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COMPUTATION OF PSEUDO-DIFFERENTIAL OPERATORS*

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Abstract. A simple algorithm is described for computing general pseudo-differential operator actions. Our approach is based on the asymptotic expansion of the symbol together with the fast Fourier transform (FFT). The idea is motivated by the characterization of the pseudo-differential operator algebra. We show that the algorithm is efficient through analyzing its complexity. Some numerical experiments are also presented.

Key words. pseudo-differential operators, fast Fourier transform, spatially varying filters, microlocal cut-off, data processing

AMS subject classifications. 35S05, 65T20, 86A22

1. Introduction. The theory of pseudo-differential operators (ΨDOs) has made many important contributions to the development of partial differential equations. It provides a natural way to decompose a differential operator, which may be difficult to study directly, into several pieces with a simple structure. A precise way to describe propagation of singularities for differential equations is in terms of ΨDOs. Pseudo-differential operators may be viewed as spatially varying filters with simple asymptotics at high frequencies. Pseudo-differential operators differentiate waves and wave-like signals according to directions of propagation. Pseudo-differential operators also arise naturally in diverse fields (often under different names!) such as wave propagation, electrical engineering, and geophysics.

Although the theory of ΨDOs, or, more generally, microlocal analysis, has been well established since the '60s, little attention appears to have been paid to the computation of ΨDOs. In this paper, we present a simple algorithm for the computation of general ΨDO actions. Our idea is based on the following characterization of ΨDOs.

Fact. The ΨDO algebra is generated by all differential operators and all powers of the Laplacian.

More precisely, ΨDOs and many functions of these (inverse, powers, ...) are included in ΨDOs in the high frequency asymptotic sense.

See Kohn and Nirenberg [3] for a detailed discussion.

2. Pseudo-differential operators. Here, we shall give a brief introduction to a class of ΨDOs. For a complete account of ΨDOs, as well as the calculus, the reader is referred to Taylor [5], Nirenberg [4], or Hörmander [2].

We begin with the introduction of the Fourier transform and the inverse Fourier transform. The Fourier transform acting on a "nice" function u defined in $\mathbf{R}^n$ is

$$\mathcal{F}(u) = \hat{u} = (2\pi)^{-n} \int u(x) e^{-ix\cdot\xi} dx,$$

and the inverse Fourier transform is defined by

$$\mathcal{F}^{-1}(u) = \int \hat{u}(\xi) e^{ix\cdot\xi} d\xi \ .$$

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Remark. A number of algorithms for the numerical computation of (discrete) Fourier transforms have been made available. We shall use a version of the FFT in our numerical work. A detailed description may be found in Conte and De Boor [1]. See also Van Loan [6] for the most recent development in the field.

Pseudo-differential operators are usually defined in terms of symbols, which are smooth functions of both space and frequency variables satisfying certain estimates. More precisely, $q(x, \xi)$ is a member of the symbol class $S^m_{1,0}(\mathbf{R}^n)$ iff $q(x, \xi)$ is a smooth function and for any compact subset K of $\mathbf{R}^n$, and real α, β, there exists a constant $C_{K,\alpha,\beta}$, such that

$$|D_x^\alpha D_\xi^\beta q(x, \xi)| \leq C_{K,\alpha,\beta}(1 + |\xi|)^{m-|\beta|} \tag{2.1}$$

for all $x \in K$ and $\xi \in \mathbf{R}^n$.

In this paper, we shall confine ourselves to a subclass of $S^m_{1,0}$, the class S^m, which is the most natural class and sufficient for many applications. A function $q(x, \xi)$ is in S^m if $q(x, \xi) \in S^m_{1,0}$ and there are smooth $q_{m-j}(x, \xi)$, homogeneous of degree $m - j$ in ξ for $|\xi| \geq 1$; i.e.,

$$q_{m-j}(x, r\xi) = r^{m-j} q_{m-j}(x, \xi), \quad |\xi| \geq 1\ , \quad r \geq 1 \tag{2.2}$$

such that

$$q(x, \xi) \sim \sum_{j \geq 0} q_{m-j}(x, \xi)\ , \tag{2.3}$$

in the sense that

$$q(x, \xi) - \sum_{j=0}^{N} q_{m-j}(x, \xi) \in S^{m-N-1}_{1,0}\ , \tag{2.4}$$

where $q_m(x, \xi)$ is called the principal symbol or principal part of $q(x, \xi)$ that carries the most important information about q.

Then the operator Q defined by

$$Q(x, D_x)u = \int q(x, \xi)\hat{u}(\xi)e^{ix\cdot\xi}d\xi \tag{2.5}$$

is called a ΨDO of order m or $Q \in OPS^m(\mathbf{R}^n)$.

In particular, differential operators with smooth coefficients are ΨDOs. Indeed, for such a differential operator of order m, the corresponding symbol is a polynomial in ξ of degree m, and consequently is a symbol in S^m. The asymptotic expansion of a symbol (2.3) is unique up to smoothing operators.

3. Algorithm. In this section we describe the algorithm explicitly. Its complexity will be examined in the section that follows. For the sake of simplicity, we shall only describe the idea of computing two-dimensional ΨDOs. Some obvious modifications may be made to compute ΨDOs of arbitrary dimension. Throughout, we shall always assume that the action of Q on u is meaningful. The precise conditions may be found in any one of the references [2]-[5].

