscous and Joule dissipations are included and the flow is driven by a constant pressure gradient. The nonlinear set of momentum and energy equations are solved by using finite element method (FEM) with the implementation of Newton’s method for nonlinearity. Accordingly, FEM solutions are obtained for various values of the problem parameters to ensure the efficiency of the underlying scheme. The FEM results obtained in this study \cite{1,2} are not only in good agreement with, but also extends, the results in the literature \cite{3,4} in terms of accuracy and intervals of the problem parameters.

This study aims to investigate the problem of controlling the steady flow by using the physically significant parameters of the problem as control variables: Hartmann number (Ha), Brinkmann number (Br), Hall parameter (\(m\)) and viscosity parameter (\(B\)) in the case of temperature dependent viscosity. For the case of power law fluid the control parameters are Ha and the flow index (\(n\)). The optimization is implemented by the discretize-then-optimize approach with a gradient based algorithm. Starting with an initial estimate the optimization loop to calculate new estimates for optimal solution repeated until the norm of the gradient of the reduced cost function is less than a predefined tolerance. Control variables are considered as single and pairwise as well. Numerical results ensure that the proposed control approach is effective at driving the flow to prescribed velocity profiles as well as isolines.

Bibliography


\cite{2} Cansu Evcin, Ömür Uğur, and Münnevver Tezer-Sezgin. Controlling the power law fluid flow and heat transfer under the external magnetic field using the flow index and the Hartmann number. International Journal of Computational Methods, 2018.


The present study focuses on the boundary type method solution of the magnetohydrodynamic (MHD) flow which is governed by the nonlinear convection-diffusion type equations coupled in velocity and magnetic field. The numerical method is based on the use of boundary element method (BEM) with two different formulations, namely domain BEM (DBEM) and dual reciprocity BEM (DRBEM) in the spatial discretization; and a backward finite difference scheme is adopted for the time integration. These MHD equations are decoupled first into two transient convection-diffusion equations, and then into two modified Helmholtz equations by using suitable transformations. Then, the DBEM or the DRBEM is used to transform these equations into equivalent integral equations by employing the fundamental solution of either steady-state convection-diffusion or modified Helmholtz equations. Thus, the resulting BEM integral equations contain a domain integral whose kernel involves the multiplication of the fundamental solution with the first order time derivative of the unknown. In DBEM this domain integral is kept and treated by numerical integration, while it is transformed into a boundary integral by means of radial basis functions in DRBEM. The obtained DBEM and DRBEM results are compared and visualized in terms of equi-velocity and current lines at steady-state and transient levels for several values of Hartmann number $M$ and the inclination angle of magnetic field at arbitrary wall conductivities. The numerical results reveal that the well-known characteristics of MHD flow are captured. That is, as $M$ increases the velocity decreases and becomes stagnant at the center of the duct; and boundary layers are formed near the corners in the direction of the applied magnetic field for both $V$ and $B$. DBEM and DRBEM with the fundamental solution of convection-diffusion equation give better results than the ones with the fundamental solution of modified Helmholtz equation in the sense of increasing $M$. Moreover, DBEM gives reasonably well results for higher values of $M$ when compared to DRBEM.
Computational Modeling of Durability Phenomena in Concrete

Mehran Ghasabeh\(^1\), Serdar Göktepe\(^2\)

\(^1\) Dep. of Civil Engineering, Middle East Technical University, Ankara, Turkey
    mehran.ghasabeh@metu.edu.tr

\(^2\) Dep. of Civil Engineering, Middle East Technical University, Ankara, Turkey
    sgoktepe@metu.edu.tr

A sound understanding and predictive computational modeling of potential durability problems in concrete are of main concern for evaluating the service life of concrete structures. The durability-related phenomena are inherently associated with a set of physico-chemical events, collectively referred to as the hydration. The degree of hydration, in turn, governs the evolution of mechanical, physical, thermal properties, among many others, of hardening concrete through the so-called aging equations. In early age concrete, different types of coupling between the hydration reactions, the temperature evolution and, deformation may lead to induced cracking. The concentration of tensile stresses in hardening concrete often results from uneven volume changes due mainly to the high temperature gradients in mass concrete, the different types of shrinkage because of the reduction in the relative humidity, or the alkali-silica reactions resulting in gels with excessive swelling capacity, to mention a few. The prediction of crack initiation and propagation in concrete structures is of a major concern which contributes to estimate strength and durability of structures during their service lives.

