Solving SLAEs in Integration of the Initial Boundary Value Problems

V.P. Il'in

Institute of Computational Mathematics
and Mathematical Geophysics SB RAS
Novosibirsk State University

2-nd International CONFERENCE
"Multiscale Methods
and High Performance Scientific Computing"

August, 15–17 2018 г.
Moscow

Content

- **Statement of the Problem**
- **Approximation of the Initial Boundary Value Problems (IBVP)**
- **Features of SLAEs in Implicit Schemes**
- **Choosing the Initial Guess**
- **Algebraic and Geometric DMM**
- **Multi - Precondioned SCR Methods**
- **Parallel Processes in IBVP**

References

1. Il'in V. P. Mathematical Modeling,Part I:Continuous and Discrete Models. Novosi- birsk, SBRAS Publ., 2017 (in Russian).
2. Il'in V. P. Methods of Solving the Ordinary Differential Equations. Novosibirsk, NSU Publ., 2017 (in Russian).
3. Il'in V. P. Least Squares Methods in Krylov Subspaces. Journal of Mathematics Sciences. 224(6), 2017, 900-910.
4.Gander M. J. 50 years of time parallel integration in "Multiple Shooting and Time Domain Decomposition". T. Carraro, ed., Springer Verlag, Berlin, 2015,69-114.
5.Gander M. J. ,Neumuller M. Analysis of a new space-time parallel multigrid algorithm for parabolic problems, SIAM J. Sci. Comput. Vol. 38, №4, 2016, A2173-A2208.
6.Dolean V., Jolivet P., Nataf F. An Introduction to Domain Decomposition Methods: algorithms, theory and parallel implementaion. Philadelphia: SIAM, 2015.
7. Il'in V. P. Problems of parallel solution of large systems of linear algebraic equations. J. of Mathem. Sci. 216, 6, 2016, 795–804.

Statement of Initial Boundary Value Problems

$$\frac{\partial u}{\partial t} + L(u) = f(\vec{x}, t), \quad \vec{x} \in \Omega \subset \mathcal{R}^d, \quad d \geq 2,$$
$$\bar{\Omega} = \Omega \cup \Gamma, \quad 0 < t \leq T_e < \infty, \quad u \mid_{t=0} = u^0(\vec{x}), \tag{1}$$
$$l(u) \mid_\Gamma = g(\vec{x}, t), \quad \vec{x} = (x_1, \ldots, x_d),$$

$$Lu = -\sum_{i,j=1}^{n} \frac{\partial}{\partial x_i}\left(a_{i,j}(\vec{x}) \frac{\partial u}{\partial x_j}\right) + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x_i} + cu = f(\vec{x}). \tag{2}$$

$$\alpha_k u + \beta_k \sum_{i,j=1}^{d} a_{i,j} \frac{\partial u}{\partial x_j} \cos(\vec{n}, x_j) = g_k, \quad |\alpha_k| + |\beta_k| \neq 0, \quad \vec{x} \in \Gamma_k, \tag{3}$$

Space - Time Approximations

$$B\dot{u}^h + Au^h = f^h, \qquad (4)$$

$$\dot{u}^h, u^h, f^h \in \mathcal{R}^N; \quad B, A \in \mathcal{R}^{N,N},$$

$$f^h = \{f_l\},\ B = \{b_{l,l}\},\ \ A = \{a_{l,l}\},\ u^h = \{u_l^h\},\ (u)^h = \{u(\vec{x}_l)\}$$

$$B(\dot{u})^h + A(u)^h = (f)^h + \psi^h, \quad \psi = O(h^\gamma), \qquad (5)$$

$$(Au^h)_l \equiv a_{l,l}u_l + \sum_{l' \in \omega_l} a_{l,l'}u_{l'} = f_l, \quad l \in \Omega^h,\ l' = 1, \ldots, N_l, \qquad (6)$$

$$l = 1, \ldots, N,\ N_l \ll N,\ N \approx 10^7 - 10^{10}\ ,\ N_l \approx 100$$

Explicit and Implicit Methods
Crank - Nikolson Approximation

$$B\frac{u^{n+1}-u^n}{\tau_n}+\theta(Au^{n+1}-f^{n+1})=(1-\theta)(f^n-Au^n), \quad (7)$$

$$\theta\in[0,1], \qquad n=0,1,\dots,$$

$\theta=1/2$ $\psi^\tau=O(\tau^2)$, $\tau=\max_n\{\tau_n\}$, $\psi^n=\psi^\tau+\psi^h$

$$B\frac{(u)^{n+1}-(u)^n}{\tau_n}+\theta[A(u)^{n+1}-(f)^{n+1}]=(1-\theta)[(f)^n-A(u)^n]+\psi^n, \quad (8)$$

