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Computational Modeling of Wave Fields for Engineering Applications

A.T. de Hoop

Introduction

The computational modeling of acoustic, electromagnetic, and elastic wave fields is a major branch of research and development in engineering sciences. High-speed, large-storage-capacity digital computers provide the tools to study in detail a considerable number of basic features of technical configurations before actual design, manufacturing, and testing take place. The complexity of the structures involved reflects itself in the complexity of the accompanying computer programs, and this complexity necessitates the development of more or less fully automated computer codes to do the job. Some typical applications are: the seismic prospecting for fossile energy resources in the subsurface of the earth, electromagnetic exploration methods in the search for minerals and ground water, the non-destructive evaluation of mechanical structures where acoustic waves probe the interior for the presence of mechanical defects (cracks, bubbles, inclusions), and the analysis of ElectroMagnetic Interference (EMI) and ElectroMagnetic Compatibility (EMC) of electric and electronic devices, the performance of which may be degraded by unwanted electromagnetic radiation.

Mathematical formulation of the wave field problem

The basic mathematical equations that describe, on a macroscopic scale, electromagnetic wave phenomena in vacuum and in matter, acoustic wave phenomena in fluids, and elastic wave phenomena in solids have the following, common, form:

(1) $(D_x + M\,\partial_t)F = Q.$

Here, F stands for the wave field quantities that are the physical observables, M represents the physical properties of the medium in which the wave field occurs, and Q symbolizes the action of the sources (either man-made or natural) that generate the wave field. The operator D_x is a differential operator acting on the spatial variables x and ∂_t represents differentiation with respect to time t. Notice that in this basic form the field equation (1) interrelates the spatial and temporal changes of the field in space-time, rather than the field values themselves. Each of the quantities in Equation (1) is a multicomponent one, the number of components being directly related to the dimension of the space in which the wave phenomena occurs. The number of components is four for acoustic waves in fluids, six for electromagnetic waves, and nine for elastic waves in solids.
One can show that for media that vary (piecewise) continuously in space, the pointwise exact (or so-called "strong") solutions of Equation (1) are *analytic* in nature, i.e., their construction requires an infinity of arithmetic operations of infinite precision. However, any computational procedure is of an *algebraic* nature, i.e., it can only carry out a finite number of arithmetic operations of a finite precision. This implies that the computed field is always an approximate version of the exact one, while in the process of computation Equation (1) is necessarily discretized. Now, the computational solution can, in its turn, be envisaged as an exact solution to a certain approximate problem that resembles in some sense the one posed by Equation (1), and the central question is: How good is the approximation? Such exact solutions to an approximated problem are also denoted as "weak" solutions. In the solution to Equation (1) one distinguishes between the following categories: the direct wave field problem, where M and Q are known, and F is unknown, the inverse source problem, where M is known, F is only partly known, and Q is unknown, the inverse constituency problem, where Q is known, F is only partly known, and M is unknown.

Field reciprocity and weak solutions

As point of departure it is taken that the field reciprocity theorems associated with Equation (1) do serve as the most general basis for constructing weak solutions of wave problems. Field reciprocity relations have been formulated by H.A. Lorentz for electromagnetic waves (in 1896), by Lord Rayleigh for acoustic waves in fluids (in 1894), and by Betti and Lord Rayleigh (in 1871-1872/1873) for elastic waves in solids (for details, see De Hoop 1987, 1988, and De Hoop and Stam 1988). In general terms, a reciprocity relation yields a quantitative measure for the interaction of two different wave field states that could occur in one and the same domain in space-time. The media properties and the source distributions in the two states may differ. Let the superscripts "A" and "B" denote the two states that could occur in the common domain D with boundary surface ∂D, then the reciprocity relation has the general form:

(2) $$\langle F^A, N, F^B\rangle_{\partial D} - \langle F^B, N, F^A\rangle_{\partial D} = -\langle F^A, M^B, F^B\rangle_D + \langle F^B, M^A, F^A\rangle_D + \langle F^A, Q^B\rangle_D - \langle F^B, Q^A\rangle_D,$$

where the term on the left-hand side, with the unit normal operator N on ∂D, is representative for the wave field interaction at the boundary ∂D, while the first two terms on the right-hand side are representative the wave field interaction in D through the difference in media properties in the two states, and the last two terms on the right-hand side are representative for the wave field interaction in D through the source distributions in the two states.

