

A finite difference approach to solve obstacle-type problems using complementarity models

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This paper focuses on elaborating practical finite difference schemes to reduce the computational cost incurred in the construction of large sparse matrices. Our methodology generates a sequence of lower-dimensional vectors to mitigate this cost. In addition, we test our approach on obstacle-type problems in its equivalent version of a complementarity model.

Keywords. Finite difference method, Complementarity models, obstacle problems.

1 Introduction

The finite difference method (FDM) is a numerical technique used to obtain approximate solutions to differential equations, [1]. FDM has a high computational cost because this method replaces the derivatives in the differential equation with finite-difference approximations and leaves a large but finite algebraic system of equations. We employ FDM to solve obstacle-type problems (OTP) [2]; however, we do not solve this problem directly but in its associated complementarity version. Generally, a solution to an optimization problem is the solution to the complementarity problem; however, the converse is not always correct. To validate the reciprocal, deep regularity analyzes are necessary, thus obtaining the equivalence between optimization and complementarity problems. This equivalence facilitates multiple and varied applications, as mentioned in [2, 3].

Our proposal reduces the cost of processing high-dimensional sparse matrices by building them based on a sequence of lower-dimensional vectors. We detail the construction of these vectors in the appendix. In addition, we validate the numerical schemes with two obstacle-type problems, such as the **Porous dam problem** [4] and the **Elastoplastic torsion problem** [5]. We write the Porous Dam problem as a linear complementarity problem. In comparison, the Elastoplastic torsion problem, we formulate as a mixed nonlinear complementarity problem.

Many methods are applied to solve complementarity problems, among which smoothing methods [6], projection methods [7], and interior point algorithms [8] stand out. In particular, Herskovits and Mazonche [8], introduced the FDA-NCP and FDA-MNCP algorithms that solve complementarity problems in simple and mixed versions. FDA-NCP and FDA-MNCP stand out for their versatility and potential to solve problems with high computational costs.

This paper is organized as follows: in Section 2, we introduce the preliminaries related to a basic notation and the complementarity models explored in this paper. A concise finite difference scheme is present in Section 3. In Section 4, we describe two applications in obstacle-type problems. One of them is the porous dam problem, and the other is the elastoplastic torsion problem. Finally, the conclusions are addressed in Section 5, and the Appendix detail the construction of the vectors that formulate our numerical scheme.

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2 Preliminaires

We write \mathbb{R}^m to represent the Euclidean space of dimension m . In particular, $\mathbf{1}_m$ and $\mathbf{0}_m$ are vectors whose all components are ones and zeros, respectively. We write x' to represent the transpose of the vector $x \in \mathbb{R}^m$. Given a vector $x \in \mathbb{R}^m$, we denote $x \geq 0$ to represent a vector where all components are non-negatives. In addition, $\langle x, y \rangle$ represents the usual inner product between the vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$ and $\|x\| = \sqrt{\langle x, x \rangle}$ denote the Euclidean norm of x .

Given the vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$, $x \bullet y$ represents the Hadamard product between them. The space of real matrices of m rows and n columns is denoted by $\mathbb{R}^{m,n}$. Also, $\text{diag}(x) \in \mathbb{R}^{n,n}$ represents the diagonal matrix composed by elements of the vector $x \in \mathbb{R}^n$. We write $X \otimes Y \in \mathbb{R}^{mp,nq}$ to denote the Kronecker product of the matrices $X \in \mathbb{R}^{m,n}$ and $Y \in \mathbb{R}^{p,q}$.

Considering a differentiable application $\mathfrak{F} : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}^m$, we denote by $J_x \mathfrak{F} \in \mathbb{R}^{m,m}$ and $J_y \mathfrak{F} \in \mathbb{R}^{n,m}$ to represent the Jacobian matrices concerning the variables x and y respectively. Furthermore, we present below the complementarity problems used in this paper.

