MODELING AND NUMERICAL SIMULATION OF FIRST AND SECOND ORDER DISTRIBUTED PARAMETERS PROCESSES, USING THE (M_{dpx}) OPERATING MATRIX

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Abstract: Continuing the papers (Colosi *et al*, 2002; Colosi *et al*, 2003; Bogdan, 2005), are presented significant aspects of modeling and numerical simulation of some categories of processes, defined by partial differential equations (pde) of I and II order, with frequent applications in technique. The originality of the paper is the definition and the use of the (\mathbf{M}_{dpx}) operating matrix, which, beside the disadvantage of a relatively high volume of calculus, cumulate as the main advantage the *quasi-general applicability* of the method for a large category of (pde), linear or nonlinear. This main advantage is attested by numerous examples, run on computer

Keywords: partial differential equations, state variables, Taylor series, modeling and numerical simulation

1. INTRODUCTION

For general forms of (pde) of I and II order:

 $\begin{array}{l} a_{0000} x_{0000} + a_{1000} x_{1000} + a_{0100} x_{0100} + a_{0010} x_{0010} + a_{0001} x_{0001} = \\ = \phi(t, p, q, r) \end{array}$ (1)

respectively

 $\begin{array}{l} a_{0000} x_{0000} + a_{1000} x_{1000} + a_{2000} x_{2000} + a_{1100} x_{1100} + a_{0200} x_{0200} + \\ + a_{0110} x_{0110} + a_{0020} x_{0020} + a_{0011} x_{0011} + a_{0002} x_{0002} + a_{1001} x_{1001} \\ + a_{1010} x_{1010} + a_{0101} x_{0101} + a_{0101} x_{0101} = \phi(t, p, q, r), \end{array}$ (2)

are considered four independent variables: time (t) and the spatial variables (p), (q) and (r).

For the partial differentials is adopted the obvious notation:

$$\mathbf{x}_{\text{TPQR}} = \frac{\partial^{\text{T+P+Q+R}} \mathbf{y}}{\partial \mathbf{t}^{\text{T}} \cdot \partial \mathbf{p}^{\text{P}} \cdot \partial \mathbf{q}^{\text{Q}} \cdot \partial \mathbf{r}^{\text{R}}},$$
(3)

where the dependent variable y = y(t, p, q, r) and the function $\varphi(t, p, q, r)$ respects the continuity conditions in Cauchy sense. If, for example, T = 0, P = 0, Q = 0 and R = 0, or T = 0, P = 1, Q = 0 and R = 0, or T = 1, P = 0, Q = 1, R = 0, then results

$$\mathbf{x}_{0000} = \mathbf{y},\tag{4}$$

$$\mathbf{x}_{0101} = \frac{\partial \mathbf{y}}{\partial \mathbf{p} \cdot \partial \mathbf{r}} \tag{5}$$

and

$$\mathbf{x}_{1010} = \frac{\partial^2 \mathbf{y}}{\partial \mathbf{t} \cdot \partial \mathbf{q}} \tag{6}$$

Respectively.

Of course, (1) and (2) can be limited to three independent variables, for example (t, p, q), resulting:

$$a_{000} x_{000} + a_{100} x_{100} + a_{010} x_{010} + a_{001} x_{001} = \varphi(t, p, q)$$
(7)

respectively

 $\begin{array}{l} a_{000} x_{000} + a_{100} x_{100} + a_{200} x_{200} + a_{110} x_{110} + a_{020} x_{020} + a_{011} x_{011} \\ + a_{002} x_{002} + a_{101} x_{101} = \phi(t, p, q). \end{array}$

(8)

If (1) and (2) is limited to two independent variables, for example (t, p), then results:

 $a_{00} x_{00} + a_{10} x_{10} + a_{01} x_{01} = \varphi(t, p)$ (9)

respectively

$$a_{00} x_{00} + a_{10} x_{10} + a_{20} x_{20} + a_{11} x_{11} + a_{02} x_{02} = \varphi(t, p).$$
(10)

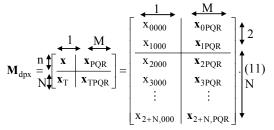
All the coefficients $(a_{...})$ from (1), (2), (7), (8), (9) and (10) are considered constants, and in the hypothesis of numerical integration with respect to time, considered in the present work, the elements of the state vector (\mathbf{x}) is presented in Table 1.

