Deflated Krylov Iterations in Domain Decomposition Methods

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1 Introduction

The goal of this research is an investigation of some advanced versions of algebraic approaches to parallel domain decomposition algorithms for solving sparse large systems of linear algebraic equation (SLAEs) with nonsymmetric sparse matrices arising from some approximation of the multi-dimension boundary value problems (BVPs) in complicated computational domains on non-structured grids.

Algebraic domain decomposition methods (DDMs) are the main tool to provide high performance computing when solving very large SLAEs which is the bottleneck of the modern interdisciplinary tasks. There are many publications on this topic, see Toselli and Widlund [2005], Dolean et al. [2015], Dubois et al. [2012], Gurieva and Il'in [2015] and literature cited there, for example. They present a manifold of mathematical and technological contradictory problems. On the one hand, high convergence rate of iterative processes leads to high computational complexity of algorithms. On the other hand, performance of applied program packages depends on used data structures and code adaptation to a particular parallel architecture.

We describe some essential aspects of the algorithms implemented on the basis of the multi-preconditioned semi-conjugate residual method and the coarse grid correction procedure with basic functions of different orders. In some sense, the proposed approaches present a further development of the ideas considered in papers by Saad [2003], Bridson and Greif [2006].

This paper is organized as follows. Section 2 contains the formulation of the problems to be solved. Section 3 is devoted to the parallel structure of algorithms. Section 4 deals with demonstration of the numerical results. In conclusion, the results obtained are described.

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2 Statement of the problem

Let us have a boundary value problem

$$Lu = f(\mathbf{r}),\ \ \mathbf{r} \in \Omega,\ \ lu|_{\Gamma} = g(\mathbf{r}), \tag{1}$$

in a computational open domain Ω with a boundary Γ and a closure $\bar{\Omega} = \Omega \bigcup \Gamma$, where L and l are some linear differential operators. We suppose that (1) has a unique solution $u(\mathbf{r})$ which is smooth enough.

Let us decompose Ω into P subdomains (with or without overlapping):

$$\begin{array}{l} \Omega = \bigcup\limits_{q=1}^{P} \Omega_q,\ \ \bar{\Omega}_q = \Omega_q \bigcup \Gamma_q, \\ \Gamma_q = \bigcup\limits_{q' \in \omega_q} \Gamma_{q,q'},\ \ \Gamma_{q,q'} = \Gamma_q \bigcap \bar{\Omega}_{q'},\ \ q' \neq q. \end{array} \tag{2}$$

Here Γ_q is the boundary of Ω_q which is composed from the segments $\Gamma_{q,q'}$, $q' \in \omega_q$, and $\omega_q = \{q_1, \ldots, q_{M_q}\}$ is a set of M_q contacting, or conjuncted, subdomains. We can denote also by $\Omega_0 = R^d/\Omega$ the external subdomain:

$$\bar{\Omega}_0 = \Omega_0 \bigcup \Gamma,\ \ \Gamma_{q,0} = \Gamma_q \bigcap \bar{\Omega}_0 = \Gamma_q \bigcap \Gamma,\ \ \Gamma_q = \Gamma_q^i \bigcup \Gamma_{q,0}, \tag{3}$$

where $\Gamma_q^i = \bigcup\limits_{q' \neq 0} \Gamma_{q,q'}$ and $\Gamma_{q,0} = \Gamma_q^e$ mean internal and external parts of the boundary of Ω_q. We define also an overlapping $\Delta_{q,q'} = \Omega_q \bigcap \Omega_{q'}$ of the neighbouring subdomains. If $\Gamma_{q,q'} = \Gamma_{q',q}$ and $\Delta_{q,q'} = 0$ then overlapping of Ω_q and $\Omega_{q'}$ is empty.

The idea of DDM includes the definition of sets of boundary value problems for all subdomains which should be equivalent to the original problem (1):

$$\begin{array}{l} Lu_q(\mathbf{r}) = f_q,\ \ \mathbf{r} \in \Omega_q,\ \ l_{q,q'}(u_q)\big|_{\Gamma_{q,q'}} = g_{q,q'} \equiv l_{q',q}(u_{q'})\big|_{\Gamma_{q',q}}, \\ q' \in \omega_q,\ \ l_{q,0}u_q|_{\Gamma_{q,0}} = g_{q,0},\ q = 1, \ldots, P. \end{array} \tag{4}$$