Problem 1 (Nonlinear Complementarity Problem). *Given $\mathfrak{F} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ a differentiable application, the Nonlinear Complementarity Problem consists in determine $x \in \mathbb{R}^m$ such that $x \geq 0$, $\mathfrak{F}(x) \geq 0$ and $x \bullet \mathfrak{F}(x) = 0$.*

Problem 2 (Mixed Nonlinear Complementarity Problem). *Given $\mathfrak{F} : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}^m$ and $\mathfrak{G} : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ differentiable applications, the Mixed Nonlinear Complementarity Problem consists in determine $x \in \mathbb{R}^m$ and $y \in \mathbb{R}^n$ such that $x \geq 0$, $\mathfrak{F}(x, y) \geq 0$, $x \bullet \mathfrak{F}(x, y) = 0$ and $\mathfrak{G}(x, y) = 0$.*

This work applies the FDA-NCP and FDA-MNCP to calculate the solutions to the abovementioned problems. These algorithms generate a sequence of interior points whose limit value is a solution to the complementarity problem. We briefly summarize these algorithms in the next.

Algorithm 1: FDA-NCP

Input: The parameters $\alpha, \beta, \text{tol} \in (0, 1)$ and $\varepsilon > 0$.

Output: A solution to Problem 1.

- **Step 1:** Initialize with $x^0 \in \Omega_\varepsilon = \{x \in \mathbb{R}^m : \phi(x) \leq \varepsilon\}$, where $\phi(x) = \langle x, \mathfrak{F}(x) \rangle$. Assign $x \leftarrow x^k$, $y \leftarrow y^k$ and $k \leftarrow k + 1$.

For each $k = 1, 2, \dots$, follows

- **Step 2:** Compute the vector $d^k \in \mathbb{R}^m$ by solving

$$[\text{diag}(\mathfrak{F}(x)) + \text{diag}(x)J_x \mathfrak{F}] d^k = [-x \bullet \mathfrak{F}(x, y) + \alpha \cdot \mathbf{1}_m].$$

- **Step 3** Obtain the first element $\beta^* \in \{1, \beta, \beta^2, \dots\}$ such that

$$x + \beta^* d_x^k \geq 0 \quad , \quad \mathfrak{F}(x + \beta^* d_x^k) \geq 0 \quad \text{and} \quad \phi(x + \beta^* d_x^k) \leq \varepsilon.$$

- **Step 4:** Assign $x \leftarrow x + \beta^* d_x^k$. If $\phi(x) \leq \text{tol}$ then x is a solution to Problem 1, otherwise, return to **Step 2**.
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Algorithm 2: FDA-MNCP

Input: The parameters $\alpha, \beta, \text{tol} \in (0, 1)$ and $\varepsilon > 0$.

Output: A solution to Problem 2.

- **Step 1:** Initialize with $(x^0, y^0) \in \Omega_\epsilon = \{(x, y) \in \mathbb{R}^m \times \mathbb{R}^n : \phi(x) \leq \epsilon\}$, where $\phi(x, y) = \langle x, \mathfrak{F}(x, y) \rangle + \|\mathfrak{G}(x, y)\|^2$. Assign $x \leftarrow x^k, y \leftarrow y^k$ and $k \leftarrow k + 1$.

For each $k = 1, 2, \dots$, follows

- **Step 2:** Compute the vector $d^k = \begin{bmatrix} d_x^k \\ d_y^k \end{bmatrix} \in \mathbb{R}^{n+m}$ by solving

$$\begin{bmatrix} \text{diag}(\mathfrak{F}(x, y)) + \text{diag}(x)J_x\mathfrak{F} & \text{diag}(x)J_y\mathfrak{F} \\ J_x\mathfrak{G} & J_y\mathfrak{G} \end{bmatrix} d^k = \begin{bmatrix} -x \bullet \mathfrak{F}(x, y) + \alpha \cdot \mathbf{1}_m \\ -\mathfrak{G}(x, y) \end{bmatrix}.$$