Table 1.						
Order		Ι			II	
Pde	(1)	(7)	(9)	(2)	(8)	(10)
X	X ₀₀₀₀	x ₀₀₀	X ₀₀	X ₀₀₀₀	x ₀₀₀	X ₀₀
				x ₁₀₀₀	X100	x ₁₀

It can be observed that for I order (pde) corresponds $\mathbf{x}(1 \times 1)$ and for II order (pde) corresponds $\mathbf{x}(2 \times 1)$. Multiple versions can present initial conditions $\mathbf{x}_{IC} = \mathbf{x}(t_0, \dots)$, final conditions $\mathbf{x}_{FC} = \mathbf{x}(t_f, \dots)$ and boundary conditions, for example $\mathbf{x}_{BC} = \mathbf{x}(t, p_0, \dots)$ or $\mathbf{x}_{BC} = \mathbf{x}(t, p_f, \dots)$.

2. OPERATOR MATRIX (Mdpx)

The definition and the detailed presentation of the operating matrix (\mathbf{M}_{dpx}) is exposed in (Colosi *et al*, 2003), which for (2) leads to the particular form:



For n = 2, the (\mathbf{M}_{dpx}) matrix is partitioned as follows:

- a) The state vector $\mathbf{x}(2 \times 1)$;
- b) The Nth with respect to time derived state vector $\mathbf{x}_{T}(N \times 1)$;
- c) The $\mathbf{x}_{PQR}(2 \times M)$ matrix, which contains (M) successive partial differentials of the state vector $\mathbf{x}(2 \times 1)$, with respect to the independent variables (p, q, r), for combinations of order 0, 1, 2, ... Because at the start of calculus (t = t₀) the two state variables $x_{0000}(t_0, p, q, r)$ and $x_{1000}(t_0, p, q, r)$ are known initial conditions, the analytical partial differentials with respect to (p, q, r) is

recommended to be calculated for as high order is possible;

d) The $\mathbf{x}_{TPQR}(N \times M)$ matrix is successively calculated from the first element of the vector \mathbf{x}_T , which results from (2), at $t = t_0$, respectively

$$\begin{split} x_{2000} &= \frac{1}{a_{2000}} \left[\phi(t_0, p, q, r) - \left(a_{0000} \cdot x_{0000} + \right. \\ &+ a_{1000} \cdot x_{1000} + a_{1100} \cdot x_{1100} + a_{0200} \cdot x_{0200} + \\ &+ a_{0110} \cdot x_{0110} + a_{0020} \cdot x_{0020} + a_{0011} \cdot x_{0011} + \\ &+ a_{0002} \cdot x_{0002} + a_{1001} \cdot x_{1001} + a_{1010} \cdot x_{1010} + \\ &+ a_{0101} \cdot x_{0101} \right) \right]_{t_0} \end{split}$$

(12)

As a result, all the components $(\mathbf{x}_{...})$ from the right side are known from $\mathbf{x}(t_0, p, q, r)$ and $\mathbf{x}_{PQR}(t_0, p, q, r)$, which represents the two rows above the element (\mathbf{x}_{2000}) from (12). To calculate the first line of the matrix (\mathbf{x}_{TPQR}) , respectively (\mathbf{x}_{2PQR}) , are operated successive partial differentials on (\mathbf{x}_{2000}) from (12), with respect to (p, q, r), with an adequate high order, with the note that all these partial results are obtained from the previous calculated rows, disposed above this first row of (\mathbf{x}_{TPOR}) .

In the following is calculated (x_{3000}), by derivation of (12) with respect to (t), after which the successive partial derivation is repeated with respect to (p, q, r), formally identical with (x_{2000}). The note that all the partial results will be takes over from the previous calculated rows, disposed above the second row of (x_{TPQR}), remain valuable.

