

On Richardson Extrapolation for Finite Difference Methods on Regular Grids[★]

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Summary. Difference solutions of partial differential equations can in certain cases be expanded by even powers of a discretization parameter h . If we have n solutions corresponding to different mesh widths h_1, \dots, h_n we can improve the accuracy by Richardson extrapolation and get a solution of order $2n$, yet only on the intersection of all grids used, i.e. normally on the coarsest grid. To interpolate this high order solution with the same accuracy in points not belonging to all grids, we need $2n$ points in an interval of length $(2n-1)h_1$.

This drawback can be avoided by combining such an interpolation with the extrapolation by h . In this case the approximation depends only on grid points in an interval of length $\frac{3}{2}h_1$. The length of this interval is independent of the desired order.

By combining this approach with the method of Kreiss, boundary conditions on curved boundaries can be discretized with a high order even on coarse grids.

Subject Classifications: AMS(MOS): 65B05, 65N05, 65D05, 41A05; CR:G1.8.

Preliminaries

The numerical solution of a boundary value problem

$$\begin{aligned} \Delta u &= f & \text{on } \Omega \subset \mathbb{R}^N \\ u &= g & \text{on } \partial\Omega \end{aligned} \tag{1}$$

by a suitable regular discretization of the independent variable(s) x depends in a well predictable way on the coarseness of the discretization. Under certain

[★] This paper is based on a lecture held at the 5th Sanmarinian University Session of the International Academy of Sciences San Marino, at San Marino, 1988-08-27–1988-09-05

conditions the approximative solution is known to possess an asymptotic expansion by even powers of the mesh width h of the discretizing grid. This fact can be exploited to increase the precision order of the solution by Richardson extrapolation (see Richardson [7]) from $O(h^2)$ to $O(h^{2N})$ (compare Marchuk and Shaidurov [5]).

Traditional Richardson extrapolation is possible only in those points x where several approximations, corresponding to different values of h , are known. These points are at most the points of the coarsest grid used, e.g. if h is taken from the *Romberg* sequence, $h = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \dots$

Therefore, the increased accuracy by extrapolation is paid for by a reduction of the domain. For an interpolation of the high-order solution only coarse grid points are available, so the interpolation error can be expected to be large. Furthermore, interpolation with the desired order of $O(h^{2n})$ requires $2n$ collinear points in the grid, thereby restricting the largest mesh width h_1 ; so it may be necessary to use finer grids than would be appropriate, which increases the computational effort. No use is made of the information in the values in fine-grid-only points.

To exploit this information we could compute in these points values of the coarse grid solutions, e.g. by interpolation on these grids; this, however, leads to the same problems, viz. lack of points and high errors.

These problems impose restrictions especially on *Kreiss'* method [3] for the discretization of boundary conditions; here the numerical solution must be interpolated with high accuracy in intersection points of the boundary with grid lines.

Combined Interpolation by Spatial Coordinates and Discretization Parameter

We assumed for the numerical solutions u_h of the boundary value problem (1) the existence of an asymptotic expansion by h^2 :

$$u_h(x) = u(x) + \sum_{k>0} h^{2k} U_k(x). \quad (2)$$

Under suitable assumptions the functions U_k can be expanded by Taylor in the spatial coordinates. We consider only the expansion by *one* coordinate t , e.g. on a grid line or diagonal, and have

$$u_h(x_0 + t) = \sum_{j,k \geq 0} a_{jk} t^j h^{2k} \quad (3)$$

$$\text{with } a_{00} = u(x_0).$$

When we use (3) to approximate the value of a certain grid function u_h in a certain point $(x_0 + t)$ all support points needed can be chosen in the neighborhood of x_0 , so $t = O(h)$. Therefore the order of the interpolation is determined by the non-vanishing terms with the smallest $j + 2k$ (compare Steffensen [8]). To achieve an order of $2N$ by extrapolation we must find a linear combination of known approximations on several grids, with all terms with $j + 2k$ less than

$2n$ eliminated; i.e. we have an interpolation problem in two variables (the parameter h and a spatial coordinate t). The terms to be approximated form the silhouette S of the interpolating polynomial.

h^{2n-2}	$t h^{2n-2}$							
h^{2n-4}	$t h^{2n-4}$	$t^2 h^{2n-4}$	$t^3 h^{2n-4}$					
h^{2n-6}	$t h^{2n-6}$	$t^2 h^{2n-6}$	$t^3 h^{2n-6}$	$t^4 h^{2n-6}$	$t^5 h^{2n-6}$			
h^{2n-8}	$t h^{2n-8}$	$t^2 h^{2n-8}$	$t^3 h^{2n-8}$	$t^4 h^{2n-8}$	$t^5 h^{2n-8}$	$t^6 h^{2n-8}$	$t^7 h^{2n-8}$	
...								