Given a ΨDO $Q(x, z, D_x, D_z) \in OPS^m$ whose symbol is $q(x, z, \xi, \eta)$ and a function $u(x, z)$, our goal is to compute the action Qu efficiently. Let us assume that the asymptotic expansion of the symbol is given by

$$q(x, z, \xi, \eta) \sim \sum_{j \geq 0} q_{m-j}(x, z, \xi, \eta)\ , \tag{3.1}$$

where $q_{m-j}(x, z, r\xi, r\eta) = r^{m-j}q_{m-j}(x, z, \xi, \eta)$ for $(|\xi|, |\eta| \geq 1)$. Again, q_m denotes the principal symbol of q.

Knowing the asymptotic expansion of q we compute the ΨDO action Qu through computing $Q_{m-j}u$ for $j \geq 0$. We describe the calculation for $j = 0$, as it is representative. That is, we will describe an algorithm for computing the action of the principal part of a ΨDO. Evidently this algorithm could be applied recursively to compute general ΨDO actions. However, the principal part gives the dominant effect on high frequency inputs, which is most important for our intended applications. Thus, for us, computation of the principal part above is sufficient.

Let

$$\xi = \omega\cos\theta\ , \quad \eta = \omega\sin\theta\ , \quad \omega = \sqrt{\xi^2 + \eta^2}\ . \tag{3.2}$$

The homogeneity of q_m in ξ and η yields

$$q_m(x, z, \xi, \eta) = q_m(x, z, \omega\cos\theta, \omega\sin\theta) = \omega^m\tilde{q}_m(x, z, \theta)\ , \tag{3.3}$$

where $\tilde{q}_m(x, z, \theta)$ is defined to be $q_m(x, z, \cos\theta, \sin\theta)$.

Since $\tilde{q}_m$ is periodic in θ, it has a Fourier series expansion as follows:

$$\begin{aligned}\tilde{q}_m(x, z, \theta) = \sum_{l=-\infty}^{\infty} c_l(x, z)e^{il\theta} &\simeq \sum_{l=-K/2}^{K/2} c_l(x, z)e^{il\theta} \\ &= \sum_{l=-K/2}^{K/2} c_l(x, z)(\cos\theta + i\sin\theta)^l\ ,\end{aligned} \tag{3.4}$$

where K is an indicator of the number of terms in the expansion.

It follows from the definition of ΨDO (2.5) that

$$\begin{aligned}Q_m u &\simeq \int\int d\xi d\eta e^{i(x\xi+z\eta)} \sum_{l=-K/2}^{K/2} \omega^m c_l(x, z)(\cos\theta + i\sin\theta)^l\hat{u}(\xi, \eta) \\ &= \sum_{l=-K/2}^{K/2} c_l(x, z) \int\int d\xi d\eta\omega^m e^{i(x\xi+z\eta)}(\cos\theta + i\sin\theta)^l\hat{u}(\xi, \eta) \\ &= \sum_{l=-K/2}^{K/2} c_l(x, z)\mathcal{F}^{-1}[\omega^{m-l}(\xi + i\eta)^l\hat{u}(\xi, \eta)],\end{aligned} \tag{3.5}$$

where, to obtain the last equality, we have used the relations $\cos\theta = \xi/\omega$ and $\sin\theta = \eta/\omega$ in (3.2). Observe that ω^{m-l} is the symbol of the $(m-l)/2$-power of the (negative) Laplacian, while ξ and η are symbols of differential operators $D_x = -i\partial_x$ and $D_z = -i\partial_z$, respectively.

The procedure implicit in the above formulae leads to an algorithm to evaluate $Q_m u$ approximately, as follows. Assume that u is sampled on a discrete grid,

$$\begin{gathered}U_{i,j} = u(x_0 + (i-1)\Delta x, z_0 + (j-1)\Delta z)\ , \\ i = 1, \ldots, M, \quad j = 1, \ldots, N\ ,\end{gathered} \tag{3.6}$$

with spacings $\Delta x, \Delta z > 0$. Assume similarly that a sampling of $\tilde{q}_m$ is given

$$\begin{gathered}Q_{i,j,k} = \tilde{q}_m(x_0 + (i-1)\Delta x, z_0 + (j-1)\Delta z, k\Delta\theta)\ , \\ i = 1, \ldots, M,\ j = 1, \ldots, N,\ k = -K/2, \ldots, K/2\ .\end{gathered} \tag{3.7}$$

With $X = (M-1)\Delta x$, $Z = (N-1)\Delta z$, the sample rates in the frequency domain are $\Delta\xi = 1/X$, $\Delta\eta = 1/Z$, so the (unaliased) samples of the symbols of the Laplacian, D_x, and D_z are

$$\Omega_{p,r} = 2\pi\sqrt{(p\Delta\xi)^2 + (r\Delta\eta)^2}\ , \tag{3.8}$$

$$\Xi_{p,r} = 2\pi p\Delta\xi\ , \tag{3.9}$$

$$Z_{p,r} = 2\pi r\Delta\eta\ , \tag{3.10}$$

$$p = -M/2, \dots, M/2,\ r = -N/2, \dots, N/2\ ,$$

respectively.

PROCEDURE FOR COMPUTING $Q_m u$

1. Compute the discrete Fourier transform $\hat{U}$ of U.
2. For each $i \in \{1, \dots, M\}$ and $j \in \{1, \dots, N\}$, compute the discrete Fourier transform $\hat{Q}_{i,j} = \{Q_{i,j,l}\}_{l=-K/2}^{K/2}$ of $Q_{i,j} = \{Q_{i,j,k}\}_{k=-K/2}^{K/2}$.
3. Initialize $(QU)_{i,j} = 0.0$, for $i = 1, \dots, M$, $j = 1, \dots, N$.
   DO $l = -K/2,\ K/2$
   a compute the inverse Fourier transform $\{R^l_{i,j}\}_{i=1,j=1}^{M,N}$ of
   $$\Omega^{m-l}_{p,r}(\Xi_{p,r} + iZ_{p,r})^l\hat{U}_{p,r}$$
   for $p = -M/2, \dots, M/2$ and $r = -N/2, \dots, N/2$.
   b accumulate
   $$(QU)_{i,j} = (QU)_{i,j} + \hat{Q}_{i,j,l}R^l_{i,j}$$
   END DO

4. Complexity analysis. We return to the general case. The complexity will be analyzed by the number of multiplications. We also make a few remarks about the accuracy of the algorithm.