- **Step 3** Obtain the first element $\beta^* \in \{1, \beta, \beta^2, \dots\}$ such that

$$x + \beta^* d_x^k \geq 0, \quad \mathfrak{F}(x + \beta^* d_x^k, y + \beta^* d_y^k) \geq 0 \quad \text{and} \quad \phi(x + \beta^* d_x^k, y + \beta^* d_y^k) \leq \varepsilon.$$

- **Step 4:** Assign $x \leftarrow x + \beta^* d_x^k$ and $y \leftarrow y + \beta^* d_y^k$. If $\phi(x, y) \leq \text{tol}$ then (x, y) then is a solution to Problem 2 otherwise, return to **Step 2**.
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3 Finite difference schemes

Given $\Omega = \{(x, y) \in \mathbb{R}^2 : a \leq x \leq b \text{ and } c \leq y \leq d\}$ and $u : \Omega \rightarrow \mathbb{R}, u = 0, \forall (x, y) \in \partial\Omega$. We write N to represents the number of sub-intervals in $[a, b]$ and $[c, d]$ and $U_{i,j}$ to represent approximate value of $u(x_i, y_j), \forall i, j = 0, \dots, N + 1$. Using the boundary condition, we obtain $U_{0,i} = U_{N+1,i} = U_{i,0} = U_{i,N+1} = 0, \forall i = 0, \dots, N + 1$. Finally, we employ FDM to obtain a numerical scheme to Laplacian and gradient vector norm as functions of $M = N^2$ variables.

$$\Delta u(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} + \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{k^2}, \quad (1)$$

$$\|\nabla u(x_i, y_j)\| \approx \sqrt{\left(\frac{U_{i+1,j} - U_{i-1,j}}{2h}\right)^2 + \left(\frac{U_{i,j+1} - U_{i,j-1}}{2k}\right)^2}, \quad (2)$$

where $h = \frac{b-a}{N+1}$ and $k = \frac{d-c}{N+1}$. We order these variables row by row, starting with $U_{1,1}, \dots, U_{N,1}$, continuing with $U_{1,2}, \dots, U_{N,2}$, until we complete $U_{1,N}, \dots, U_{N,N}$ and define a new variable, so it depends on only one index, by the form $U^\ell = U_{i,j}$, whenever $i = \frac{\ell-j}{N} + 1$ and $j = \ell \bmod N$. Denoting $U = [U^1, \dots, U^M]' \in \mathbb{R}^M$, we write (1) and (2), in a more concise form

$$\begin{bmatrix} \Delta u(x_1, y_1) \\ \vdots \\ \Delta u(x_N, y_N) \end{bmatrix} \approx \mathcal{P}U \quad \text{and} \quad \begin{bmatrix} \|\nabla u(x_1, y_1)\| \\ \vdots \\ \|\nabla u(x_N, y_N)\| \end{bmatrix} \approx \sqrt{(\mathcal{Q}U) \bullet (\mathcal{Q}U) + (\mathcal{R}U) \bullet (\mathcal{R}U)}, \quad (3)$$

where \mathcal{P}, \mathcal{Q} and \mathcal{R} are square matrices of dimension M , define by

$$\mathcal{P} = \sum_{\ell=1}^M e(\ell) \otimes \left(\frac{1}{h^2} a'(\ell) + \frac{1}{k^2} b'(\ell)\right), \quad \mathcal{Q} = \sum_{\ell=1}^M \frac{1}{2h} e(\ell) \otimes c'(\ell), \quad \text{and} \quad \mathcal{R} = \sum_{\ell=1}^M \frac{1}{2k} e(\ell) \otimes d'(\ell).$$

The computations of these matrices are detailed in the appendix.

4 Applications

In this section, we illustrate our propose with two obstacle-type problems.

