Fourth order, full-stencil immersed interface method for elastic waves with discontinuous coefficients

Chaoming Zhang[*] *William W. Symes*[†]

ABSTRACT

We present fourth order, full-stencil immersed interface finite difference methods for elastic wave equations with discontinuous coefficients. Jump conditions are built into the stencil for special finite difference formulas on uniform Cartesian grids. While this gives solutions of fourth order accuracy, $(4,4)$ or $(4,2)$, at all grid points, the full-stencil immersed interface method is far less demanding in terms of the smoothness of the interface, and is simpler in deriving the numerical jump condition than a minimum-stencil method.

1. INTRODUCTION

High accuracy simulations of wave propagation in heterogeneous media draw considerable interest in many applications. Many *first order* and a few *second order* methods for wave propagation in discontinuous media have been developed, e.g. [Bouchon et al.,1989], [Brown, 1984], [Card and Allen, 1995], [LeVeque, 1995], [Symes and Sei, 1994], [Wojcik et al., 1993], [Zhang and LeVeque, 1997], [Zhang and Symes, 1998], and [Zhang (1996,1997)]. First order methods create unwanted "stair-step" diffraction at an interface or discontinuity. Second order methods improve over the first order methods in accuracy (reduce the diffraction). Given computational resources and the availability of the data, however, *fourth order* methods are often highly desired, and sometimes even required (for practical reasons). The presence of the interfaces between discontinuous materials, however, makes it difficult to achieve this high accuracy.

Zhang and Symes [Zhang and Symes, 1998] extended the work of Zhang and LeVeque [Zhang and LeVeque, 1997] on second order immersed interface method, and gave solutions of fourth order accuracy to acoustic wave equations with discontinuous coefficients. In this paper we develop the full-stencil immersed interface method to

[*]Western Geophysical, 10001 Richmond AVE, Houston, TX 77042 chaoming.zhang@waii.com
[†]TRIP, CAAM, Rice University, Houston, TX 77005 symes@caam.rice.edu

solve elastic wave problems with discontinuous coefficients. By full-stencil method, we mean that maximum number of grid points are used in the stencil for the special finite difference formula. In [Zhang and Symes, 1998] and [Zhang and LeVeque, 1997] minimum number of grid points are used in the stencil for the special formula (we refer this as minimum-stencil method for convenience in this paper). Compared with a minimum-stencil immersed interface method, the full-stencil immersed interface method is far less demanding in terms of the smoothness of the interface, and more manageable in deriving the correct numerical jump conditions.

For this *fourth* order method, we only require the numerical jump conditions derived for a *second* order, minimum-stencil method. At grid points away from the interface, any standard finite difference method can be used. This flexibility maintains the efficiency of the computation on non-interface grid points (the overwhelming majority of the computation). At grid points near the interface, we built the numerical jump conditions into a special stencil, and obtained a set of coefficients for a special finite difference method. This method gives fourth order accuracy at all grid points, including those near the interface.

The fourth order method presented here can be combined with even higher order method to give much improved accuracy near the interface.

2. ELASTIC WAVE EQUATIONS

Consider the two dimensional wave equations of linear elasticity

$$
\begin{aligned}
v_{1t} &= \frac{1}{\rho}\left(\sigma_{11x} + \sigma_{12y}\right) \\
v_{2t} &= \frac{1}{\rho}\left(\sigma_{12x} + \sigma_{22y}\right) \\
\sigma_{11t} &= (\lambda + 2\mu)v_{1x} + \lambda v_{2y} \\
\sigma_{12t} &= \mu(v_{1y} + v_{2x}) \\
\sigma_{22t} &= \lambda v_{1x} + (\lambda + 2\mu)v_{2y}
\end{aligned}
\tag{1}
$$

with the discontinuous coefficients

$$
(\rho,\ \lambda,\ \mu) = \begin{cases} (\rho^-,\ \lambda^-,\ \mu^-) & \text{if} \quad \mathcal{F}_{\text{int}}(x,y) < 0, \\ (\rho^+,\ \lambda^+,\ \mu^+) & \text{if} \quad \mathcal{F}_{\text{int}}(x,y) > 0 \end{cases}
$$

at the interface $\mathcal{C}$, defined by $\mathcal{F}_{\text{int}}(x,y) = 0$. Here, v_1 and v_2 are the two components of the velocity in x (the first coordinate) and y (the second coordinate), respectively, σ_{11}, σ_{12} and σ_{22} are the three stress components in two dimensional problems, ρ is the density, and λ and μ are Lamé constants. $(\rho^-,\ \lambda^-,\ \mu^-)$ and $(\rho^+,\ \lambda^+,\ \mu^+)$ are two sets of constants.

