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A Finite Difference Procedure for a Class of Free Boundary Problems

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Finite difference schemes loose accuracy when free boundaries cross over rectangular grids. For a class of second-order equations, the leading error term at such a boundary can be eliminated by a simple correction strategy. This procedure works in any number of space dimensions and offers an alternative to (more costly and complicated) adaptive grid techniques.

1. INTRODUCTION

We consider equilibrium equations of the form

$$L\psi + f^+(\psi) = 0, \tag{1}$$

where

$$f^+(\psi) = \begin{cases} 0 & \text{if} \quad \psi \leqslant 0 \\ \left.\begin{matrix} \lambda\psi + O(\psi^2) \\ \text{or} \\ \mu + O(\psi) \end{matrix}\right\} & \text{if} \quad \psi > 0. \end{cases} \tag{2}$$

Here, ψ is a function of any number of space variables, L a linear (or locally linearizable) second-order elliptic differential operator (with lower order terms allowed) and λ (>0) and μ ($\neq 0$) smooth functions of the space variables (and/or of low derivatives of ψ).

An important equation of this form is the Grad–Schlüter–Shafranov equation describing magnetohydrodynamic equilibria in plasma physics, cf. [1, 2]. Reference [2] investigates the discretization errors of standard difference schemes for this equation and describes an early implementation of the present correction method.

Straightforward numerical approximation of (1) with centered, second-order finite differences will give second-order accuracy away from the free boundary (along which $\psi = 0$), but only first- or zeroth-order (dependent on the character of $f^+(\psi)$ at the interface) whenever any "leg" of the finite difference stencil happens to cross over this boundary. Since the large errors occur only on a set of one order lower dimensionality than the full solution space, the global error will be one order higher, i.e., second or first order, respectively. In both cases, the error level will have increased significantly and the error will depend in a very irregular way on the location of the free boundary relative to the grid. This damages the convergence rate of, for example, multi-grid and makes enhancements like Richardson extrapolation or deferred correction impractical.

The purpose of this paper is to point out a simple strategy to eliminate the leading error term at the free boundary. Figures 1–3 illustrate the general procedure in the special case of

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \lambda\psi^+ = 0 \tag{3}$$

with

$$\lambda = 1, \qquad \psi^+ = \begin{cases} 0 & \text{if} \quad \psi < 0 \\ \psi & \text{if} \quad \psi \geqslant 0. \end{cases} \tag{4}$$

Figure 1 displays one particular solution to this equation. Figure 2 shows the residual obtained when this solution is substituted into the standard second-order finite difference approximation to (3). Smooth second-order residuals arise

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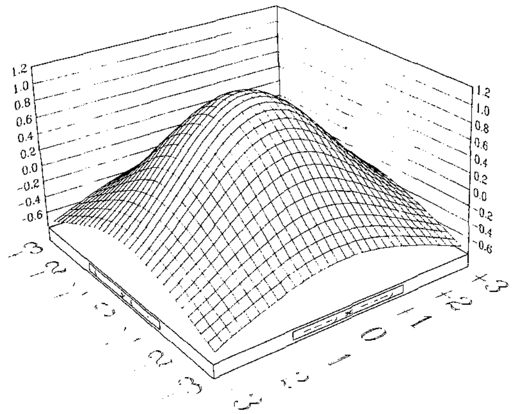

FIG. 1. Example of free boundary problem (demonstration problem 1):

Equation.

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\psi^+=0.$$

Solution shown.

$$\psi(x,y)=\begin{cases}J_0(r) & r\leqslant r_c\\ A\times\log(r/r_c) & r>r_c,\end{cases}$$

where

$$r=(x^2+y^2)^{1/2}$$

$J_0(r)$, Bessel function of order zero

r_c, first zero of $J_0(r)$, ≈ 2.404826

$A=r(d/dr)\,J_0(r)|_{r=r_c}\approx -1.248459.$

Free boundary. $\psi(x,y)=0$ along the circle $x^2+y^2=r_c^2$.