The direct method of computing the ΨDO action is by straightforward discretization of the definition

$$\begin{aligned} Q_m u &= \int\int q_m(x,\xi)\hat{u}(\xi)e^{ix\cdot\xi}d\xi \\ &= \mathcal{F}^{-1}[q_m(x,\xi)\hat{u}(\xi)]\ . \end{aligned}$$

Let us assume that the input function is discretized on a regular d-dimensional grid, as is the symbol q_m. We denote by N the number of grid points in each direction, assuming these are roughly similar. Assuming also that the discrete Fourier transforms are computed using an FFT algorithm. We then have the following result.

LEMMA 4.1. *The direct algorithm has $O(N^{2d}\log N)$ complexity.*

This is an immediate consequence of the well-known fact that the FFT exhibits $O(N\log N)$ complexity, where N is the length of the input sequence.

We next discuss the complexity of the new algorithm. For simplicity, we once again consider the two-dimensional case. The approximate complexity orders of the steps in the algorithm proposed above are

1. $N^2\log N$;
2. $N^2K\log K$; and
3. a. $KN^2\log N$, b. KN^2.

Hence the total complexity is $O(KN^2(\log N + \log K))$ in two dimensions.

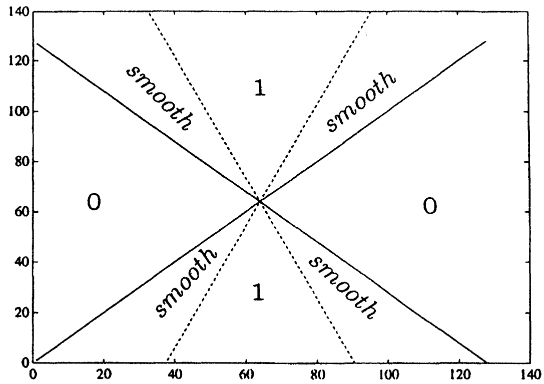


FIG. 1. *The symbol of a convolutional operator.*

In general, when the number of dimensions is d, a similar calculation will give Lemma 4.2.

LEMMA 4.2. *The new algorithm exhibits $O(K^{d-1}N^d(\log N + \log K))$ complexity.*

Remarks. The new algorithm is significantly superior to the direct method. In practice, the number of terms K in the finite θ-Fourier series approximation of q_m (3.4) ought to be chosen properly to make the sup-norm error small. If this is the case, the error in the computation of Q_m, modulo compact operators, will also be small (Taylor [5], p. 52). In particular the error will be small for oscillatory inputs u. Note that K is completely independent of N in this regard. Thus, in effect, the complexity of our algorithm is $O(N^d \log N)$!

In actual applications, N is usually big. When N and K are given, the numbers of multiplications involved in our algorithm and the direct method may be calculated easily. What makes the real difference is the number K. The theory and our numerical experiments both indicate that the number K depends only on the smoothness of the symbol, is insensitive to N, and can always be small.

5. Numerical experiments. In this section, we present the results of some numerical experiments carried out with the ΨDO algorithm. The class of ΨDO of great importance in our applications are microlocal cutoff operators, i.e., operators whose symbols are asymptotically one in some conic set and asymptotically zero in the complement of a slightly bigger conic set (essential support or aperture). These are the simplest undecomposable order zero ΨDOs. Our numerical experiments exhibit some interesting features of ΨDOs.

We begin with convolutional ΨDOs, which are ΨDOs that are independent of spatial variables. Convolutional operators are natural extensions of differential operators with constant coefficients. For this class of operators, it is easy to show that

$$\mathcal{F}(Qu) = Q(\xi)\hat{u}(\xi) \ . \tag{5.1}$$

This simple identity is useful in verifying the code. In fact, according to (5.1), one can recover the symbol from $\mathcal{F}(Qu)$ and $\hat{u}$. A symbol that characterizes a microlocal cutoff is specified by Figure 1, where the symbol is designed to be a C^2 function. Figure 2 displays the symbol function in terms of the angle θ. From this one-dimensional array, the ΨDO algorithm may be employed to compute the action, and hence the two-dimensional symbol function Q. The result, Figure 3, shows the symbol when the number of terms in Fourier series expansion of the symbol $K = 4$. It is easy to see that the symbol in Figure 3 illustrates the right direction

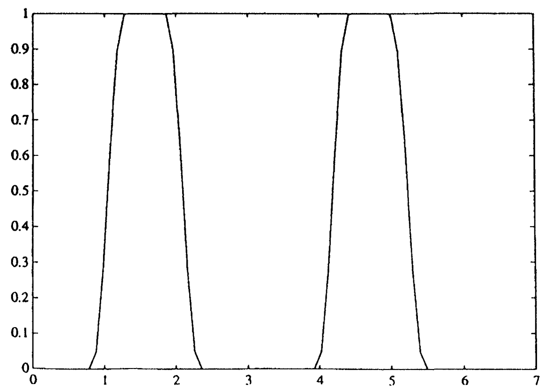
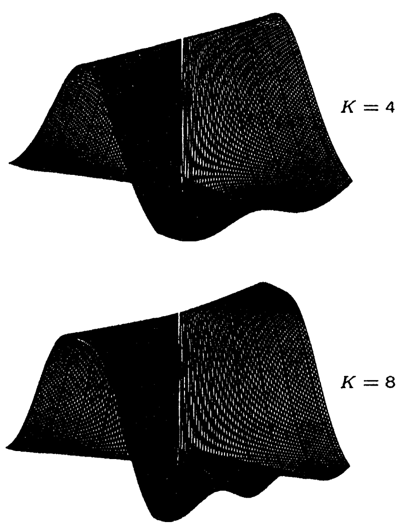


