

Natural Factor Based Solvers

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1 Summary

We consider parametric families of partial differential equations–PDEs where the parameter κ modifies only the (1,1) block of a saddle point matrix product of a discretization below. The main goal is to develop an algorithm that removes some of the dependence of iterative solvers on the parameter κ . The algorithm we propose requires only one matrix factorization which does not depend on κ , therefore, allows to reuse it for solving very fast a large number of discrete PDEs for different κ and forcing terms. The design of the proposed algorithm is motivated by previous works on natural factor formulation of the stiffness matrices and their stable numerical solvers. As an application, in two dimensions, we consider an iterative preconditioned solver based on the null space of Crouzeix-Raviart discrete gradient represented as the discrete curl of P_1 conforming finite element functions. For the numerical examples, we consider the case of random coefficient pressure equation where the permeability is modeled by an stochastic process. We note that contrarily from recycling Krylov subspace techniques, the proposed algorithm does not require fixed forcing terms.

2 Introduction

The general form of a saddle point system of linear equations we consider is

$$\begin{bmatrix} D(\kappa)^{-1} & G \\ G^T & 0 \end{bmatrix} \begin{bmatrix} q \\ u \end{bmatrix} = \begin{bmatrix} r \\ b \end{bmatrix}, \quad (1)$$

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where the matrix D is symmetric positive definite. This form is standard in the formulation of mixed finite elements. What is not very well-known, as pointed out by Argyris and Brønlund [1], is that classical conforming and nonconforming finite element methods – FEMs can also be written in the form (1) with $r = 0$; see Section 3 for the case of Crouzeix-Raviart FEM and Section 4 for P_1 conforming FEM. We show that the stiffness matrix, associated to the Crouzeix-Raviart FEM element discretization for the PDE (2) with isotropic coefficients $\kappa(x)$, has the natural factor of the form $A_{CR} = G_{CR}^T D(\kappa) G_{CR}$, where G_{CR} is the discrete gradient (not affected by the parameter κ) and $D(\kappa)$ is a diagonal matrix with entries depending of the integration of κ in each element, hence, it is easy to update the natural factor if κ is modified. Due to the superior numerical stability with respect to roundoff errors when operating with G^T , $D(\kappa)$ and G rather than the assembled stiffness matrix, several works [5, 4, 3, 2] were dedicated in solving the saddle point problem (1) or associated SVD and diagonalization. In Sections 5 and 6 we review some aspects of these works. The methods start by representing q on the range of the matrix $[G \ Z]$ where Z is such that $Q = [G \ Z]$ is a square invertible matrix; two common choices of Z are $Z^T G = 0$ or $Z^T D^{-1} G = 0$. These works generate very stable algorithms for ill-conditioned κ , however, they do not remove the dependence on D of the factorizations, hence, they do not fit our goal of reusing the same factorization for different values of κ . In Section 7 we propose our method, we first use discrete Hodge Laplacian ideas to choose $Z = C_L$ as the curl of P_1 conforming piecewise linear basis functions, hence $G_{CR}^T C_L = 0$. Then we consider the coupled system

$$(\text{grad } u_{CR} + \text{curl } w_{P_1}, \kappa (\text{grad } v_{CR} + \text{curl } v_{P_1}))_{L^2(\Omega)}$$

as a preconditioner for the uncoupled system

$$(\text{grad } u_{CR}, \kappa \text{ grad } v_{CR})_{\kappa} + (\text{curl } w_{P_1}, \kappa \text{ curl } v_{P_1})_{L^2(\Omega)}.$$

3 Crouzeix-Raviart nonconforming finite elements

Consider the heterogeneous diffusion equation

$$\begin{cases} -\partial_1(\kappa(x)\partial_1 u(x)) - \partial_2(\kappa(x)\partial_2 u(x)) = f(x), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases} \quad (2)$$

where $\Omega \subseteq \mathbb{R}^2$ and $\kappa : \Omega \rightarrow \mathbb{R}^+$, $f : \Omega \rightarrow \mathbb{R}$ are given.