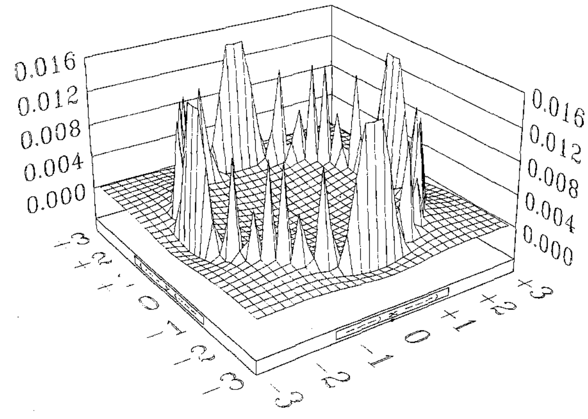

FIG. 2. Calculation of residual in demonstration problem 1: Residual when the solution $\psi(x,y)$ (with the square $-3\leqslant x, y\leqslant 3$ corresponding to array locations $f(i,j)$, $-15\leqslant i,j\leqslant 15$) is substituted into the standard finite difference approximation to the equation:

```
:
:
dx = 0.2
for i = -15 to 15 step +1
  for j = -15 to 15 step +1
    res(i,j) = (f(i+1,j) + f(i-1,j) + f(i,j+1) + f(i,j-1)
         - 4.0*f(i,j))/dx**2
    if f(i,j) > 0.0 then res(i,j) = res(i,j) + f(i,j)
    next j
  next i
:
:
```

(*Negative of Residual shown*).

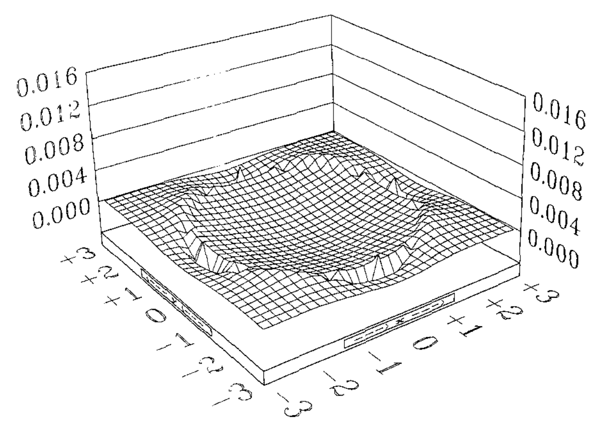

FIG. 3. Calculation of boundary corrected residual in demonstration problem 1:

Correction for free boundary. Immediately before the *next j*—statement closing the innermost loop in Fig. 2, add the following lines:

```
:
c = 2.0/(3.0*((f(i+1,j) - f(i-1,j))**2 + (f(i,j+1) - f(i,j-1))**2))
if f(i,j)*f(i+1,j) < 0.0 then res(i,j) = res(i,j) + c*abs(f(i+1,j))**3
if f(i,j)*f(i-1,j) < 0.0 then res(i,j) = res(i,j) + c*abs(f(i-1,j))**3
if f(i,j)*f(i,j+1) < 0.0 then res(i,j) = res(i,j) + c*abs(f(i,j+1))**3
if f(i,j)*f(i,j-1) < 0.0 then res(i,j) = res(i,j) + c*abs(f(i,j-1))**3
(next j)
```

(*Negative of Residual shown*).

throughout the domain. Regarding the large first-order ones along the free boundary, we note

i. they are of the same sign everywhere (suggesting that no "local averaging" procedure is likely to work, nor are favorable cancellations likely to occur in applications), and

ii. they depend very much on just how the boundary cuts across each finite difference stencil (over 1 or 2 "legs" of it, where along the "legs," at what angles etc.).

Figure 3 illustrates, how a correction procedure, applied to each "leg" separately, all but removes the errors. The procedure, in this special case, is derived in Section 2 below. The concluding Section 3 discusses different generalizations (to more general elliptic operators, variable coefficients, more space dimensions, etc.). Two more test cases are also presented.