FIG. 2. *The same symbol as a function of* θ: *The angle with the horizontal axis.*



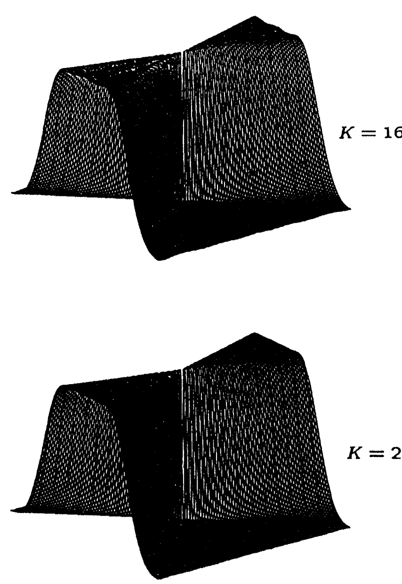


FIG. 3. *Symbol recovery*: $k = 4$.

FIG. 4. *Symbol recovery*: $k = 28$.

but wrong amplitude within the aperture. As the number of terms K increases, the recovery of the symbol becomes better and better. Figure 4 shows that the symbol is perfectly recovered after several steps. Again, we want to emphasize that the number K only depends on the smoothness of the symbol, and particularly is independent of the grid size N.

Another numerical experiment of ours concerns the rotation of apertures for convolutional operators. The function plotted in Figure 5 is a slightly smoothed characteristic function of a circle. We apply a ΨDO cutoff, whose symbol is given in Figure 6, to this function. Just as the theory predicts, the high frequency information of the resulting function (Figure 7) is well preserved within the aperture. We then rotate the symbol (Figures 8 and 10), and again the high frequency information is preserved in Figures 9 and 11, respectively. These examples are only illustrative, as the discrete Fourier transform allows a very simple and fast computation of convolution operators.

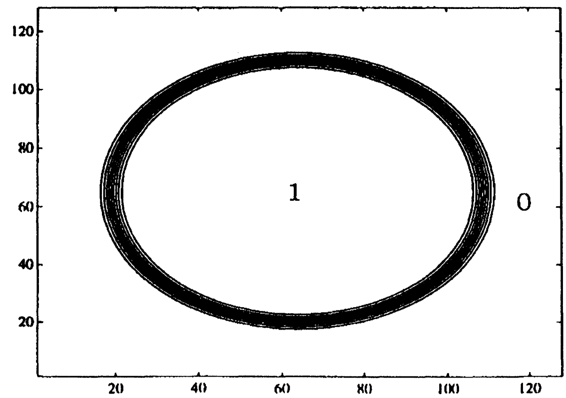


FIG. 5. *Function u.*

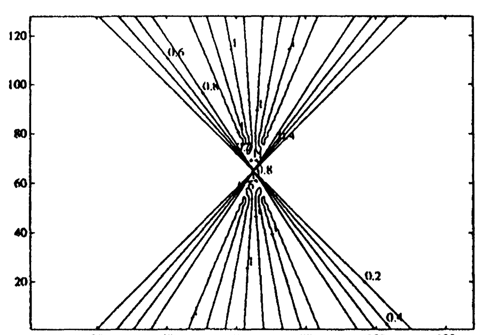


FIG. 6. *Symbol* q_0.

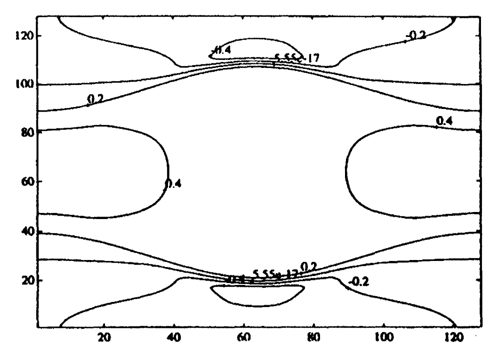


FIG. 7. *The action* $q_0 u$.

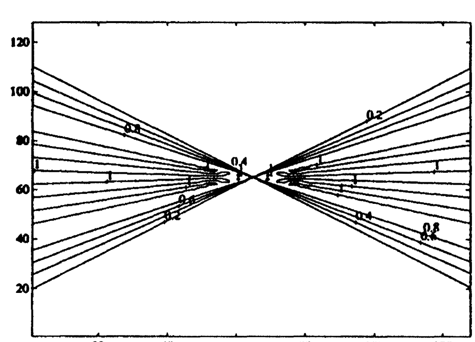


FIG. 8. *Symbol rotation* 1.

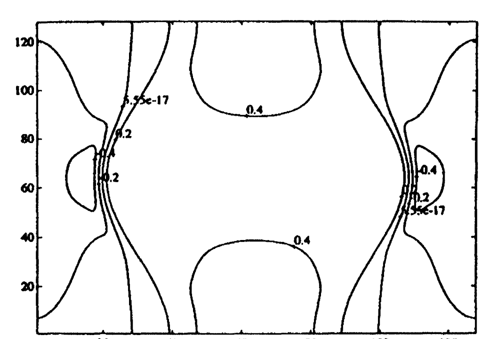


FIG. 9. *The action for rotation* 1.