4.1 Porous dam problem

This problem focuses on the filtration of liquids through a rectangular porous dam between two different heights reservoirs. This problem focuses on the filtration of liquids through a rectangular porous dam between two different heights reservoirs. This problem aims to determine the curve that limits the wet and dry areas. In [4], the construction of this problem as a simple complementarity model was presented in detail.

Application 1. Given $\Omega = \{(x, y) \in \mathbb{R}^2 : 0 \leq x \leq L \text{ and } 0 \leq y \leq H_1, 0 < H_0 < H_1\}$, the Porous Dam problem consists in determine $u : \Omega \rightarrow \mathbb{R}$ such that

$$-\Delta u \geq 1, \text{ in } \Omega, \quad u \geq 0, \text{ in } \Omega, \quad (-\Delta u + 1) \cdot u = 0, \text{ in } \Omega \quad \text{and} \quad u = g, \text{ on } \partial\Omega, \quad (4)$$

where

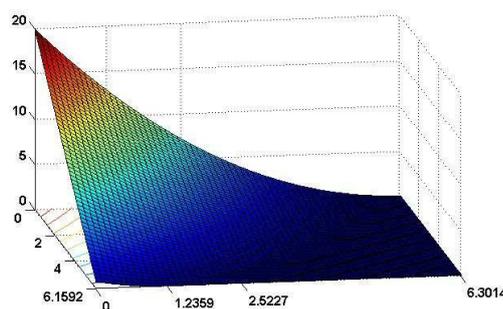
$$g(x, y) = \begin{cases} \frac{x}{2L}(H_0 - y)^2 + \frac{L-x}{2L}(H_1 - y)^2 & , 0 \leq y \leq H_0, \\ \frac{L-x}{2L}(H_1 - y)^2 & , H_0 \leq y \leq H_1. \end{cases}$$

Also, the wet region is $\Omega_{wet} = \{(x, y) \in \mathbb{R}^2 : y \leq \varphi(x)\}$, where $\varphi : [0, L] \rightarrow \mathbb{R}$ is a decreasing function such that $\varphi(0) = H_1$ and $\varphi(L) > H_0$.

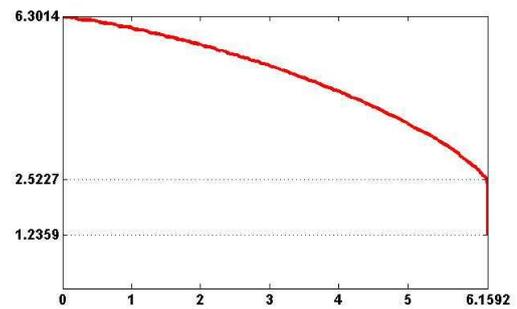
Let the parameters $H_1 = 6,3014$, $H_0 = 1,2359$ and $L = 6,1592$, we write (4) as Problem 1 and define $\mathfrak{F} : \mathbb{R}^M \rightarrow \mathbb{R}^M$ by

$$\mathfrak{F}(x) = -\mathcal{P}x + \mathbf{1}_M. \quad (5)$$

Considering $N = 50$, and consequently $M = 2500$, we replace this value in (5) to apply FDA-NCP and obtain a numerical solution of Application 1. In Figure 1(a) we show the function $u : \Omega \rightarrow \mathbb{R}$, and Figure 1(b) illustrates the function $\varphi : [0, L] \rightarrow \mathbb{R}$ that separates the wet and dry regions.



(a) Representation of the function $u : \Omega \rightarrow \mathbb{R}$.



(b) Representation of the curve φ that separate the dry region with flow region of Ω .

Figure 1: Numerical solution of (4) with $H_0 = 6,3014$, $H_1 = 1,2359$, $L = 6,1592$ and $M = 2500$.

4.2 Elastoplastic torsion problem

Considering an isotropic and homogeneous elastic cylinder with a cross-section subject to a torsion applied at the ends and the lateral boundary stress-free. After applying torque, the resulting configuration separates the cross-section into an elastic and plastic region. The objective of this problem is to determine these regions.