Note that this silhouette is *saturated*; i.e. with every term it contains the whole rectangle spanned by it and the lower left corner:

$$t^j h^{2k} \in S \Rightarrow \forall \begin{cases} l: 0 \leq l \leq k \\ i: 0 \leq i \leq j \end{cases} : t^i h^{2l} \in S.$$

To prove the existence of the interpolating function, according to Bulirsch and Rutishauser [1] one can try to arrange the available grid points t and mesh widths h in such a way that the *associated point grid* is identical to the silhouette of the polynomial; i.e. to index the points t and the grids G (mesh widths h) in such a way that

$$h^{2i} t^k \in S \Leftrightarrow t_k \in G_i.$$

According to [1] (Sect. 6.2.3) we have

Lemma 1. *If the silhouette of an interpolating polynomial is saturated and identical to the grid associated to the support points, the polynomial exists and is uniquely determined by its values in these points.*

The normal case is to “follow the distribution of points and construct from it the polynomial” [1]. Contrarily we here can choose from an ample set of points to interpolate with a given polynomial, viz. a complete polynomial of certain degree (with even powers of h only).

For the support point configuration to be saturated each h_i must be a multiple of h_{i+1} ; so we choose the h_i from the Romberg sequence. The grids are indexed starting with the finest one, $G_1 \supset G_2 \supset \dots$. The points t_k must be indexed in such a way that

$$\exists i: t_{k_1} \in G_i, t_{k_2} \notin G_i \Rightarrow k_1 < k_2$$

so the points of the coarser grids come first. Such an ordering exists because of $G_i \supset G_{i+1}$; yet it is not unique. It may be derived from the geometric ordering by reversing the binary representation of $k-1$, possibly with some points skipped (compare Fig. 1).

The number of points on each grid must be chosen according to the silhouette, namely $2(n-i)$ points on G_i . n grids are needed.

triangular, with blocks corresponding to the grids, so it can be solved grid after grid, starting with the finest one.

To prove this, it is important to know how the support values influence the interpolation. We consider general two-dimensional interpolation on a saturated point grid in an (x, y) -space (here $y = h^2$).

Let $L_{ik}(x, y)$ be the two-dimensional Lagrange polynomials with $L_{ik}(x_j, y_l) = \delta_{ij} \cdot \delta_{kl}$. Kuntzmann [4] gives (with some misprints) these polynomials for the case of regular (equidistant) grids in an explicit form, expressed by one-dimensional Lagrange polynomials. This case is not applicable here; we have, however,

Lemma 2. *Let the associated point grid of a two-dimensional interpolation problem in x and y have n different values of y and for $1 \leq v \leq n$ m_v different support points $(x_1, y_v), \dots, (x_{m_v}, y_v)$, with $m_1 > m_2 > \dots > m_n$. Then the Lagrange polynomials $L_{ik}(x, y)$ vanish identically for $y = y_v, v < k$. In other words, the values of an interpolation polynomial on a $y = y_v$ line are not influenced by support values in (x, y_k) with $k > v$.*

Applied to Kreiss' method, this means that support values on coarser grids do not influence interpolation on finer grids, so the system is block-triangular.

Proof. by induction for k from n down to 1 (from coarse to fine). $x^{(m_v-1)}$ is the maximal power of x appearing together with y^{v-1} in the polynomial.

Let $k = n$;

the polynomial $L_{in}, 1 \leq i \leq m_n$ is

$$L_{in}(x, y) = \prod_{j=1, j \neq i}^{m_n} \frac{x - x_j}{x_i - x_j} \cdot \prod_{l=1}^{n-1} \frac{y - y_l}{y_n - y_l}$$

for this polynomial is of degree $m_n - 1$ in x and of degree $n - 1$ in y , so it is a candidate for the interpolation, and obviously it possesses the values of the Lagrange polynomial. As for $l < n$ it contains the factor $(y - y_l)$ it vanishes identically for $y \in \{y_1, \dots, y_{n-1}\}$.