![Figure 1: The crack pattern of the RCC dam under coupled thermo-mechanical effect, and the concrete ring subjected to the relative humidity variation of environment [7], [8].](image)

In this contribution, coupled constitutive models furnished by robust computational framework are developed to address the durability problems that arise due to the uneven chemical heating through
hydration in mass concrete [7] and the non-uniform shrinkage by means of the reduction in relative humidity [8]. In the case of mass concrete structures such as dams, the coupling between the hydration reaction, temperature evolution, and deformation at early ages may lead to cracking. In many hydraulic and building structures, located in a region with a great temperature variation between day and night, the problem of the humidity diffusion mostly refers to temperature effect. The parameters governing shrinkage can be classified in three groups (i) Environmental parameters (relative humidity, temperature, rate of moisture loss, duration of moisture loss), (ii) geometry of the concrete element (surface area to volume ratio, thickness), (iii) cementitious paste parameters (water-cementitious material ratio, amount and composition of the cementitious material, degree of hydration). Hence, the proposed approaches account for the chemo-thermo-mechanical coupling [1, 2] to investigate the cross effects between the evolution of temperature due to hydration and stresses through the deformation in mass concrete for the former problem, while the latter class of problems are tackled by the coupled hygro-thermo-mechanical models incorporating shrinkage-induced stress concentrations either in hardening or hardened concrete within the framework of Reactive Porous Media based on the coupled problem of Darcy-Biot-type fluid transport [3, 4]. These coupled models are further supplemented by the Phase Field models [5, 6] to predict the crack initiation and propagation under the considered coupled effects.

Bibliography

A Modulus Gradient Model for Nano–Reinforced Composites

Hasan Gülüşık¹, Serdar Göktepe², Ercan Gürses³

¹ Department of Aerospace Engineering, Middle EastTechnical University, Ankara, Turkey
² Department of Civil Engineering, Middle East Technical University, Ankara, Turkey
³ Department of Aerospace Engineering, Middle East Technical University, Ankara, Turkey

A new gradient elasticity formulation, so called E-grad model, is proposed for a one-dimensional linear elastic inhomogeneous rod [1]. In the new formulation, similar to the differential relation between the local strain and the gradient enhanced strain in the classical models of gradient elasticity, a differential relation is proposed for the Young’s modulus. The E-grad model is extended to more general three-dimensional inhomogeneous materials with isotropic linear elastic constituents [2]. In addition to the constitutive equations and balance relations, differential relations for the material parameters of isotropic linear elasticity are provided. The finite element formulation for axisymmetric problems is derived and a model problem of a soft cylindrical rod with a stiff spherical inclusion is solved. It is seen that discontinuities and/or very sharp changes in the modulus, displacement, strain and stress fields that exist in local formulations are smoothed with the proposed model. It is shown, as expected, that increasing internal length scale parameter increases the stiffness of the model. The proposed model is compared with a micromechanical model from literature and experiments conducted with polyimide/silica nanocomposites. The results obtained by the proposed approach capture the experimentally measured values of the nanocomposite modulus. Finally, the model is extended to obtain anisotropic macroscopic response by choosing different length scale parameters in different directions.

Bibliography

Numerical Aspects of POD-Based Reduced-Order Modeling for Darcy–Brinkman Equations

Fatma G. Eroglu¹, Songül Kaya Merdan²

¹ Middle East Technical University, Mathematics Department, Ankara, Turkey, Bartın University, Mathematics Department, Bartın, Turkey, fguler bartin.edu.tr
² Middle East Technical University, Mathematics Department, Ankara, Turkey, smerdan metu.edu.tr

We propose, analyze and test a reduced order modeling with proper orthogonal decomposition (POD) method for the modeling to flows governed by double diffusive convection, which models flow driven by two potentials with different rates of diffusion. We present a theoretical analysis of the method and give results for various numerical tests on benchmark problems that will demonstrate both the theory and the effectiveness of the proposed method.
Heuristic Optimization of Three–Dimensional Structures for Diverse Electromagnetic Applications