This algorithm is repeated for $(N \ge 4)$ number of rows and $(M \ge 10)$, after which it is obtained the operator matrix at the sequence (k-1), respectively:

$$\mathbf{M}_{dpx,k-1} = \begin{bmatrix} \mathbf{1} & \mathbf{M} \\ \mathbf{x}_{k-1} & \mathbf{x}_{PQR,k-1} \\ \mathbf{x}_{T,k-1} & \mathbf{x}_{TPQR,k-1} \end{bmatrix} \mathbf{\uparrow}_{N}^{2} \mathbf{13}$$

The elements of the matrix $(\mathbf{M}_{dpx,k-1})$ from (13) allows the approximation of the vector (\mathbf{x}_k) and the matrix $(\mathbf{x}_{PQR,k})$ by (truncated) Taylor series from the obvious series:

$$\mathbf{x}_{k} = \mathbf{x}_{k-1} + \sum_{T=1}^{\omega} \frac{\Delta t^{T}}{T!} \mathbf{x}_{T,k-1}$$
(14)
$$\mathbf{x}_{PQR,k} = \mathbf{x}_{PQR,k-1} + \sum_{T=1}^{\omega} \frac{\Delta t^{T}}{T!} \mathbf{x}_{TPQR,k-1} ,$$
(15)

where to the sequences (k-1) and (k) corresponds the time (t_{k-1}) and $t_k = t_{k-1} + \Delta t$, respectively, with the integration step (Δt) small enough and $\omega \ge 4$.

With the results (14) and (15) are completed the first two rows of the vector $(\mathbf{M}_{dpx,k})$ for the new (k) sequence:

$$\mathbf{M}_{dpx,k} = \begin{bmatrix} \mathbf{1} & \mathbf{M} \\ \mathbf{x}_{k} & \mathbf{x}_{PQR,k} \\ \mathbf{x}_{T,k} & \mathbf{x}_{TPQR,k} \end{bmatrix} \mathbf{\uparrow}^{2}_{N} \quad (16)$$

The calculus details for $(\mathbf{x}_{T,k})$ and $(\mathbf{x}_{TPQR,k})$ are the same with the previous sequence (k-1) calculus, in conformity with the equations (12), (13), resulting the matrix (16) at the new sequence (k) and time (t_k), formally identical with the matrix (13), considered at the previous sequence (k-1) and time (t_{k-1}).

3. EXAMPLES RUN ON COMPUTER

For the two pde examples, considered for general forms (1) and (2), it was considered:

- a) $t_0=0$; $p_0=0$; $q_0=0$; $r_0=0$; $t_f=1$; $p_f=1$; $q_f=1$; $r_f=1$. b) The coefficients $a_{0000}=1$; $a_{000}=1$ and $a_{00}=1$.
- c) The analytical solution $y_{AN}(t, p, q, r)$, necessary for the validation of the errors cumulated in percent (ercp) and for the start of calculus, is considered of exponential form, usual in various technical applications, respectively:

$$y_{AN}(t, p, q, r) = y_{0000} + \left(J_{0T} + J_{1T} \cdot \varepsilon^{-t/T_1} + J_{2T} \cdot \varepsilon^{-t/T_2}\right) \left(J_{0P} + J_{1P} \cdot \varepsilon^{-p/P_1} + J_{2P} \cdot \varepsilon^{-p/P_2}\right).$$

$$\cdot \left(J_{0Q} + J_{1Q} \cdot \varepsilon^{-q/Q_1} + J_{2Q} \cdot \varepsilon^{-q/Q_2}\right) \cdot \left(J_{0R} + J_{1R} \cdot \varepsilon^{-t/R_1} + J_{2R} \cdot \varepsilon^{-t/R_2}\right) \cdot K_u \cdot u$$
(17)

which can be particularized for $y_{AN}(t,p,q)$ if $J_{1R}=0$, $J_{2R}=0$ and $J_{0R}=1$, respectively for $y_{AN}(t,p)$ if – supplementary – $J_{1Q}=0$, $J_{2Q}=0$ and $J_{0Q}=1$.

d)Using the following abbreviations:

$$\begin{split} \lambda_t &= \frac{T_2}{T_1} > 1 \,; \quad \lambda_p = \frac{P_2}{P_1} > 1 \,; \quad \lambda_q = \frac{Q_2}{Q_1} > 1 \,; \\ \lambda_r &= \frac{R_2}{R_1} > 1 \,; \quad \mu_t = \frac{t_f}{T_1 + T_2} \ge 2 \,; \\ \mu_p &= \frac{p_f}{P_1 + P_2} \ge 2 \,; \quad \mu_q = \frac{q_f}{Q_1 + Q_2} \ge 2 \,; \\ \mu_r &= \frac{r_f}{R_1 + R_2} \ge 2 \,; \quad J_{0T} = J_{0P} = -J_{0Q} = -J_{0R} = 1 \,; \\ J_{1T} &= -\frac{T_1}{T_1 - T_2} \,; \quad J_{2T} = -\frac{T_2}{T_2 - T_1} \,; \\ J_{1P} &= -\frac{P_1}{P_1 - P_2} \,; \quad J_{2P} = -\frac{P_2}{P_2 - P_1} \,; \\ J_{1Q} &= -\frac{Q_1}{Q_1 - Q_2} \,; \quad J_{2Q} = -\frac{Q_2}{Q_2 - Q_1} \,; \end{split}$$

