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POSITIVITY PRESERVING DISCONTINUOUS GALERKIN METHOD FOR DRIFT-DIFFUSION SYSTEM

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We consider drift-diffusion models describing the classical transport of charge carriers in a semiconductor coupled with a Poisson equation for electric potential. The difficulties of solving this problem numerically are that the numerical scheme should conserve the total charge inside the device, any negative numerical density is unphysical, and the numerical scheme should respect monotonicity of the solution. Here we present a method for solving the drift-diffusion system uses a Discontinuous Galerkin (DG) finite element algorithm, which combines features of both finite element and finite volume methods, and it is particularly suitable for problems satisfying the conservation laws. Furthermore, we have applied a post-processing technique with a bound preserving limiter [1] to insure that the solution satisfies a global positivity. To demonstrate the capabilities of this new method combined with the adaptive mesh refinement technique, and evaluate the trade-offs in computational speed, cost and solution accuracy we also present results for the same test using the Finite Element Method (FEM) which uses the artificial entropy viscosity stabilization scheme.

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ELECTROMAGNETIC CHARACTERISATION OF OBJECTS USING POLARIZABILITY TENSORS

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The low cost characterisation and detection of conducting, dielectric and magnetic objects is important for a range of applications including security screening, land mine detection, medical imaging, archeological searches, ensuring food safety and non–destructive testing. In these applications, the ability to describe an object in terms of a small number of parameters using polarization/polarizability tensors hold great promise for the low-cost solution of electromagnetic inverse problems based on magnetic induction, ground penetrating radar, electrical impedance tomography and optical tomography modalities.

Asymptotic expansions, which describe the perturbation in electromagnetic fields caused by the presence of an object as its size tends to zero, have been obtained for the full Maxwell system [3], the eddy current model [1, 4] and electrical impedance tomography [2]. These expansions describe the shape and material properties of an object in terms of polarizability tensors, which are independent of an object's position. We have recently obtained new results that describe the interrelationship between classes of (magnetic) polarizability tensors for different problems and the role the topology of an object has on its coefficients [5]. In the presentation we will summarise these recent developments.

In order to compute the polarizability tensor coefficients (vectorial) transmission problems must be solved. In the presentation we will also describe how the *hp* finite element can be applied to the solution of the transmission problems and the computation of the tensor coefficients thus allowing for the generation of a library for the characterisation potential objects and inclusions.

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SCALABLE HIGH-ORDER SIMULATIONS FOR TRANSPORT EQUATIONS

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Efficient and scalable algorithms are critical to deliver numerical PDE solutions fast for important scientific applications. This talk will discuss recent development on high-order spectral-element/spectral-element discontinuous Galerkin discretizations for solving wave, Poisson, and convection-diffusion type equations arising in electromagnetics and fluid systems [1, 2, 3, 4, 5]. Discussion will include the algorithmic strategies on fast operator evaluations and minimizing communcation cost that are key components to achieve a fast simulation on CPUs/GPUs on the advanced computing facilities.

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TIME DEPENDENT SCATTERING FROM A DIFFRACTION GRATING

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Computing the electromagnetic field in a periodic grating due to light from the sun is critical for assessing the performance of thin film solar voltaic devices. This calculation needs to be performed for many angles of incidence and many frequencies across the solar spectrum. To compute at multiple frequencies one approach is to use a broad band incoming wave and solve the time domain scattering problem for a grating. The frequency domain response for a band of frequencies can then be computed by a Fourier transform.

In this presentation we discuss a two dimensional model problem derived from Maxwell's equations by assuming that the fields and grating are translation invariant in one coordinate direction. This results in a wave equation with coefficients appearing as convolutions in the time domain. Assuming plane wave incidence, and a suitable space-time transformation we then arrive at a time dependent second order hyperbolic problem posed on a infinite strip with periodic boundary conditions. Two complications occur: first, materials used in practical devices have frequency dependent coefficients. In fact, at optical frequencies, commonly used metals have a frequency domain permittivity with negative real part but positive imaginary part which describes conductivity. Secondly the spatial domain for the problem is an infinite strip.

Using Laplace transform, we provide a proof of existence and uniqueness in the time domain for a general class of such frequency dependent materials. In the Laplace domain we can also derive a simple expression for the Dirichlet-to-Neumann map (D-t-N), and hence reduce the Laplace domain problem to a bounded domain containing the grating. Then using Convolution Quadrature we can construct a discrete D-t-N map to truncate the spatial computational domain after time discretization, and we prove fully discrete error estimates using a class of multistep methods in time and finite elements in space. Because of the use of Convolution Quadrature, the discrete time domain D-t-N map is perfectly matched to the time stepping scheme.

