Westervelt Equation Simulation on Manifold using DEC

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Abstract

The Westervelt equation is a model for the propagation of finite amplitude ultrasound. The method of discrete exterior calculus can be used to solve this equation numerically. A significant advantage of this method is that it can be used to find numerical solutions in the discrete space manifold and the time, and therefore is a generation of finite difference time domain method. This algorithm has been implemented in C++.

Keywords: Westervelt equation, Laplacian operator, Discrete exterior calculus, Manifold, Numerical simulation.

MSC(2010): 35J05, 65M12, 65M08, 53A25.

1 Introduction

The nonlinear effects are important in medical ultrasound and also plays a role in diagnostic program. Some of diagnostic ultrasound instruments have implemented harmonic imaging into their devices by receiving the harmonics in the reflected ultrasound caused by nonlinear distortion of the signal propagating through the biological tissue. Meanwhile, we should pay attention to observing hygienic limits of ultrasound exposition to avoid heating the unwanted tissue. The ability to predict the effects of nonlinear ultrasound propagation therefore becomes important. Numerical simulations are

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currently the best means of making predictions of nonlinear ultrasound propagation. Two of the numerical techniques suitable for providing solutions to the propagation problem are the finite difference time domain(FDTD) method [1–3] and the discrete exterior calculus(DEC) [4–12].

The Westervelt equation is a model for the propagation of finite amplitude ultrasound, deriving from the equation of fluid motion by keeping up to quadratic order terms [13,14]. In this paper, an conditional stable scheme for this equation using the techniques in DEC is proposed. A significant advantage of this scheme is that it can be used to find numerical solutions on the discrete space manifold and the time, therefore is a generation of FDTD. In order to refine the space mesh to improve the accuracy of the solution given by the this scheme, the amount of work involved increases rapidly, since the length of time step should also be reduced. Hence, two unconditional stable schemes are also proposed, namely the implicit and semi-implicit DEC schemes for Westervelt equation on manifold.

2 DEC schemes for Westervelt equation

Discrete Laplace operator

The 2D or 3D space manifold can be approximated by triangles or tetrahedrons, and the time by line segments. Suppose each simplex contains its circumcenter. The circumcentric dual cell $D(\sigma_0)$ of simplex σ_0 is

$$D(\sigma_0) := \bigcup_{\sigma_0 \in \sigma_1 \in \cdots \in \sigma_r} \operatorname{Int}(c(\sigma_0)c(\sigma_1) \cdots c(\sigma_r)),$$

where σ_i is all the simplices which contains $\sigma_0,...$, σ_{i-1} , and $c(\sigma_i)$ is the circumcenter of σ_i . A discrete differential k-form, $k \in \mathbb{Z}$, is the evaluation of the differential k-form on all k-simplices. Dual forms, i.e., forms evaluated on the dual cell. In DEC, the exterior derivative d is approximated as the transpose of the incidence matrix of k-cells on k + 1-cells, the approximated Hodge Star * scales the cells by the volumes of the corresponding dual and primal cells, and the Laplace operator is approximated as

$$\Delta \approx *^{-1}d^T * + d^T * d.$$

Take Fig.1 as an example for a part of 2D mesh, in which 0,..., C are vertices, 1, 2, 3 are the circumcenters of triangles, a, b, c are the circumcenters of edges. Denote l_{ij} as the length of line segment (i,j) and A_{ijkl} as the area of

quadrangle (i, j, k, l).

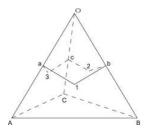


Figure.1. A part of 2D mesh

Define

$$l_{12} := l_{1b} + l_{2b}, \ l_{23} := l_{2c} + l_{3c}, \ l_{31} := l_{3a} + l_{1a},$$

and

$$P_{123} := A_{01ab} + A_{02bc} + A_{03ac}.$$

In Fig.1, the discrete Laplace operator acting on p at vertex 0 is

$$\Delta p_0 \approx \frac{1}{P_{123}} \left(\frac{l_{13}}{l_{A0}} (p_A - p_0) + \frac{l_{12}}{l_{B0}} (p_B - p_0) + \frac{l_{23}}{l_{C0}} (p_C - p_0) \right). \tag{1}$$

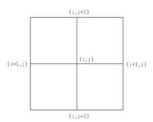


Figure.2. A part of 2D rectangular mesh

In Fig.2, scheme (1) reduces to

$$\Delta p_{i,j} \approx \frac{p_{i,j+1} + p_{i,j-1} + p_{i+1,j} + p_{i-1,j} - 4p_{i,j}}{(\Delta s)^2},$$

where Δs is the uniform space step length.