At each segment of the internal boundaries of subdomains, the interface conditions in the form of the Robin boundary condition are imposed:

$$\begin{array}{l} \alpha_q u_q + \beta_q \frac{\partial u_q}{\partial \mathbf{n}_q}\big|_{\Gamma_{q,q'}} = \alpha_{q'} u_q + \beta_{q'} \frac{\partial u_{q'}}{\partial \mathbf{n}_{q'}}\big|_{\Gamma_{q',q}}, \\ |\alpha_q| + |\beta_q| > 0, \quad \alpha_q \cdot \beta_q \geq 0. \end{array} \tag{5}$$

Here $\alpha_{q'} = \alpha_q, \beta_{q'} = \beta_q$ and $\mathbf{n}_q$ means the outer normal to the boundary segment $\Gamma_{q,q'}$ of the subdomain Ω_q.

We consider the iterative additive Schwarz method which can be interpreted as a sequential recomputation of the boundary condition:

$$Lu_q^n = f_q,\ \ l_{q,q'}u_q^n|_{\Gamma_{q,q'}} = l_{q',q}u_{q'}^{n-1}|_{\Gamma_{q',q}}. \tag{6}$$

In order to solve the considered problem numerically we need to perform its dicretization. We introduce the grid computational domain Ω^h which consists of a set of the numbered nodes Q_l, $l = 1, \ldots, N$, where N is the total number of mesh points. Then we divide Ω^h into P grid subdomains Ω_q^h

$$\bar{\Omega}^h = \bigcup_{q=1}^{P} \bar{\Omega}_q^h, \;\; \bar{\Omega}^h = \Omega_h \bigcup \Gamma^h, \;\; \bar{\Omega}_q^h = \Omega_q^h \bigcup \Gamma_q^h, \tag{7}$$

In the case of a non-overlapping decomposition, for $q' \neq q''$ we have $\Omega_{q'}^h \bigcap \Omega_{q''}^h = \emptyset$, and $\Gamma_{q',q''}^h = \bar{\Omega}_{q'}^h \bigcap \bar{\Omega}_{q''}^h$ is the common boundary (a grid separator) between the contacting subdomains $\Omega_{q'}^h, \Omega_{q''}^h$.

After an approximation of the original continuous problem (1) on the non-structured grid Ω^h, one can obtain a SLAE

$$Au \equiv \sum_{l' \in \bar{\omega}_l} a_{l,l'} u_{l'} = f, \;\; A = \{a_{l,l'}\} \in \mathcal{R}^{N,N}, \;\; u = \{u_l\}, \;\; f = \{f_l\} \in \mathcal{R}^N, \tag{8}$$

where the matrix A is supposed to be invertible and nonsymmetric in general. We consider the nodal grid equations only, i.e. each vector component u_l or f_l corresponds to some mesh point $Q_l \in \Omega^h$. Here $\bar{\omega}_l$ is the stencil of the grid point Q_l, and $N_{\omega_l} \ll N$ is the corresponding number of the neighbouring nodes. Also, we denote by N_q and $N_{q,q'}$ the numbers of the grid nodes in the grid subdomain Ω_q^h and the boundary segment $\Gamma_{q,q'}^h$ respectively.

3 Deflated DDM in Krylov subspaces

From here after, we consider a decomposition of the grid computational domain without mesh separators. It means that the continuous internal boundaries $\Gamma_{q,q'}$ for $q \neq 0$ do not contain mesh points, and $\Gamma_{q,q'}^h \neq \Gamma_{q',q}^h$.

If we denote by $\hat{u}_q, \hat{f}_q \in \mathcal{R}^{N_q}$, $q = 1, \ldots, P$ the subvectors corresponding to a subdomain Ω_q, the system (8) can be written in the following block form

$$A_{q,q}\hat{u}_q = f_q - \sum_{r \in \omega_q} A_{q,r}\hat{u}_r \equiv \hat{f}_q, \;\; A_{q,r} \in \mathcal{R}^{N_q,N_r}, \;\; q = 1, \ldots, P. \tag{9}$$

The additive Schwarz method is then described by the following formula:

$$\begin{aligned} &B_{q,q}\hat{u}_q^n \equiv (A_{q,q} + C_{q,q})\hat{u}_q^n = \\ &= f_q + C_{q,q}\hat{u}_q^{n-1} - \sum_{r \in \omega_q} A_{q,r}\hat{u}_r^{n-1}, \;\; n = 1, 2, \ldots \end{aligned} \tag{10}$$

Here we suppose that the preconditioning matrices $B_{q,q}$ are nonsingular ones and hence for $n \to \infty$ the iterative process (10) converges to a unique solution $u = \{\hat{u}_q\}$ of SLAE (8). The matrix $C_{q,q}$ in (10) is responsible for the interface condition between the subdomains and has nonzero entries for the near-boundary nodes of Ω_q only.