We end with some preliminary numerical results that demonstrate the convergence and stability of the scheme. We show that using the Backward Differentiation Formula-2 (BDF2) in time and finite elements in space we can compute the time dependent solution for a metal modeled by a Drude law, and for a dielectric modeled by the Sellmeier equation.

NUMERICAL APPROXIMATION OF THE LAPLACE EIGENVALUES WITH MIXED BOUNDARY DATA

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Eigenfunctions of the Laplace operator with mixed Dirichet-Neumann boundary conditions may possess singularities, especially if the Dirichlet-Neumann junction occurs at angles $\geq \frac{\pi}{2}$. This suggests the use of boundary integral strategies to solve such eigenproblems. As with boundary value problems, integral-equation methods allow for a reduction of dimension, and the resolution of singular behaviour which may otherwise present challenges to volumetric methods.

In this talk, we present a novel integral-equation algorithm for mixed Dirichlet-Neumann eigenproblems. This is based on joint work with Oscar Bruno and Eldar Akhmetgaliyev (Caltech).

For domains with smooth boundary, the singular behaviour of the eigenfunctions at Dirichlet-Neumann junctions is incorporated as part of the discretization strategy for the integral operator. The discretization we use is based on the high-order Fourier Continuation method (FC).

For non-smooth (Lipschitz) domains an alternative high-order discretization is presented which achieves high-order accuracy on the basis of graded meshes.

In either case (smooth or Lipschitz boundary), eigenvalues are evaluated by examining the minimal singular values of a suitably stabilized discrete system. This is in the spirit of the modification proposed by Trefethen and Betcke in the modified method of particular solutions.

The method is conceptually simple, and allows for highly accurate and efficient computation of eigenvalues and eigenfunctions, even in challenging geometries. If time permits, we also present results on the mixed Stekhlov-Neumann problem.

NUMERICAL MODELLING OF EVANESCENT AND PROPAGATING MODES IN PHONONIC STRUCTURES

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The phononic plates are periodic structures made of elastic components with large differences in their elastic coefficients, the soft phase being distributed in a form of inclusions embedded in a stiff matrix. The homogenization approach of such elastic structures occupying domain Ω with the "dual porosity" type of the scaling ansatz applied in the inclusions [1] leads to the following problem describing the acoustic wave propagation in a homogenized medium: Find polarization $\boldsymbol{q} \in Q(\Omega)$, $\boldsymbol{q}(x) \in \mathbb{R}^d$ for $x \in \Omega$ ($Q(\Omega)$ is the admissibility set reflecting boundary conditions), such that

$$-\omega^2 \mathbb{M}(\omega^2)\boldsymbol{q} + \mathbb{K}\boldsymbol{q} = \boldsymbol{f}(\omega^2) \;, \quad \text{in } \Omega \;, \tag{1}$$

where $\omega \in \mathbb{R}$ is a fixed frequency, $\mathbb{M} : \mathbb{R}^d \mapsto \mathbb{R}^d$ is the mass tensor (real symmetric, but possibly indefinite, depending on $\omega \in \mathbb{R}_+$) and $\mathbb{K}$ is the 2nd order (elliptic) differential operator, the stiffness. For the 3D elasticity problem (with $\boldsymbol{q} = \boldsymbol{u} = (u_i)$, $i = 1, 2, 3$) $\mathbb{K}$ attains the form $(\mathbb{K})_{ij} = -\partial_k D_{ikjl} \partial_j$ with D_{ikjl} being the usual symmetric positive definite elasticity tensor. The problem for a phononic Reissner-Mindlin plate which is issued in the paper attains the same form, although $\boldsymbol{q}$ involves plate deflections and rotations and the $\mathbb{K}$ and $\mathbb{M}$ have a more complex structure.