Sadri Güler¹, Özgür Ergül²

¹ Electrical and Electronics Eng., METU, Ankara, Turkey
² Electrical and Electronics Eng., METU, Ankara, Turkey

guler.sadri@metu.edu.tr
ozergul@metu.edu.tr

Communication, imaging, sensing, energy harvesting, and similar technologies involve electromagnetic applications that require optimal devices for performing the desired operations in the most efficient and reliable ways. As the optimality in these applications cannot be represented analytically, heuristic optimization techniques are useful to design high-performance structures. These techniques can be supported by full-wave electromagnetic solvers to make simulations accurate while they must be accelerated via fast solution algorithms. Such a robust optimization mechanism, based on genetic algorithms, flexible modification tools, and the multilevel fast multipole algorithm, is presented in this study. Flexible modifications, such as extraction, addition, free deformation, and regularization, are achieved by an automated mesh generation that is interacting with the full-wave solver. The developed design environment not only provides on-off optimization for designing efficient RFID antennas [1] and nano-optical arrays for imaging [2], but also enables complex optimization of three-dimensional helical metamaterials, gradient-index lenses, and nanostructures, without resorting to geometric simplification. The optimization mechanism including the mesh generation algorithms, as well as its application to design diverse nano–optical structures, will be presented.

Bibliography

Stability Analysis of Time Dependent MHD Flow Equations in a Rectangular Duct

Merve Gürbüz¹, Münevver Tezer-Sezgin²

¹ Department of Management, Baskent University, Ankara, 06790, Turkey
mervegurbuz@baskent.edu.tr

² Department of Mathematics, Middle East Technical University, Ankara, 06800, Turkey
munt@metu.edu.tr

The unsteady magnetohydrodynamic (MHD) flow equations [1] are solved in a rectangular duct by using the radial basis function (RBF) approximation. The inhomogeneities in the coupled velocity and induced magnetic field equations are approximated by using thin plate splines (r²lnr) [2]. Then, particular solution is found satisfying both the MHD equations and the boundary conditions which are the no-slip and insulated wall conditions. The explicit forward finite difference is used for advancing the solution to steady-state together with a relaxation parameter for achieving stable solution. It is found that, as Hartman number (M) increases the flow develops boundary layers on the Hartmann walls (perpendicular to the applied magnetic field) and side walls (parallel to the magnetic field). The induced magnetic field also exhibits boundary layers at the Hartmann walls. The velocity magnitude drops and the fluid becomes stagnant at the center of the duct with an increase in the Hartmann number. These are the well-known characteristics of the MHD flow. The stability analysis is carried in terms of spectral radius of the coefficient matrix in the final discretized system. The numerical procedure which is forward in time - radial basis function approximation in space gives stable solution by using quite large time increment and relaxation parameter although the time integration scheme is an explicit method.

Bibliography

Application of Finite Element Method by HYDRUS 1D for Assessing the Effects of Irrigation by Contaminated Groundwater in Turkey

Y. Güray Hatipoğlu¹, Zöhre Kurt²

¹ Department of Earth System Science, METU, Ankara, Turkey e171894@metu.edu.tr
² Department of Environmental Engineering, METU, Ankara, Turkey zkurt@metu.edu.tr

Pump and fertilize, while removing nitrate in the groundwater, can also reduce nitrate requirement. There are many aquifers contaminated with nitrate in Turkey, and a considerable amount of the cases have more than 50 mg/L nitrate concentration [1,2], the maximum allowed limit for drinking water. In this study, we constructed groundwater models via HYDRUS 1D for one-hectare maize field in prevalent soils in Turkey and Eskişehir, Adana, Şanlıurfa, Düzce similar climates, assessed the most likely promising conditions for pump and fertilize, and found that even in 50 mg/L nitrate concentrations, this process is beneficial, especially in Şanlıurfa similar climates (687 TL gain/year). Nitrogen leaching loss was more in highly permeable soils, (loamy sand (350.2 cm/d), sand (712.8 cm/d), sandy loam (106.1 cm/d) hydraulic conductivities). Additionally, in Şanlıurfa similar climate, silty clay loam has also a quite high nitrate leaching due to the stress experienced by plants from too much water, even though the soil’s hydraulic conductivity is the lowest (1.68 cm/d) among investigated 15 soil types. With this study, we found out the soils and climate in which nitrogen use efficiency by plants are high, nitrate leaching is low, denitrification is less effective and overall nitrate removal is high. cambisol was best in Eskişehir, cambisol and sandy loam were best in Adana and Şanlıurfa and none of them were suitable in Düzce similar climate. As a result, Şanlıurfa similar high irrigation water requiring climates and sandy loam and cambisol similar soils are the most suitable places for realizing pump and fertilize.

