GEOPHYSICS, VOL. 55, NO. 1 (JANUARY 1990); P. 107–110, 5 FIGS., 1 TABLE.

Short Note

On the construction and efficiency of staggered numerical differentiators for the wave equation

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INTRODUCTION

Finite-difference (FD) techniques have established themselves as viable tools for the numerical modeling of wave propagation. The accuracy and the computational efficiency of numerical modeling can be enhanced by using high-order spatial differential operators (Dablain, 1986).

FD operators for numerical differentiation are conventionally designed with the criterion of maximizing numerical accuracy order (Richtmeyer and Morton, 1967). The staggered-grid formulation (Virieux, 1986; Levander, 1988) exhibits smaller grid dispersion and grid anisotropy than centered-grid schemes for solving the first-order partial differential system of acoustics (elastodynamics). Recently, Holberg (1987) introduced a formulation for designing optimal convolutional differentiators for staggered schemes. His formulation is based on maximizing the spectral frequency band for which a peak relative error is bounded by a specified value. Holberg's differentiators have the largest possible dispersion-bounded bandwidth for a given operator length. To implement his formulation, Holberg goes through a constrained optimization procedure.

In the first section of this note, we present an alternative construction which makes use of minimax ideas to simplify the computation of Holberg's operators, thereby rendering easier their use and the analysis of their effectiveness. We also present a new closed form for the fourth-order operator and a useful truncated series expansion of Holberg's convolutional weights in terms of powers of the error bound.

In the second section of this note, Holberg's differentiators are briefly compared, in terms of the computational cost of numerical first-order differentiation for the same amount of numerical dispersion, with high-order conventional staggered FD and pseudospectral (Kosloff et al., 1984) differentiators. We determine which differentiator to use from a strictly computational viewpoint, depending on the required error bound and on the dimensionality of the problem.

DISPERSION-BOUNDED NUMERICAL DIFFERENTIATION

The frequency response of the first-order derivative operator d/dx is ik where $i = \sqrt{-1}$ and k is the spatial frequency or wavenumber. The frequency response of the generic staggered numerical differentiator $\delta/\delta x$ with weights $d_{2\ell-1}$,

$$\frac{\delta f}{\delta x} = \sum_{\ell=1}^{L/2} d_{2\ell-1} \frac{f[x+(2\ell-1)\Delta x/2]-f[x-(2\ell-1)\Delta x/2]}{\Delta x}, \tag{1}$$

is given (apart from the multiplicative factor $\sqrt{-1}$) by

$$D(k) = \sum_{\ell=1}^{L/2} d_{2\ell-1} \frac{\sin[(2\ell-1)k\Delta x/2]}{\Delta x/2}, \tag{2}$$

where L is the length of the differentiator and Δx is the spatial grid spacing.

A measure of the relative error in the frequency response of the differentiator is introduced by Holberg as

$$\varepsilon(k) = D'(k) - 1, \tag{3}$$

where $D'(k) = \partial D(k)/\partial k$. As indicated in Holberg's (1987) paper, if

$$|\varepsilon(k)| \le E \quad \text{for} \quad 0 \le k \le K_c, \tag{4}$$

then in the semidiscretization of the wave equation with the differentiator (2), the relative error in the group velocity is bounded by E for all wavenumbers below K_c.

The function $D'(k)$ in the interval $0 \le k \le \pi/\Delta x$ has $L/2$ extrema $\{k_n\}$ (see dotted line in Figure 1 for the case $L = 6$). Apart from the fixed extremum at $k = k_1 = 0$, the other members of the set $\{k_n\}$ depend on the weights $\{d_{2\ell-1}\}$.