2. DERIVATION OF CORRECTION PROCEDURE

We consider first the special case of Eq. (3). To keep the notation simple, let the grid be uniform with spacing h in both directions. Assume further that the free boundary cuts two "legs" of a stencil centered at the origin (cf. Fig. 4a). "Locally," $\psi(x, y)$ behaves like a plane which cuts the x-y-plane along the straight line $\psi(x, y)=0$. With this assumption of local linearity (implying $2\psi_0=\psi_1+\psi_3=\psi_2+\psi_4$; stencil points numbered as in Fig. 4a), the line $\psi(x, y)=0$ intersects the x- and y-axes at $x=-2h\psi_0/(\psi_1-\psi_3)$ and $y=-2h\psi_0/(\psi_2-\psi_4)$, respectively. Its equation is therefore

$$\frac{\psi_1-\psi_3}{2h}x+\frac{\psi_2-\psi_4}{2h}y+\psi_0=0. \tag{5}$$

Figure 4a shows a rectilinear ξ-η-coordinate system, where η is aligned with the free boundary and the ξ-axis is pointing into the area where ψ is positive. Noting the formula for the distance between a point and a line (Fig. 4b), the magnitudes of the ξ-coordinates at the five grid points (at locations (0, 0), (h, 0), (0, h), etc.) become

$$|\xi_i|=|\psi_i|/D^{1/2}, \qquad i=0, 1, 2, ..., 4, \tag{6}$$

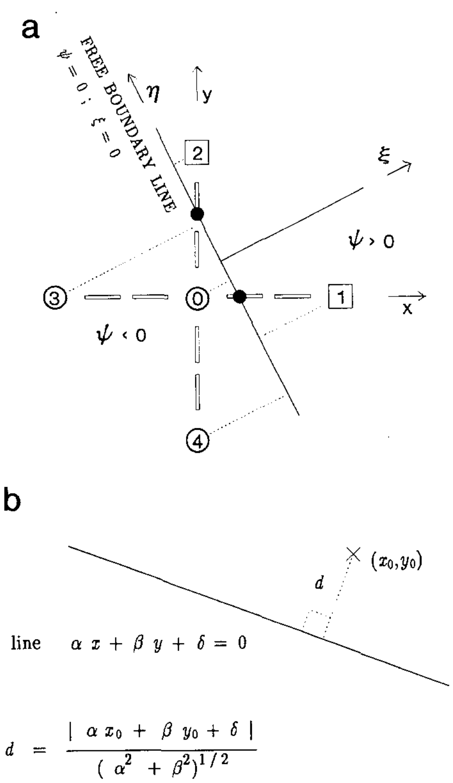

FIG. 4. (a) Notations used in the case of a 2D, 5-point finite difference stencil. (b) Distance between a point and a line.

where

$$D=\left(\frac{\psi_1-\psi_3}{2h}\right)^2+\left(\frac{\psi_2-\psi_4}{2h}\right)^2. \tag{7}$$

The slope $\partial\psi/\partial\xi$ between the $\psi(x, y)$-plane and the x-y-plane can be calculated in any of a number of ways, e.g., $(\psi_2-\psi_3)/(|\xi_2|+|\xi_3|)$, $(\psi_2-\psi_4)/(|\xi_2|+|\xi_4|)$, $(\psi_2-\psi_0)/(|\xi_2|+|\xi_0|)$, etc., all giving $\partial\psi/\partial\xi=D^{1/2}$. Since (3) takes the same form in ξ, η- as in x, y-coordinates, the "sudden" activation of ψ^+ as ξ increases through zero causes a jump of size $-\lambda D^{1/2}$ in $\partial^3\psi/\partial\xi^3$. In the case shown in Fig. 4a, the values of ψ_i, $i=1, 2$, are therefore

$$\lambda D^{1/2}|\xi_i|^3/6=\frac{\lambda}{6D}|\psi_i|^3 \tag{8}$$

less than what they would have been, had no free boundary been present. In the difference stencil approximating the Laplacian, these entries get divided by h^2. Every occurrence of the free boundary crossing a "leg" therefore reduces the residual by

$$\frac{\lambda}{6h^2D}|\psi_i|^3. \tag{9}$$

To restore full second-order accuracy, these corrections must be added back into the difference scheme.

Other alignments between the boundary and the stencil can be considered, e.g., $\psi_0>0$ (i.e., with the ψ^+-term included in the basic approximation), boundary crossing only one "leg" etc. It is easily verified that (9) takes the same form in all such cases. The code in Fig. 3 amounts to a direct implementation of (9).

