The Multipliers-Free Dual-Primal Domain Decomposition Methods for Symmetric and Non-symmetric Matrices:Implementation Issues

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Summary. This paper corresponds to the second talk given in the minisymposium devoted to present the multipliers-free domain decomposition method. After supplying an overview of such methods, in Paper 1, implementation issues are here discussed. Some details related with code development are explained and then computational and numerical experiments are carried out. The results here contained confirm the advantages that these methods possess as was claimed in Paper1. Unified matrix formulas for the different algorithms that are applicable to both symmetric and non-symmetric matrices. simplified code development that can be 100% implemented in parallel; such methods also permit the construction of very robust codes; and state-of-the-art convergence rate.

1 Introduction

Nowadays it is standard to treat preconditioned non-overlapping domain decomposition methods with recourse to Lagrange-multipliers using a saddle point formulation [1]-[3]. This artifice, no doubt, has been quite valuable since it has permitted dealing with a large variety of problems; however, it is an indirect approach that bypasses many details of the problems considered and it is not free of shortcomings, as it was explained in paper 1 of this minisymposium [4]. Actually two approaches are possible when formulating DDMs:

1. Avoid the introduction of discontinuous functions, keeping the treatment within spaces of continuous functions, and deal with the problem as one of constrained optimization by means of a Lagrange multipliers formulation; or
2. Enlarge the functions-space considered to one whose members are generally discontinuous and contains the continuous-functions-space as a linear subspace.

When research on domain decomposition began the first option was preferred and the second option had remained unexplored up to now in spite of the many years elapsed.
Recently, a systematic program of research to fill this gap has been carried out [5]-[9] and the purpose of this Minisymposium, entitled the Multipliers-Free Dual-Primal Domain Decomposition Methods for Symmetric and Non-symmetric Matrices, is to summarize its results. In paper 1, an overview of this approach was presented, while this second article is devoted to explain with certain details its numerical and computational properties.

2 Parallelization Properties of the Multipliers-free DDMs

The developments of this Section are done in $\tilde{D}\left(\bar{\Omega}\right)$, the extended space of vectors, whose members are generally discontinuous and contains the continuous-vectors-space, $\tilde{D}\left(\Omega\right)$, as a subspace. Hence, all vectors here considered belong to $\tilde{D}\left(\bar{\Omega}\right)$. In paper 1, the matrix $\underline{\underline{A}}$ was written as

$$\underline{\underline{A}} \equiv \begin{pmatrix} \underline{\underline{A}}_{\Pi\Pi} \underline{\underline{A}}_{\Pi\Delta} \\ \underline{\underline{A}}_{\Delta\Pi} \underline{\underline{A}}_{\Delta\Delta} \end{pmatrix} \tag{1}$$

The notation here is such that

$$\begin{cases} \underline{\underline{A}}_{\Pi\Pi} : \tilde{D}^{DP}\left(\Pi\right) \to \tilde{D}^{DP}\left(\Pi\right), & \underline{\underline{A}}_{\Pi\Delta} : \tilde{D}\left(\Delta\right) \to \tilde{D}^{DP}\left(\Pi\right) \\ \underline{\underline{A}}_{\Delta\Pi} : \tilde{D}^{DP}\left(\Pi\right) \to \tilde{D}\left(\Delta\right), & \underline{\underline{A}}_{\Delta\Delta} : \tilde{D}\left(\Delta\right) \to \tilde{D}\left(\Delta\right) \end{cases} \tag{2}$$

Also, $\tilde{D}\left(\Delta\right) \subset \tilde{D}\left(\bar{\Omega}\right)$ is the linear space of vectors of $\tilde{D}\left(\bar{\Omega}\right)$ that vanish at every *derived node* that is not a *dual node*, while $\tilde{D}\left(\Pi\right)$ is the linear space of vectors that vanish at every dual node (i.e., they vanish at Δ). Furthermore,

$$\tilde{D}^{DP}\left(\bar{\Omega}\right) = \tilde{D}^{DP}\left(\Pi\right) \oplus \tilde{D}\left(\Delta\right) \tag{3}$$

We now define $\Sigma \equiv I \cup \Delta$, and in a similar fashion shall write

$$\underline{\underline{A}} \equiv \begin{pmatrix} \underline{\underline{A}}_{\Sigma\Sigma} \underline{\underline{A}}_{\Sigma\pi} \\ \underline{\underline{A}}_{\pi\Sigma} \underline{\underline{A}}_{\pi\pi} \end{pmatrix} \tag{4}$$

