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APPROXIMATION OF SOLUTION OF DIFFERENTIAL EQUATIONS AND OF THEIR DERIVATIVES

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1. Introduction. A Numerical method for simple boundary value problems is described which allows to calculate bounds for the absolute error ε of an approximate solution v for the wanted solution u; it is supposed, that monotonicity principles hold; in this case the described method are in many cases the only one's which admit to calculate bounds one can guarantee. Examples for the method are given in many papers, (f.i. Bohl [74], J. Schröder [80], Collatz [81] a.o.); therefore we restrict ourselves to a very brief description, omitting many details.

Here recent results are given, especially for singular boundary value problems and for calculating of derivatives.

2. Operators of monotonie type. Let us consider the boundary value problem for a function $u(x)=u(x_1,\dots,x_n)$ in a domain B of the n-dimensional point-space $\mathbb{R}^n$:

(2.1) $Lu = r(x)$ in B

(2.2) $Su = \gamma(x)$ on the boundary ∂B.

L and S may be linear oder nonlinear differential operators, S may be a vector of several components, r,γ may be given, f.i. continuous functions (a more detailed description f.i. in Collatz [68], Bohl [74], Schröder [80] a.o.). We introduce the operator T with Lu and Su as components

(2.3) $Tu = (Lu, Su)$.

and correspondingly $\rho(x) = (r(x),\gamma(x))$.

Let D be the domain of definition of the operator T.

Definition: We call the operator Tu an "operator of monotonic type",

(2.4) if $Tv \le Tw$ has the consequence $v \le w$ in B for every pair $v,w\in D$.

Here the sign $\le$ means the classical ordering of real numbers(Kantorowitsch-Akilow [64], Bohl [74] a.o.) and the inequalities are understood as pointwise for every component and for every point of B, resp. of ∂B.

Then one has the obvious

<u>Error-Principle:</u>

(2.5) From $Tv \le \rho(x) \le Tw$ follows $v \le u \le w$ in B.

The pointwise monotonicity was proved for wide classes of linear and nonlinear ordinary and partial differential equations of elliptic and parabolic type (Nickel [58], Redheffer [67], Walter [70], Glashoff-Werner [79] and many others) and for certain types of problems with hyperbolic equations (Gloistehn [63], Hofmann [73] a.o.).

<u>3. Approximation and optimization.</u> We let v and w depend on parameters a_ν, b_μ

$$v = v(x,a),\ w = w(x,b),\ a = (a_1,\ldots,a_p),\ b = (b_1,\ldots,b_q)$$

and determine the a_ν, b_μ from the optimization

$$(3.1)\ \begin{cases} -\delta_1 \le w(x,b) - v(x,a) \le \delta_2,\ Tv(x,a) \le \rho(x) \le Tw(x,b) \\ \delta_1 \ge 0,\ \delta_2 \ge 0,\ \delta_1 + \delta_2 = \text{Min.} \end{cases}$$

and we get the lower and upper bound for the solution

$$(3.2)\qquad v(x) \le u(x) \le w(x) \text{ in } B.$$

<u>Example:</u> On can combine the procedure with an iteration. We consider the nonlinear boundary value problem for a function u(x,y)

$$(3.3)\ \begin{cases} -\Delta u = -\dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial^2 u}{\partial y^2} = 1 + 2u^2 \text{ in } B = \{(x,y),\ r^2=x^2+y^2<1\} \\ u = 0 \qquad\qquad \text{on } \partial B = \{(x,y),\ r=1\}. \end{cases}$$

u(x,y) may be interpreted as temperature of a liquid or a gaze in a circular domain under the influence of chemical reactions, we suppose as nonlinear corresponding to the term $2u^2$.

We assume two approximate solutions v_o, w_o in the form

$$(3.4)\quad v_o = \sum_{\nu=1}^{p} a_\nu (1-r^2) r^{2\nu-2},\quad w_o = \sum_{\nu=1}^{p} b_\nu (1-r^2) r^{2\nu-2}$$

and determine the real constants a_ν, b_ν from the optimization problem

$$(3.5)\ \begin{cases} w_1 - v_1 \le \delta,\ \delta = \text{Min.} \\ 0 \le v_o \le v_1 \le w_1 \le w_o,\ -\Delta v_1 = 1+2v_o^2, \\ -\Delta w_1 = 1+2w_o^2 \text{ in B}, \end{cases}$$

v_o, v_1, w_1, w_o satisfy the boundary condition on ∂B.