Bibliography
In this study, metallic nanoantenna arrays are rigorously designed to obtain high power-enhancement capabilities in the visible light spectrum. Nanoantennas are known to have an extensive ability of trapping and focusing electromagnetic waves in subwavelength regions. We use their ability to design effective nanoantenna arrays for particle sensing and optical imaging applications. For this purpose, a full-wave electromagnetic solver is developed to simulate the plasmonic behaviors of metals at optical frequencies. Lorentz-Drude Model is used to represent metals as penetrable structures with electric permittivity values in the frequency domain [1]. Scattering problems are investigated by a modified combined tangential formulation (MCTF), which was developed for very accurate analysis of penetrable objects with negative real permittivity [2]. MCTF is discretized by using the Rao-Wilton-Glisson (RWG) functions, while the obtained matrix systems are solved iteratively with the multilevel fast multipole algorithm (MLFMA). By means of accurate simulations of finite structures, the effects of the used material, geometry, frequency, as well as the array parameters are investigated in detail for reaching optimal nanoantenna configurations in the context of particle sensing applications.

Bibliography

Computational Electromagnetic Simulations of Three-Dimensional Structures with Exotic Material Properties

Hande İbili¹, Özgür Ergül²

¹ Electrical and Electronics Eng., METU, Ankara, Turkey
² Electrical and Electronics Eng., METU, Ankara, Turkey

In this study, computational analysis of three-dimensional metamaterial structures that induce negative and zero permittivity and permeability values in the host environment, as well as plasmonic materials at optical frequencies, is presented. All these electromagnetic problems are challenging since effective material properties become negative/zero, while numerical solvers are commonly developed for ordinary positive parameters. In real life, three-dimensional metamaterial structures, involving split-ring resonators, thin wires, and similar subwavelength elements, are designed to exhibit single negativity (imaginary refractive index) and double negativity (negative refractive index) behaviors. However, metamaterial elements have small details with respect to wavelength and they operate when they resonate. Then, their numerical models lead to large matrix equations that are also ill-conditioned, making their solutions extremely difficult, if not impossible [1]. If performed accurately, homogenization simplifies the analysis of metamaterials, while new challenges arise due to negative parameters. For example, a combination of zero-index and near-zero-index materials with ordinary media (metals, free space, etc.) results in a high-contrast problem, and numerical instabilities occur particularly due to huge values of wavelength. Similar difficulties arise when considering the plasmonic effects of metals at optical frequencies since they must be modeled as penetrable bodies with negative real permittivity, leading to imaginary index values. In this work, different surface-integral-equation formulations [2] are extensively tested for accurate and efficient numerical solutions of zero-index, near-zero-index, and imaginary-index materials. In addition to canonical problems, real-life applications, including but not limited to subwavelength focusing, energy harvesting, bio-sensing, and electromagnetic tunneling, are considered in the context of their fast and accurate solutions.

Bibliography

Computational Electromagnetic Simulations of Electrically Large Structures

Barışcan Karaosmanoğlu\textsuperscript{1}, Özgür Ergül\textsuperscript{2}

\textsuperscript{1} Department of Electrical and Electronics Engineering, METU, Ankara, Turkey \textsuperscript{2} Department of Electrical and Electronics Engineering, METU, Ankara, Turkey

In radar applications, the electrical size of the airborne targets exceeds 1000 wavelengths. It is possible to use high-frequency techniques, e.g., physical optics, geometric diffraction, and ray tracing, for the electromagnetic analysis of such large targets \cite{1}. However, these techniques may not yield sufficiently accurate results for the analysis of complex geometries, especially involving cavities and resonant parts. Furthermore, the presence of material coating, antennas, and other electronic devices on large platforms makes the high-frequency techniques inapplicable. On the other hand, the application of full-wave solvers, such as method of moments, to electrically large objects is inefficient even on powerful computer systems. Since these direct solutions require unaffordable levels of memory usage and solution time, there is a need for fast algorithms, such as multilevel fast multipole algorithm (MLFMA) \cite{1,2}.

In this study, MLFMA-based implementations for efficient and accurate solutions of electromagnetic problems involving electrically large targets are presented. These solvers are built on linear systems of equations, which are obtained by the discretization of integral equations applied on the target geometries. The solutions are obtained by using iterative solvers and the required matrix-vector multiplications are calculated via MLFMA. The solutions obtained demonstrate the effectiveness of the developed implementations.