Our next example is meant to illustrate the success of our algorithm with nonconvolutional ΨDOs. Figure 12 shows the symbol of a two-dimensional ΨDO, which is spatially varying (in the z-direction). The symbol can be generated from $q(z, \theta) = q_0(\theta + \delta\theta \sin(\pi z / z_{\max}))$, where q_0 is given in Figure 6, $\delta\theta$ is selected to be $\pi/2$, and $z \in [0, z_{\max}]$. Thus, as z increases, the symbol rotates smoothly; in particular the symbol will be equal to q_0 when z reaches its

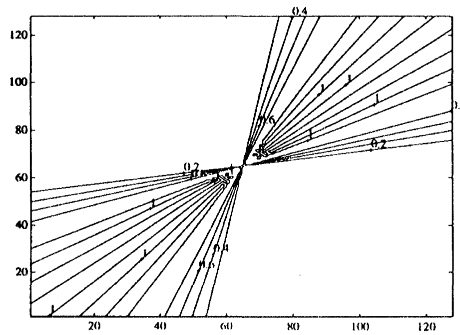


FIG. 10. *Symbol rotation* 2.

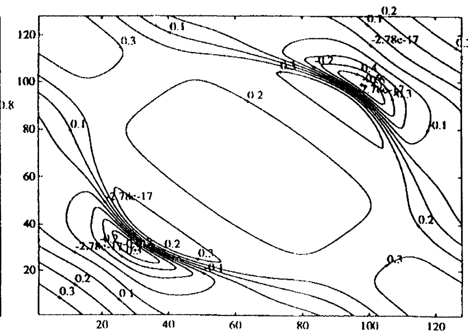


FIG. 11. *The action for rotation* 2.

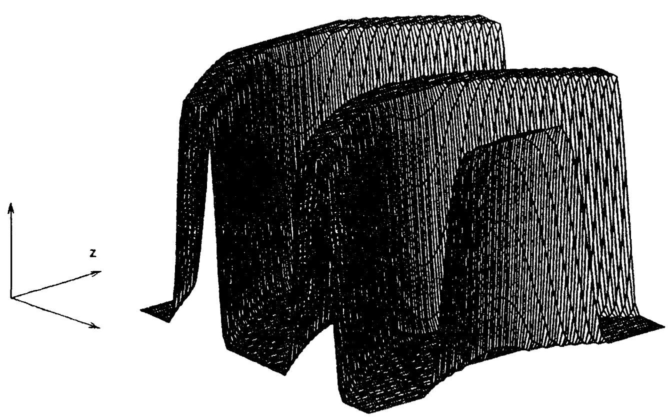


FIG. 12. *A spatially varying symbol.*

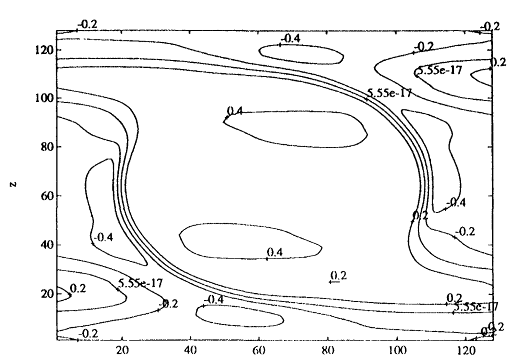


FIG. 13. *The action for the spatially varying symbol.*

maximum. Once again, the function u is the same as before in Figure 5. The result, as shown in Figure 13, agrees with the theory. Observe that the aperture is vertical for z near 0. The symbol rotates as z increases, so we start to see some high frequency horizontal components. When z is getting close to its maximum, the symbol rotates back, and the aperture becomes vertical again.

Our final example demonstrates an important application of the ΨDO algorithm to the seismic data processing in reflection seismology. The basic objective of all seismic processing is to convert the information recorded in a field into a form that most greatly facilitates geological interpretation of such a field. Evidently, real reflection data, which carry most of the information of the mechanical properties of the earth, are what geophysicists are most interested in obtaining through this process. Thus, an essential object of the processing is to eliminate or suppress all signals not associated with reflections. Figure 14 displays a seismogram, i.e., the recorded seismic data at receivers on the surface of the earth after an energy source is fired. The dark region that can be seen clearly contains very strong signals. These signals represent the early arrivals (direct and head waves). In the region below, there are other signals (reflections) which are not nearly as strong as the early arrivals. Unfortunately, the direct and head waves do not penetrate the earth; hence they contain no information about the subsurface about which we are interested. What contains useful information is the reflection energy in the lower region. This can be observed more clearly if one increases the amplitude of the seismogram as in Figure 15. The question arises: can one remove the early arrivals and yet keep the useful information of reflections? Applying the ΨDO computation algorithm, we design a microlocal cutoff (ΨDO) whose action on the seismogram is shown in Figure 16. The result appears to be very encouraging. The amplitude of the early arrivals is reduced dramatically, and meanwhile information of reflections is well preserved. We apply the same ΨDO filter to the data set once more to obtain an even better result shown in Figure 17. Now, the early arrivals are essentially gone, while again most of the reflections are preserved. We believe the noise left in the region where the early arrivals resided is caused by numerical scales; hence they can be eliminated. This processing technique is actually used in reflection seismology, where it is called "f-k dip filtering," e.g., Yilmaz [7], pp. 69–78. Our ΨDO algorithm yields an accurate and efficient means of "spatially variable dip filtering," for which we envision numerous uses. However, the enormous amount of computations of ΨDOs by the direct method makes any practical application impossible. Note that in the above examples, the grid size is taken to be 256 in each direction, which should be much bigger in real applications. However, the number K may be chosen much smaller than N due to the fact that K is independent of N.