$$J_{1R} = -\frac{R_1}{R_1 - R_2}; \quad J_{2R} = -\frac{R_2}{R_2 - R_1}; \quad K_u = 1$$

and u=1, the evolution of the analytical solution $y_{AN}(t, p, q, r)$ is limited inside of a (super)cube with unitary length. (T₁) and (T₂) are time constants, and (P₁, P₂, Q₁, Q₂, R₁ and R₂) can be interpreted as "length" constants" if (p, q and r) are spatial coordinates

e) The performance indicator of numerical integration is defined by the cumulated relative error in percent (crep) by form:

crepy =
$$100 \cdot \frac{\sum_{k_0}^{k_f} |\Delta x_{00...k}|}{\sum_{k_0}^{k_f} |y_{ANk}|}$$
 (18)

where $\Delta x_{00...k} = |y_{ANk} - x_{00...k}|$ represent the absolute value of the sequential error between the analytical solution (y_{ANk}) and the numerical approximated solution $(x_{00...k})$, between the limits $k_0=0$ and $k_f=t_f/\Delta t$. The integration step is $\Delta t \approx \frac{t_f}{100}$ in a minimal version or $\Delta t \approx \frac{T_1}{100}$ in a more restrictive version, where $T_1 < T_2$.

In the following, in conformity with the pde solving method exposed in 2), satisfying the conditions presented in 3) in paragraphs a, b, ..., e, are presented the results, obtained by numerical simulation.

3.1. <u>Pde I(t, p, q, r) by form (1)</u>

		Table 2		
t	X ₀₀₀₀	$y_{\rm AN}$	\dot{y}_{AN}	crep
0.01	1.0371	1.0371	3.6358	5·10 ⁻⁶
0.1	1.3367	1.3368	2.4372	0.0024
0.2	1.5208	1.5210	1.7004	0.0058
0.3	1.6608	1.6611	1.1398	0.0099
0.4	1.7546	1.7550	0.7640	0.0136
0.5	1.8175	1.8180	0.5121	0.0167
0.6	1.8597	1.8602	0.3433	0.0190
0.7	1.8880	1.8885	0.2301	0.0206
0.8	1.9071	1.9075	0.1543	0.0212
0.9	1.9199	1.9202	0.1034	0.0208
1	1.9287	1.9287	0.0693	0.0194

The results from Table 2 corresponds to $p=p_i=1$; $q=q_i=1$; $r=r_i=1$. With respect to the time constant $a_{1000}=T_1=t_1/4=0.25$, the integration step $\Delta t=0.01$

represents $\frac{\Delta t}{T_1} = \frac{1}{25}$, a relatively high value. Still,

(crep) is maintained in very low limits, which highlight the correctness of the method.

3.2. <u>Pde I(t, p, q) by form (7)</u>

Table 3						
t	x ₀₀₀₀	y_{AN}	Υ _{ΑΝ}	crep		
0.01	1.0378	1.0378	3.7037	3.10-5		
0.1	1.3430	1.3430	2.4826	$1.7 \cdot 10^{-3}$		
0.2	1.5305	1.5307	1.7321	$4.1 \cdot 10^{-3}$		
0.3	1.6732	1.6734	1.1610	$7 \cdot 10^{-3}$		
0.4	1.7688	1.7691	0.7783	9.9·10 ⁻³		
0.5	1.8329	1.8333	0.5217	$1.25 \cdot 10^{-2}$		
0.6	1.8758	1.8763	0.3497	$1.49 \cdot 10^{-2}$		
0.7	1.9046	1.9051	0.2344	$1.7 \cdot 10^{-2}$		
0.8	1.9238	1.9244	0.1571	$1.88 \cdot 10^{-2}$		
0.9	1.9368	1.9374	0.1053	$2.04 \cdot 10^{-2}$		
1	1.9454	1.9461	0.0706	$2.18 \cdot 10^{-2}$		

The results from Table 3 corresponds to $p=p_f=1$; $q=q_f=1$. With respect to the time constant $a_{100}=T_1=t_f/4=0.25$, the integration step $\Delta t=0.01$ represents $\frac{\Delta t}{T_1} = \frac{1}{25}$, a relatively high value in this case to. Still, (crep) is maintained in very low limits, which highlight the correctness of the method.