In the case of a decomposition without overlapping, the global solution vector is the direct sum of its subvectors, i.e. $u = \hat{u}_1 \oplus \ldots \oplus \hat{u}_P$. In general, the formulae of the iterative method within the Schwarz approach can differ from that above, and we use RAS (Restricted Additive Schwarz, see Toselli and Widlund [2005], Dolean et al. [2015]) for a definition of the iterative process. Here we have to construct the grid domain decomposition in two steps. Firstly, we define a decomposition into some non-intersected subdomains, see (7). Let us denote by Γ_q^0 the grid boundary of Ω_q^h and define an extended subdomain $\Omega_q^1 = \Omega_q^h \bigcup \Gamma_q^0 = \bar{\Omega}_q^h$. At the second step we extend each subdomain layer-by-layer and define a set of the embedded subdomains:

$$\begin{array}{l} \Gamma_q \equiv \Gamma_q^0 = \{l' \in \omega_l,\ \ l \in \Omega_q,\ \ l' \notin \Omega_q,\ \ \Omega_q^1 = \bar{\Omega}_q^0 = \Omega_q \bigcup \Gamma_q^0\}, \\ \Gamma_q^t = \{l' \in \omega_l,\ \ l \in \Omega_q^{t-1},\ \ l' \in \Omega_q^{t-1},\ \ \Omega_q^t = \bar{\Omega}_q^{t-1} = \Omega_q^{t-1}\Gamma_q^{t-1}\}, \\ t = 1, \ldots, \Delta_q. \end{array} \tag{11}$$

Here Δ_q is a measure parameter of the extension of the subdomain $\Omega_q^{\Delta_q}$. The RAS iterative process can be described as $u_{RAS}^n = \{u_l^n,\ \ l \in \Omega_q^0\}$.

The conventional additive Schwarz (AS) method can be rewritten in more general form as

$$B_n(u^n - u^{n-1}) = f - Au^{n-1} \equiv r^{n-1},\ \ n = 1, 2, \ldots, \tag{12}$$

where the preconditioning matrix B_n = block-diag $\{B_{q,q}^n\}$ may be chosen differently at each iteration.

To solve SLAE (1), we apply a preconditioned iterative process in the Krylov subspaces instead of (12) . In particular, we use multi-preconditioned semi-conjugate residual (MPSCR) method (Gurieva and Il'in [2015]), which is the unification of the ideas presented in (Bridson and Greif [2006], Il'in and Itskovich [2007], Eisenstat et al. [1983], Yuan et al. [2004]). Let us have some rectangular matrices and vectors of iterative parameters

$$P_n = (p_1^n \ldots p_{m_n}^n) = \{p_k^n\} \in \mathcal{R}^{N,m_n},\ \ \bar{\alpha}_n = (\alpha_{n,1} \ldots \alpha_{n,m_n})^T = \{\alpha_k^n\} \in \mathcal{R}^{m_n}.$$

Then MPSCR iterations are defined by the recursions for $n = 0, 1, \ldots$:

$$r^0 = f - Au^0, u^{n+1} = u^n + P_n\bar{\alpha}_n,\ \ r^{n+1} = r^n - AP_n\bar{\alpha}_n. \tag{13}$$

Let us suppose that at each n-th iteration we have m_n different nonsingular matrix preconditioners $B_n^{(k)}, k = 1, \ldots, m_n$. In this case the initial search vectors are chosen as $p_k^0 = (B_0^{(k)})^{-1}r^0$. Let these vectors be linearly independent and let the matrices P_n in (13) have full ranks m_n. Then under the orthogonality conditions

$$(Ap_k^n, Ap_{k'}^{n'}) = \rho_{n,k}\delta_{k,k'},\ \ \rho_{n,k} = (Ap_k^n, Ap_k^n), \tag{14}$$

where $\delta_{n,n'}$ is the Kronecker symbol, the formulas (13), with the coefficients

$$\alpha_k^n = (r^n, A(B_n^{(k)})^{-1} r^n)/\rho_{n,k}, \;\; k = 1, \ldots, m_n, \tag{15}$$

provide the minimal norm $||r^n||$ of the residual in the block Krylov subspaces $\mathrm{Span}\{AP_1, \ldots, AP_n\}$. The matrices P_i, $i = 1, \ldots, n+1$, are defined as

$$\begin{aligned} &P_{n+1} = Q_{n+1} - \sum_{k=0}^{n} \sum_{l=0}^{m_k} \beta_{k,l}^n p_l^k, \;\; Q_{n+1} = \{q_k^{n+1} = (B_{n+1}^{(k)})^{-1} r^{n+1}\}, \\ &\beta_{k,l}^n = (Ap_l^k, A(B_n^{(k)})^{-1} r^n)\rho_{n,l}, \;\; k = 1, \ldots, m_n. \end{aligned} \tag{16}$$