Discretization for Westervelt equation

The Weservelt equation can be written in the following form:

$$\Delta p - \frac{1}{c_0^2} \frac{\partial^2 p}{\partial t^2} + \frac{\delta}{c_0^4} \frac{\partial^3 p}{\partial t^3} + \frac{\beta}{\rho_0 c_0^4} \frac{\partial^2 p^2}{\partial t^2} = 0, \tag{2}$$

where p is the acoustic pressure, ρ_0 is the are the ambient density, and c_0 is the ultrasound speed, δ is the diffusivity of ultrasound, β is the coefficient of nonlinearity.

For some situations, a source having azimuthal symmetry about its axis is considered. In this case, 2D triangular discrete manifold as the space is only need to be considered. And the Eq.(2) on 3D space manifold and the time can also be solved numerically, using a similar approach.

The temporal partial derivatives with discrete differences, which can be obtained from Taylor series expansions about each node of the computational mesh. Temporal derivatives present in Eq.(2) can be calculated as follows:

$$\frac{\partial^2 p^n}{\partial t^2} \approx \frac{1}{(\Delta t)^2} (p^{n+1} - 2p^n + p^{n-1})$$

$$\frac{\partial^3 p^n}{\partial t^3} \approx \frac{1}{(\Delta t)^3} (p^n - 3p^{n-1} + 3p^{n-2} - p^{n-3})$$

$$\frac{\partial^2 (p^2)^n}{\partial t^2} \approx \frac{1}{(\Delta t)^2} ((p^2)^n - 2(p^2)^{n-1} + (p^2)^{n-2}),$$

where Δt is the time step length, n is the time coordinate. Let

$$\begin{array}{ll} Lp_0^{n-1} & := & \frac{1}{(c_0\Delta t)^2}(p_0^n - 2p_0^{n-1} + p_0^{n-2}) - \frac{\delta}{c_0^4(\Delta t)^3}(p_0^{n-1} - 3p_0^{n-2} + 3p_0^{n-3} \\ & - p_0^{n-4}) - \frac{\beta}{\rho_0 c_0^4(\Delta t)^2}((p_0^2)^{n-1} - 2(p_0^2)^{n-2} + (p_0^2)^{n-3}) \end{array}$$

The explicit DEC scheme for Eq.(2) is

$$\frac{\frac{l_{13}}{l_{A0}}(p_A^{n-1} - p_0^{n-1}) + \frac{l_{12}}{l_{B0}}(p_B^{n-1} - p_0^{n-1}) + \frac{l_{23}}{l_{C0}}(p_C^{n-1} - p_0^{n-1})}{P_{123}} = Lp_0^{n-1}.$$
 (3)

If refining the space mesh, the amount of work involved increases rapidly, since the length of time step should satisfy the stable condition. Now, two unconditional stable schemes are proposed, namely the implicit DEC scheme (4) and semi-implicit DEC scheme (5).

$$\frac{1}{P_{123}} \left(\frac{l_{13}}{l_{A0}} (p_A^n - p_0^n) + \frac{l_{12}}{l_{B0}} (p_B^n - p_0^n) + \frac{l_{23}}{l_{C0}} (p_C^n - p_0^n) \right) = L p_0^{n-1} \tag{4}$$

$$\frac{1}{P_{123}} \left(\frac{l_{13}}{l_{A0}} (p_A^{n-1} - p_0^n) + \frac{l_{12}}{l_{B0}} (p_B^{n-1} - p_0^n) + \frac{l_{23}}{l_{C0}} (p_C^{n-1} - p_0^n) \right) = L p_0^{n-1} \quad (5)$$

The higher order accuracy scheme for temporal derivatives can also be used in schemes (3-5).

3 Stability, convergence and accuracy

The first two terms in (2) describe linear wave propagation at the small-signal sound speed. The third term describes the loss due to he viscosity and thermal conduction of the media. The fourth term describes the non-linear distortion of the traveling wave due to amplitude effects. Since the coefficients of third and fourth terms in Eq.(2) are small compared with the coefficient of second term, the effect of $\frac{\partial^3 p}{\partial t^3}$ and $\frac{\partial^2 p^2}{\partial t^2}$ on the stability of the scheme (3) can be ignored. Therefore, the stable condition for the wave equation

$$\Delta p - \frac{1}{c_0^2} \frac{\partial^2 p}{\partial t^2} = 0$$

is need to be satisfied. The wave equation can be discretized as

$$Right(1)^{n-1} = \frac{1}{(c_0 \Delta t)^2} (p_0^n - 2p_0^{n-1} + p_0^{n-2})$$
 (6)

The stable condition condition for scheme (6) [12] is

$$c_0 \Delta t \le \min_{\forall 0 \in \text{vertices}} \sqrt{\frac{2}{\frac{1}{P_{123}} \left(\frac{l_{13}}{l_{A0}} + \frac{l_{12}}{l_{B0}} + \frac{l_{23}}{l_{C0}}\right)}}.$$
 (7)

In Fig.2, the inequality (7) reduces to

$$c_0 \Delta t \le \frac{\sqrt{2}}{2} \Delta s,$$

which is the stable condition for scheme (6) on square grid. The analysis of unconditional stability for schemes (4) and (5) can also be proved as the wave equations.

