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An algorithm to compute the electro-elastic fields for layers of unrestricted anisotropy. Konrad Bojar, *Industrial Research Institute for Automation and Measurements, Warsaw, Poland*
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We present an algorithm to compute the Green's function and the coupled electro-elastostatic fields in a 2D piezoelectric layer of unrestricted anisotropy and containing a distribution of straight line defects. Currently only three types of boundary conditions for the layer are accepted by the algorithm: mechanically uncoupled boundaries, clamped boundaries, one boundary clamped and one boundary mechanically uncoupled. In addition, it is assumed that the layer is adjoined to dielectric subspaces of known dielectric permittivities. The algorithm presented computes the result using the inverse Fourier transform. It is well-known that the Fourier amplitudes of the Green's function and the corresponding electro-elastostatic fields for a single defect in a medium of any anisotropy class may contain essential singularities at $k=0$. For example, for clamped boundaries there are poles of order 1 for any symmetry class [1], for mixed boundary conditions there are no singularities irrespective of possible anisotropy [1], and for a layer of cubic symmetry with uncoupled boundaries there are poles of order 1, 2, and 3 [2]. Other boundary conditions have been investigated in [1], but the results obtained there contain some errors and cannot be implemented until the formulas are corrected. The poles mentioned above exclude direct application of simple quadratures or the IFFT (the inverse FFT).
The first step of the algorithm is to calculate constants c for all poles of the form c/k^n, $n = 1,2,3$. Once all such constants are known, the singularities are removed from the amplitudes by a simple subtraction. The singular part of the solution which corresponds to the subtracted term does not need to be computed; it was shown in [2, 3] that although the Green's function diverges polynomially when $x \to \infty$ (far from the defects), the electro-elastostatic fields exhibit a regular behavior at infinity if and only if all forces and force moments are equilibrated.
The second step of the algorithm is to compute the IFFT of the remainder of the above subtraction. Given the desired precision, the appropriate sampling frequency is calculated using the analytical estimate of the Filon-type quadrature error [4]. The remainder is sampled at the chosen sampling frequency and fed into the IFFT function (e.g. from the FFTW library). The same procedure is applied for every defect of the layer and the final result is obtained by summing the partial solutions.
The proposed algorithm is a building block of a future modeling tool where continuum and discrete solutions are combined by means of the Teodosiu semi-discrete method [5]. Such a tool may appear powerful for designers of multilayered piezoelectric transducers, HFETs, and alike active elements. This tool will easily outperform the FEM and BEM methods in precision, resolution, and computation time.

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Keywords: anisotropic piezoelasticity, singularities, computer algorithm development

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DFT studies of 2-Methyl-6-[2-(trifluoromethyl) phenyl-iminomethyl]phenol: in gas phase and solvent media. Ümit Ceyaln, Hasan Tanak, Recep Tapramaz, *Department of Physics,Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.*
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Schiff bases are of interest because they are known to show photochromism and thermochromism in the solid state; this may involve reversible proton transfer from the hydroxyl-O atom to the imine-N atom. In general, O-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and keto-amine (or quinoid) forms. Depending on the tautomers, two types of intra-molecular hydrogen bonds are possible: O—H···N in benzenoid and N—H···O in quinoid tautomers. The H atom in title compound (I) is located on atom O1, thus the phenol-imine tautomer is favored over the keto-amine form, as indicated by the C2—O1 and C8—N1 bond lengths [1]. These values are in good agreement with the related compound [2]. The dihedral angle between the aromatic rings is 38.79 (5)º. The molecular structure is stabilized by an intramolecular O—H…N hydrogen bond, which generates an S(6) ring. In addition, there is an intramolecular short C—H…F contact [1].
The experimental geometry of 2-Methyl-6-[2(trifluoromethyl) phenyliminomethyl]phenol obtained from single-crystal X-ray diffraction [1] was compared with those obtained from DFT methot in gas phase. In order to evaluate the energetic and dipole moment behavior of the title compound in solvent, we carried out optimization calculations in the three kinds of solvent (chloroform, ethanol and water). The methodology used in this investigation is centered on Onsager's reaction field theory.

[1] H. Tanak, M.Yavuz, and O. Büyükgüngör, Acta Cryst., 2009, E65, o2949. [2] E. Temel, Ç. Albayrak, M. Odabaşoğlu, and O. Buyukgungor Acta Cryst., 2007, E63, o374.

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The molecular dipole moment of a non linear optical compound The 4,4 DiMethyl Cyano Biphenyl (DMACB) : Theoretical and X-ray diffraction study. Abdelkader CHOUAIH, Naima BOUBEGRA, Mokhtaria DRISSI & Fodil HAMZAOUI, *Laboratoire SEA2M – Facultés des Sciences & Technologies – University of . Mostaganem Algeria.*
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We present here results of comparative study of electron charge density distribution in the 4,4 dimethylamino-cyanobiphenyl (DMACB) compound from X-ray data experiment and theoretical investigation using Ab initio Hartree Fock (HF) and density functional theory (DFT) employing B3LYP/ B3PW91 exchange correlation levels of