In particular, in the target application $\kappa(x)$ is a random field that describes the permeability and allows modeling the lack of data and uncertainties of the problem (e.g., subsurface flow). The forcing term f may also be a random field. In general, in many practical situations we must solve (2) for a large family of coefficients κ and forcing terms f . See Section 8.

Let us introduce a triangulation \mathcal{T}^h of Ω . Discretize (2) by the Crouzeix-Raviart (CR) non-conforming finite element space. Define the CR space \widetilde{V}^{CR} as the space of

all piecewise linear functions with respect to \mathcal{T}^h that are continuous at interior edges midpoints. The degrees of freedom are located in the midpoint of the edges of \mathcal{T}^h . Let $V_{CR} \subseteq \tilde{V}^{CR}$ the subspace of functions in \tilde{V}^{CR} with zero value at the midpoint of boundary edges. The approximation $u_{CR} \in V_{CR}$ of the solution of (2) is the solution of

$$\sum_{T \in \mathcal{T}^h} \int_T \kappa(x) (\partial_1 u_{CR}(x) \partial_1 v(x) + \partial_2 u_{CR}(x) \partial_2 v(x)) dx = \int_{\Omega} f(x) v(x) dx,$$

for all $v \in V^{CR}$. The linear system of the CR approximation is given by

$$A_{CR} u_{CR} = b_{CR}, \quad (3)$$

where $A_{CR} = [a_{ei}^{CR}]_{e,i=1}^{N_e}$ and $b_{CR} = [b_e]_{e=1}^{N_e}$. Here, N_e denotes the number of interior edges of \mathcal{T}^h , $b_e = \int_{\Omega} f(x) \varphi_e^{CR}(x) dx$ and

$$a_{ei}^{CR} = \sum_{T \in \mathcal{T}^h} \int_T \kappa(x) (\partial_1 \varphi_e^{CR}(x) \partial_1 \varphi_i^{CR}(x) + \partial_2 \varphi_e^{CR}(x) \partial_2 \varphi_i^{CR}(x)) dx.$$

Let x_T denote the barycenter of triangle $T \in \mathcal{T}^h$. Piecewise gradients of functions in V^{CR} are piecewise constant vector functions and then

$$a_{ei}^{CR} = \sum_{T \in \mathcal{T}^h} \kappa_T |T| \partial_1 \varphi_e(x_T) \partial_1 \varphi_i(x_T) + \sum_{T \in \mathcal{T}^h} \kappa_T |T| \partial_2 \varphi_e(x_T) \partial_2 \varphi_i(x_T) \quad (4)$$

where κ_T is the average value of $\kappa(x)$ in T . Therefore, we can write (see [1])

$$A_{CR} = G_{CR}^T D G_{CR} = G_{CR,1}^T D_1 G_{CR,1} + G_{CR,2}^T D_2 G_{CR,2}$$

where $G_{CR,l} = [g_{e,T}^{CR,l}]_{N_T \times N_e} = [\sqrt{|T|} \partial_l \varphi_e^{CR}(x_T)]_{N_T \times N_e}$, and N_T denotes the number of triangles in \mathcal{T}^h and $l = 1, 2$. Furthermore, write,

$$D_l = \text{diag}(\kappa_T)_{T \in \mathcal{T}^h}, \quad D = \text{diag}(D_1, D_2) \quad \text{and} \quad G_{CR} = \begin{bmatrix} G_{CR,1} \\ G_{CR,2} \end{bmatrix}_{2N_T \times N_e}. \quad (5)$$

We can write the matrix formulation as

$$G_{CR}^T D G_{CR} u_{CR} = b_{CR}. \quad (6)$$

We see that problem (6) is the Schur complement of the saddle point problem

$$\begin{bmatrix} D^{-1} & G_{CR} \\ G_{CR}^T & 0 \end{bmatrix} \begin{bmatrix} q \\ u_{CR} \end{bmatrix} = \begin{bmatrix} 0 \\ -b_{CR} \end{bmatrix}. \quad (7)$$