We apply MPSCR method with two types of preconditioners ($B_n^{(s)}$ and $B_n^{(c)}$) at each iteration. The first one corresponds to the block Jacobi–Schwarz preconditioner from (10) and (12), and the second one is responsible for a coarse grid correction, or aggregation, or deflation approach (Toselli and Widlund [2005], Dolean et al. [2015]). This procedure is based on the low rank approximation of the original matrix A (Gurieva and Il'in [2015]):

$$\begin{aligned} &(B_n^{(c)})^{-1} \equiv \tilde{A}_n = W_n \hat{A}_n^{-1} W_n^T, \;\; \hat{A}_n = W_n^T A W_n \in \mathcal{R}^{N_n^{(c)}, N_n^{(c)}}, \\ &W_n = (w_1 \ldots w_{N_n^{(c)}}) \in \mathcal{R}^{N, N_n^{(c)}}, \;\; N_n^{(c)} \ll N. \end{aligned} \tag{17}$$

Here W_n are some full rank rectangular matrices whose columns consist of the entries presenting the values of the finite basis functions $w_q(\mathbf{r})$ defined at some coarse grid with the number of the macro-nodes $N_n^{(c)} \ll N$ (this number can have different value at different iterations). This macrogrid can be independent of the domain decomposition, but we use $N_n^{(c)} = P$ and $w_q(\mathbf{r})$ with the entries equal one in Ω_q and the zero entries in other subdomains.

One disadvantage of SCR is the long recursions and high memory requirements to compute the search vectors p_k^n. More lightweight approach is in an application of the BiCGStab (Saad [2003]) with a deflation to improve the residual at the first iteration only. Having initial guess u^{-1}, we compute

$$\begin{aligned} &u^0 = u^{-1} + (B_0^{(c)})^{-1} r^{-1}, \;\; r^{-1} = f - Au^{-1}, \\ &r^0 = f - Au^0, \;\; p^0 = r^0 - (B_0^{(c)})^{-1} r^0, \end{aligned} \tag{18}$$

where $B_0^{(c)}$is defined by (17). This trick provides the orthogonality properties $W_0^T r^0 = 0$, $W_0^T A p^0 = 0$. The next iterations are implemented by the corresponding steps of the conventional BiCGStab method.

4 Numerical experiments

Consider solving a model Dirichlet boundary value problem for 2D and 3D diffusion-convection equation with constant coefficients p, q, r:

$$\begin{aligned} &\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + p\frac{\partial u}{\partial x} + q\frac{\partial u}{\partial y} + r\frac{\partial u}{\partial z} = f(x,y,z), \\ &(x,y,z) \in \Omega,\ u|_\Gamma = g(x,y,z),\ \Omega = [0,1]^3. \end{aligned} \tag{19}$$

Problem (19) is discretized by the monotone exponential finite volume scheme (Il'in [2003]) on a square (cubic) mesh with $N = N_x^d$ degrees of freedom, for different values of N_x. The stopping criterion for external iterations was $||r^n|| \le \varepsilon^e = 10^{-7}$. All the experiments were carried out on the hybrid cluster NKS-30T where every MPI process was run on Intel Xeon E5450 processor.

The implementation of DDM was made via the hybrid programming with two levels of a parallelization. At the upper level, the iterative Krylov process over P subdomains has been organized on the basis of MPI approach which forms one MPI-process for every subdomain and provides data communications. The auxiliary SLAEs in subdomains were solved by PARDISO from Intel MKL which uses multithreading, thus giving one more level of parallelism.