The statement be valid for $k + 1, \dots, n$:
the polynomials

$$\prod_{j=1, j \neq i}^{m_k} \frac{x - x_j}{x_i - x_j} \cdot \prod_{l=1}^{k-1} \frac{y - y_l}{y_k - y_l}, \quad 0 \leq i \leq m_k$$

are of degree $m_k - 1$ in x and of degree $k - 1$ in y . They have for $y = y_v, v \leq k$ the values of the Lagrange polynomial and vanish identically for $y = y_v, v < k$. L_{ik} can be written as a sum of such a polynomial and Lagrange polynomials $L_{\mu v}$ with $v > k$ which, from induction hypothesis, vanish for $y \in \{y_1, \dots, y_{v-1}\}$. This completes the proof. \square

The proof also shows that the saturation of the point grid is not a necessary condition.

Reduction to One-Dimensional Interpolation

Since in our application of combined inter/extrapolation one of the interpolation coordinates, namely $y = h^2$, takes only fixed values (0 or y_v), it is natural to

reduce the problem to one-dimensional interpolation in the other coordinate. To this end, we consider the one-dimensional grids belonging to the values of y :

Let S be the saturated silhouette of a two-dimensional interpolating polynomial in x and y , with support points $(x_1, y_1), (x_2, y_1), \dots, (x_1, y_2), \dots$; as before, let m_v again be the number of points with $y=y_v$, n the number of different y_v .

Let further $K_v := \{x_1, \dots, x_{m_v}\} \subset G_v$ be the sets of x -coordinates for which $(x, y_v) \in S$; from the saturation of S it follows that $K_1 \supset K_2 \supset \dots \supset K_n$. Let $P_{\mu v}$, $1 \leq \mu \leq m_v \leq n$, be one-dimensional interpolating polynomials of the function u in the x direction for $y=y_\mu$ and $x \in K_v$, i.e. $x = x_1, \dots, x_{m_v}$:

$$\begin{matrix} P_{11} \\ P_{12} & P_{22} \\ P_{13} & P_{23} & P_{33} \\ \dots & \dots & \dots & \dots \end{matrix}$$

Then the two-dimensional interpolating polynomial \mathbb{P}_n of u has a representation as a linear combination of the polynomials $P_{\mu v}$.

The *proof* is constructive and inductively sets up divided differences:

$n = 1$: The desired interpolation polynomial \mathbb{P}_1 is equal to the polynomial P_{11} .

$n - 1 \rightarrow n$:

According to the induction hypothesis, the problem on the $n - 1$ grids G_1, \dots, G_{n-1} has a solution, i.e. the interpolation polynomial \mathbb{P}_{n-1} is a linear combination of the $P_{\mu v}$:

$$\mathbb{P}_{n-1}(x, y) = \sum_{v=1}^{n-1} \sum_{\mu=1}^{m_v} c_{\mu v}(y) \cdot P_{\mu v}(x)$$

the coefficients $c_{\mu v}$ being dependent on y but not on x . In the points of the grid G_n , \mathbb{P}_{n-1} has values that in general are different from u ; it can be made equal to \mathbb{P}_n by corrections in these points:

$$\begin{aligned} \mathbb{P}_n(x, y) &= \mathbb{P}_{n-1}(x, y) - \left(\mathbb{P}_{n-1}(x, y_n) = P_{nn}(x) \right) \cdot \prod_{l=1}^{n-1} \frac{y - y_l}{y_n - y_l} \\ &= \sum_{v=1}^{n-1} \sum_{\mu=1}^{m_v} \left(c_{\mu v}(y) \cdot P_{\mu v}(x) - c_{\mu v}(y_n) \cdot P_{\mu n}(x) \cdot \prod_{l=1}^{n-1} \frac{y - y_l}{y_n - y_l} \right) \\ &\quad + P_{nn}(x) \cdot \prod_{l=1}^{n-1} \frac{y - y_l}{y_n - y_l}. \end{aligned}$$