4 Conforming finite elements P_1

Let $\tilde{V}^L = P_1(\mathcal{T}^h) = \{v : \Omega \rightarrow \mathbb{R} \mid v|_T \text{ is linear for all } T \in \mathcal{T}^h\} \cap C^0(D)$. The space \tilde{V}^L has a base $\{\varphi_i^L\}_{i=1}^{\tilde{N}_v}$, where \tilde{N}_v is the number of vertices and φ_i^L is the

function that takes value 1 at the i -th node and 0 at the other nodes. Also define $V^L = \tilde{V}^L \cap H_0^1(\Omega)$ and N_v the number of interior vertices.

The approximation u_L of the solution of (2) is: find $u_L \in V^L$ such that

$$\int_{\Omega} \kappa(x) (\partial_1 u_L(x) \partial_1 v(x) + \partial_2 u_L(x) \partial_2 v(x)) dx = \int_{\Omega} f(x) v(x) dx,$$

for all $v \in V^L$, with matrix form $A_L u_L = b_L$, where, $A_L = [a_{ij}^L]_{i,j=1}^{N_v}$ and $b_L = [b_i^L]_{i=1}^{N_v}$ with $b_i^L = \int_D f(x) \varphi_i^L(x) dx$ and $a_{ij}^L = \int_{\Omega} \kappa(x) (\partial_1 \varphi_i^L(x) \partial_1 \varphi_j^L(x) + \partial_2 \varphi_i^L(x) \partial_2 \varphi_j^L(x)) dx$. As before, we have (see [1])

$$A_L = G_L^T D G_L = G_{L,1}^T D_1 G_{L,1} + G_{L,2}^T D_2 G_{L,2}$$

where $G_{L,l} = [g_{e,v}^{L,l}]_{N_T \times N_v} = [\sqrt{|T|} \partial_l \varphi_v^L(x_T)]_{N_T \times N_v}$ and $G_L = \begin{bmatrix} G_{L,1} \\ G_{L,2} \end{bmatrix}_{2N_T \times N_v}$.

We can write the matrix formulation as

$$G_L^T D G_L u_L = b_L, \quad (8)$$

and the corresponding saddle point problem is $\begin{bmatrix} D^{-1} & G_L \\ G_L^T & 0 \end{bmatrix} \begin{bmatrix} q \\ u_L \end{bmatrix} = \begin{bmatrix} 0 \\ -b_L \end{bmatrix}$.

5 The null space method

A method for solving the saddle point problem (1) is called the null space method, see [3]. We split (1) into two equations, $D^{-1}q + Gu = r$ and $G^T q = b$. The null space method consists in finding Z that represents the null space of G^T , $G^T Z = 0$, and such that $[G \ Z]$ is a non-singular square matrix. Therefore, we can change variables to potentials χ and ψ such that

$$q = [G \ Z] \begin{bmatrix} \chi \\ \psi \end{bmatrix} = G\chi + Z\psi. \quad (9)$$

From (9) and $G^T Z = 0$ we have $G^T q = G^T G\chi$ and from $G^T q = b$ we have $b = G^T G\chi$ which gives $\chi = (G^T G)^{-1} b$, that can be pre-computed. On the other hand, from $D^{-1}q + Gu = r$ and (9) we have that $D^{-1}G\chi + D^{-1}Z\psi + Gu = r$ which gives $Z^T D^{-1}Z\psi = Z^T r - Z^T D^{-1}G\chi$ and if we call $c = Z^T r - Z^T D^{-1}G\chi$, we can write the system

$$Z^T D^{-1}Z\psi = c. \quad (10)$$

This is the null space system and it is similar to the Schur complement of (1). See (8).

6 Range null-space hybrid

Now we combine the first equation of (1) and (9). We have $D^{-1}(G\chi + Z\psi) + Gu = r$ which gives $Z\psi + DGu = Dr - G\chi$ and it allows us to write the system ([4, 5])

$$[DG \ Z] \begin{bmatrix} u \\ \psi \end{bmatrix} = Dr - G\chi. \quad (11)$$

We note that the matrix $[DG \ Z]$ is a square matrix and this system is called range space scaled system. The related matrix $[G \ D^{-1}Z]$ is called null space scaled matrix. This algorithm is called “hybrid” because uses both the range-space and the null-space. See [4, 5].