To maximize the range $0 \le k \le K_c$, for which $|\varepsilon(k)| \le E$,

Manuscript received by the Editor February 15, 1989; revised manuscript received July 3, 1989.
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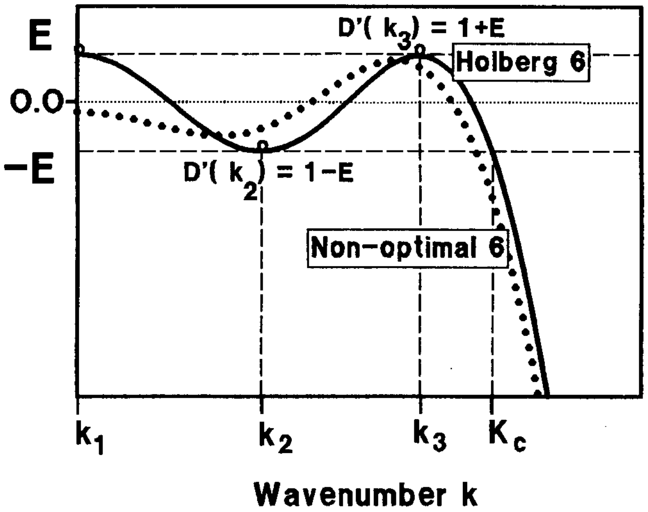

FIG. 1. Relative error in the frequency response of a sixth-order nonoptimal numerical differentiator (dotted line) and of Holberg's sixth-order differentiator with maximal dispersion-bounded bandwidth K_c (continuous line): $k_1 = 0$, k_2, and k_3 are the locations of the three extrema of the group-velocity error $\varepsilon(k)$ for Holberg's operator.

we impose the following simple requirement (see the continuous line in Figure 1 for the case $L = 6$):

$$D'(k_n) = 1 + (-1)^{n+L/2}E, \qquad n = 1, 2, \ldots, L/2. \tag{5}$$

The above requirement, supplemented with

$$D''(k_n) = 0, \qquad n = 2, 3, \ldots, L/2, \tag{6}$$

constitutes a system of $L - 1$ transcendental equations which defines the $L/2$ weights $\{d_{2\ell-1}\}$ and the locations $\{k_n\}$ of the $(L/2 - 1)$ extrema for a given error bound E and a given differentiator length L. A variant of Newton's method can be used to solve the system, and it converges in a few iterations to Holberg's weights defined by the constrained optimization procedure described in Holberg (1987). Figure 2 shows the behavior of Holberg's weights for different values of E; note that Holberg's weights converge to the conventional staggered FD weights as $E \to 0$.

For the case $L = 4$, system (5) and (6) can be reduced to a single cubic equation, which has one admissible root and which generates a simple closed form for Holberg's weights $\{d_{2\ell-1}\}$ in terms of the threshold E; i.e.,

