



# Hierarchical Matrices and Inexact GMRES

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# Chapter 1

## Iterative Methods and Krylov's Subspace

### 1.1 Iterative Methods and motivation

Iterative methods appear as an alternative to direct solution methods, where the direct solution to a problem usually scales with  $\mathcal{O}(m^3)$  complexity, where  $m$  is the dimension of the input matrix. Since larger matrices are usually employed in practise, the direct algorithms become inefficient and a more reliable approach is desired.

The idea of the iterable methods is to find, after a certain number of iterations, a sequence  $x_k$  that converges to  $x$ , the exact solution of the problem 1.1, all while making the large-scale computations faster, i.e. obtaining a complexity smaller than  $\mathcal{O}(m^3)$ , and keeping a maximum tolerance between the iterable solution and the exact one.

$$x = \lim_{k \rightarrow \infty} x_k \quad (1.1)$$

The method stops after  $k$  iterations, where  $x_k$  is the first element of the sequence to satisfy the condition 1.2.

$$\frac{\|x_k - x\|}{\|x\|} \leq \epsilon \quad (1.2)$$

Where  $\epsilon$  is a tolerance defined by who is applying the algorithm.

Usually  $x$  isn't known, so 1.2 gets modified for 1.3, where  $A$  is the system's matrix and  $b$  is the RHS(right hand side).

$$\frac{\|Ax_k - b\|}{\|b\|} \leq \epsilon \quad (1.3)$$

The first iterative methods used a decomposition of  $A$  as a combination of two matrices 1.4, where  $A_1$  isn't singular, and each iteration is defined as 1.5.

$$A = A_1 - A_2 \quad (1.4)$$

$$A_1 x_{k+1} = b + A_2 x_k \quad (1.5)$$

With a substitution of the others  $x_k$ , 1.5 gives 1.6, which converges for every initial solution if and only iff  $\rho(A_2 A_1^{-1}) < 1$ , or  $\rho(X)$  is the spectral radius of  $X$  [5].

$$x_{k+1} = A_1^{-1}(b + A_2 x_k) = A_1^{-1}(b + A_2 A_1^{-1}(b + A_2 x_{k-1})) \dots = A_1^{-1} \left[ \sum_{i=0}^k (A_2 A_1^{-1})^i b \right] \quad (1.6)$$

If  $A_1 = I$  and  $A_2 = I - A$  in 1.4, the sequence found in 1.6 is:  $x_1 = b, x_2 = 2b - Ab, x_3 = 3b - 3Ab + A^2 b, \dots$

Even if the condition  $\rho(A - I) \leq 1$  is strong [5], it shows that one approximation  $x_k$  could be represented as 1.7.

$$x_k \in \text{span}(b, Ab, A^2 b, \dots, A^{k-1} b) \quad (1.7)$$

## 1.2 Krylov's Subspace

Be  $A \in \mathbb{K}^{n \times n}$  a matrix and  $b \in \mathbb{K}^n$ . To each  $k \leq n$  the Krylov's Subspace  $\mathcal{K}_k = \mathcal{K}_k(A, b)$  associated to  $A, b$  is defined as 1.8.

$$\mathcal{K}_k(A, b) = \text{span}(b, Ab, A^2 b, \dots, A^{k-1} b) \quad (1.8)$$

These Subspaces also have the following property:  $k < l \rightarrow \mathcal{K}^k \subset \mathcal{K}^l$  [5].

The subspace  $\mathcal{K}_k(A, b)$  is also the subspace of all the vectors from  $\mathbb{R}^m$  which could be written as  $x = p(A)b$ , where  $p(A)$  is a polynom of degree less than  $k - 1$  which  $p(0) = 1$ .

The problem with using  $A^k b, k \in 0, 1, 2, \dots$  as a base comes from the fact that successive products of  $A$  make vectors that are *approximately colinear*, since those are really close of the eigenvector with the largest eigenvalue of  $A$ .

## 1.3 Arnoldi's Method

With the task of obtaining an orthonormal basis to  $\mathcal{K}_k(A, b)$ , the method searches for a unitary matrix  $Q$  for which the expression 1.9 is valid.  $H_k = h_{ij}$  is an Hessenberg's matrix.

$$AQ_k = Q_{k+1} H_k \quad (1.9)$$

For each column-vector of  $Q$ ,  $q_i$ , 1.9 could be written as 1.10, where the representation of  $\mathcal{K}_k(A, b)$  with an orthonormal basis becomes more evident. In a pratical application,  $Q$  is initialized with  $q_1 = \frac{b}{\|b\|}$ .

$$Aq_m = h_{1m} q_1 + h_{2m} q_2 + \dots h_{m+1,m} q_{m+1} \quad (1.10)$$

An algorithm for the method can be found in 1.