Using the spectral decomposition of $\mathbb{M}$, see [2], the wave equation (1) can be transformed to a "diagonalized" form,

$$-\omega^2 \left\langle \boldsymbol{\Lambda\xi},\, \boldsymbol{\zeta} \right\rangle_\Omega + a_\Omega\left(\boldsymbol{\xi},\, \boldsymbol{\zeta}\right) = \left\langle \boldsymbol{b}(\omega^2),\, \boldsymbol{\zeta} \right\rangle_\Omega \;, \quad \text{for all } \boldsymbol{\zeta} \in W_0(\Omega) \;, \tag{2}$$

where $a_\Omega\left(,\right)$ is an elliptic bilinear form and $\boldsymbol{\Lambda} = \boldsymbol{\Lambda}^+ + \boldsymbol{\Lambda}^-$ is the spectral matrix associated with $\mathbb{M}$, decomposed into the positive and the negative parts. This is the basis for introducing two subspaces by solving eigenvalue problems which depend on the imposed frequency. Projections of (2) into these bases yield a system which allows us to resolve the propagating and evanescent modes (when $\boldsymbol{\Lambda}^- \neq \boldsymbol{0}$).

In the conference paper, this approach to the wave dispersion analysis in the phononic media based on the outlined spectral decomposition will be compared with other methods of modelling the wave propagation in homogenized periodic structures. In particular, solving the dynamic problem in the time domain, thus, involving time convolutions, due to the presence of $\mathbb{M}(\omega^2)$, will be discussed. The research was supported by the Czech Scientific Foundation project GACR P101/12/2315.

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NUMERICAL SIMULATIONS OF PHOTOVOLTAIC SOLAR CELLS

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Devices containing a periodically corrugated metallic backreflector have become of interest since surface gratings are able to enhance the electromagnetic field due to the excitation of multiple surface plasmon polariton waves. Design of this type of structure requires a rapid and reliable way to simulate the optical characteristics for wide ranges of wavelength and angle of incidence.

Recently, several simulations of wave-guide concentrators and solar cells ([1, 2, 3]) have been performed using two different numerical methods: the rigorous coupled-wave approach (RCWA) and the finite element method (FEM). In this work we compare the performance of these methods. RCWA is fast and flexible, but FEM has predictable convergence even for discontinuous constitutive properties.

On the other hand, for devices involving shallow-surface relief gratings, we numerically test the accuracy of an asymptotic model which replaces the shallow grating by a planar interface with suitable transmission conditions ([5]).

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THE HELMHOLTZ EQUATION IN HETEROGENEOUS MEDIA: WAVENUMBER-EXPLICIT BOUNDS

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We consider the Helmholtz equation with variable wavenumber, i.e.

$$\Delta u + \kappa^2 n u = f$$

where $\kappa > 0$ is a constant and n (the refractive index) is a function of position. Under a condition on n (which has a natural interpretation as a *non-trapping* condition), we prove bounds that are explicit in κ, $n_{\min}$, and $n_{\max}$ on the solution of the following Helmholtz boundary value problems:

1. the interior impedance problem when the 2- or 3-d domain is Lipschitz and star-shaped with respect to a ball,

2. the exterior Dirichlet problem when the 2- or 3-d obstacle is Lipschitz and star-shaped,

3. the exterior Neumann problem when the 2-d obstacle is C^2 and has strictly positive curvature.

The bounds in 1 and 2 are sharp in their κ dependence, whereas the bound in 3 is $\kappa^{2/3}$ away from being sharp.

WINDOW GREEN FUNCTION METHODS FOR THE SOLUTION OF WAVE PROPAGATION PROBLEMS IN PERIODIC MEDIA

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We present a simple and highly efficient algorithm for evaluation of quasi-periodic Green functions that is seamlessly incorporated into a boundary integral equation numerical method for the solution of wave scattering problems by bi-periodic arrays of scatterers in three-dimensional space. Except at certain "Wood frequencies" at which the quasi-periodic Green function ceases to exist, the proposed approach, which is based on use of smooth windowing functions, gives rise to lattice sums which converge to the Green function superalgebraically fast—that is, faster than any power of the number of terms used—in sharp contrast with the extremely slow convergence exhibited by the corresponding sums in absence of smooth windowing. A variety of numerical results, in turn, demonstrate the practical efficiency of the proposed approach.

APPLICATION OF FINITE ELEMENTS IN NANO-OPTICS

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In this presentation we give an overview of the application of finite elements for the design of nano-optical devices. This ranges from single photon emitters, lightning (LEDs), scatterometry, solar cells, photomasks to silicon photonics. The physical modelling involves a basic understanding of quantum field theory and a deep insight in wave propagation and coherence theory. Numerically, we need to combine various concepts such as high order hp-Finite Elements, transparent boundary conditions, shape optimizer and the Reduced Basis method for fast parameter scans.