Computational procedure

To use Equation (2) for a computational procedure, State A is identified with suitably chosen discretized representations of the wave field, the medium parameters and the source distributions present in the actual configuration. Let the unknown quantities be parameterized by $NP \geq 1$ expansion coefficients. Next, State B is identified with a succession of $NQ \geq 1$ of computational states, and for each value of NQ Equation (2) is invoked. This procedure leads to a system of NQ equations in NP unknowns. In practice this system is very large (cases are known for NQ = 500.000), and is, hence, solved on the computer, usually by an *iterative* procedure. For details, see De Hoop (1990a, 1990b, 1991).

Error criteria

In the discretization procedure applied to the actual State A (with the *simplex* as the fundamental subdomain in space-time), a *first error criterion* quantifies the descrepancy between the actual and the computational values of the known quantities. For example, the global root-mean-square (RMS) value, over the domain of computation, can serve as such. Further, the iterative solution procedure to solve the systems of equations can be stopped as soon as the system is satisfied to within a prescribed accuracy, for which a *second error criterion* is employed. It is observed that the latter error criterion can elegantly be used to generate an iterative solution procedure associated with it (see Van den Berg 1991 and Kleinman and Van den Berg 1991). Thirdly, the question remains how accurate the final answer to the wave problem is. An estimate of this is usually obtained by applying the computational procedure to a canonical configuration for which analytic solutions can be constructed in an independent manner, and a *third error criterion* quantifies the discrespancy.
Up to now, RMS error criteria have been used as standard tools in the entire analysis. However, this criterion is not based on the physics of the problem. It is felt that more physics-related error criteria could be preferable alternatives, especially as far as the first and third error criteria are concerned. For example, an energy-related criterion could serve as a point of departure. As far as the second error criterion is concerned, it is observed that this stems from the metric in the mathematical space in which the numerical solution is constructed. The RMS error is, in this respect, related to the Euclidean metric, and it sometimes leads to slowly convergent iteration schemes. It is conjectured that a generalization to a Riemannian metric could lead to a more rapidly convergent scheme. These are subjects for future research at the Delft Laboratory of Electromagnetic Research.

References

A.T. de Hoop 1987, "Time-domain reciprocity theorem for electromagnetic fields in dispersive media", Radio Science, Volume 22, Number 7, December 1987, pp. 1171-1178.

A.T. de Hoop 1988, "Time-domain reciprocity theorems for acoustic wave fields in fluids with relaxation", Journal of the Acoustical Society of America, Vol. 84, No. 5, November 1988, pp. 1877-1882.

A.T. de Hoop and H.J. Stam 1988, "Time-domain reciprocity theorems for elastodynamic wave fields in solids with relaxation and their application to inverse problems", Wave Motion 10, 1988, pp. 479-489.

A.T. de Hoop 1990a, "Reciprocity, discretization and the numerical solution of direct and inverse acoustic radiation and scattering problems", In: *Inverse Methods in Action*, P.C. Sabatier (Ed.), Proceedings of the Multicentennials Meeting on Inverse Problems, Montpellier, November 27th-December 1st, 1989, Springer-Verlag, Berlin, 1990, pp. 268-284.

A.T. de Hoop 1990b, "Reciprocity, discretization and the numerical solution of elastodynamic propagation and scattering problems", In: *Elastic Waves and Ultrasonic Nondestructive Evaluation*, S.K. Datta, J.D. Achenbach and Y.S. Rajapakse (Eds.), Proceedings of the IUTAM Symposium on Elastic Wave Propagation and Ultrasonic Evaluation, Boulder, Colorado, U.S.A., July 30 - August 3, 1989, Elsevier Science Publishers B.V. (North-Holland), 1990, pp. 87-92.

A.T. de Hoop 1991, "Reciprocity, discretization, and the numerical solution of direct and inverse electromagnetic radiation and scattering problems", Proceedings of the IEEE, Vol. 79, No. 11, November 1991.

P.M. van den Berg 1991, "Iterative schemes based on minimization of a uniform error criterion", In: PIER 5: *Application of Conjugate Gradient Method to Electromagnetics and Signal Analysis*, T.K. Sarkar (Ed.), Elsevier, New York, 1991, pp.27-66.

R.E. Kleinman and P.M. van den Berg 1991, "Iterative methods for solving integral equations", In: PIER 5: *Application of Conjugate Gradient Method to Electromagnetics and Signal Analysis*, T.K. Sarkar (Ed.), Elsevier, New York, 1991, pp.67-102.