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A Robust Nested Krylov Subspace Method for Solving Sparse Symmetric Indefinite Linear Systems

Murat Manguoğlu¹, Volker Mehrmann²

¹ Department of Computer Engineering, Middle East Technical University, Ankara, Turkey
manguoglu@ceng.metu.edu.tr

² Institut für Mathematik, Technische Universität Berlin, Berlin, Germany
mehrmann@math.tu-berlin.de

Sparse linear systems of equations that are symmetric and indefinite are an important class of problems that arise in a variety of applications including optimization, computational physics and chemistry. We propose a novel 2-level nested Krylov subspace scheme for symmetric indefinite systems where the coefficient matrix has only few negative eigenvalues. The proposed scheme consists of outer Minimum Residual (MINRES) iterations with a deflated preconditioner. Deflated systems involving the preconditioner are solved via inner Conjugate Gradient (CG) iterations with an indefinite preconditioner. The robustness of the proposed scheme is illustrated via realistic linear systems that arise in a variety of applications.
Subspace Frameworks for Eigenvalue Optimization and Applications

Emre Mengi¹, Fatih Kangal², Karl Meerbergen³, Wim Michiels⁴

¹ Koç University  emenge@ku.edu.tr
² Koç University  fkaengal@ku.edu.tr
³ KU Leuven, Belgium  karl.meerbergen@cs.kuleuven.be
⁴ KU Leuven, Belgium  Wim.Michiels@cs.kuleuven.be

We deal with a Hermitian matrix depending on parameters, and the minimization of its jth largest eigenvalue (for a prescribed j) over the set of admissible parameter values. Such problems have drawn substantial interest starting around the 1980s due to their connection with semi-definite programs, more recently due to applications in robust control.

A major hurdle today is how to cope with such problems in the large-scale setting, that is when the parameter-dependent matrix is large. The talk describes procedures to construct small subspaces such that the projection and restriction of the parameter-dependent matrix into these subspaces lead to reduced eigenvalue optimization problems that approximate the original optimization problem well. The proposed subspace procedures are greedy interpolatory approaches; they are designed to achieve rapid global convergence with respect to the subspace dimension in theory.

We present the adaptations of the procedures for large-scale semi-definite programs and to maximize the robust stability of large-scale linear dynamical systems.
Due to the difficulties of experimental studies in practical medicine, there is a great need for the mathematical models that explain the nature of the heart. With the use of these models, new diagnostic and therapeutic approaches can be developed by cardiologists and researchers from different disciplines. Moreover, individualization of these mathematical models helps the medical doctors treat the disease of each specific patient accurately. In order to improve the individualization techniques, accurate physical definitions of the problems, generalization of the heart geometries and efficient mathematical and numerical tools are required. Electrocardiogram (ECG), one of the most popular diagnostic tools in clinics, is used to assess the electrical activity of the heart. The motivation of this study is to propose numerically efficient approaches to decrease the computational cost of the forward problem of electrophysiology for the integrated heart models including the torso.

In this contribution, the bimaterial problem of the integrated cardiac electrophysiology in the bidomain setting is solved [1, 2]. The torso, in this model, is assumed to be a linear conductor and it surrounds the nonlinear model of the cardiac tissue. While the excitation of the cardiac tissue involves two field variables, the transmembrane potential and the extracellular potential, the electrical activity of the torso involves the extracellular potential field only [3, 4]. The electrophysiological behavior of the cardiac tissue is governed by a set of two partial differential equations. One of these equations contains
a highly non-linear ionic current term that is modeled by the celebrated ten Tusscher model including 17 ODEs [5, 6]. The linear and time-independent nature of the differential equations describing the electrical behavior of the torso motivates us to propose computationally efficient approaches.

The first approach is the condensation of the stiffness matrix for an entirely Finite Element Method (C-FEM). Owing to the linear behavior of the torso, the conductivity matrix of the surrounding tissue is constant and can be assembled once and for all. Consequently, we can rearrange the overall coefficient matrix to decrease the total number of degrees of freedom. The second approach is to solve the problem using hybrid Finite Element Method - Boundary Element Method (FEM-BEM) [7]. With this approach, we exploit the linear differential equation of the torso and solve it by using the BEM. The coupling between the nonlinear equations of cardiac tissue and the equations of the torso is achieved on the surface of the heart by the FEM-BEM approach. The efficiency of the proposed approaches is demonstrated through the representative numerical examples. In particular, the ECGs obtained from these examples are compared to the existing numerical results [1, 2, 8].