$(u)^n=\tilde{u}^n=\{u(\vec{x}_i,t_n)\}$ $-$ **vector of exact solution**

$$r^n=(1-\theta)(\tilde{f}^n-A\tilde{u}^n)-B\frac{\tilde{u}^{n+1}-\tilde{u}^n}{6\quad\tau_n}+\theta(A\tilde{u}^{n+1}-\tilde{f}^{n+1}). \quad (9)$$

Runge - Kutta - Radau Implicit Schemes, I Discontinuus Galerkin Methods (DGM) for ODES

$$\partial_t u(t) + Au(t) = f(t),\ \ t \in (0,\ \ T),\ \ u(0) = u_o,$$
$$u,\ \ f \in \mathcal{R}^{N_h},\ \ A \in \mathcal{R}^{N_h,N_h}$$
$$u_r^{n+1} \in \mathcal{P}_{N_\tau}(t_n,\ \ t_{n+1}), v_r^{n+1} \in \mathcal{P}_{N_t}(t_n,\ \ t_{n+1})$$
$$-\int_{t_n}^{t_{n+1}}, u_{n+1}^{\tau}(t)\partial_t v_\tau^{n+1}(t)dt + u_\tau^{n+1} v_\tau^{n+1}(t_{n+1})+$$
$$A\int_{t_n}^{t_{n+1}} u_\tau^{n+1}(t)v_\tau^{n+1}(t)v_\tau^{n+1}(t)dt =$$
$$\int_{t_n}^{t_{n+1}} f(t)dt + u_\tau^{n}(t_n)v_\tau^{n+1}(t_n)$$

Runge - Kutta - Radau Implicit Schemes, II

$$(K_\tau + AM_\tau)u^{n+1} = f^{n+1} + C_\tau u^n, \;\; n = 0, \; 1, \ldots, N-1$$

$$u^{n+1} \in \mathcal{R}^{N_t * N_h}, \;\; f^{n+1} = \{f_l^{n+1} = \int\limits_{t_n}^{t_{n+1}} f(t)\Psi_l^n(t)dt\},$$

$$\int\limits_{t_n}^{t_{n+1}} f(t)dt \approx r\sum_{k=1}^{s} b_k f(t_n + c_k\tau), \;\; c_1 = 0.$$

Estimate of the Total Error

$$C_1 u_{n-1} = C_2 u^n + g^n, \quad g = \tau_n[\theta f^{n+1} + (1-\theta) f^n],$$

$$C_1 = B + \theta \tau_n A, \quad C_2 = B - (1-\theta)\tau_n A.$$

$$z^{n+1} = (u)^{n+1} - \tilde{u}^{n+1}$$

$$C_1 z^{n+1} = C_2 z^n + \tau_n(\psi^n - r^n),$$

$$\tau_n(\psi^n - r^n)\| \leq \tau \|\psi\| \|z^{n+1}\| \leq \rho \|z^n\| + \tau \rho_1 \|\psi\| => $$

$$\rho = \|C_1^{-1} C_2\|, \quad \rho = \|C_1^{-1}\|.$$

$$\rho = 1 + O(\tau) => ||z^h|| \leqslant C(||z^0|| + ||\psi||)$$

Choosing the Initial Guess

- **simple shift** $\quad u^{n+1,\ 0} = u^n + O(\tau)$
- **linear extrapolation**

$$u^{n+1} = u^n + (u^n - u^{n-1})\tau_n/\tau_{n-1} + O(\tau^2). \tag{10}$$

- **predictor - corrector schemes**

$$B(\hat{u}^{n+1} - u^n) = \tau_n(f^n - Au^n) \equiv \tau_n r^n, \tag{11}$$

$$B(u^{n+1,s} - u^n) = \tau_n[\theta(f^{n+1} - Au^{n+1,s-1}) + (1-\theta)(f^n - Au^n)],$$

$$u^{n+1,\ 0} = \hat{u}^{n+1}$$

,

$$s = 1, \dots, m :$$

$$r^{n+1,s} = \tau_n[\theta(f^{n+1} - Au^{n+1,s-1}) + (1-\theta)\tau_n] - B(u^{n+1,s} - u^n)$$