3. GENERALIZATIONS

What makes the simple one-term correction we have just described for Eqs. (3) and (4) more than just a curiosity is that the equation can be made very much more general without the correction procedure becoming more complicated. For example:

i. $f^+(\psi)$ may be discontinuous when $\psi=0$ (rather than having a discontinuous derivative)

ii. L may include lower order terms (first derivatives etc.)

iii. L may include variable coefficients; $\lambda\psi^+$ may be generalized to $f^+(\psi)$

iv. The second-order part of L may include mixed derivatives and have different coefficients in front of the dif-

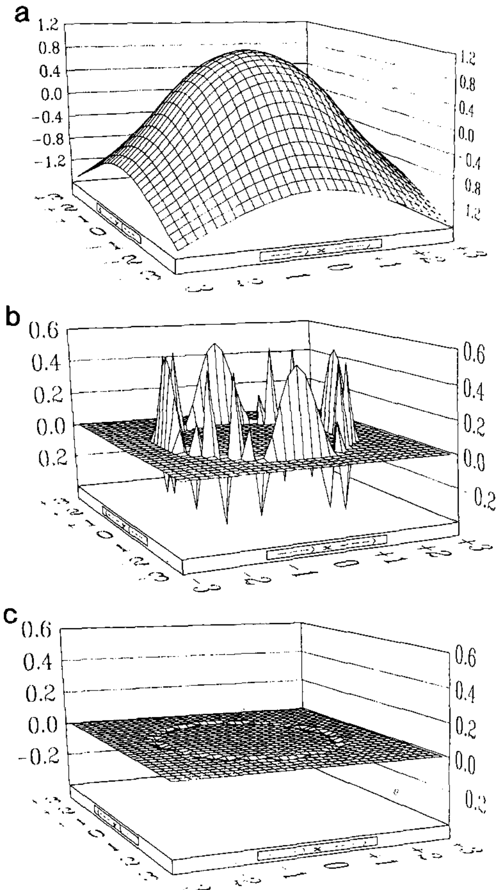

FIG. 5. (a) Solution to demonstration problem 2; (b) Residual in demonstration problem 2; (c) Corrected residual in demonstration problem 2.

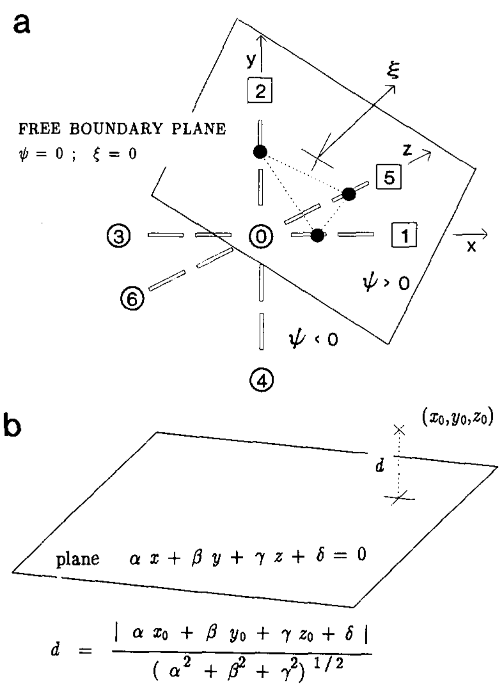

FIG. 6. (a) Notations used in the case of a 3D, 7-point finite difference stencil. (b) Distance between a point and a plane.

ferent terms. Also, the grid spacing may differ in the different spatial directions

v. There can be more (or fewer) than two space dimensions.

To address these issues in turn:

i. If the boundary irregularity in (3) and (4) is modified to

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \mu H(\psi) = 0 \tag{10}$$

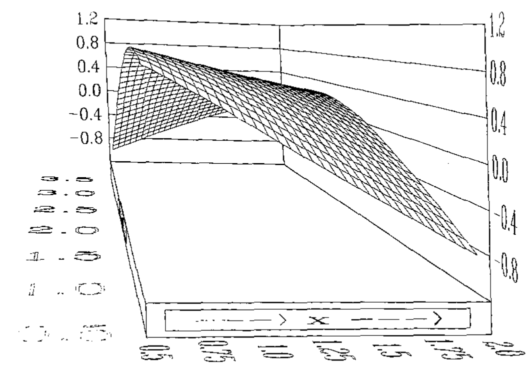

FIG. 7. Example of free boundary problem (demonstration problem 3): *Equation.*

$$CXX\frac{\partial^2\psi}{\partial x^2} + CXY\frac{\partial^2\psi}{\partial x\,\partial y} + CYY\frac{\partial^2\psi}{\partial y^2}$$