3.3. <u>Pde I(t, p) by form (9)</u>

Table 4						
t	X ₀₀₀₀	$y_{\rm AN}$	Υ _{AN}	crep		
0.01	1.0385	1.0385	3.7728	$3 \cdot 10^{-12}$		
0.1	1.3494	1.3494	2.5290	$1.21 \cdot 10^{-11}$		
0.2	1.5406	1.5406	1.7644	$1.54 \cdot 10^{-11}$		
0.3	1.6860	1.6860	1.1827	$1.65 \cdot 10^{-11}$		
0.4	1.7835	1.7835	0.7928	$1.63 \cdot 10^{-11}$		
0.5	1.8488	1.8488	0.5314	$1.55 \cdot 10^{-11}$		
0.6	1.8926	1.8926	0.3562	$1.45 \cdot 10^{-11}$		
0.7	1.9220	1.9220	0.2388	$1.34 \cdot 10^{-11}$		
0.8	1.9417	1.9417	0.1601	$1.23 \cdot 10^{-11}$		
0.9	1.9549	1.9549	0.1073	$1.12 \cdot 10^{-11}$		
1	1.9637	1.9637	0.0719	1.03.10-11		

The results from Table 4 corresponds to $p=p_f=1$. In this case to, with respect to the time constant $a_{10}=T_1=t_f/4=0.25$, and the integration step $\Delta t=0.01$

which represents $\frac{\Delta t}{T_1} = \frac{1}{25}$, a relatively high value,

the performance indicator (crep) is maintained at negligible values, which attest the correctness of the method.

3.4. <u>Pde II(t, p, q, r) by form (2)</u>

for all a...=1; T₁=0.15t_f; T₂=0.2t_f; P₁=0.15p_f; P₂=0.2p_f; Q₁=0.15q_f; Q₂=0.2q_f; R₁=0.15r_f; R₂=0.2r_f; n=2; N=6; M=25 and Δt =0.01.

Table 5						
t	x ₀₀₀₀	$y_{\rm AN}$	У _{АN}	crep		
0.01	1.0015	1.0015	0	0		
0.1	1.1241	1.1241	2.8891	$1.6 \cdot 10^{-5}$		
0.2	1.2976	1.2976	2.5462	$1.09 \cdot 10^{-4}$		
0.3	1.4787	1.4787	1.6892	$2.6 \cdot 10^{-4}$		
0.4	1.6219	1.6219	1.0157	$3 \cdot 10^{-4}$		
0.5	1.7258	1.7259	0.5744	$1.1 \cdot 10^{-3}$		
0.6	1.7974	1.7978	0.3144	$3.5 \cdot 10^{-3}$		
0.7	1.8452	1.8459	0.1686	8·10 ⁻³		
0.8	1.8764	1.8774	0.0892	$1.4 \cdot 10^{-2}$		
0.9	1.8970	1.8977	0.0468	$1.8 \cdot 10^{-2}$		
1	1.9117	1.9106	0.0244	1.9·10 ⁻²		

The results from Table 5 corresponds to $p=p_f=1$; $q=q_f=1$; $r=r_f=1$. The integration step $\Delta t=0.01$ represents only $\frac{\Delta t}{T_1} = \frac{0.01}{0.15} = \frac{1}{15}$ from the smallest time constant (T₁), but the performance indicator (crep) is maintained at sufficiently low limits, which highlight the correctness of the method.

3.5. Pde II(t, p, q) by form (8)

for all a...=1; T₁=0.15t_f; T₂=0.1t_f; P₁=0.15p_f; P₂=0.1p_f; Q₁=0.15q_f; Q₂=0.1q_f; n=2; N=6; M=30 and Δt =0.01.