Where

$$\begin{cases} \underline{\underline{A}}_{\Sigma\Sigma} : \tilde{D}\left(\Sigma\right) \to \tilde{D}\left(\Sigma\right), & \underline{\underline{A}}_{\Sigma\pi} : \tilde{D}\left(\pi\right) \to \tilde{D}\left(\Sigma\right) \\ \underline{\underline{A}}_{\pi\Sigma} : \tilde{D}\left(\Sigma\right) \to \tilde{D}\left(\pi\right), & \underline{\underline{A}}_{\pi\pi} : \tilde{D}\left(\pi\right) \to \tilde{D}\left(\pi\right) \end{cases} \tag{5}$$

It can be verified that

$$\underline{\underline{A}}_{\Sigma\Sigma} \equiv \begin{pmatrix} \underline{\underline{A}}_{II} \underline{\underline{A}}_{I\Delta} \\ \underline{\underline{A}}_{\Delta I} \underline{\underline{A}}_{\Delta\Delta} \end{pmatrix} = \sum_{\alpha=1}^{E} \begin{pmatrix} \underline{\underline{A}}_{II}^{\alpha} \underline{\underline{A}}_{I\Delta}^{\alpha} \\ \underline{\underline{A}}_{\Delta I}^{\alpha} \underline{\underline{A}}_{\Delta\Delta}^{\alpha} \end{pmatrix} \tag{6}$$

When making use of the multipliers-free domain-decomposition methods, the formulas that need to be applied are:

$$\textit{For the Schur complement}: \underline{\underline{aS}}\underline{u}_\Delta = \underline{f}_{\Delta 2} \textit{ and } \underline{\underline{j}}\underline{u}_\Delta = 0 \tag{7}$$

$$\textit{For Neumann}-\textit{Neumann}: \underline{\underline{aS}}^{-1}\underline{\underline{aS}}\underline{u}_\Delta = \underline{\underline{aS}}^{-1}\underline{f}_{\Delta 2} \textit{ and } \underline{\underline{j}}\underline{u}_\Delta = 0 \tag{8}$$

$$\textit{For non}-\textit{preconditioned FETI}: \underline{\underline{S}}^{-1}\underline{\underline{j}}\underline{u} = -\underline{\underline{S}}^{-1}\underline{\underline{j}}\underline{\underline{S}}^{-1}\underline{f}_{\Delta 2} \textit{ and } \underline{\underline{aS}}\underline{u} = 0 \tag{9}$$

$$\textit{For preconditioned FETI}: \underline{\underline{S}}^{-1}\underline{\underline{jSj}}\underline{u} = -\underline{\underline{S}}^{-1}\underline{\underline{jSjS}}^{-1}\underline{f}_{\Delta 2} \textit{ and } \underline{\underline{aS}}\underline{u} = 0 \tag{10}$$

So, when iterating we need to have codes for computing the action of the following matrices $\underline{\underline{a}}$, $\underline{\underline{j}}$, $\underline{\underline{S}}$ and $\underline{\underline{S}}^{-1}$. The actions $\underline{\underline{a}}\underline{u}$ and $\underline{\underline{j}}\underline{u}$ of the *average* and *jump matrices* on any vector $\underline{u} \in \tilde{D}(\bar{\Omega})$, which for every $\underline{u} \in \bar{\Omega}$ are given by

$$\underline{u}(q,\beta) = \frac{1}{m(q)} \sum_{\alpha \in Z(q)} \underline{u}(q,\alpha) \textit{ and } \underline{\underline{j}}\underline{u} = \underline{u} - \underline{\underline{a}}\underline{u}, \tag{11}$$

are so easy to compute that its parallelization is not an issue.

2.1 Parallel Computation of $\underline{\underline{S}}$.

As for the action of $\underline{\underline{S}}$, recall that

$$\underline{\underline{S}} \equiv \underline{\underline{A}}_{\Delta\Delta} - \underline{\underline{A}}_{\Delta\Pi}\underline{\underline{A}}_{\Pi\Pi}^{-1}\underline{\underline{A}}_{\Pi\Delta} \tag{12}$$

Here only the parallelization of the action of $\underline{\underline{A}}_{\Pi\Pi}^{-1}$ requires further explanation. Given $\underline{w} \in \tilde{D}(\Pi)$, let $\underline{v} \in \tilde{D}(\Pi)$ be such that $\underline{v} = \underline{v}_I + \underline{v}_\pi \equiv \underline{\underline{A}}_{\Pi\Pi}^{-1}\underline{w}$. Then, since

$$\underline{\underline{A}}_{\Pi\Pi}\underline{v} \equiv \begin{pmatrix} \underline{\underline{A}}_{\mathrm{II}}\underline{\underline{A}}_{\mathrm{I}\pi} \\ \underline{\underline{A}}_{\pi\mathrm{I}}\underline{\underline{A}}_{\pi\pi} \end{pmatrix} \begin{pmatrix} \underline{v}_{\mathrm{I}} \\ \underline{v}_\pi \end{pmatrix} = \begin{pmatrix} \underline{w}_{\mathrm{I}} \\ \underline{w}_\pi \end{pmatrix} \tag{13}$$