Application 2. Considering $\Omega \subset \mathbb{R}^2$ and γ plasticity coefficient according to the material, the Elastoplastic torsion problem consists in determine $u : \Omega \rightarrow \mathbb{R}$ such that

$$-\Delta u - \tau \geq 0, \text{ in } \Omega, \quad \gamma - \|\nabla u\| \geq 0, \text{ in } \Omega \quad \text{and} \quad (-\Delta u - \tau)(\gamma - \|\nabla u\|) = 0, \text{ in } \Omega. \quad (6)$$

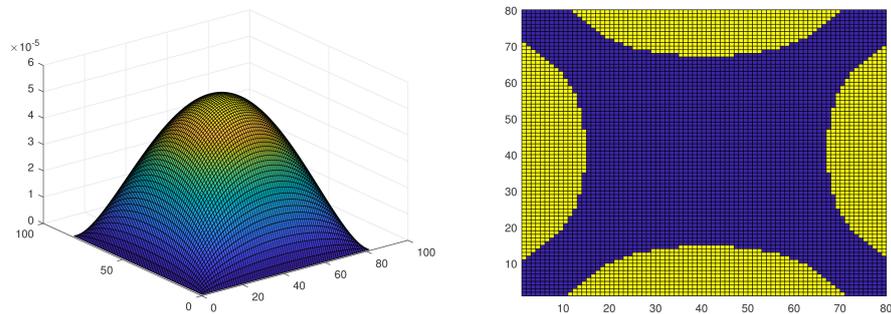
Also, the elastic and plastic regions are denoted by Ω_E and Ω_P , and defined as follows:

$$\begin{aligned} \Omega_E &= \{(x, y) \in \Omega : \|\nabla u(x, y)\| < \gamma\}, \\ \Omega_P &= \{(x, y) \in \Omega : \|\nabla u(x, y)\| = \gamma\}. \end{aligned}$$

Let $\Omega =]0, 1[\times]0, 1[$, $\gamma = 1$ and $\tau = 5$, we formulate (6) as Problem 2, and define $\mathfrak{F} : \mathbb{R}^M \rightarrow \mathbb{R}^M$ and $\mathfrak{G} : \mathbb{R}^M \rightarrow \mathbb{R}^M$ as follows

$$\begin{aligned} \mathfrak{F}(x, y) &= \gamma \cdot \mathbf{1}_M - \sqrt{(\mathcal{Q}y) \bullet (\mathcal{Q}y) + (\mathcal{R}y) \bullet (\mathcal{R}y)}, \\ \mathfrak{G}(x, y) &= -x - \mathcal{P}y - \tau \cdot \mathbf{1}_M. \end{aligned} \quad (7)$$

We use FDA-MNCP with $M = 6400$ to obtain the numerical solution of (6), see Figure 2(a). While in Figure 2(b) we illustrate the plastic region and elastic region.



(a) Representation of the function $u : \Omega \rightarrow \mathbb{R}$. (b) Representation of plastic region Ω_P (blue) and elastic region Ω_E (yellow).

Figure 2: Numerical solution of (6) with $\gamma = 1$, $\tau = 5$, $\Omega = [0, 1] \times [0, 1]$ and $M = 6400$.

5 Conclusions

We propose a practical and versatile finite difference scheme to solve numerically obstacle-type problems in their version of complementarity. This approach determines the differentiable applications \mathfrak{F} and \mathfrak{G} computed in terms of matrices of high dimensions. However, we use a sequence of lower-dimensional vectors to mitigate this computational cost caused by the increased memory used when defining these matrices of high dimensions. Our approach makes the FDA-NCP and FDA-MNCP more robust and efficient.