Let

$$U = \begin{pmatrix} v_1(x,y,t) \\ v_2(x,y,t) \\ \sigma_{11}(x,y,t) \\ \sigma_{12}(x,y,t) \\ \sigma_{22}(x,y,t) \end{pmatrix},$$

$$A = -\begin{pmatrix} 0 & 0 & (1/\rho) & 0 & 0 \\ 0 & 0 & 0 & (1/\rho) & 0 \\ (\lambda+2\mu) & 0 & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 & 0 \\ \lambda & 0 & 0 & 0 & 0 \end{pmatrix}.$$

We can express equation (1) in the form of first order system (with B appropriately defined similar to A):

$$U_t + AU_x + BU_y = 0. \tag{2}$$

The full-stencil method can be used to obtain a second order method for this system, with simpler formulations. Here we demonstrate it for fourth order (both (4,4) and (4,2)) accuracy solutions to this system. This method and the work in [Zhang and Symes, 1998] share some similar procedures, for which we condense the illustration in this paper. Emphasis will be made on the differences.

3. THE ALGORITHM

To solve equation (2), in the region where A and B are smooth, we can use any standard numerical scheme of the form:

$$U_{ij}^{n+1} = U_{ij}^{n} + \text{update terms}, \tag{3}$$

where the *update terms* can be from any standard solver. Equation (3) is valid at regular points, where all the points in the stencil lie on the same side of the interface.

The difficulty arises at irregular points, where some of the points of the stencil are on opposite sides of the interface. At these points, a 25-point difference scheme of the form

$$U_{ij}^{n+1} = U_{ij}^{n} + \sum_{l=1}^{25} \Gamma_{ij,l} U_{ij,l}^{n} \tag{4}$$

is used.

The Γ's are 5×5 matrices, and the $U_{ij,l}$ ($l = 1, 2, ..., 25$) are values at points

$$U_{rs}, \quad (i-2 \le r \le i+2, j-2 \le s \le j+2).$$

The choice of the $U_{ij,l}$ corresponds to a full stencil. This is in contrast to earlier work of using a minimum stencil in immersed interface method, where a 15-point stencil is used. We want to choose the Γ's so that fourth order accuracy is maintained. Taylor series expansion gives, at point (i,j), that

$$U_{ij}(t+\Delta t) = U_{ij}(t) + \Delta U_{ij}(t) + \mathrm{O}(\Delta t^{K+1}), \tag{5}$$

with

$$\Delta U_{ij}(t) = \sum_{s=1}^{K} \frac{\partial^s U_{ij}(t)}{\partial t^s}\Delta t^s, \tag{6}$$

where $K=4$ for a $(4,4)$ scheme (fourth order in space, fourth order in time) and $K=2$ for a $(4,2)$ scheme (fourth order in space, second order in time). Comparing (4) with (5), we note that approximating ΔU_{ij} in (5) by

$$\sum_{l=1}^{25} \Gamma_{ij,l} U_{ij,l}^n \tag{7}$$

to 4th order in space, we can obtain a fourth order method. The difficulty is: how to approximate a set of derivatives of up to fourth order at points near the interface, where a standard difference approximation will fail? Our approach can be summarized as follows.

1) Since the physical jump conditions are expressed in the directions normal and tangential to the interface, the numerical jump conditions have the simplest form in a local coordinate system. Pick any point P on the interface near point (i,j) as the origin of the local coordinates (ξ,η) (in the directions normal and tangential to the interface at P). It can easily be verified that wave equations (2) in coordinate system (ξ,η) remain of the same form

$$U_t + AU_\xi + BU_\eta = 0 \tag{8}$$

for the same matrices A and B.