So we get for the $c_{\mu v}$:

$$\begin{aligned} c_{vv}(y) &= \prod_{l=1}^{v-1} \frac{y - y_l}{y_v - y_l} \\ c_{\mu v}(y) &= - \prod_{l=1}^{v-1} \frac{y - y_l}{y_v - y_l} \left(\sum_{\lambda=\mu}^{v-1} c_{\mu \lambda}(y_v) \right), \quad \mu = 1, \dots, v - 1. \end{aligned}$$

Table 1a. $c_{\mu\nu}(y_\nu)$ ($y_\nu=4^{\nu-1}$)

ν	μ			
	0	1	2	3
0	1			
1	-1	1		
2	4	-5	1	
3	-64	84	-21	1

Table 1b. $c_{\mu\nu}(0)$

ν	μ				
	0	1	2	3	
0	1				
1	1	-1			/3
2	4	-5	1		/45
3	64	-84	21	-1	/2835

The $c_{\mu\nu}(y)$ for different y therefore differ by a factor which depends on ν but not on μ :

$$\frac{c_{\mu\nu}(y_a)}{c_{\mu\nu}(y_b)} = \prod_{l=1}^{\nu-1} \frac{y_a - y_l}{y_b - y_l}, \quad \mu = 1, \dots, \nu. \quad \square$$

Especially, the $c_{\mu\nu}(y)$ for arbitrary y are easily computed from $c_{\mu\nu}(y_\nu)$:

$$c_{\mu\nu}(y) = c_{\mu\nu}(y_\nu) \prod_{l=0}^{\nu-1} \frac{y - y_l}{y_\nu - y_l} = c_{\mu\nu}(y_\nu) \cdot c_{\nu\nu}(y)$$

and the interpolating polynomial depends on values on the grid G_ν only via a polynomial Q_ν , which is independent of y :

$$\begin{aligned} \mathbb{P}_n &= \sum_{\nu=1}^n \sum_{\mu=1}^{\nu} c_{\mu\nu}(y) \cdot P_{\mu\nu} = \sum_{\nu=1}^n c_{\nu\nu}(y) \cdot \left(\sum_{\mu=1}^{\nu} c_{\mu\nu}(y_\nu) \cdot P_{\mu\nu} \right) \\ &=: \sum_{\nu=1}^n c_{\nu\nu}(y) \cdot Q_\nu(x). \end{aligned}$$

For our application with $y=h^2$ we can without restriction set $y_1=1$ since the $c_{\mu\nu}$ are unaffected by scaling of y . For $y_\nu=4^{\nu-1}$ (Romberg) we get the values shown in Table 1a and for $y=0$ the values shown in Table 1b.

Adaptation of Boundary Conditions on Coarser Grids

We have seen that the linear system resulting from Kreiss' method is block-triangular and can be solved grid after grid, values on grids coarser than G_k

having no influence on $\mathbb{P}_k(y_k)$. So the representation of the interpolation polynomial \mathbb{P}_k by the one-dimensional polynomials Q_v gives us for the boundary condition (value R) in a point x :

$$R = \mathbb{P}_k(y_k) = \sum_{v=1}^k c_{v,v}(y_k) \cdot Q_v, \quad k = 1, 2, \dots$$

From this we can show by induction that for all $v > 1$ the value of Q_v on the boundary must be zero, from which we get a condition for $P_{v,v}$ to be used as the new discrete boundary condition on G_v :

$k = 1$:

$$R = \mathbb{P}_1(y_1) = Q_1 = P_{1,1}$$

$k \rightarrow k + 1$:

$$\begin{aligned} R = \mathbb{P}_{k+1}(y_{k+1}) &= \sum_{v=1}^{k+1} c_{v,v}(y_{k+1}) \cdot Q_v = (\text{from the induction hypothesis}) \\ &= c_{1,1}(y_{k+1}) \cdot Q_1 + c_{k+1,k+1}(y_{k+1}) \cdot Q_{k+1} \\ &= R + c_{k+1,k+1}(y_{k+1}) \cdot Q_{k+1} \\ &\Rightarrow Q_{k+1} = 0 \quad (\text{from the above we see that } c_{k+1,k+1} \neq 0). \end{aligned}$$

The boundary value problem (1) can be solved with the new boundary conditions. The solutions can be improved by Richardson extrapolation up to $O(h^{2^n})$, even though boundary interpolation on G_k used only $2(n-k)$ support points.