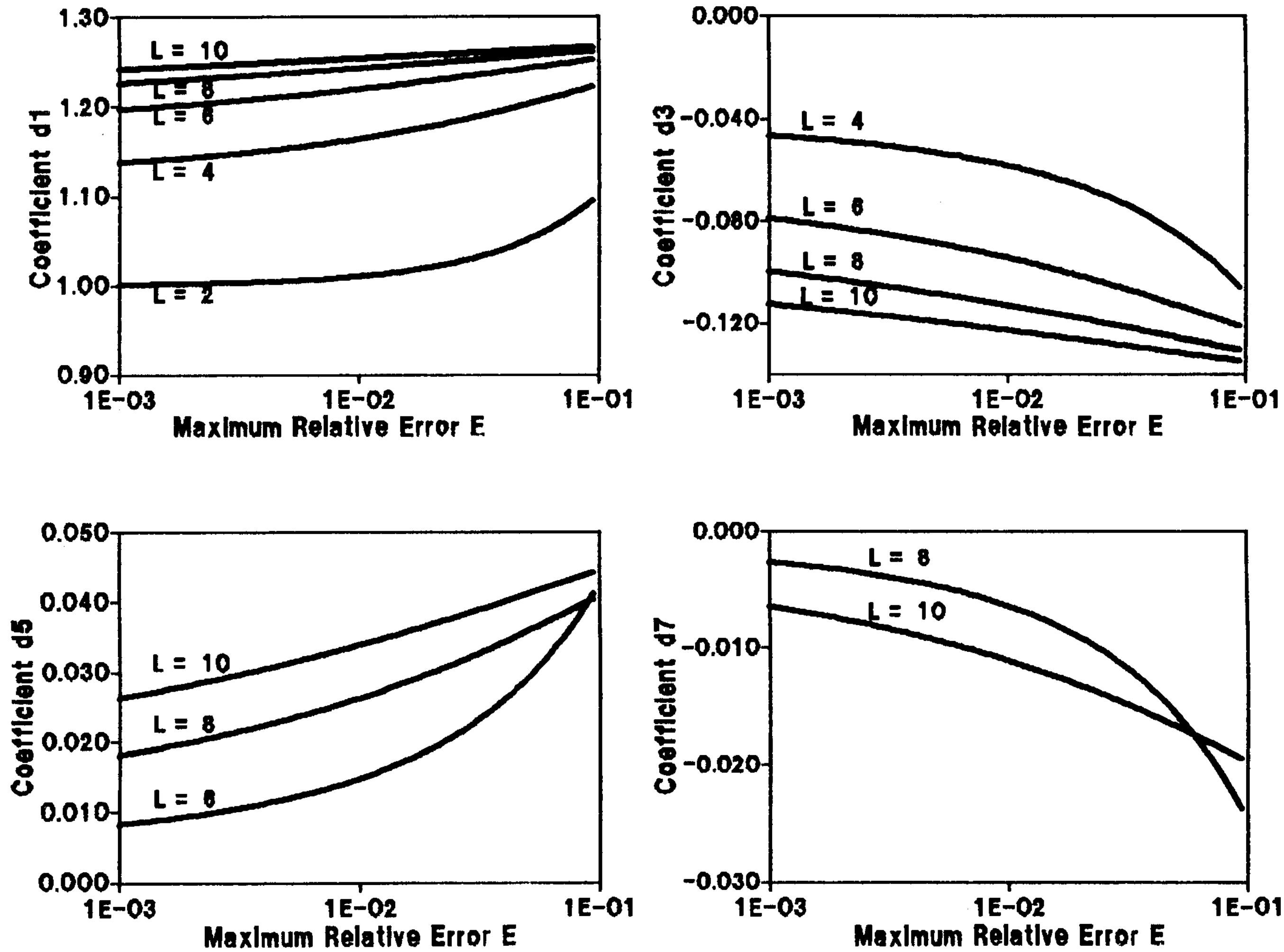

FIG. 2. Weights $\{d_{2\ell-1}\}$ of Holberg's numerical differentiators of orders $L = 2, 4, 6, 8, 10$ plotted as functions of the error threshold E. As $E \to 0$, the weights converge to those of the conventional staggered differentiators.

$$d_1 = \frac{9}{8}(1-E) + \frac{3}{8}f \tag{7}$$

and

$$d_3 = \frac{-1}{24}(1-E) - \frac{1}{8}f, \tag{8}$$

with

$$f = (1+E)^{2/3}(\mathrm{Re}\, w + \sqrt{3}\, \mathrm{Im}\, w) - (1-E) \tag{9}$$

and

$$w = (1 - E + i2\sqrt{E})^{1/3}. \tag{10}$$

Useful approximations of Holberg's weights can be obtained by expanding equations (5) and (6) in fractional powers of E, and by equating their coefficients, with the help of symbolic manipulation tools (Griesmer, J. H., Jenks, R. D., and Yun, D. Y. Y., IBM Research report RA 70); namely,

$$d^{(L)}_{2\ell-1} = \sum_{r=0} b^{(L)}_{\ell r} E^{2r/L}, \qquad \ell = 1, 2, \ldots, L/2\,. \tag{11}$$

The coefficients of the leading terms of the expansions $b^{(L)}_{\ell r}$ are given in Table 1. Note that the zeroth order terms of the expansion coincide with the conventional staggered differentiators.