2) The derivatives with respect to t can be replaced by those with respect to ξ and η by using equation (8) (repeatedly for derivatives of order two or higher), thus for a $(4,4)$ scheme (6) can be expressed as

$$\begin{aligned}
\Delta U_{ij} = & -(AU_\xi + BU_\eta)\Delta t \\
& + (A^2U_{\xi\xi} + (AB+BA)U_{\xi\eta} + B^2U_{\eta\eta})\,\Delta t^2 \\
& - (A^3U_{\xi\xi\xi} + (A^2B + ABA + BA^2)U_{\xi\xi\eta} \\
& + (B^2A + BAB + AB^2)U_{\xi\xi\eta} + B^3U_{\eta\eta\eta})\,\Delta t^3 \\
& + (A^4U_{\xi\xi\xi\xi} + B^4U_{\eta\eta\eta\eta} \\
& + (A^3B + A^2BA + ABA^2 + BA^3)U_{\xi\xi\xi\eta} \\
& + (A^2B^2 + ABAB + BA^2B \\
& + AB^2A + BABA + B^2A^2)U_{\xi\xi\eta\eta} \\
& + (B^3A + B^2AB + BAB^2 + AB^3)U_{\xi\eta\eta\eta})\,\Delta t^4
\end{aligned} \tag{9}$$

As for a $(4,2)$ scheme, we simply need drop terms of Δt^3 and Δt^4 in (9). Note that the values of U and its derivatives on the right hand side of (9) are evaluated at point (i,j). We Taylor expand each term of ΔU_{ij} and its derivatives on the right hand side in (9) at point P on the interface. We need to keep only terms of up to fourth order derivatives of U at point P, since we are only interested in the terms having a contribution to up to fourth order terms. We will not give the explicit expression after the Taylor expression. Instead, we give the expansion of one term, U_ξ, as an example:

$$\begin{aligned}[U_\xi]_{ij} &= [U_\xi]_P + [\xi U_{\xi\xi} + \eta U_{\xi\eta}]_P \\ &+\frac{1}{2}\left[\xi^2 U_{\xi\xi\xi} + 2\xi\eta U_{\xi\xi\eta} + \eta^2 U_{\xi\eta\eta}\right]_P \\ &+\frac{1}{6}\left[\xi^3 U_{\xi\xi\xi\xi} + 3\xi^2\eta U_{\xi\xi\xi\eta}\right. \\ &\left.+3\xi\eta^2 U_{\xi\xi\eta\eta} + \eta^3 U_{\xi\eta\eta\eta}\right]_P\end{aligned} \tag{10}$$

The subscript ij and P indicate that the terms are evaluated at points (i,j) and P respectively. Thus after the Taylor expansions, ΔU_{ij} linearly depends on the limiting values of the fifteen U and its derivatives evaluated at point P (with subscript P omitted):

$$\begin{aligned}&U, U_\xi, U_\eta, U_{\xi\xi}, U_{\xi\eta}, U_{\eta\eta}, U_{\xi\xi\xi}, U_{\xi\xi\eta}, \\ &U_{\xi\eta\eta}, U_{\eta\eta\eta}, U_{\xi\xi\xi\xi}, U_{\xi\xi\xi\eta}, U_{\xi\xi\eta\eta}, U_{\xi\eta\eta\eta}, U_{\eta\eta\eta\eta}.\end{aligned} \tag{11}$$

More precisely, ΔU_{ij} (after the expansion) depends on only the fourteen derivative terms because the U term does not appear on the right hand side in (9).

3) Now our task is to approximate ΔU_{ij} (after the expansion) by (7) up to fourth order accuracy. We Taylor expand each of $U_{ij,l}$ $(l = 1, 2, ..., 25)$ in (7) at point P. Since some of $U_{ij,l}$ lie on the opposite sides of the interface, (7) depends on up to thirty terms (limiting values from both sides of the interface for the fifteen terms in (11)). Given 25 Γ's to choose for the full-stencil method, we must reduce the terms on which (7) depends from 30 to 25. We can achieve this by using the following jump conditions to express values of the six terms, $U, U_\xi, U_\eta, U_{\xi\xi}, U_{\xi\eta}, U_{\eta\eta}$ on one side of the interface as those from the other side (see [Zhang, 1996]):