Then, $\underline{v}_\pi \in \tilde{D}(\pi)$ is the solution of

$$\underline{\underline{a}}^\pi \left(\underline{\underline{A}}_{\pi\pi} - \underline{\underline{A}}_{\pi\mathrm{I}}\underline{\underline{A}}_{\mathrm{II}}^{-1}\underline{\underline{A}}_{\mathrm{I}\pi}\right)\underline{v}_\pi = \underline{w}_\pi - \underline{\underline{A}}_{\pi\mathrm{I}}\underline{\underline{A}}_{\mathrm{II}}^{-1}\underline{w}_{\mathrm{I}} \textit{ together with } \underline{\underline{j}}^\pi\underline{v}_\pi = 0 \tag{14}$$

While

$$\underline{v}_{\mathrm{I}} = \underline{\underline{A}}_{\mathrm{II}}^{-1}\left(\underline{w}_{\mathrm{I}} - \underline{\underline{A}}_{\mathrm{I}\pi}\underline{v}_\pi\right) \tag{15}$$

We observe that the problem of Eq.14 is the usual DDM problem, except that it is formulated in the vector space $\tilde{D}(\pi)$ whose dimension is much smaller. Due to this fact, it can be treated in parallel by many methods.

2.2 Parallel Computation of the Inverse $\underline{\underline{S}}$.

Given $\underline{u}_\Delta \in \tilde{D}(\Delta)$, set $\underline{w}_\Delta \equiv \underline{\underline{S}}^{-1}\underline{u}_\Delta$ and write $\underline{w} \equiv \underline{w}_\pi + \underline{w}_\Sigma$ for the *dual-primal harmonic* extension of $\underline{w}_\Delta$. Then,

$$\begin{pmatrix} \underline{\underline{A}}_{\Sigma\Sigma}\underline{\underline{A}}_{\Sigma\pi} \\ \underline{\underline{A}}_{\pi\Sigma}\underline{\underline{A}}_{\pi\pi} \end{pmatrix} \begin{pmatrix} \underline{w}_\Sigma \\ \underline{w}_\pi \end{pmatrix} = \begin{pmatrix} \underline{u}_\Delta \\ 0 \end{pmatrix} \tag{16}$$

Using Eqs.6 and 16, it can be seen that

$$\begin{cases} \left(\underline{\underline{A}}_{\pi\pi} - \underline{\underline{A}}_{\pi\Sigma}\underline{\underline{A}}_{\Sigma\Sigma}^{-1}\underline{\underline{A}}_{\Sigma\pi}\right)\underline{w}_\pi = -\underline{\underline{A}}_{\pi\Sigma}\underline{\underline{A}}_{\Sigma\Sigma}^{-1}u_\Delta = -\underline{\underline{A}}_{\pi\Sigma}\left(\underline{\underline{A}}_{\Delta\Delta} - \underline{\underline{A}}_{\Delta I}\underline{\underline{A}}_{II}^{-1}\underline{\underline{A}}_{I\Delta}\right)u_\Delta \\ \underline{\underline{j}}^\pi \underline{w}_\pi = 0 \end{cases} \tag{17}$$

Only the parallelization of the action of $\underline{\underline{A}}_{\Sigma\Sigma}^{-1}$ requires further explanation, which in turn is clear since, by virtue of Eq.6, $\underline{\underline{A}}_{\Sigma\Sigma}^{-1}$ is the sum of local inverses. As before, we observe that the problem of Eq.17 is the usual DDM problem, this time formulated in the vector space $\tilde{D}(\pi)$ whose dimension is again much smaller. Once $\underline{w}_\pi$ has been obtained, one applies

$$\underline{w}_\Sigma = \underline{\underline{A}}_{\Sigma\Sigma}^{-1}\left(\underline{u}_\Delta - \underline{\underline{A}}_{\Sigma\pi}\underline{w}_\pi\right) \tag{18}$$

This completes the parallel computation of $w_\Delta = (\underline{w}_\Sigma)_\Delta = \underline{\underline{S}}^{-1}\underline{u}_\Delta$.
It should be observed that the number of primal nodes usually selected is quite small, which allows the matrices $\left(\underline{\underline{A}}_{\pi\pi} - \underline{\underline{A}}_{\pi\mathrm{I}}\underline{\underline{A}}_{\mathrm{II}}^{-1}\underline{\underline{A}}_{\mathrm{I}\pi}\right)$ and $\left(\underline{\underline{A}}_{\pi\pi} - \underline{\underline{A}}_{\pi\Sigma}\underline{\underline{A}}_{\Sigma\Sigma}^{-1}\underline{\underline{A}}_{\Sigma\pi}\right)$ to be completely computed if desired; since both are banded. Indeed, they can be factored and the local inverses can be directly applied in each CGM or DQGMRES iteration.