Alternatively, we can write $Z^T(D^{-1}q + Gu) = Z^T r$ which gives $Z^T D^{-1}q = Z^T r$ and together with (9) gives the system

$$\begin{bmatrix} G^T \\ Z^T D^{-1} \end{bmatrix} q = \begin{bmatrix} b \\ Z^T r \end{bmatrix}. \quad (12)$$

Note that matrices (11) and (12) have a dependence on D , however, for numerical stability purpose is very efficient since the matrix is based on discrete gradient times D rather than the assembled second-order derivatives with D .

7 An auxiliary problem and 2×2 systems

Recall that for a scalar w , $\overrightarrow{\text{curl}} w = (\partial_2 w, -\partial_1 w)$ and for a vector $\vec{q} = (q_1, q_2)$, $\text{curl } \vec{q} = \partial_1 q_2 - \partial_2 q_1$. Consider now the elliptic equation

$$\begin{cases} -\text{curl}(\kappa(x)\overrightarrow{\text{curl}} w(x)) = g(x), & x \in \Omega, \\ \kappa(x)\overrightarrow{\text{curl}} w(x) \cdot \tau = 0, & x \in \partial\Omega, \end{cases}$$

where τ is the tangential vector on the boundary of Ω . Note that we have $\text{curl}(\kappa(x)\overrightarrow{\text{curl}} w(x)) = -\partial_1(\kappa(x)\partial_1 w(x)) - \partial_2(\kappa(x)\partial_2 w(x))$ and $\kappa(x)\overrightarrow{\text{curl}} w(x) \cdot \tau = -n_2\kappa(x)\partial_1 w(x) - n_1\kappa(x)\partial_2 w(x) = -\kappa(x)\nabla w(x) \cdot \eta$, where η is the normal vector. We approximate this problem by conforming elements. Let $\tilde{V}^L = P_1(\mathcal{T}^h) = \{v : \Omega \rightarrow \mathbb{R} \text{ such that } v|_T \text{ is linear for all } T \in \mathcal{T}^h\} \cap C^0(\Omega)$. The approximation of the problem above is: Find $\tilde{w}_L \in \tilde{V}^L$ such that

$$\int_{\Omega} \kappa(x)\overrightarrow{\text{curl}} \tilde{w}_L(x) \cdot \overrightarrow{\text{curl}} v(x) dx = \int_{\Omega} g(x)v(x) dx \quad \text{for all } v \in \tilde{V}^L,$$

with additional requirement that $\int_{\Omega} \tilde{w}_L(x) dx = 0$. The matrix form is

$$\tilde{A}_L \tilde{w}_L = \tilde{b}_L,$$

where $\tilde{A}_L = [a_{ij}^L]_{\tilde{N}_v \times \tilde{N}_v}$ and $\tilde{b}_L = [b_i^L]_{\tilde{N}_v \times 1}$ with entries defined by $a_{ij}^L = \int_{\Omega} \kappa(x) \overrightarrow{\text{curl}} \varphi_i^L(x) \cdot \overrightarrow{\text{curl}} \varphi_j^L(x) dx$ and $b_i^L = \int_{\Omega} g(x) \varphi_i^L(x) dx$. Here \tilde{N}_v is the number of vertices in \mathcal{T}^h . As before, we have

$$\tilde{A}_L = \tilde{C}_L^T D \tilde{C}_L = \tilde{G}_{L,2}^T D_1 \tilde{G}_{L,2} + (-\tilde{G}_{L,1})^T D_2 (-\tilde{G}_{L,1})$$

where $\tilde{G}_{L,l} = [g_{e,v}^{L,l}]_{N_T \times \tilde{N}_v} = [\sqrt{|T|} \partial_l \varphi_v^L(x_T)]$ and $\tilde{C}_L = \begin{bmatrix} \tilde{G}_{L,2} \\ -\tilde{G}_{L,1} \end{bmatrix}_{2N_T \times \tilde{N}_v}$. Note

that (u_{CR}, \tilde{w}_L) satisfy the 2×2 system $\begin{bmatrix} A_{CR} & 0 \\ 0 & \tilde{A}_L \end{bmatrix} \begin{bmatrix} u_{CR} \\ \tilde{w}_L \end{bmatrix} = \begin{bmatrix} b_{CR} \\ \tilde{b}_L \end{bmatrix}$.