Minimization of the Initial Residual

q – step least squares method (LSM)

$$u^{n+1,0} = u^n + c_1 v_1 + \ldots + c_q v_q = u^n + Vc, \tag{12}$$

$$v_l = u^n - u^{n-l}, \quad l = 1, \ldots, q, \tag{13}$$

$$c = (c_1, \ldots, c_q)^T \in \mathcal{R}^q, \qquad V = (v_1, \ldots, v_q) \in \mathcal{R}^{N,q}.$$

$$Cu^{n+1} \equiv (\tau_n^{-1} B + \theta A) u^{n+1} = g^n, \tag{14}$$

$$g^n = [\tau_n^{-1} B + (1-\theta) A] u^n.$$

$$r^{n+1,0} = r^n - CVc, \ \ r^n = g^n - Cu^n, \tag{15}$$

Least Squares Method

$$r^{n+1,0} \approx 0 : Wc \equiv CVc = r^n, \quad W \in \mathcal{R}^{N,q}. \tag{16}$$

$$Gc \equiv W^T Wc = W^T \tau^n, \quad G = V^T C^T CV \in \mathcal{R}^{q,q}. \tag{17}$$

$$W^T r^{n+1,0} = 0. \tag{18}$$

deflation:

$$V^T r^{n+1,0} = 0. \tag{19}$$

$$Hc \equiv V^T CVc = V^T c, \quad H \in \mathcal{R}^{q,q}. \tag{20}$$

iterative refinement:

$$\|r^{n+1,m}\| = \|g^n - Cu^{n+1,m}\| \leq \varepsilon \|g^n\| \tag{21}$$

$$\varepsilon \ll 1, u^{n+1} = u^{n+1,m}$$

Algebraic and Geometric DDM for IBVP

$$\Omega = \bigcup_{q=1}^{P} \Omega_q, \;\; \bar{\Omega}_q = \Omega_q \bigcup \Gamma_q, \;\; \Gamma_q = \bigcup_{q' \in \omega_q} \Gamma_{q,q'}, \;\; \Gamma_{q,q'} = \Gamma_q \bigcap \bar{\Omega}_{q'}, \; q' \neq q. \tag{22}$$

$$\bar{\Omega}_0 = \Omega_0 \bigcup \Gamma, \;\; \Gamma_{q,0} = \Gamma_q \bigcap \bar{\Omega}_0 = \Gamma_q \bigcap \Gamma, \;\; \Gamma_q = \Gamma_q^i \bigcup \Gamma_{q,0}, \tag{23}$$

$$\Gamma_q^i = \bigcup\nolimits_{q' \neq 0} \Gamma_{q,q'} \;\; \Gamma_{q,0} = \Gamma_q^e \;\; \Delta_{q,q'} = \Omega_q \bigcap \Omega_{q'}$$

$$\frac{\partial u_q}{\partial t} + Lu_q(\vec{x}) = f_q, \quad \vec{x} \in \Omega_q, \quad l_{q,q'}(u_q)\,|_{\Gamma_{q,q'}} = g_{q,q'} \equiv l_{q',q}(u_{q'})\,|_{\Gamma_{q',q}}, \quad q' \in \omega_q, \quad l_{q,0} u_q\,|_{\Gamma_{q,0}} = g_{q,0}, \quad q = 1, \ldots, P. \tag{24}$$