Table 6						
t	X ₀₀₀₀	$y_{\rm AN}$	У _{АN}	crep		
0.01	1.0031	1.0031	0	0		
0.1	1.2232	1.2232	2.8783	0		
0.2	1.4763	1.4763	2.5367	10 ⁻⁴		
0.3	1.6884	1.6884	1.6919	5.7·10 ⁻⁴		
0.4	1.8221	1.8220	1.0120	$1.7 \cdot 10^{-3}$		
0.5	1.8999	1.8997	0.5723	$3.5 \cdot 10^{-3}$		
0.6	1.9433	1.9429	0.3132	$5.8 \cdot 10^{-3}$		
0.7	1.9666	1.9664	0.1679	$7.4 \cdot 10^{-3}$		
0.8	1.9787	1.9788	0.0888	$7.2 \cdot 10^{-3}$		
0.9	1.9842	1.9854	0.0466	$1.07 \cdot 10^{-2}$		
1	1.9859	1.9889	0.0243	2.15·10 ⁻²		

In this case to, the integration step (Δt) represents only $\frac{\Delta t}{T_2} = \frac{0.01}{0.10} = \frac{1}{10}$ from the smallest time constant

 (T_2) , but the performance indicator (crep) is not greater than 0.0215%.

3.6. <u>Pde II(t, p) by form (10)</u>

for all a...=1; T₁=0.15t_f; T₂=0.1t_f; P₁=0.15p_f; P₂=0.1p_f; n=2 ; N=6; M=20 and Δt =0.01.

Table 7						
t	X ₀₀₀₀	y_{AN}	Υ _{AN}	crep		
0.01	1.0031	1.0031	0	0		
0.1	1.2240	1.2240	2.8999	$3.7 \cdot 10^{-7}$		
0.2	1.4781	1.4781	2.5557	$8.8 \cdot 10^{-7}$		
0.3	1.6910	1.6910	1.7046	$1.4 \cdot 10^{-6}$		
0.4	1.8251	1.8251	1.0195	1.9·10 ⁻⁶		
0.5	1.9031	1.9031	0.5766	$2.4 \cdot 10^{-6}$		
0.6	1.9465	1.9465	0.3156	$2.8 \cdot 10^{-6}$		
0.7	1.9700	1.9700	0.1692	$3.2 \cdot 10^{-6}$		
0.8	1.9825	1.9825	0.0895	$3.8 \cdot 10^{-6}$		
0.9	1.9891	1.9891	0.0469	1.6·10 ⁻⁵		
1	1.9925	1.9926	0.0245	$1.5 \cdot 10^{-5}$		

In this case to, the integration step (Δt) represents only $\frac{\Delta t}{T_2} = \frac{0.01}{0.10} = \frac{1}{10}$ from the smallest time constant

 (T_2) , but the performance indicator (crep) is negligible.

This form (10) of pdeII(t, p) was particularized in the versions:

- elliptic: $a_{11}^2 4a_{20} \cdot a_{02} < 0$;
- parabolic: $a_{11}^2 4a_{20} \cdot a_{02} = 0$;
- hyperbolic: $a_{11}^2 4a_{20} \cdot a_{02} > 0$,

obtaining the same negligible values for (crep).

4. CONCLUSIONS

- 4.1. The present paper deals with general and complete forms of pde I and II, with for variables (t, p, q r), which are than particularized for three variables (t, p, q) and two variables (t, p), in the last case including the elliptic, parabolic or hyperbolic versions. The numerical integration is operated with respect to time, for (p), (q) and (r) constants.
- 4.2. The integration interval is framed in unitary reported measures, which limits the integration space inside of a (super)cube with unitary size, with the note that this size can be easily modified.
- 4.3. The considered examples operates with forced solutions, by exponential form (17), usual in technique.
- 4.4. All the examples are solved in a unitary and systematized manner, using the operator matrix (\mathbf{M}_{dpx}) method, considered original, with the advantages and disadvantages presented in the Abstract of this paper.

- 4.5. The numerical simulation performances, using this method, are defined by the cumulative relative error in percent (crep), which for N=6, M=(23-30) and $\Delta t=10^{-2}=t_{\rm f}/100$ (relatively high values), leads to crep $\leq 0.022\%$.
- 4.6. The logical scheme, based on this method, is simple and flexible, without special programming problems.

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