3 Numerical Results

The uniformity of the formulas of Eqs.7 to 10 allows the development of very robust codes, since the developments stem from the *original matrix* independently of the problem that motivated it. In this manner, for example, the same code was applied to treat 2-D and 3-D problems; the only routine of the code that had to be changed, when going from one class of problems to the other, was that defining the geometry and that is a very small part of it.
The problems implemented have the form:

$$\begin{aligned} &-\underline{\underline{a}}\nabla^2 u + \underline{b}\cdot\nabla u + cu = f(x) \quad x \in \Omega \\ &u = g(x) \quad x \in \partial\Omega \\ &\Omega = \textstyle\prod_{i=1}^{d}(\alpha_i, \beta_i) \end{aligned} \tag{19}$$

where $a, c > 0$ are constants, $b = (b_1, ..., b_d)$ is a constant vector and $d = 1, 2, 3$. The family of subdomains $\{\Omega_1, ..., \Omega_E\}$ is assumed to be a partition of the set

$\Omega \equiv \{1, ..., N\}$. In the applications we present N is equal to the number of degrees of freedom (*dof*), because we use linear functions and only one of them is associated with each *original* internal node (see, Table 1).

Iteration Table							
				Symmetric Case		Non-Symmetric Case	
Vertices	Subdomains	dof	Primals	Schur	FETI	Schur	FETI
2	4	9	1	2	1	2	1
4	16	225	9	7	7	9	8
6	36	1,225	25	9	9	13	12
8	64	3,969	49	10	10	15	14
10	100	9,801	81	11	11	17	15
12	144	20,449	121	12	11	18	17
14	196	38,025	169	12	12	19	18
16	256	65,025	225	13	12	20	19
18	324	104,329	289	13	13	21	19
20	400	159,201	361	13	13	21	20
22	484	233,289	441	13	14	22	20
24	576	330,625	529	14	14	23	21
26	676	455,625	625	14	14	23	22
28	784	613,089	729	14	14	23	22
30	900	808,201	841	15	14	24	22

Discretization is accomplished using central finite differences and the original problem is then to solve:

$$\widehat{A} \cdot \widehat{u} = \widehat{f} \tag{20}$$

In each domain Ω_α the local matrix $A^{\alpha}_{(i,\alpha),(j,\alpha)}$ is defined as in [8] as:

$$A^{\alpha}_{(i,\alpha)(j,\alpha)} = \frac{1}{m(i,j)} \widehat{A}_{ij} \tag{21}$$

where $m(i,j)$ is the minimum of the multiplicities of i and j. The total matrix A^t then satisfies the criteria:

$$\begin{array}{l} A^t = \sum_{\alpha=1}^{E} A^{\alpha} \\ \widehat{w} \cdot \widehat{A} \cdot \widehat{u} = \tau(\widehat{w}) \cdot A^t \cdot \tau(\widehat{u}) \end{array} \tag{22}$$

The DQGMRES algorithm [10] was implemented for the iterative solution of the non-symmetric problem 19.

4 Conclusions

Paper 1 of this Minisymposium was devoted present an overview of the *multipliers-free domain decomposition methods*, while this Paper 2 presents implementation issues. In Section 2 of the present paper a procedure that permits to develop 100% parallelized algorithms was explained and in Section 3 computational experiments were carried out. The four matrix-formulas that unify the non-overlapping domain decomposition methods and extend them to non-symmetric matrices, Eqs.7 to 10, were applied to symmetric and non-symmetric problems. Through these computational experiments the following features of the *multipliers-free methods* were verified:

1. The very same unifying matrix-formulas are applicable to both symmetric and non-symmetric problems. As a matter of fact, they yield domain decomposition methods that converge nearly as fast for non-symmetric matrices as they do for symmetric ones;
2. Simplified code development;
3. 100% parallelizable algorithms;
4. Very robust codes can be developed. A code was developed that was applied in 2-D and 3-D problems [8][9], something that is not possible when other approaches are used;
5. In the case of symmetric matrices, the rate of convergence of the preconditioned algorithms is at least as good as other state-of-the-art DDMs; and
6. For non-symmetric matrices there is little to compare with, since the literature on DDMs for non-symmetric matrices is relatively limited (see [2], [11]-[15], for some background material on this subject). However, the multipliers-free methods work nearly as efficiently for non-symmetric matrices as they do for symmetric ones.

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