Computation starts on the finer grids so that the finer solutions are available for interpolation on the coarser grids. The same savings in points are possible as for extrapolation towards $h \rightarrow 0$ (compare Föbmeier [2]). For any desired order of convergence, it is sufficient to use support points from an interval of length $\frac{3}{2}h_1$. For instance, to achieve an order of $O(h^6)$, only the points

G_3	*	*		
G_2	*	*	*	*
G_1	*	*	*	*

are required, instead of

G_3	*	*	*	*	*	*	*
G_2	*	*	*	*	*	*	*
G_1	*	*	*	*	*	*	*
	0	$\frac{3}{2}h_1$					$5h_1$

Comparison to Defect Correction

According to Pereyra et al. [6] the accuracy of a difference solution for a partial differential equation can be increased also by *defect correction*. To this end,

the defect of a numerical solution is determined with a high-order discretization, and a correction is computed with a method of lower order. This procedure approximates a solution whose error possesses the (higher) order of the defect discretization.

As an advantage versus extrapolation, defect correction operates on a single grid. Furthermore, the numerical solution need not have an error expansion; without one, however, it is normally not possible to give a higher-order discretization, so this advantage is not practically significant.

On the other hand, defect correction has two major drawbacks:

a) The high order solution can be computed on the whole domain, but not on parts of it. If it is desired only in a few points, the computational effort is disproportionate.

b) The higher-order discretization necessary to determine the defect normally for each point uses values from a somewhat extended neighborhood, e.g. in a distance of $2h$ or even $3h$. For points near the boundary some of these values are unknown and have to be approximated since an error in these points would not only influence the solution locally but pollute it on the whole domain.

c) The effort for the higher order discretization grows with the dimension of the problem. Contrarily, interpolation for points on grid lines or diagonals can be one-dimensional. Especially, boundary interpolation for the Kreiss method is always possible in one dimension.

Numerical Examples

The following examples were carried out on a Hewlett-Packard HP 9000/800 computer in double precision. The machine uses IEEE standard floating point arithmetic. Programs were written in the C programming language.

1. The first example is:

$$\begin{aligned} \Delta u(x, y) &= 0 && \text{on } \Omega_1 \\ u(x, y) &= g(x, y) && \text{on } \partial\Omega_1 \end{aligned} \quad (\text{P1})$$

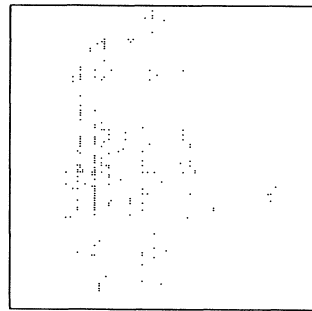
with

$$\begin{aligned} g(x, y) &= \sin x \cdot \sinh y \\ \Omega_1 &= (0, 1) \times (0, 1). \end{aligned}$$

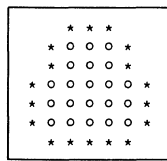
The exact solution of the problem is equal to g . The problem was solved using standard five-point discretization on grids with $K = 8/16/32/64$ meshes, and the solutions were interpolated by one-dimensional polynomials in the point (0.49; 0.50). Two different techniques were compared:

a) u_K was interpolated with degree 8 on all grids (which is possible because Ω is the unit square, so all points in the 8×8 grid can be used for interpolation); the results were extrapolated for $h \rightarrow 0$ (Richardson).

b) The interpolation polynomials $P_{\mu\nu}$, as defined above, were formed and combined using the coefficients from Table 1 b.



$h = 1/128$ (9859 internal points)



$h = 1/8$
(21 internal points)



$h = 1/4$
(one internal point)

Fig. 2. The egg-shaped domain Ω_2 (* = point near the boundary – difference operator not applicable, \circ = internal point – difference operator applicable)

Table 2. ($P1, \Omega_2$)

4	$1.1_{10^{-1}}$			
8	$2.7_{10^{-2}}$	$5.5_{10^{-4}}$		
16	$6.8_{10^{-3}}$	$3.5_{10^{-5}}$	$1.3_{10^{-6}}$	$1.0_{10^{-7}}$
32	$1.7_{10^{-3}}$	$2.3_{10^{-6}}$	$1.1_{10^{-7}}$	

The results compare with the exact value u_{ex} as follows:

$$u_{ex} = 2.3001633502186$$

$$u_a = 2.300163350301$$

$$u_b = 2.300163350300$$

The error of method b) is a little smaller, owing to the reduced support of the interpolation polynomials on the coarser grids. The main advantage, however, is that method b) would have been applicable even if the domain Ω would have been too small to offer enough support points for method a).