Bibliography


In this study, dual reciprocity boundary element method (DRBEM) solutions of magnetohydrodynamic (MHD) flows in single and coupled ducts with conducting thick walls are investigated. The effect of the slip velocity condition on the walls, parallel to the applied magnetic field, is also presented. The coupled MHD equations in terms of the velocity and the induced magnetic field of the fluid and Laplace equations for the induced magnetic field of the thick walls are discretized by the DRBEM and solved in one stroke using coupled conditions on the shared boundaries. The influences of wall thickness, conductivity ratio, Hartmann number and slip length are presented. The numerical results reveal the efficiency of the DRBEM in solutions of MHD flow in ducts with velocity slip and coupled induced magnetic field boundary conditions.

Bibliography

Large Eddy Simulation of Blood Flow Inside Vessels for Acoustic Diagnosis of Atherosclerosis

Cüneyt Sert¹, Kamil Özden², Yiğit Yazıcıoğlu³

¹ Mechanical Engineering, Middle East Technical University csert@metu.edu.tr
² Mechanical Engineering, Middle East Technical University kozden@metu.edu.tr
³ Mechanical Engineering, Middle East Technical University yigit@metu.edu.tr

Atherosclerosis is a cardiovascular disease, in which plaque builds up inside a blood vessel, narrowing it down and forming a stenosis that adversely affects flow. Because of the constriction, turbulent flow occurs at the post-stenotic region, which leads pressure fluctuations on the vessel wall. The murmur caused by this interaction propagates through the surrounding tissue and reaches the skin surface. These sounds emitted from the stenosed vessels are evaluated as a sign of stenosis. In this study, large eddy simulations are conducted to investigate the turbulence-induced wall pressure fluctuations and resulting acoustic emission. The two main parameters considered for this purpose are the stenosis severity and shape. The results show that stenosis severity under a certain level does not cause disturbance at the post-stenotic region. For constrictions above this critical level, increasing stenosis severity has an intensifying effect on the wall pressure fluctuations. Eccentric stenosis morphology causes more severe fluctuations than the axisymmetric one. Different stenosis shapes affect both the magnitude of fluctuations and the duration in which the fluctuations are intense during the pulsatile cycle. Obtained pressure fluctuations are converted into sound and investigated in terms of sound levels and patterns. Sounds emitted from the vessels with different stenosis severities and shapes have different sound characteristics, and they can provide important information about the constriction. Therefore, both the stenosis severity and the shape must be taken into account for development of an acoustic-based diagnostic system.

Keywords: Cardiovascular biomechanics, Pressure fluctuation, Non-invasive diagnosis of stenosis, Acoustic radiation, Stenosis severity, Stenosis shape, Large Eddy Simulation (LES)
A Numerical and Experimental Investigation of Crack Propagation Mechanisms in Ductile Metal Plates

Cihan Tekoğlu¹, Hatice Duran², Mert Efe³, Kim Lau Nielsen⁴

¹ Department of Mechanical Engineering, TOBB University of Economics and Technology cihantekoglu@etu.edu.tr
² Department of Materials Science and Nanotechnology Engineering, TOBB University of Economics and Technology hduran@etu.edu.tr
³ Metallurgical and Materials Engineering, Middle East Technical University mefe@metu.edu.tr
⁴ Department of Mechanical Engineering, Solid Mechanics, Technical University of Denmark kin@mek.dtu.dk

Ductile fracture mainly occurs through the stages of nucleation, growth and coalescence of micron scale voids. The micro cracks that initiate through coalescence of micro voids propagate and lead to overall failure of structural components. Measuring the crack growth resistance of large structural components under approximated service conditions is an expensive and difficult task, if possible. Consequently, predicting the crack growth resistance of structural members requires numerical simulations. The finite element method (FEM) is widely used for that purpose.

The three experimentally observed crack propagation mechanisms in the ductile failure of metal plates are: i-) slanted, ii-) cup-cone, and iii-) cup-cup crack growth. In real life applications, cracks usually show a mixture of different propagation modes. The present work investigates the effects of volume fraction, size, and distribution of second phase particles on the crack propagation mechanisms. Both experimental and numerical (FE analysis) analyses are performed for this purpose. In the FE calculations, the plate is subjected to quasi-static uniaxial tensile loading by imposing displacements boundary conditions on its top and bottom surfaces. The random spatial/dimensional distribution of the voids (nucleated by the second phase particles) in the fracture process zone of the plate are represented by using the Gurson-Tvergaard-Needleman (GTN) porous plasticity, see e.g. [1]. The results show that, a few number of small particles tend to lead to cup-cup crack growth, while the presence of a large number of big particles leads to slanted or cup-cone crack morphologies.