$$\begin{aligned}U^+ &= Q_1 U^- \\ U^+_\eta &= Q_1 U^-_\eta + R_1 U^- \\ U^+_\xi &= Q_2 U^-_\xi + Q_3 U^-_\eta + R_2 U^- \\ U^+_{\eta\eta} &= Q_1 U^-_{\eta\eta} + R_3 U^-_\xi + R_4 U^-_\eta + R_5 U^- \\ U^+_{\xi\eta} &= Q_2 U^-_{\xi\eta} + Q_3 U^-_{\eta\eta} \\ &+ R_6 U^-_\xi + R_7 U^-_\eta + R_8 U^-, \\ U^+_{\xi\xi} &= Q_4 U^-_{\xi\xi} + Q_5 U^-_{\xi\eta} + Q_6 U^-_{\eta\eta} \\ &+ R_9 U^-_\xi + R_{10} U^-_\eta + R_{11} U^-,\end{aligned} \tag{12}$$

where the Q's and R's are 5×5 matrices, functions of λ, μ and ρ, and the superscripts $+$ and $-$ represent the limiting values of U and its derivatives on the $+$ and $-$ side of the interface respectively. We can choose any five of the six jump conditions in (12). Different choice of the five jump conditions will lead to slightly different formulations. A simple and good choice is to use the first five jump conditions in (12), since the sixth conditions is the most complicated and thus the most dispensable. By replacing the 5 terms on one side with those on the other side, we reduce the 30 terms to 25 on which (7) depends: all 15 terms on one side plus 10 terms on the other side.

4) Equating each of the coefficients of the 25 terms in (7) and (9) after the Taylor expansions, we are able to approximate (9) with (7) up to fourth order accuracy. Then we obtain a system of twenty five linear algebraic equations in Γ's

$$\sum_{l=1}^{25} \Gamma_l \hat{Q}_{sl} = F_s, \quad s = 1, 2, ..., 25, \tag{13}$$

where both $\hat{Q}$ and F are 5×5 matrices, with $\hat{Q}$'s depending on the Q's and R's in (12), and the local coordinates of the twenty five points, and F's depending on $A, B, \Delta t$ and the local coordinates of point (i, j); We dropped the subscripts ij from Γ for simplicity. Both $\hat{Q}_{sl}$ and F_s, too, should have subscripts ij to indicate point (i, j), but we dropped them for the same reason. Taking the transpose of (13), we get

$$\sum_{l=1}^{25} \hat{Q}'_{sl} \Gamma'_l = F'_s, \quad s = 1, 2, ..., 25,$$

which is equivalent to

$$\hat{Q}\hat{\Gamma} = \hat{F}, \tag{14}$$

where Q is a block 25×25 matrix, with element (s, l) being $\hat{Q}'_{sl}$, and $\hat{\Gamma}$ and $\hat{F}$ are block 25×1 matrices, with element l being Γ'_l and F'_s respectively. Solving for the system of equations (14) is equivalent to solving for 5 systems of 125×125 linear equations, with the 5 systems having the same coefficient matrix $\hat{Q}$.

5) Solve the linear systems of (14). The Γ's available now can be used to advance the solution by one time step using the finite difference method (4). In practice, in every time step, we can compute values on all grid points using a standard solver. Then we recompute the values at irregular points using previous time step's values. The advantage of computing on all grid points using a standard solver maintains the efficiency and robustness of a standard solver.

The Γ's depend on media properties on both sides of the interface, the interface geometry, grid size and time-step size. Once the Γ's are obtained, the wave propagation is computed in two steps. The first step updates solutions on all grid points including irregular points. The second step obtains the correct values on irregular points using equation (4). The first step retains the flexibility of using any standard solver, maintaining the solver's efficiency and robustness. The second step updates values on a very small fraction of all computational grid points ($O(m)$ in our problem, with $O(m^2)$ being the total number of grid points).

Because the derivation of the special fourth order formula is independent of whatever standard solver is used, and its use is separated from the standard solver in updating solutions, this method can be combined with a standard solver of accuracy higher than fourth order. While the computation of the Γ's (one-time cost) and updating the solutions near the interface (small fraction of total grid points) will add to only insignificant computational cost to the overall cost, the special formula can provide the combined method with a much improved solutions near the interface and therefore much better overall accuracy.