$$+ CX\frac{\partial\psi}{\partial x} + CY\frac{\partial\psi}{\partial y} + CPL\,\psi^+ = 0,$$

where CXX etc. depend on x and y as follows:

$$CXX = 16x^2 - 24xy + 8y^2 + 2x - 2y$$
$$CXY = 32x^2 - 48xy + 16y^2 + 8x - 8y$$
$$CYY = 16x^2 - 24xy + 8y^2 + 8x - 8y$$
$$CX = 2x - 2y + 1$$
$$CY = 2x - 2y + 2$$
$$CPL = 2x - 2y.$$

Solution shown.

$$\psi(x, y) = \begin{cases} \cosh[(-r)^{1/2}] & r \leqslant 0 \\ \cos(r^{1/2}) & 0 < r \leqslant \pi^2/4 \\ \pi/2 - r^{1/2} & r > \pi^2/4 \end{cases}$$

where

$$r = x^2 - 2xy + y^2 + 2x - y.$$

Free boundary. $\psi(x, y) = 0$ along the curve $r = \pi^2/4$. (*Note.* Although changing analytical form, the solution remains smooth across the curve $r = 0$.)

with

$$H(\psi)=\begin{cases}0 & \text{if } \psi<0\\ 1 & \text{if } \psi\geqslant 0,\end{cases} \tag{11}$$

the appropriate correction for each "leg" that crosses the free boundary becomes a slight modification of (9), namely,

$$\frac{\mu}{2h^2D}\psi_i\,|\psi_i|. \tag{12}$$

Figures 5a, b, and c show the equivalent results to Figures 1, 2, and 3 when the correction (12) is applied to

$$\psi(x,y)=\begin{Bmatrix}1-r^2/4, & r\leqslant 2\\ \log(4/r^2), & r>2\end{Bmatrix}, \quad r=(x^2+y^2)^{1/2}, \tag{13}$$

which solves (10) and (11) in the case of $\mu=1$.

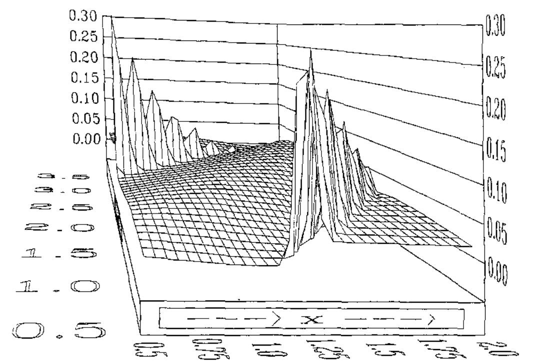

FIG. 8. Calculation of residual in demonstration problem 3: Residual when the solution $\psi(x,y)$ (with the rectangle $0.5\leqslant x\leqslant 2.0$, $0.5\leqslant y\leqslant 3.5$ corresponding to array locations $f(i,j)$, $0\leqslant i,j\leqslant 30$) is substituted into the standard nine point finite difference approximation:

```
   :
dx = 0.05
dy = 0.10
  for i = 0 to 30 step +1
    for j = 0 to 30 step +1
      w(-1,  1) = -cxy(i,j) * 0.25/(dx* dy)
      w( 0,  1) =  cyy(i,j) / dy**2            + cy(i,j) * 0.5/dy
      w( 1,  1) =  cxy(i,j) * 0.25/(dx* dy)
      w(-1,  0) =  cxx(i,j) / dx**2            - cx(i,j) * 0.5/dx
      w( 0,  0) = -cxx(i,j) * 2.0/dx**2        - cyy(i,j) * 2.0/dy**2
      w( 1,  0) =  cxx(i,j) / dx**2            + cx(i,j) * 0.5/dx
      w(-1, -1) =  cxy(i,j) * 0.25/(dx* dy)
      w( 0, -1) =  cyy(i,j) / dy**2            - cy(i,j) * 0.5/dy
      w( 1, -1) = -cxy(i,j) * 0.25/(dx* dy)
        res(i,j) = 0.
      for k = -1 to 1 step +1
        for l = -1 to 1 step +1
          res(i,j) = res(i,j) + w(k,l)* f(i+k,j+l)
          if f(i,j) > 0. then res(i,j) = res(i,j) + cpl(i,j)*f(i,j)
          next l
        next k
      next j
    next i
   :
```