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Appendix

First, we write $e_k(\ell) = 1$ whenever $k = \ell$, otherwise $e_i(\ell) = 0$. For each $\ell = 1, \dots, M$, we obtain the vector $a(\ell)$, $b(\ell)$, $c(\ell)$, and $d(\ell)$, as follows:

- If $\ell = 1$ then $c_{\ell+1}(\ell) = 1$, $c_k(\ell) = 0$, $\forall k \neq \ell + 1$, $d_{\ell+N}(\ell) = 1$, and $d_k(\ell) = 0$, $\forall k \neq \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell = N$ then $c_{\ell-1}(\ell) = -1$, $c_k(\ell) = 0$, $\forall k \neq \ell - 1$, $d_{\ell+N}(\ell) = 1$, and $d_k(\ell) = 0$, $\forall k \neq \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell = M - N + 1$ then $c_{\ell+1}(\ell) = 1$, $c_k(\ell) = 0$, $\forall k \neq \ell + 1$, $d_{\ell-N}(\ell) = 1$, and $d_k(\ell) = 0$, $\forall k \neq \ell - N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell = M$ then $c_{\ell-1}(\ell) = -1, c_k(\ell) = 0, \forall k \neq \ell - 1, d_{\ell-N}(\ell) = -1, d_k(\ell) = 0, \forall k \neq \ell - N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell \in \{2, 3, \dots, N - 1\}$ then $c_{\ell-1}(\ell) = -1, c_{\ell+1}(\ell) = 1, c_k(\ell) = 0, \forall k \neq \ell - 1, \ell + 1, d_{\ell+N}(\ell) = 1, \text{ and } d_k(\ell) = 0, \forall k \neq \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell \in \{rN + 1, r = 1, \dots, N - 2\}$ then $c_{\ell+1}(\ell) = 1, c_k(\ell) = 0, \forall k \neq \ell + 1, d_{\ell-N}(\ell) = -1, d_{\ell+N}(\ell) = 1, \text{ and } d_k(\ell) = 0, \forall k \neq \ell - N, \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ -1 & , k = \ell - N \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell \in \{rN, r = 2, \dots, N - 1\}$ then $c_{\ell-1}(\ell) = -1, c_k(\ell) = 0, \forall k \neq \ell - 1, d_{\ell-N}(\ell) = -1, d_{\ell+N}(\ell) = 1, \text{ and } d_k(\ell) = 0, \forall k \neq \ell - N, \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ -1 & , k = \ell - N \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

- If $\ell \in \{M - N + r, r = 2, \dots, N - 1\}$ then $c_{\ell-1}(\ell) = -1, c_{\ell+1}(\ell) = 1, c_k(\ell) = 0, \forall k \neq \ell - 1, \ell + 1, d_{\ell-N}(\ell) = -1, \text{ and } d_k(\ell) = 0, \forall k \neq \ell - N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - N \\ 0 & , \text{otherwise} \end{cases}$$

- For internal points, $c_{\ell-1}(\ell) = -1, c_{\ell+1}(\ell) = 1, c_k(\ell) = 0, \forall k \neq \ell - 1, \ell + 1, d_{\ell-N}(\ell) = -1, d_{\ell+N}(\ell) = 1, \text{ and } d_k(\ell) = 0, \forall k \neq \ell - N, \ell + N$. Also,

$$a_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - 1 \\ 1 & , k = \ell + 1 \\ 0 & , \text{otherwise} \end{cases} \quad \text{and} \quad b_k(\ell) = \begin{cases} -2 & , k = \ell \\ 1 & , k = \ell - N \\ 1 & , k = \ell + N \\ 0 & , \text{otherwise} \end{cases}$$

Finally,

$$\mathcal{P} = \sum_{\ell=1}^M e(\ell) \otimes \left(\frac{1}{h^2} a'(\ell) + \frac{1}{k^2} b'(\ell) \right), \quad \mathcal{Q} = \sum_{\ell=1}^M \frac{1}{2h} e(\ell) \otimes c'(\ell), \quad \text{and} \quad \mathcal{R} = \sum_{\ell=1}^M \frac{1}{2k} e(\ell) \otimes d'(\ell).$$