Bibliography


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This study gives numerical solution of the Magnetohydrodynamic (MHD) flow in a square duct under several combinations of insulated and perfectly conducting, and partly insulated partly conducting walls with either Hartmann walls or side walls or all the walls exhibit slip. The finite element method (FEM) is used with SUPG stabilization in solving the coupled MHD equations, and the velocity and induced magnetic field are simulated for Hartmann number values in the range $M \leq 100$ and for several values of the slip length. The results show that, as $M$ increases the well-known MHD characteristics are observed as the flattening of the flow and the enlargement of the core region (where the fluid is stagnant) for the case of no-slip walls. As the slip length increases the velocity of the fluid increases, the core region gets smaller and the slip is more pronounced when the slip ratio $\geq 1$. When the Hartmann walls exhibit slip and are insulated, side layers become thicker than the ones obtained in no-slip Hartmann walls. However, the case of conducting Hartmann walls weaken the slip velocity as well as the Hartmann layers considerably as $M$ increases. The flow is concentrated symmetrically in front of the side walls when the side walls are insulated and exhibit slip. In partly insulated partly conducting Hartmann walls the main flow is concentrated between the parabolic layers emanating from the points where the conductivity changes. The stabilized FEM procedure captures the physical changes in the flow and the induced current due to the variation of the slip lengths and the conductivity changes on the duct walls.
In this talk, we consider a stabilized finite element approximation of the Stokes eigenvalue problems stated in the two-field (displacement-pressure) and the three-field (stress-displacement-pressure) formulations. The method is motivated in a subgrid scale framework, and it is based on the approximation of the unresolvable scales of the continuous solution. Thus, a residual based term is added to the standard Galerkin formulation. On the other hand, the application of such a residual based stabilization method transform the linear eigenvalue problem to a quadratic problem in discrete form. To solve this issue, the space of the unresolved subscales is taken as orthogonal to the finite element space in the present work. In this way, the residual is simplified and the use of term by term stabilization is allowed, and hence, the linear eigenproblem is recovered appropriately. The convergence behaviour of the method is studied, and the error estimates for the eigenvalues and the eigenfunctions are presented. Numerical tests on various problem domains will be reported to validate the theoretical results. Furthermore, several issues raised in approximating the eigenspace of the Stokes operator which remain as topics for future research will be addressed.
On the Solution of Generalized Allen–Cahn Equation

Murat Uzunca\textsuperscript{1}, Bülent Karasözen\textsuperscript{2}, Hamdullah Yücel\textsuperscript{3}

\textsuperscript{1} Department of Mathematics, Sinop University, Sinop, Turkey
\textsuperscript{2} Institute of Applied Mathematics, METU, 06800, Ankara, Turkey
\textsuperscript{3} Institute of Applied Mathematics, METU, 06800, Ankara, Turkey

We consider generalized Allen–Cahn (AC) equation with a nonlinear mobility and advection term:

\[
\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = M(u) \left( \epsilon \Delta u - \frac{1}{\epsilon} F'(u) \right).
\]

The AC equation was first introduced by Allen and Cahn to describe the motion of anti-phase boundaries in crystalline solids. It has been now widely used in various areas, especially for many phase-field models of multi-component fluid flows, and the diffuse interface approach for phase transitions and interfacial dynamics in materials science. The nonlinear degenerate mobility $M(u)$ is used to describe the physics of the phase separation more accurately. The potential function $F(u)$ stands for the commonly used polynomial free energy or the logarithmic free energy. The most important property of the AC equation is that it is an $L^2$-gradient flow with the energy functional $\mathcal{E}(u)$:

\[
\mathcal{E}(u) = \int_{\Omega} \left[ \frac{1}{2} \epsilon |\nabla u|^2 + \frac{1}{\epsilon} F(u) \right] \, dx, \quad \frac{d}{dt} \mathcal{E}(u) \leq 0.
\]

The choice of a numerical solver for the AC equation is crucial in the sense that the discrete approximations should also satisfy the above nonlinear energy stability. In our study, we use interior penalty discontinuous Galerkin (IPG) method for the space discretization, and average vector field (AVF) as the time integrator. The IPG method is a well-known method to preserve the local physical quantities, on the other hand, the AVF method preserves the dissipative structure.