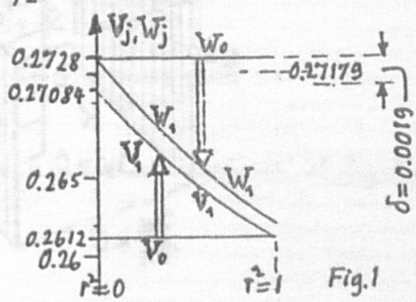

Fig.1

We take just for illustration only one term in (3.4), p=1:

$$v_1 = \frac{1-r^2}{36}\left[9+a_1^2\phi(r)\right], \quad w_1 = \frac{1-r^2}{36}\left[9+b_1^2\phi(r)\right],$$

with $\phi(r) = 11 - 7r^2 + 2r^4$

and get $a_1=0.2612$, $b_1=0.2728$, $\delta=0.0019$,

f.i. $0.27084 \le u(0.0) \le 0.27274$ or $|0.27179-u(0.0)| \le 0.00095 = \frac{1}{2}\delta$

Fig. 1 shows with

$$v_j = (1-r^2)\, V_j, \quad w_j = (1-r^2)\, W_j \quad (j = 0.1)$$

the iteration process, going from V_o to V_1 and from W_o to W_1.

The Schauder's fixed point theorem gives the existence of at least one solution u(x,y) in the strip $\langle v_1(x,y),\ w_1(x,y)\rangle$ as in (3.2).

Of course it is easy to improve the numerical results by taking more terms in (3.4): p>1.

Many other examples have been calculated on compüters, (f.i. Collatz [81] a.o.)

4. Three-dimansional singularities. Singular boundary value problems occur frequently in applications and are treated often numerically (Collatz [77], Whiteman [83] and theoretically (f.i. Tolksdorf [83] a.o.) In the last years 3-dimensional problems became interesting.

Let us consider a simple example of distribution of the temperature u(x,y,z) in a room, which covers the unit-cube K in a x-y-z-space: $K = \{(x,y,z),\ |x| < 1,\ |y| < 1,\ |z| < 1\}$, fig. 2

with a wall

$$\Gamma_1 = \{(x,y,z),\ 0 \le x \le 1,\ y = o,\ |z| \le 1\}.$$

u satisfies the potential equation

(4.1) $\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$ in $B = k-\Gamma_1$ and the boundary conditions

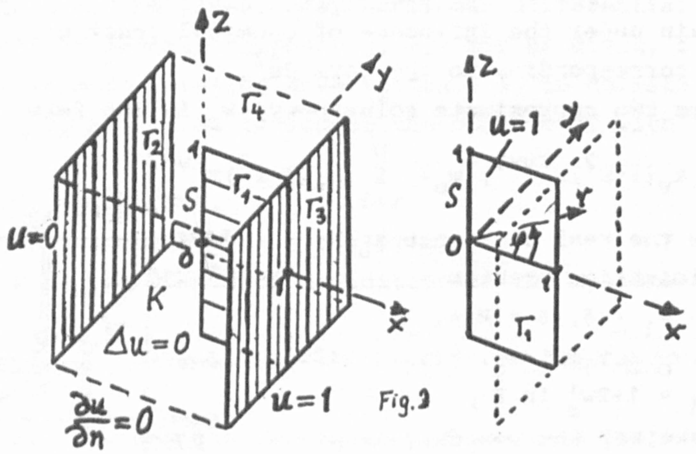

Fig.2

$$
(4.2)\quad \begin{cases} u = 0 \text{ on } \Gamma_2 : x = -1 \\ u = 1 \text{ on } \Gamma_1 \text{ and } \Gamma_3 : x = 1 \\ \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma_4 = \partial K - \Gamma_2 - \Gamma_3 \text{ (or } |x|<1, \text{ and } y=\pm 1 \text{ or } z=\pm 1) \end{cases}
$$

with n as outer normal.

The singular line S is given by $S = \{(x,y,z),\ x=y=0,\ |z|<1\}$. We introduce polarcoordinates r,ϕ with

$x = r\cos\phi,\ y = r\sin\phi,$ fig. 2;

The singularity along S has the form

$$
(4.3)\qquad \psi = \sum_{j=1}^{p} a_j \psi_j \text{ with } \psi_j = r^{j-\frac{1}{2}} \sin\left[(j-\tfrac{1}{2})\phi\right];
$$

and is locally determined and independent of the values, which are prescribed in a finite distance of S, for instance of the values of u at Γ_2 and Γ_3 (Tolksdorf [83], Dobrowolski [84], Schnack [84]). (In this special case u is independent of z, but the form for the approximate solution with v_j as harmonic polynomials

$$
(4.4)\qquad u \approx v(x,y,z) = \sum_{j=1}^{p} a_j \psi_j + \sum_{j=1}^{q} b_j h_j \text{ with } \Delta h_j = 0
$$

would also possible in the case, that the values of u on Γ_2 and Γ_3 depend on z.).