Denote

$$\hat{A} = \begin{bmatrix} A_{CR} & 0 \\ 0 & \tilde{A}_L \end{bmatrix}, \quad \hat{u} = \begin{bmatrix} u_{CR} \\ \tilde{w}_L \end{bmatrix} \quad \text{and} \quad \hat{b} = \begin{bmatrix} b_{CR} \\ \tilde{b}_L \end{bmatrix} \quad (13)$$

and introduce the matrices $H = [G_{CR} \quad \tilde{C}_L]$ and

$$M = H^T D H = \begin{bmatrix} A_{CR} & G_{CR}^T D \tilde{C}_L \\ \tilde{C}_L^T D G_{CR} & \tilde{A}_L \end{bmatrix}. \quad (14)$$

The preconditioned system is given by

$$M^{-1} \hat{A} \hat{u} = M^{-1} \hat{b}. \quad (15)$$

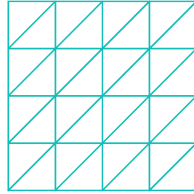


Fig. 1: Triangulation of $D = [0, 1]^2$.

For any planar triangulation (with triangular elements) of a simply connected domain we have $2N_T = N_e + \tilde{N}_v - 1$ (where N_e is the number of interior edges and \tilde{N}_v is the number of vertices). See Figure 1 for the particular case of $\Omega = [0, 1]^2$ and \mathcal{T}^h constructed by dividing Ω into n^2 squares and further dividing each square into two triangles by adding an edge from the left-bottom vertex to right-top one. The following lemma shows that no extra computation is required to obtain basis of null spaces. Also, recall that $G^T G$ is the stiffness matrix of the Laplace operator.

Lemma 1. We have: (a) $H = [G_{CR} \quad \widetilde{C}_L]$ is a square matrix of size $2N_T \times 2N_T$. (b) $G_{CR}^T \widetilde{C}_L = 0$. (c) Because of (b), H is non singular and \widetilde{C}_L spans the kernel of G_{CR}^T . Also G_{CR} spans the kernel of \widetilde{C}_L^T . (d) $M = H^T D H$ is the product of three square matrices. Therefore the solution of $M\widehat{v} = \widehat{r}$ can be computed as $\widehat{v} = H^{-1} D^{-1} H^{-T} \widehat{r}$.

Proof: We prove (b). Let e be an interior edge and v a vertex of \mathcal{T}^h . Then

$$\begin{aligned} (G_{CR}^T \widetilde{C}_L)_{e,v} &= \sum_{T \in \mathcal{T}^h} g_{e,T}^{CR,1} g_{v,T}^{L,2} - \sum_{T \in \mathcal{T}^h} g_{e,T}^{CR,2} g_{v,T}^{L,1} \\ &= \sum_{T \in \mathcal{T}^h} |T| [\partial_1 \varphi_e^{CR}(x_T) \partial_2 \varphi_v^L(x_T) - \partial_2 \varphi_e^{CR}(x_T) \partial_1 \varphi_v^L(x_T)] \\ &= \sum_{T \in \mathcal{T}^h} \int_T \nabla \varphi_e^{CR}(x) \cdot \overrightarrow{\text{curl}} \varphi_v^L(x) dx \\ &= \sum_{T \in \mathcal{T}^h} \int_{\partial T} \varphi_e^{CR}(x) \overrightarrow{\text{curl}} \varphi_v^L(x) \cdot \boldsymbol{\eta} dx = 0. \end{aligned}$$

We have the following condition number bound.