4. FULL-STENCIL VS. MINIMUM-STENCIL

The major difference between a full-stencil immersed interface method and a minimum-stencil is in 3) above. With a minimum-stencil method, for a fourth order scheme, we would need a 15-point stencil since there are 15 U and its derivative terms on one side. The cost is that we would need jump conditions of up to fourth order derivatives, which is very demanding. With the full-stencil method, we need only minimum number of numerical jump conditions (5 in this problem). This enables us to build the numerical jump conditions (which was developed for a second order scheme) into the finite difference scheme to give a fourth order method. Since higher order numerical jump conditions mean higher order differentiability of the interface, the full-stencil method is the least demanding in the smoothness of the interface (given the order of accuracy). Another advantage, the ease in deriving the numerical jump conditions, is greatly beneficial.

With a full-stencil method we need to solve larger systems of linear equations for the twenty five Γ's for every irregular point, and a full-stencil method requires more matrix multiplications (25 vs. 15) in updating solutions at an irregular point. However, the impact of the extra computation on the overall computational cost is insignificant for several reasons. First, solving for the Γ's is only a one-time cost, since we need only compute the Γ's *once* before time stepping, and the Γ's can be used in each time step. Also note that in solving the system of linear equations for the Γ's, we can decouple it into smaller systems before solving for the Γ's. Moreover, the total number of irregular points is only a small fraction of the total computational grid points, making updating solutions at irregular points inexpensive.

Note that there can be variations on the *number* of stencils, depending on how many numerical jump conditions are used. For example, we can use all the six jump conditions in (12), and use a 24-point stencil instead of that of a 25-point in the full-stencil method. Since the inclusion of the sixth jump condition do not demand higher order differentiability of the interface, it can provide a similarly viable scheme . The inclusion of any additional jump conditions allows a stencil of fewer points, but it will need high order of differentiability of the interface. Full-stencil and minimum-stencil represent two extremes of the variations on the number of stencils.

5. CONCLUSIONS

We developed a fourth order, full-stencil immersed interface method for elastic wave equations in heterogeneous media. This full-stencil method demands far less smoothness in the interface than a minimum-stencil method, and the derivation of the numerical jump conditions is significantly simpler. The method gives fourth order accuracy, even on points near the discontinuity. This method can be combined with other high order standard solver to give improved solutions near the interface.

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REFERENCES

Bouchon, M., Campillo, M., and Gaffet, S., 1989, A boundary integral equation – discrete wavenumber representation method to study wave propagation in multilayered media having irregular interfaces: Geophysics, **54**, 1134–1140.

Brown, D. L., 1984, A note on the numerical solution of the wave equation with piecewise smooth coefficients: Math. Comput., **42**, 369–391.

Card, C. L., and Allen, M. B., 1995, Difference approximations for wave equations via finite elements: I. Construction and performance: Numer. Meth. PDE, **11**, 127–146.

LeVeque, R. J., 1995, Wave Propagation Algorithms for Multi-dimensional Hyperbolic Systems, submitted.

Symes, W., and Sei, A., 1994, Error analysis of numerical schemes for the wave equation in heterogeneous media: Applied Numerical Mathematics, **15**, 465–480.

Wojcik, G. L., Vaughan, D. K., Abboud, N., and J. Mould, Jr., 1993, Electromechanical modeling using explicit time-domain finite elements: Electromechanical modeling using explicit time-domain finite elements:, IEEE, IEEE Ultrasonics Symposium Proceedings.

Zhang, C., and LeVeque, R. J., 1997, The immersed interface method for acoustic wave equations with discontinuous coefficients: Wave Motion, **25**, 237–263.

Zhang, C., and Symes, W. W., 1998, Fourth order methods for acoustic waves with discontinuous material, to appear in the Proceedings of International Conference on Mathematical and Numerical Aspects of Wave Propagation.

Zhang, C., 1996, The immersed interface methods for elastic wave propagation in heterogeneous materials, Trip Annual Report, 1997, No. 7, submitted to *Wave Motion*.

———, 1996, Immersed interface methods for hyperbolic systems of partial differential equations with discontinuous coefficients, *PhD Dissertation*, University of Washington,
(`ftp://amath.washington.edu/pub/chaoming /dissertation.ps.Z`).