The operator $T\phi = (-\Delta\phi$ in B, ϕ on $\{\Gamma_1, \Gamma_2, \Gamma_3\}, \frac{\partial\phi}{\partial n}$ on $\Gamma_4)$ is of monotonic type. We look on a lower bound v as in (4.4) and an upper bound $w = \sum_j b_j \psi_j + \sum_j B_j h_j$ with $h_j = \mathrm{Re}(x+iy)^j$ and use the optimization (3.1); Here a is the vector $a=(a_1,\dots,a_p,A_1,\dots,A_q)$ and analogously b. Then we have (3.2) and $0 \le w-v \le \delta$.

The following table gives the error bound in dependence of the number p of singularities and the number q of polynomial terms.

Table for δ

Number of singularities

	p \ q	0	1	2	3
number of polynomial terms	1	1	1	0.11501	0.09408
	4	0.5	0.15291	0.07979	0.05414
	6	0.5	0.14341	0.02024	0.01270
	7	0.5	0.10179	0.00769	0.00441

This means f.i. for p=7, q=3 the inclusion of the solution u:

$$
\left|\frac{v+w}{2} - u\right| \le 0.00221 \quad (= \tfrac{1}{2}\delta)
$$

It may be sufficient, to give the values of a_j, A_j; the values of b_j, B_j are only slightly different.

The parameters a_j, A_j are

$a_1 = -0.760\ 652$	$A_1 = 0.998\ 580$	$A_4 = 0.017\ 448$
$a_2 = 0.206\ 860$	$A_2 = 0.014\ 152$	$A_5 = 0.006\ 282$
$a_3 = 0.035\ 281$	$A_3 = -0.039\ 148$	$A_6 = 0.001\ 387$
		$A_7 = -0.001\ 080$

Fig. 3 gives some curves u=const.

The value $-\frac{a_1+b_1}{2} = 0.75927$ has as "stress-intensity factor" a physical meaning.

I thank Mr. Uwe Grothkopf for the numerical calculation on a computer.

5. Vectormonotonicity. A generalization of the monotonicity of (2.4), (2.5) is the vectormonotonicity. The general scheme is the following; Let be given a domain $B \subset \mathbb{R}^n$ and subsets B_j of dimension $d_j \leq n$; if $d_j < n$ the subsets are usually boundaries or interfaces. $(j=1,\ldots k)$ Furthermore there are given operators $T_j, \tilde{T}_j$ on B_j and restrictions $M_\mu = 0$ on B_j $(j=1,\ldots,q)$ (B_j possible multiple counted).

Let be u,v,w functions on B, satisfying certain conditions about continuity and differentiability.

I. For linear problems: "Vectormonotonicity" means:

$$(5.1)\quad \begin{array}{|l|}\hline T_j u \geq 0 \text{ on } B_j \\ M_\mu u = 0 \text{ on } B_\mu \\ \hline \end{array} \xrightarrow{\text{implies}} \begin{array}{|l|}\hline \tilde{T}_j u \geq 0 \text{ on } B_j \\ \hline \end{array} \quad \begin{array}{l}(j=1,\ldots,k)\\ (\mu=1,\ldots,q)\end{array}$$

II. For nonlinear problems:

$$(5.2)\quad \begin{array}{|l|}\hline T_j v \geq T_j w \text{ on } B_j \\ M_\mu v = M_\mu w \\ \hline \end{array} \xrightarrow{\text{implies}} \begin{array}{|l|}\hline \tilde{T}_j v \geq \tilde{T}_j w \text{ on } B_j \\ \hline \end{array} \quad \begin{array}{l}(j=1,\ldots,k)\\ (\mu=1,\ldots,q)\end{array}$$

Let us explain this on the example of a linear or nonlinear elliptic operator L: Then the classical monotonicity principle was proved under rather general restrictions (compare f.i. Redheffer [67], Collatz [68] a.o.):

$$\begin{array}{|l|}\hline L \text{ elliptic in } B \subset \mathbb{R}^n \\ Lv \geq Lw \text{ in } B \\ v \geq w \text{ on } \Gamma_1 \\ \frac{\partial v}{\partial n} \geq \frac{\partial w}{\partial n} \text{ on } \Gamma_2 \\ \hline \end{array} \xrightarrow{\text{implies}} \begin{array}{|l|}\hline v \geq w \text{ in } B \\ \hline \end{array}$$

Suppose that L satisfies this monotonicity, then we split the condition $v \geq w$ on Γ_1 in two parts, corresponding to a part Γ_1^* of Γ_1 and the rest $\Gamma_1 \setminus \Gamma_1^*$ and we have the consequence:

(5.3) $\boxed{\begin{array}{l} Lv \geq Lw \text{ in } B \\ v = w \text{ on } \Gamma_1^* \ [c\Gamma_1] \\ v \geq w \text{ on } \Gamma_1 \setminus \Gamma_1^* \\ \frac{\partial v}{\partial n} \geq \frac{\partial w}{\partial n} \text{ on } \Gamma_2 \end{array}}$ implies $\longrightarrow \boxed{\begin{array}{l} v \geq w \text{ in } B \\ \frac{\partial v}{\partial n} \geq \frac{\partial w}{\partial n} \text{ on } \Gamma_1^* \end{array}}$

In this way we can get inclusions also for certain derivatives.

Example

We consider a very simple problem only for illustration of the method: the torsion problem for a beam with a square B as cross section:

$$(5.4)\begin{cases} \Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \text{ in } B \ (|x| < 1, |y| < 1) \\ u = \frac{1}{4}(x^2 + y^2) \quad \text{on } \partial B \end{cases}$$

we are interested on the normal derivative η at the point $P(x=1,y=0)$, (for calculating of tensions) $\eta = (-\frac{\partial u}{\partial x})_P$, Fig. 3

We take as Approximate solution $v = \sum_{j=0}^{p} a_j v_j(x,y)$

$v_j = \operatorname{Re}(x+iy)^{4j}$

$v_0 = 1;\ v_1 = x^4 - 6x^2y^2 + y^4;\ldots$

then one has

$$\left(\frac{\partial v}{\partial x}\right)_{(P)} = \sum_{j=0}^{p} 4j\, a_j$$

Correspondingly to (5.3) we wish, that the error $\varepsilon = v - u$ vanishes at P:

$$v(P) = u(P) \text{ or } \sum_{j=0}^{p} a_j = \frac{1}{4}$$

From $v \leq u$ on ∂B follows $v \leq u$ in B or $\varepsilon = v - u \leq 0$ in B; therefore $\varepsilon = 0$ at P implies

$$\left(\frac{\partial \varepsilon}{\partial x}\right)_{(P)} \geq 0, \quad \left(\frac{\partial v}{\partial x}\right)_{(P)} + \eta \geq 0, \quad \eta \geq \left(-\frac{\partial v}{\partial x}\right)_{(P)} = -\sum_{j=0}^{p} 4j\, a_j$$

Analogously one gets an upper bound for η.

We calculate a lower bound $\underline{v} \leq u$ with parameters $a_j = \underline{a}_j$

an upper bound $\overline{v} \leq u$ with parameters $a_j = \overline{a}_j$.

For getting bounds for η we have the optimization problem

$$\underline{v} \leq u \leq \overline{v} \text{ on } \partial B, \quad \underline{v}(P) = \overline{v}(P) = u(P), \quad \left(-\frac{\partial \overline{v}}{\partial x}\right)_{(P)} - \left(\frac{\partial \underline{v}}{\partial x}\right)_{(P)} \leq \delta, \quad \delta = \text{Min}$$

or more explicitly

$$\sum_j \underline{a}_j v_j \leq \frac{1}{4}(x^2+y^2) \leq \sum_j \overline{a}_j v_j \text{ on } \partial B, \quad \sum_j \underline{a}_j = \sum_j \overline{a}_j = \frac{1}{4}, \quad \sum_j j(\underline{a}_j - \overline{a}_j) \leq \delta, \quad \delta = \text{Min}.$$

I thank Mr. Uwe Grothkopf and Jörg Haarmeyer for numerical calculation of a computer. They get with discretizing the boundary with $h=0.01$ (that means taking $x=1$, $y=k\cdot h$, $k=0,1,\ldots,100$) for $p=1,2,3$ the following values for parameters and bounds for η:

$p=1$	$\underline{a}_1=-\frac{1}{24}\approx-0.041667$	$\bar{a}_1 = -\frac{1}{20} = 0.05$	$0.16667 \le \eta \le 0.2$
$p=2$	$\underline{a}_1 = -0.045\,215$ $\underline{a}_2 = 0.000\,817$	$\bar{a}_1 = -0.046\,739$ $\bar{a}_2 = 0.001\,087$	$0.174327\le\eta\le0.178260$
$p=3$			$0.175502\le\eta\le0.175906$

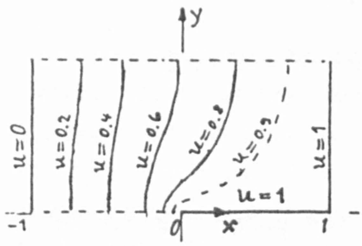

Fig.3

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