By the definition of truncation error, the exact solutions of Westervelt equation satisfy the same relation as schemes (3-5) except for an additional term $O(\Delta t)^2$. This expresses the consistency, and so the convergence for schemes (3-5) by Lax equivalence theorem (consistency + stability = convergence). The derivative in Eq.(2) is approximated by first order difference in schemes (3-5). Equivalently, p is approximated by linear interpolation function. This is to say that schemes (3-5) have first order spacial and temporal accuracy, according to the definition about accuracy of finite volume method.

4 Algorithm Implementation

The DEC schemes (3-5) for Westervelt equation was implemented in C++. The implementation consists of the following steps:

- 1. Set the simulation parameters. These are the dimensions of the computational mesh and the size of the time step, etc.;
- 2. Set the propagating media parameters.
- 3. Initialize the mesh indexes.
- 4. Assign current transmitted signal.
- 5. Compute the value of all spatial nodes and temporarily store the result in the circular buffer for further computation.
- 6. Visualize the currently computed grid of spatial nodes.
- 7. Repeat the whole process from the step 4, until reach the desired total number of iterations.

In the common practice, not every simulation step needs to be visualized, especially when the time step size is too small. In all the following examples, scheme (3) is used, and the parameters are $\delta=0.01$ $\beta=1$ $\rho=10000$. The Gaussian envelope $\frac{1}{\sqrt{2\pi}}\exp(-\frac{t^2}{2})\cos(t)$ is used as a source signal. The example in Fig.3 shows the nonlinear propagation effects and the

The example in Fig.3 shows the nonlinear propagation effects and the diffusivity in the propagation of the Gaussian envelope.

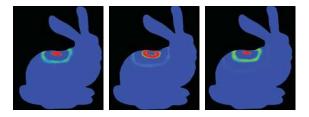


Figure.3. The propagation of Gaussian envelope on a rabbit

The example in Fig.4 shows the propagation of Gaussian envelope at a boundary of two kinds of media with different wave speeds 340 m/s and 3400 m/s.

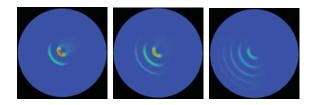


Figure.4. The propagation of Gaussian envelope on a sphere with two kinds of media

References

- [1] K.S. Yee, Numerical solution of inital boundary value problems involving Maxwell's equations in isotropic media, IEEE Trans. Ant. Prop., 14(3), 302-307, (1966).
- [2] A. Bossavit, L. Kettunen, Yee-like schemes on a tetrahedral mesh, with diagonal lumping, Int. J. Numer. Modell., 12(1-2), 129-142, (1999).
- [3] M. Cizek, J. Rozman, Acoustic Wave Equation Simulation Using FDTD, Radioelektronika, 17th International Conference, (2007).
- [4] H. Whitney, Geometric integration theory, Princeton University Press, Princeton, (1957).
- [5] D.N. Arnold, R.S. Falk, R. Winther, Finite element exterior calculus, homological techniques, and applications, Acta Numer., 15, 1-155, (2006).
- [6] M. Meyer, M. Desbrun, P. Schröder, A.H. Barr, Discrete differential geometry operators for triangulated 2-manifolds. In InternationalWorkshop on Visualization and Mathematics, VisMath, (2002).
- [7] M. Desbrun, A.N. Hirani, M. Leok, J. E. Marsden, Discrete exterior calculus, arXiv: math.DG/0508341.
- [8] J. M. Hyman, M. Shashkov, Natural discretizations for the divergence, gradient, and curl on logically rectangular grids, Comput. Math. Appl., 33(4):81-104, (1997).
- [9] R. Hiptmair, Discrete Hodge operators, Numer. Math., 90(2), 265-289, (2001).

- [10] M. Leok, Foundations of computational geometric mechanics. Ph.D. thesis, California Institute of Technology, (2004).
- [11] A. Stern, et al, Computational Electromagnetism with Variational Integrators and Discrete Differential Forms, arXiv:0707.4470.
- [12] Z. Xie, Y.J. Ma, Computation of Maxwell's equations on Manifold using DEC, arXiv:0908.4448.
- [13] M.F. Hamilton, C.L. Mofrey, Model equations, Nonlinear Acoustics, Chap.3, Academic Press, San Diego, (1998).
- [14] G. Taraldsen, A generalized Westervelt equation for nonlinear medical ultrasound, J. Acoust. Soc. Am. 109(4), 1329-1333, (2001).