For large systems, especially in 3D models, the solution of the arising linear systems from discretization becomes harder to solve by direct solvers. There is a big demand to develop suitable preconditioners for the efficient and accurate solution of large linear systems. Here, we apply the matrix reordering and partitioning technique to provide efficiency in the solution of the arising linear systems. Numerical experiments are carried out to show the efficient and accurate solution of the preconditioned system of IPG-AVF discretized AC equation.
Differential equations are the primary tool to mathematically model physical phenomena in industry and natural science and to gain knowledge about its features. Deterministic differential equations do not sufficiently model physically observed phenomena since there exist naturally inevitable uncertainties in nature. Employing random variables or processes as inputs or coefficients of the differential equations yields a stochastic differential equation which can clarify unnoticed features of physical events. Korteweg-de Vries (KdV) equation with the random input data is a fundamental differential equation for modeling and describing solitary waves occurring in nature. It can be represented by employing time dependent additive randomness into its forcing or space dependent multiplicative randomness into derivative of the solution. Since analytical solutions of the differential equation with the random data input does not exist, quantifying and propagating uncertainty employed on the differential equation are done by numerical approximation techniques.

This talk will focus on numerical investigation of the Korteweg-de Vries equation with random input data by employing stochastic Galerkin in probability space, local discontinuous Galerkin method in spatial dimension, and theta (weighted average) method in temporal dimension. In numerical implementations, both additive noise and multiplicative noise cases are considered by comparing with other numerical techniques such as Monte Carlo and stochastic collocation methods for the probability space and finite difference method for the spatial discretization.
A Projection-Based VMS Method on Linearly Extrapolated BDF2
Time-stepping Scheme for Navier-Stokes Equations

Duygu Vargün\textsuperscript{1}, Songül Kaya Merdan\textsuperscript{2}

\textsuperscript{1}Department of Mathematics, METU, 06800, Ankara, Turkey  
\texttt{e179290@metu.edu.tr}

\textsuperscript{2}Department of Mathematics, METU, 06800, Ankara, Turkey  
\texttt{smerdan@metu.edu.tr}

In this talk, we consider a projection-based variational multiscale (VMS) method based on a linearly extrapolated second order backward difference formula (BDF2) to simulate the incompressible time-dependent Navier-Stokes equations (NSE). The method concerns adding stabilization based on projection acting only on the small scales. By using this stabilization scheme for spatial discretization and the linearly extrapolated BDF2 for time discretization of NSE, we obtain the fully discrete approximation of NSE. Then, we prove the unconditional stability and convergence of the approximate solutions. Also, we present numerical experiments which confirm the theoretical results and indicate efficiency of the proposed scheme.

\textbf{Keywords:} Navier-Stokes equations; projection-based variational multiscale method; BDF2; error analysis

\textit{Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey}
Cancer is a disease caused by abnormal cell growth due to broken gene order and about half a million deaths are reported every year. Cancer-obesity relation has been revealed by American Cancer Society based on the data of 900,000 American adults, which have been collected for 16 years. Cancer cells form tumor, except for hematologic cancers, and they can be distributed in different parts of the body through vascular system and this process might be followed by metastasis. Indeed, construction of a tumor is not an instantaneous incident, but it has a history behind. Fractional differentiation and integration operators, which are the generalization of classical integer-order counterparts, are capable of capturing memory effects due to their nonlocal nature. It is a useful tool to develop suitable models for describing real-world problems which cannot be expressed by using integer-order differential equations. In this work, we propose a new mathematical model to depict the effect of obesity on cancerous tumor growth and chemotherapy as well as immunotherapy are administered with the use of time fractional derivative. Instead of imposing constant drug dose, we construct an optimal control problem to find the optimal drug doses where the objective is to minimize the difference between the number of tumor cells and normal cells together with the side effects of the treatment. Simulation results of the proposed model are shown to examine the impact of the fractional derivatives of different orders. Indeed, our model predicts the negative effect of obesity on the health of patient and we show that the most efficient treatment choice to eradicate the tumor is to apply combined therapy together with low caloric diet.
Local Discontinuous Galerkin Methods for Dirichlet Boundary Control Problems

Hamdullah Yücel

* Institute of Applied Mathematics, METU, 06800, Ankara, Turkey  
vucelh@metu.edu.tr

In this talk, we consider Dirichlet boundary control of a convection–diffusion equation with $L^2$–boundary controls subject to pointwise bounds on the control posed on a two dimensional convex polygonal domain. Local discontinuous Galerkin method is used as a discretization method since the boundary conditions can be applied weakly. We derive primal–dual weighted error estimates for the objective functional with an error term representing the mismatch in the complementary system due to the discretization. Several numerical results are provided to illustrate the effectiveness of the proposed approach.
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