6. Concluding remarks.

A simple algorithm for the computation of a class of ΨDOs is introduced in this work. We exhibit some of the features of the algorithm. The complexity analysis indicates that the algorithm is much more efficient than the direct computation. Because of the simple structure, various massive parallel computers may be used to implement this algorithm so long as a fast FFT routine and fast array operations are available. In fact, some of our numerical experiments reported in this paper were obtained by using the Connection Machine.

We anticipate many applications of this algorithm. For example, ΨDOs are expected to play an important role in regularizing a class of ill-posed problems in multidimensional wave propagation that arise naturally in seismic inversion, oil and gas exploration, and many other related geophysical problems. Our experiment indicates the usefulness of microlocal (or ΨDO) cutoff in seismic data processing, i.e., sorting of waves according to direction in seismic data.

Mathematically, this algorithm should provide a way to compute the so-called microlocal norms of microlocal Sobolev spaces, which in turn would help us test the sharpness of various results on propagation of singularities for partial differential equations. This algorithm should also have some impact on signal processing, where ΨDOs form a class of spatially varying filters.

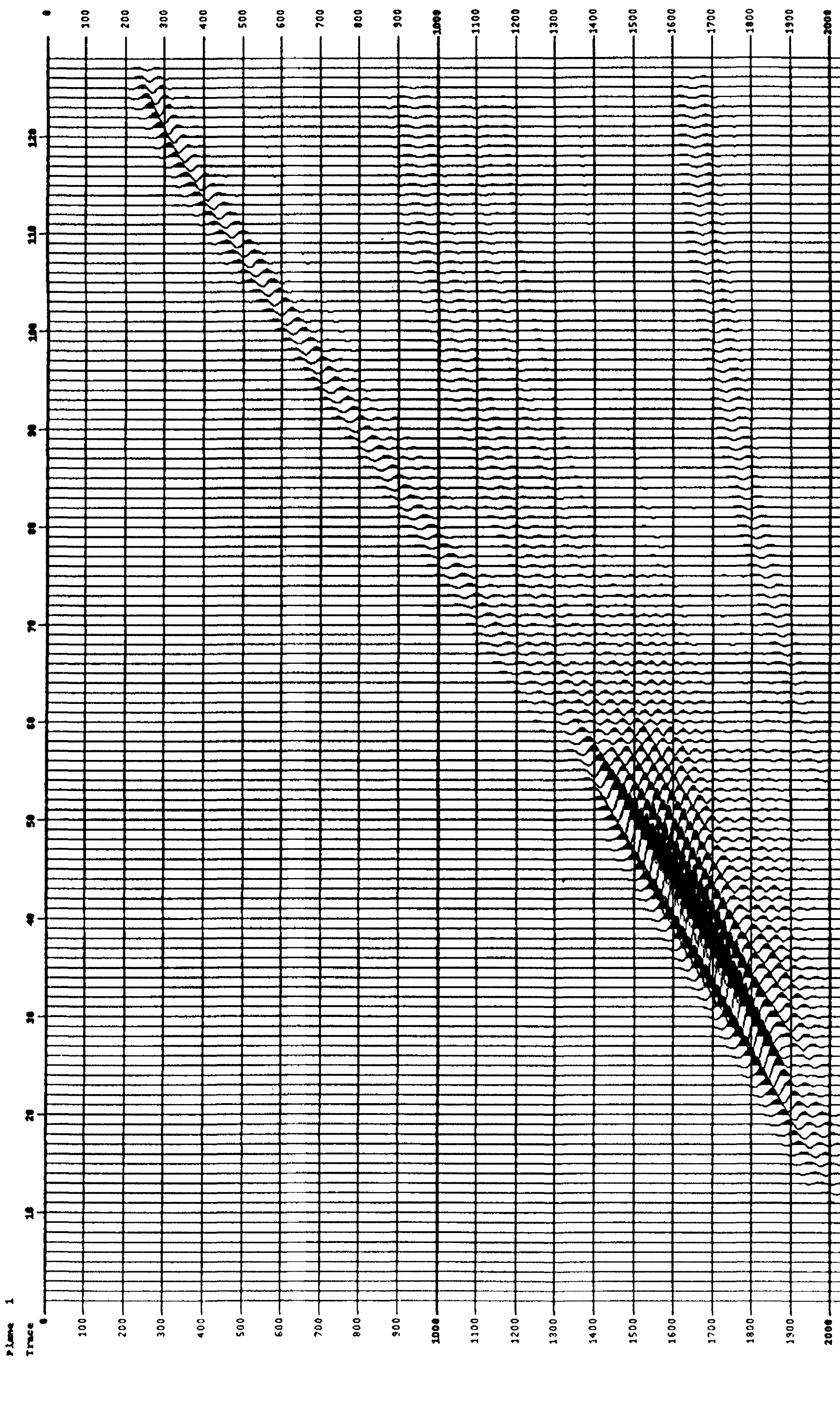


FIG. 14. *Seismogram.*

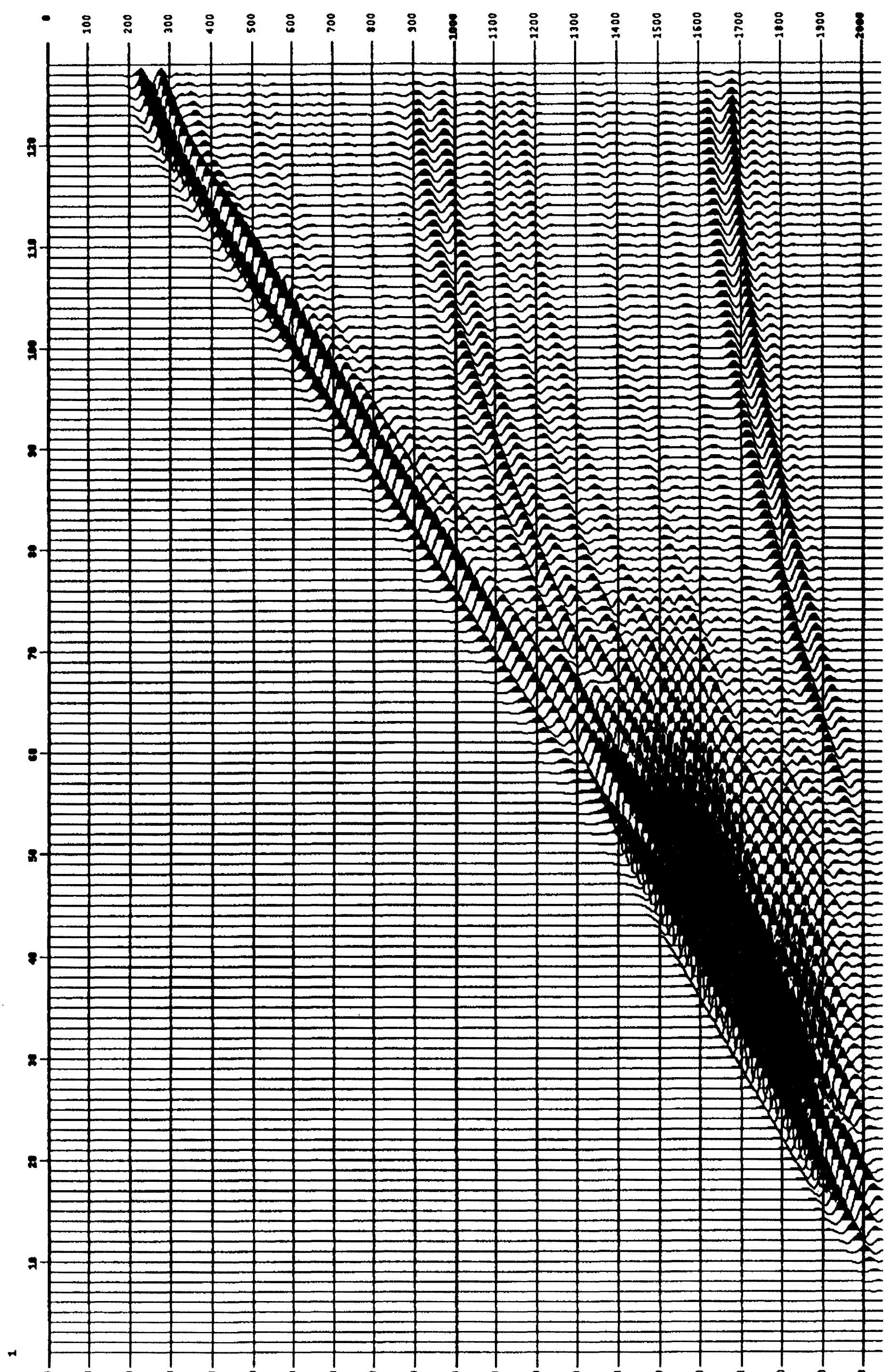


FIG. 15. *Seismogram with increased amplitude.*

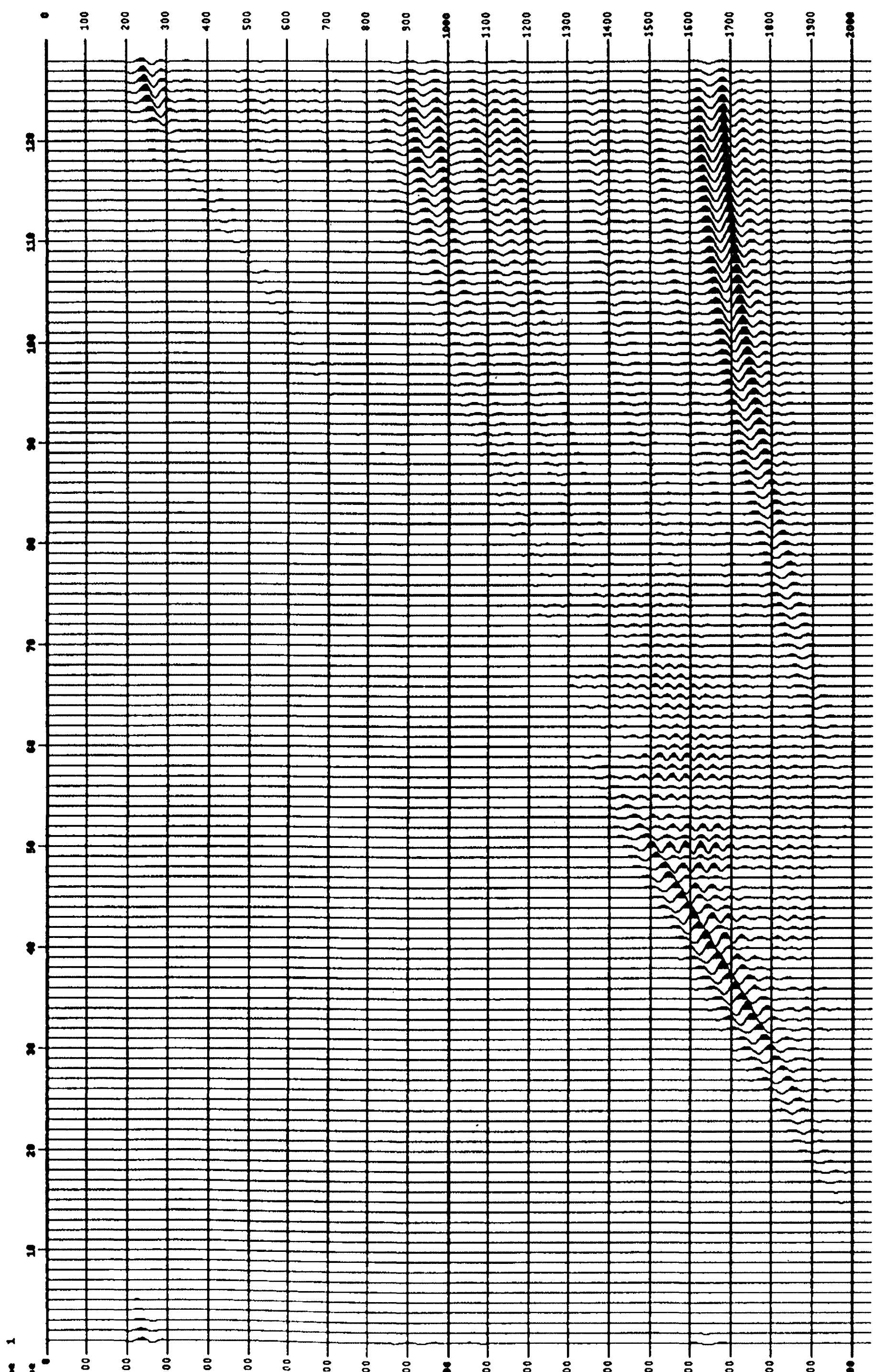


FIG. 16. *The result after applying the filter.*

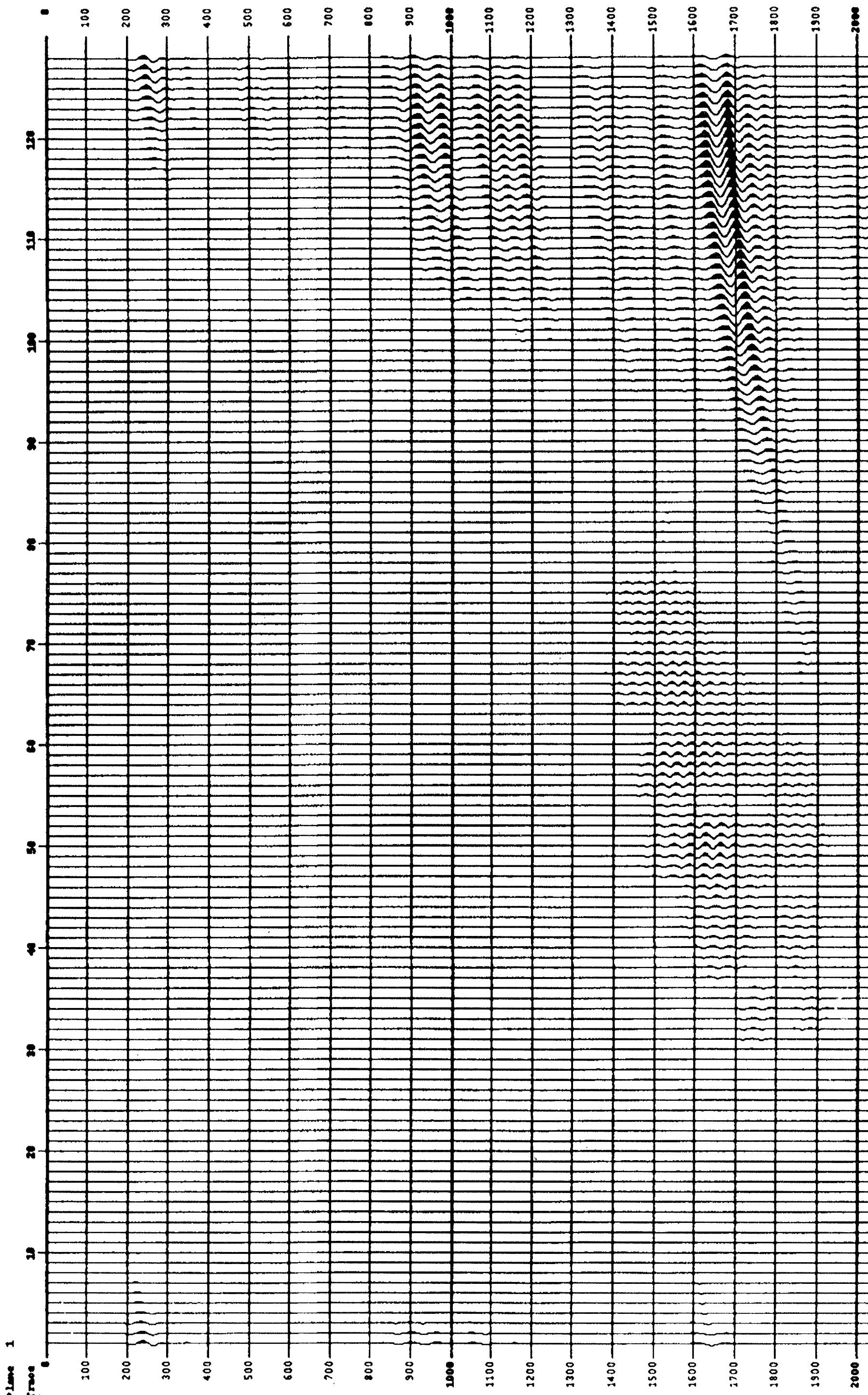


FIG. 17. *The result after applying the filter twice.*

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