Table 3. ($P1, \Omega_2$)

8	$3.0_{10^{-2}}$			
16	$7.5_{10^{-3}}$	$3.8_{10^{-5}}$		
32	$1.9_{10^{-3}}$	$2.4_{10^{-6}}$	$3.2_{10^{-8}}$	
64	$4.7_{10^{-4}}$	$1.5_{10^{-7}}$	$7.9_{10^{-10}}$	$5.0_{10^{-10}}$
Traditional Kreiss Method:				
16	$7.5_{10^{-3}}$			
32	$1.9_{10^{-3}}$	$2.3_{10^{-6}}$		
64	$4.7_{10^{-4}}$	$1.5_{10^{-7}}$	$3.1_{10^{-8}}$	

Table 4. ($P2$)

4	048 14569553504			
8	0481 9561946991	0482122 6078154		
16	04820 812904600	04821229 890470	04821230144 624	
32	04821 125822426	048212301 28368	048212301442 28	048212301442 22

2. The second example has the same solution and boundary conditions but is defined on the roughly egg-shaped domain

$$\Omega_2 = \{(x, y) \in [0, 1] \times [0, 1] \mid (y - \frac{1}{2})^2 \cdot (1 + x) + (x - \frac{1}{2})^2 < 0.24\} \quad (\text{see Fig. 2}).$$

If Ω_2 is discretized with a mesh size $h = \frac{1}{K}$, corresponding to a mesh number of $K = 4$ in the unit square, the grid contains only one inner point (see Fig. 2). Yet with values from the grids with $K = 8, 16,$ and 32 , the boundary conditions can still be approximated with $O(h^8)$. The polynomials used for boundary interpolation on the four grids were of degree 2, 4, 6, and 8 respectively. (Degrees of 1/3/5/7 would do but give higher errors.) Table 2 shows the maximum norm of the error of the computed and the extrapolated solutions. The gain in accuracy is evident.

Table 3 shows the analogous figures for grids with mesh numbers 8/16/32/64 and, for comparison, the results of the traditional Kreiss method, applicable only for $K = 16/32/64$. (For $K = 4/8$ there are not enough points.) Even though the two methods are of the same order, the improved method shows clear advantages after the second extrapolation step (for $O(h^6)$). Here on the coarser grids both the degree of the interpolation polynomial and the maximum distance between support points are smaller: for $K = 16$ with degree 4 the distance is only $\frac{1}{4}$, opposed to $\frac{1}{2}$ with degree 8. Both factors contribute to smaller error bounds for the interpolation, which here results in a reduction of the error by a factor of about 40 in the maximum norm.

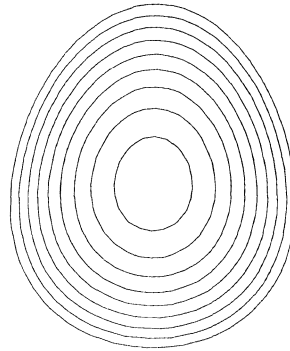


Fig. 3. The solution of example 3

3. The third example is defined on the same domain Ω_2 , the equation is:

$$\begin{aligned} \Delta u(x, y) &= 1 & \text{on } \Omega_2 \\ u(x, y) &= 0 & \text{on } \partial\Omega_2. \end{aligned} \quad (\text{P2})$$

The traditional Kreiss method with boundary interpolation of degree 8 on grids with mesh numbers 32/64/128/256 yields the value in the point $(\frac{1}{2}, \frac{1}{2})$ to be about

$$u(\frac{1}{2}, \frac{1}{2}) \approx 0.048212301442029$$

Table 4 shows how the new method approximates this value by solutions for $K = 4/8/16/32$ and their extrapolates. Accurate figures are shown in larger print. Again, convergence is clearly as predicted. Figure 3 shows the solution by contour lines with a distance of 0.005.

The examples show that the method allows the computation of extremely accurate solutions using rather coarse grids and a fairly simple interpolation and extrapolation technique. For curved boundaries, it may be difficult to find a competitive alternative.

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Received October 5, 1988 / January 18, 1989