A Symbolic Procedure for the Diagonalization of Linear PDEs in Accelerated Computational Engineering

A. R. Baghai-Wadji

Vienna University of Technology
Accelerated Computational Technology Group
Institute of Industrial Electronics and Materials Science
Gusshausstr. 27-29, A-1040, Vienna, Austria, EU
Phone: 43 1 58801 36636, Email: wadji@math.la.asu.edu

Since early 90's in the past century our research has been focused on the acceleration of computer simulations of PDEs. Another equally important and uncompromising objective has been the accuracy enhancement of the numerical results. As a first step towards these goals we have devised a symbolic procedure for systematically and conveniently diagonalizing the linear PDEs, which are commonly encountered in mathematical physics and computational engineering applications.

This presentation provides a detailed account of the ideas behind diagonalization, and discusses its consequences on designing robust, accurate and accelerated algorithms for solving boundary value problems (BVPs) in both integral- and differential form.

The discussion starts with a conjecture stating that *all linearized PDEs, as models for physically realizable systems, can be diagonalized.* As byproducts, our conjecture implies several constraints, consistent with known classical results, upon the involved constitutive equations.

Diagonalized forms are, by construction, equivalent to the originating PDEs, but distinguish the space coordinate with respect to which the diagonalization has been performed. As will be shown in this presentation diagonalized forms intrinsically allow several useful interpretations which are generally deeply hidden in their PDE counterparts.

We demonstrate the technical details by converting several PDEs into their respective diagonalized forms. In particular we consider the Laplace equation for the electrostatic and magnetostatic fields, elastostatic equations, the Helmholz equation for the scalar wave propagation, the acoustic-, piezoelectric-, and electromagnetic wave equations for vector fields in anisotropic and transversally inhomogeneous media, and finally the Schrödinger wave equation. Thereby, a symbolic notation, which can easily be automated, will enable us to replace lengthy and tedious calculations by a *simply-by-inspection* manipulatory procedure.

For reasons which will be made clear we refer to diagonalized representations as Huygens' Principle in Differential Form. We will interpret this principle and show that it can favorably be used for (i) generating novel stencils in the finite difference method (leading to our recently developed *Differential Boundary Element Method, DBEM*); (ii) constructing functionals in the finite element method; and most importantly, (iii) establishing singular surface integrals in the boundary element method.

Diagonalized forms in spectral domain transform into algebraic eigenvalue equations. Using the associated eigenpairs we suggest three procedures for constructing Green's functions associated with a given boundary value problem, keeping in mind the automatization aspect in our derivations.

We investigate the asymptotic properties of the eigenpairs in the far- and near-field in the spectral domain. In accordance with Heisenberg's uncertainty principle these asymptotic expansions correspond to the near- and far-fields in the spatial domain. Utilizing the far-field expansions in the spectral domain we propose an easy-to-implement recipie for the regularization of singular surface integrals in the boundary element formulations. For completeness, the presentation of the proposed regularization will proceed a discussion on Hadamard's definition of well-behavedness of linear operator equations, and Tikhonov's regularization technique.

Using our regularization technique we show that moments of Green's functions associated with a given BVP can be written in coordinate (geometry)-free, frequency-, and material independent forms, and therefore, they can be regarded as *universal functions* for the underlying class of problems. It turns out that the universal functions are generally astonishingly smooth; they can be precalculated, stored, and thus retrieved as often as required (data recycling). This capability allows us to separate the scientific computing efforts from the pre- and postprocessing steps in simulations, suggesting the following organization of our software: preprocessing-buffer-computational:engine-buffer-postprocessing. These considerations have resulted in the development of the Fast-MoM, which is an accelerated form of the conventional method of moments (boundary element method).

Using precalculated universal functions the computation times for the calculation of *impedance matrices* in the BEM applications reduce to the times required for retrieving data from the chosen storage medium. However, in spite of this advancement, a major drawback in the BEM still remains to be removed: the impedance matrices are dense. Several techniques have been suggested in literature for obtaining sparse matrices, each with its own limitation. We have suggested a procedure which consists of constructing problem-specific orthogonal sequences of basis functions derived from the involved Green's functions. The idea is to expand the unknowns in our problems in terms of basis functions which embed intrinsic features of the underlying PDEs in their structures: Using Meyer's orthogonalization technique and Green's functions associated with a given BVP, we construct functions which are orthonormal to their integer-translates. In the case of Laplace operator, we are able to show that the resulting functions even support a multiresolution analysis, leading to *Green's-functions-based scaling functions and wavelets*. Several numerical examples will illuminate the underlying concepts.

We continue our presentation by briefly discussing several alternative *localization* techniques for generating sparse matrices in computations, including coherent states and Wannier fucntions, originally suggested in quantum mechanics, and photonics applications, respectively.

We conclude our discussion by posing the following *existence* question: Why is it possible to diagonalize a given system of linearized PDEs in the first place?