Theorem 1. Let $\kappa_{\min} \leq \kappa(x) \leq \kappa_{\max}$ and $\eta = \kappa_{\max}/\kappa_{\min}$ the contrast. Then $\text{cond}(H^{-1} D^{-1} H^{-T} A) \leq 2\eta - 1$.

Proof: let $s = u_{CR}^T A_{CR} u_{CR} + \widetilde{w}_L^T \widetilde{A}_L \widetilde{w}_L$, using Lemma 1 (b), the result follows from $2|u_{CR}^T G_{CR}^T D \widetilde{C}_L \widetilde{w}_L| = 2|u_{CR}^T G_{CR}^T (D - D(\kappa_{\min})) \widetilde{C}_L \widetilde{w}_L| \leq (1 - 1/\eta)s$.

8 PCG for the block system and numerical experiments

We propose to solve $\widehat{A}\widehat{u} = \widehat{b}$ with \widehat{A} and \widehat{b} defined in (13) with $\widetilde{b}_L = 0$ using PCG with preconditioner M in (14). See (15). Recall that we use the construction in Section 7. For the numerical test we compute an LU or QR factorizations for H and apply $M^{-1} = H^{-1} D^{-1} H^{-T}$. Note that M^{-1} depends on the coefficient κ only through the matrix $D = D(\kappa)$. See (5).

	Condition	Iterations	Contrast
Mean	1.79	7.32	5.65
Variance	0.23	1.46	23.91

Table 1: Condition number, number of iteration and coefficient contrast in the CG method for the Monte Carlo computation of $\widehat{u}(x)$ for (2). The log-coefficient c is given by a truncated KL expansion with $K = 15$ terms with covariance function shown in (16). We use $N = 40$ elements in each direction and $R = 1000$ realizations.

Numerical tests for exponential covariance function. For problem (2) we consider the coefficient κ of the form $\kappa(x, \omega) = e^{c(x, \omega)}$, where the stochastic process c is defined by the Karhunen-Loève expansion with associated covariance function

$$\mathbf{c}(x, x') = \exp\left(-\frac{1}{2} \|x - x'\|^2\right). \quad (16)$$

We approximate the expected value $\bar{u}(x)$ of the solution (2), through Monte Carlo method with R realizations. In Table 1 we show the mean and variance of condition number of the preconditioned system, the number of iterations and the contrast $\max_x \kappa(x, \omega) / \min_x \kappa(x, \omega)$ during the Monte Carlo solve. The small variance in the condition number indicates low dependence of the method on the parameter κ .

Matérn class of covariance functions. Now, the coefficient κ is defined with the Matérn class of covariance functions

$$\mathbf{c}_{\text{Matern}}(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}\|x - x'\|}{l}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}\|x - x'\|}{l}\right) \quad (17)$$

with (probabilistic) parameters $\nu, l > 0$ and K_ν is the modified Bessel function of the second kind. With this function in the KL expansion, we obtain the results in Table 2. In Table 2 we show the dependence of the condition number, number of iteration and coefficient contrast. We note that the small variance of the number of iterations and the value of the condition number indicate that the iteration do not depend much on the parameter $\kappa(x, \omega)$. Additional experiments and results are object of current research and will be presented elsewhere.

	Condition	Iterations	Contrast
Mean	3.07	11.1	11.18
Variance	0.73	1.3	67.28

Table 2: Condition number, iterations numbers and contrast of coefficient κ in the CG method in the Monte Carlo computation of $\bar{u}(x)$ solution of (2). The log-coefficient c given as a truncated KL expansion with $K = 30$ terms constructed from the covariance function shown in (17) with $\nu = 0.5$ and $l = 1$. We use $N = 20$ elements in each direction and $R = 1000$ realizations.

Acknowledgements The authors are grateful to Professor Zlatko Drmac from Univesity of Zagreb for introducing M. Sarkis to the natural factor formulation of the stiffness matrices in finite element computations during our discussions in Rio de Janeiro. J. Galvis thanks partial support from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777778 (MATHROCKS).

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