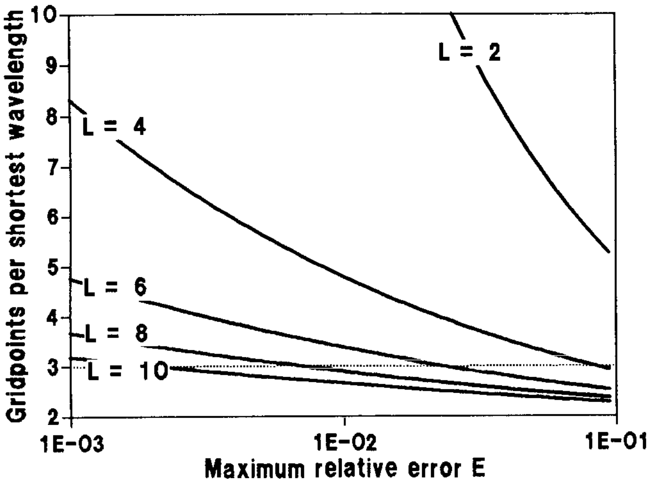

FIG. 3. Number of grid points per shortest wavelength $N_c(L, E)$ for a given error bound E needed by Holberg's convolutional differentiator. For $E = 1\%$, $N_c\,(L, E) = 15.76$, 4.80, 3.37, 2.90, 2.66 for $L = 2, 4, 6, 8, 10$, respectively.

COMPUTATIONAL COST OF NUMERICAL DIFFERENTIATION

The bandwidth K_c over which $|\varepsilon(k)| \le E$ defines the number of grid points per shortest wavelength $N_c(L, E) = 2/(K_c \Delta x/\pi)$ needed to model the wave field and thereby is a significant factor in the computational cost of the scheme. Figure 3 shows the dependence of N_c on E.

In this note we define formally, following Marfurt (1984), the computational cost for numerical first-order differentiation. The cost depends on the prescribed error bound and the FD operator accuracy and length:

$$C(d, L, E) = n_{\mathrm{op}}(L)[N_c(L, E)]^d, \qquad d = 1, 2, 3. \tag{12}$$

In equation (12) d is the dimensionality of the problem and $n_{\mathrm{op}}(L) = 3L/2 - 1$ is the number of floating-point operations needed to compute the numerical derivative ($L/2$ multiplications, $L/2$ subtractions, and $L/2 - 1$ additions). Figures 4 and 5 compare the cost of Holberg's schemes for different operator lengths L and error bounds E with conventional and pseudospectral differentiators. Holberg's operators of a given order L are always more cost-effective than conventional staggered FD of the same order. Furthermore, depending on the specified error bound and on the dimensions of the problem, an optimal Holberg scheme can be found. For example, with a specified error bound of 1%, Holberg's schemes of $L = 6$, 8 are the least costly for $d = 2$, 3, respectively. The pseudospectral scheme becomes attractive for small error bounds, especially in the three-dimensional case.

It should be clear that the proposed comparison takes an abstract computational cost viewpoint (in other terms, spe-

Table 1. Leading terms of the expansions of the Holberg's weights $\{d_{2\ell-1}\}$ given by equation (11) for the cases $L = 4, 6, 8$: the zeroth order terms of the expansions $b^{(L)}_{\ell 0}$ coincide with the conventional staggered differentiators weights. All the terms of the table are accurate to the last decimal digit, except for the terms of the first row ($L = 4$) or first column ($r = 0$), which are exact.

		$r = 0$	$r = 1$	$r = 2$	$r = 3$	$r = 4$	$r = 5$
L	ℓ	$b^{(L)}_{\ell 0}$	$b^{(L)}_{\ell 1}$	$b^{(L)}_{\ell 2}$	$b^{(L)}_{\ell 3}$	$b^{(L)}_{\ell 4}$	$b^{(L)}_{\ell 5}$
4	1	9/8	$\sqrt{3}/4$	−11/24	$4\sqrt{3}/27$		
	3	−1/24	$-\sqrt{3}/12$	−13/72	$-4\sqrt{3}/81$		
6	1	75/64	.2742	−.3006	.2637	−.2391	
	3	−25/384	−.1371	−.0100	.1077	−.0086	
	5	3/640	.0274	.0661	.0826	.0530	
8	1	1225/1024	.1987	−.2195	.2096	−.2038	.1779
	3	−245/3072	−.1192	.03929	.04049	−.05841	.04389
	5	49/5120	.03975	.04853	−.00967	−.05507	−.01117
	7	−5/7168	−.00568	−.02014	−.04039	−.04937	−.03625