Algebraic and Geometric DDMs

$$\alpha_q u_q + \beta_q \frac{\partial u_q}{\partial \vec{n}_q}\Big|_{\Gamma_{q,q'}} = \alpha_{q'} u_{q'} + \beta_{q'} \frac{\partial u_{q'}}{\partial \vec{n}_{q'}}\Big|_{\Gamma_{q',q}}, \quad |\alpha_q| + |\beta_q| > 0, \quad \alpha_q \cdot \beta_q \geq 0. \tag{25}$$

$$\begin{aligned} \Gamma_q \equiv \Gamma_q^0 &= \left\{ l' \in \hat{\omega}_l, \ \ l \in \Omega_q, \ \ l' \notin \Omega_q, \ \ \Omega_q^1 = \bar{\Omega}_q^0 = \Omega_q \bigcup \Gamma_q^0 \right\}, \\ \Gamma_q^t &= \left\{ l' \in \hat{\omega}_l, \ \ l \in \Omega_q^{t-1}, \ \ l' \in \Omega_q^{t-1}, \ \ \Omega_q^t = \bar{\Omega}_q^{t-1} = \Omega_q^{t-1} \bigcup \Gamma_q^{t-1} \right\}. \end{aligned} \tag{26}$$

$$C_{q,q} u_q + \sum_{r \in \hat{\omega}_q} C_{q,r} u_r = g_q, \quad q = 1, \ldots, P, \tag{27}$$

$$(D_{q,q} u)_l \equiv \left(c_{l,m} + \theta_l \sum_{m \notin \omega_q} c_{l,m} \right) u_l + \sum_{m \in \omega_q} c_{l,m} u_m = g_l + \sum_{m \notin \omega_q} c_{l,m} (\theta_l u_l - u_m). \tag{28}$$

$$D u^{s+1} = (D - C) u^s + g, \quad s = 0, 1, \ldots. \tag{29}$$

$$D = block - diag\{D_{l,l}\}$$

Restricted Additive Swartz Method

$$R_{q,\Delta}^T \in \mathcal{R}^{N,N_q^\Delta} \quad u_q = \{u_l,\ l \in \Omega_q^\Delta\} \in \mathcal{R}^{N_q^\Delta}$$

$$(R_{q,\Delta}^T u_q)_l = \begin{cases} (u_q)_l & \textbf{if} \quad l \in \Omega_q^\Delta, \\ 0, & \textbf{otherwise}. \end{cases}$$

$$B_{AS} = \sum_{q=1}^{P} B_{AS,q}, \quad B_{AS,q} = R_{q,\Delta}^T \hat{C}_q^{-1} R_{q,\Delta}.$$

$$B_{RAS} = \sum_{q=1}^{P} B_{RAS,q}, \quad B_{RAS,q} = R_{q,0}^T \hat{C}_q^{-1} R_{q,\Delta}.$$

- **coarse grid correction**

$$\tilde{u}^n = u^n + Vc, \ \ V = (v_1 \ldots v_{N_c}), \ \ \tilde{r}^n = r^n - Wc, \ \ W = AV,$$

$$W = (w_1, \ldots, w_{N_c}) \in \mathcal{R}^{N,N_c}, \ \ Wc \approx r^n, \ \ c = B_c^{-1} r^n,$$

$$B_c^{-1} = W \hat{C}^{-1} W^T, \ \ \hat{C} = W^T C W \in \mathcal{R}^{N_c,N_c},$$

Multi - Preconditioned SCR Methods, I

$r^0 = f^0 - Cu^0$, $B_0^{(1)}, \ldots, B_0^{(m_0)} \in \mathcal{R}^{N,\ N}$

$$P_0 = [p_1^0 \cdots p_{m_0}^0] \in \mathcal{R}^{N,m_0}, \quad p_l^0 = (B_0^{(l)})^{-1} r^0, \tag{30}$$

$$\begin{aligned} u^{n+1} &= u^n + P_n\bar{\alpha}_n = u^0 + P_0\bar{\alpha}_0 + \cdots + P_n\bar{\alpha}_n, \\ r^{n+1} &= r^n - CP_n\bar{\alpha}_n = r^0 - CP_0\bar{\alpha}_0 - \cdots - CP_n\bar{\alpha}_n. \end{aligned} \tag{31}$$

$\bar{\alpha}_n = (\alpha_n^1, \ldots, \alpha_n^{m_n})^T$, $P_n = [p_1^n \cdots p_{m_n}^n] \in \mathcal{R}^{N,m_n}$, $D_{n,n} = diag\{\rho_{n,l}\}$