ii. The value of $\partial^3\psi/\partial\xi^3$ (of $\partial^2\psi/\partial\xi^2$ in the case of $f^+(\psi)$ discontinuous at $\psi=0$) will jump at the boundary with the same amount (to leading order) even if lower order derivatives are present. Since finite difference approximations for first derivatives only involve a division by h (vs. by h^2 for second derivatives), such terms can be ignored as far as the corrections are concerned.

iii. In the case of variable coefficients, we simply use their local values at the center of the stencil. The errors that this leads to will again be of a lower order.

iv. If the second-order operator locally takes the more general form

$$a\frac{\partial^2\psi}{\partial x^2}+b\frac{\partial^2\psi}{\partial x\,\partial y}+c\frac{\partial^2\psi}{\partial y^2}, \tag{14}$$

the only essential difference that arises is that the transformation between x, y- and ξ, η-coordinates is no longer completely trivial. To accommodate for this (and for different steps h and k in the x- and y-directions), we generalize the definition of D in (7) to

$$D=a\left(\frac{\psi_1-\psi_3}{2h}\right)^2+b\left(\frac{\psi_1-\psi_3}{2h}\right)\left(\frac{\psi_2-\psi_4}{2k}\right)+c\left(\frac{\psi_2-\psi_4}{2k}\right)^2. \tag{15}$$

Although the derivation carries through slightly differently, the "end result" remains the same: the corrections are

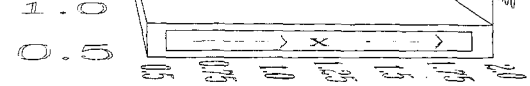

FIG. 9. Calculation of boundary corrected residual in demonstration problem 3:

Correction for free boundary. Within the loops over i and j but before the loops over k and l in the code in Fig. 8, add:

```
ddx = (f(i+1,j) - f(i-1,j))/(2.0* dx)
ddy = (f(i,j+1) - f(i,j-1))/(2.0* dy)
d   = cxx(i,j)* ddx**2 + cxy(i,j)*ddx*ddy + cyy(i,j)*ddy**2
```

Within the loops over k and l, add:

```
if f(i,j)* f(i+k,j+1) < 0.0
then res(i,j) = res(i,j) +
     w(k,l)*cpl(i,j)* abs(f(i+k,j+l))** 3/(6.0*d)
```

obtained by multiplying the (rightmost) expression in (8) with the corresponding weight in the finite difference stencil. The assumption that L is an elliptic operator (i.e., D is a positive definite form) protects against division by zero in (8) (if it were to happen that both $\psi_1 = \psi_3$ and $\psi_2 = \psi_4$, then $\psi(x, y)$ is locally independent of both x and y and no correction at all is called for).

v. The result in (8) remains the same and (15) generalizes in the obvious way. Figures 6a, b summarize the key geometric differences when going from 2D to 3D. As before, corrections have to be made for each stencil point which lies on the different side of the boundary than the center stencil point.

Figures 7–9 show an example which includes variable coefficients, lower order terms as well as different grid spacings in the two space dimensions. The corrections are even more accurate in this case than in the previous test cases (Figs. 1–3 and Fig. 5), mainly because the curvature of the free boundary is lower.

We should finally note that, in most applications, the issue is not finding the residual when ψ is given, but rather to solve for ψ (and/or λ in the case of eigenvalue problems) under given boundary conditions. The corrections described here can either be incorporated directly into iterative methods (like Newton, Gauss–Seidel, SOR, Jacobi, multi-grid, etc.) or added separately in the form of iterative improvement (deferred correction).

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2. R. Meyer-Spasche and B. Fornberg, *Numer. Math.* **59**, 683 (1991).