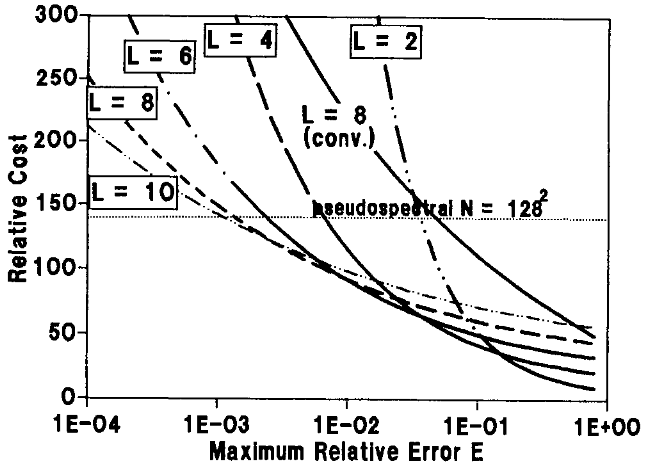

FIG. 4. Cost of numerical differentiation. Holberg's schemes of orders $2 \leq L \leq 10$ in the 2-D case as given by formula (12) correspond to the dashed curves; the solid curve corresponds to the cost of an eighth-order accurate conventional staggered FD scheme; and the dotted horizontal line represents the pseudospectral scheme (for which $E = 0$) when the number of grid points is 128^2. For $E = 1\%$, Holberg's scheme of order 6 is the most effective.

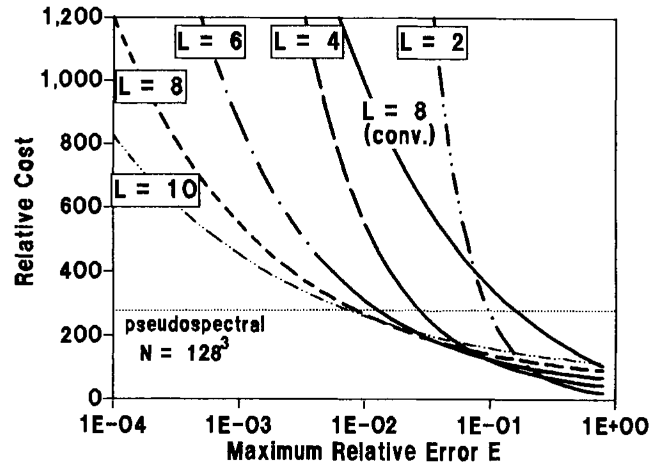

FIG. 5. Cost of numerical differentiation in the 3-D case. Holberg's schemes of orders $2 \leq L \leq 10$ as given by formula (12) correspond to the dashed curves; the solid curve represents an eighth-order accurate conventional staggered FD scheme; and the dotted horizontal line represents the pseudospectral scheme (for which $E = 0$) when the number of grid points is 128^3. For $E = 1\%$, Holberg's scheme of order 8 is the most effective.

cific hardware cost elements, such as the cost of memory access, have not been taken into account) and is strictly valid only for homogeneous media. In practice, for models involving dipping and curved interfaces, a grid resolution of roughly 3 grid points per shortest wavelength is required to ensure a reasonably accurate approximation of the interface conditions. The high spatial bandwidth of the pseudospectral method cannot be fully exploited, thus rendering Holberg's dispersion-bounded convolutional differentiators of orders 6 and 8, for which $N_c \cong 3$ (see Figure 3), competitive even at small error bounds. Furthermore, the present analysis of cost-effectiveness for a required error bound has not considered the role in the overall accuracy played by time discretization: this is the subject of Sguazzero et al.'s (1989) recent presentation.

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