- **orthogonal properties**

$$P_n^T C^T CP_k = D_{n,k} = 0 \quad \textbf{for} \quad k \neq n, \tag{32}$$

- **minimizing the residual**

$$\mathcal{K}_{M_n} = Span\{P_0, \ldots, C^{n-1}P_{n-1}\}, \quad M_n = \sum_{k=0}^{n-1} m_k \tag{33}$$

Multi - Preconditioned Methods SCR, II

$$\bar{\alpha}_n = \{\alpha_{n,l}\} = (D_{n,n}^{-1})^{-1} P_n^T C^T r^0, \tag{34}$$

$$P_{n+1} = Q_{n+1} - \sum_{k=0}^{n} P_k \bar{\beta}_{k,n}, \tag{35}$$

$$Q_{n+1} = [q_1^{n+1} \cdots q_{m_n}^{n+1}], \quad q_l^{n+1} = (B_{n+1}^{(l)})^{-1} r^{n+1}, \quad l = 1, \ldots, m_n, \tag{36}$$

$$\bar{\beta}_{k,n} = D_{k,k}^{-1} P_k^T C^T C Q_{n+1}. \tag{37}$$

Examples of Methodical Experiments

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x,t), \;\; x \in (0,\pi), \;\; t \in (0,\pi), \qquad (38)$$

$$u(x,t) = \sin x \cdot \sin \omega t, \;\; f(x,t) = \sin x(\sin t + \omega \cos \omega t), \;\; (39)$$

$$\theta = 1/2), \quad \epsilon = 10^{10}, \quad \delta \approx 10^{-5},$$

$$\triangle_n = 3 - diag\{-1, 2, -1\}/h^2,$$

$$N_h, N_\tau = 16, 32, 64, 128, 256.$$

Table 1. The total number of iterations for simple shift and predictor - corrector methods, $\theta = 1/2$, $\omega = 1$

$N_\tau \setminus N_h$	**16**	**32**	**64**	**128**	**256**
16	1361 1216	5421 4852	22012 19707	89065 79758	358699 321224
32	**1514** **1277**	**5632** **4761**	**22427** **18969**	**90301** **76403**	**363228** **307330**
64	**1742** **1389**	**5835** **4638**	**22409** **17833**	**89328** **71127**	**358413** **285429**
128	**2138** **1648**	**6194** **4587**	**22340** **16656**	**87443** **65099**	**349130** **259973**
256	**2832** **2039**	**6935** **4847**	**22621** **15579**	**85473** **58987**	**338028** **233163**

Table 2. The total number of iterations for predictor - LSM and one - step LSM, $\theta = 1/2$, $\omega = 1$

$N_\tau \setminus N_h$	16	32	64	128	256
16	131 0	790 2	5999 83	28459 415	151381 6205
32	108 0	926 11	5313 0	28268 1152	146381 6522
64	78 0	804 12	6767 75	36667 1	132951 42
128	12 0	579 14	5241 135	26731 5325	157813 13593
256	0 0	404 8	4075 184	25337 2097	144422 26339

Table 3.The total number of iterations for simple shift and predictor - corrector methods, $\theta = 1/2$, $\omega = 4$

$N_\tau \setminus N_h$	**16**	**32**	**64**	**128**	**256**
16	1465 1399	5843 5585	23717 22668	95976 91735	386535 369435
32	**1632** **1495**	**6078** **5574**	**24209** **22192**	**97478** **89362**	**392104** **359453**
64	**1878** **1646**	**6302** **5534**	**2416** **21250**	**96572** **84729**	**387493** **339976**
128	**2311** **1912**	**6705** **5601**	**24200** **20224**	**94711** **79139**	**378197** **315974**
256	**3062** **2537**	**7519** **5900**	**24549** **19399**	**92809** **73368**	**367090** **290033**

Table 4. The total number of iterationst for predictor - LSM and one - step LSM, $\theta = 1/2$, $\omega = 4$

$N_\tau \setminus N_h$	16	32	64	128	256
16	125 0	1141 0	6423 0	29083 0	153512 0
32	130 0	971 10	5611 0	37661 0	184556 2
64	79 0	814 0	5514 0	33831 10	162940 416
128	13 0	668 0	4983 9	26897 95	142330 514
256	0 0	397 1	3816 10	24243 82	135163 9480

СПАСИБО ЗА ВНИМАНИЕ

THANKS FOR ATTENTION