Table 1 presents the results for the 2D problem (19) solved by the deflated BiCGStab-DDM method at the upper level of the iterative process with the Dirichlet interface condition. Acceleration of the method was done only before the iterations by the procedure (18). The boundary conditions and the right hand side were chosen in accordance with the known exact solution $u(x,y) = 3xy^2 - x^3$. The experiments were made on the square macro-grid of P^2 equal subdomains, with the number of $(N/P)^2$ mesh points in each subdomain. Here the number of iterations are given for the grids with the numbers of their points $N = 64^2, 128^2, 256^2$. Each four columns stand for the case without deflation, the case with the piece-wise constant, the linear and the quadratic basis functions w_k taken for the deflation matrices $W_0 \in \mathcal{R}^{N,P}$, respectively. Zero initial guess and overlapping parameter $\Delta = 0, 1, 2, 3$ were taken.

Table 1 The numbers of iterations for BiCGStab method (2D problem) for different grids, macrogrids and basis functions in the deflation matrix, $\Delta = 0, 1, 2, 3$, $p = q = 4$

N	Δ	P^2											
		2^2				4^2				8^2			
64^2	0	19	21	23	17	27	27	25	19	38	34	33	26
	1	12	12	12	10	18	16	15	13	21	20	19	14
	2	9	10	9	8	13	13	11	11	17	16	14	11
	3	8	8	8	7	10	12	9	9	13	13	12	10
128^2	0	27	29	31	22	43	41	36	26	51	46	44	38
	1	16	18	18	14	24	22	21	17	30	27	25	16
	2	13	14	13	12	19	18	17	14	23	21	21	15
	3	11	12	11	10	15	15	14	12	19	18	16	11
256^2	0	42	35	46	35	65	52	45	33	98	73	65	32
	1	22	24	22	19	32	30	30	22	43	39	38	31
	2	17	20	19	14	26	25	22	18	34	31	30	24
	3	15	18	17	13	22	21	20	15	28	25	25	20

As we can see from these results, an application of the coarse grid correction gives the considerable improvement of the BiCGStab method, for different values of coefficients p, q for the single usage of the acceleration before the first iteration only. Moreover, the efficiency of the deflation procedure increases when the smoothness of the basis functions grows. Another way to decrease the number of iterations is to use small subdomain overlapping, $\Delta = 1, 2, 3$. But for big Δ values, the solution of BVPs in the subdomains becomes too expensive, and so we have the optimal parameters $\Delta \approx 4$, in the sense of the run time. These effects are especially valuable for the big numbers of subdomains and the degrees of freedom of the SLAE.

The second set of experiments is devoted to application of the SCR method with two preconditioners $B_n^{(s)}$ and $B_n^{(c)}$, the latter one formed using piecewise constant basis functions. Here we solved 3D Laplace equation ($p = q = r = f = 0$) in (19) with the exact solution $u = x^2 + y^2 + z^2$ and the initial guess $u^0 = 0$. Also, the domain decomposition was carried out without overlapping of the subdomains, with the Dirichlet interface conditions. In each cell of Table 2 we present the number of iterations and the run time for the grids $N = 32^3, 64^3, 128^3$, and for the number of subdomains (it is equal to the number of MPI-processes) $P = 4, 8, 16, 32, 64$. The results for the second set of experiments indicate that it may not be advantageous to employ coarse grid correction at every step of an iterative process, especially if low-order basis functions are used. This observation also correlates with the results obtained in the first set of experiments.

Table 2 The number of iterations and run times for SCR method with coarse grid corrections at every 5-th iteration and for block algorithm MPSCR, $p = q = r = 0$, $\Delta = 0$

N	Method	P				
		4	8	16	32	64
32^3	SCR	52 0.34	59 0.27	59 0.23	66 0.30	70 0.42
	MPSCR	45 0.48	54 0.34	54 0.32	62 0.38	67 0.48
64^3	SCR	66 4.81	82 2.71	101 1.96	102 1.72	105 2.07
	MPSCR	59 5.35	70 3.18	85 2.39	98 2.32	109 2.66
128^3	SCR	114 217.2	132 72.5	133 33.1	151 22.3	150 20.6
	MPSCR	101 226.3	111 79.1	134 43.2	156 32.8	159 30.7

5 Conclusion

The presented numerical results demonstrate that multi-preconditioned DDM in the Krylov subspaces have reasonable efficiency. Our main goal is to investigate the scalability of parallel DDM with application of multi-preconditioned SCR iterative process and the coarse grid correction approach with different order of basis functions. Our numerical experiments with the proposed

approaches have shown the valuable impovement of the methods' behaviour for the test problems considered. However, further experimental investigations are needed to understand the properties of the algorithms and to arrive at a robust high-performance code and to define a niche of the approaches presented when used for some particular applied problems.

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