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**Algorithm 1** Arnoldi's iteration
 

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```

1:  $A \in \mathbb{K}^{n \times n}$  et  $b \in \mathbb{K}^n$ 
2:  $x = 0, \beta = \|b\|, q_1 = \frac{b}{\beta}$ 
3: for  $j = 1, 2, \dots, k$  do
4:    $q_{j+1} = Aq_j$ 
5:   for  $i = 1, 2, \dots, j$  do
6:      $h_{ij} = q_{j+1}^t q_i$ 
7:      $q_{j+1} = q_{j+1} - h_{ij}q_i$ 
8:   end for
9:    $h_{j+1,j} = \|q_{j+1}\|$ 
10:   $q_{j+1} = \frac{q_{j+1}}{h_{j+1,j}}$ 
11: end for

```

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## Chapter 2

# GMRES

A projection in  $\mathcal{K}_k(A, b)$ , where the different approximations are taken as in 2.1, where  $Q_m$  is the vector in 1.9.

$$x = x_0 + Q_m y \quad (2.1)$$

With 2.1 and 1.9 the residual becomes 2.2, where  $x_0 = 0$ ,  $\beta = \|b\|$  and  $Q_{m+1}^t b = (\|b\| \ 0 \ 0 \dots)^t$  since the columns of  $Q_{m+1}$  are orthonormal vectors and  $q_1 = \frac{b}{\|b\|}$ .

$$\begin{aligned} r(y) &= \|b - Ax\| \\ &= \|b - A(Q_m y)\| \\ &= \|b - Q_{m+1} H_m y\| \\ &= \|Q_{m+1} (Q_{m+1}^t b - H_m y)\| \\ &= \|\beta e_1 - H_m y\| \end{aligned} \quad (2.2)$$

Thus,  $y$  which appears in 2.1, is found as the solution of the residual's minimisation problem in 2.2.

$$y = \min_y \|\beta e_1 - H_m y\| \quad (2.3)$$

An initial version of the GMRES is in 2. The lines 4 to 12 bring the Arnoldi's Method presented in 1.

However, 2 doesn't bring an efficient way of finding the residual in each iteration. To solve this problem and also to find a more efficient way of solving the least squares problem in 2.3, a transformation is applied to  $H_m$ , turning it into a triangular matrix.

### 2.1 Givens's Rotation

Givens's operator,  $G(i, i+1)$ , is a unitary matrix such that the column vector  $a = Gb$  has the elements  $a(i) = r \in \mathbb{R}$  and  $a(i+1) = 0$ . It has a structure as in 2.4. The coefficients  $c_i, s_i$  only appear in the rows  $i$  et  $i+1$ .

**Algorithm 2** Initial GMRES

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```

1:  $A \in \mathbb{K}^{n \times n}$  and  $b \in \mathbb{K}^n$ 
2:  $x = 0, \beta = \|b\|, q_1 = \frac{b}{\beta}$ 
3: for  $k = 1, 2, \dots$  do
4:   for  $j = 1, 2, \dots, k$  do
5:      $q_{j+1} = Aq_j$ 
6:     for  $i = 1, 2, \dots, j$  do
7:        $h_{ij} = q_{j+1}^t q_i$ 
8:        $q_{j+1} = q_{j+1} - h_{ij} q_i$ 
9:     end for
10:     $h_{j+1,j} = \|q_{j+1}\|$ 
11:     $q_{j+1} = \frac{q_{j+1}}{h_{j+1,j}}$ 
12:  end for
13:  Find  $y = \min_y \|\beta e_1 - H_m y\|$ 
14:   $x = Q_k y$ 
15:  Stop if the residual is smaller than the tolerance
16: end for

```

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$$G(i, i+1) = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c_i & s_i & & \\ & & & -s_i & c_i & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{bmatrix} \quad (2.4)$$

This operator offers a way to transform the columns in  $H_m$ , *zeroing* the elements outside the main diagonal. Since a product of unitary operators is still unitary, 2.3 can be written as 2.5, where  $R_m$  and  $g_m$  are the results from the application of multiple Givens's operators to  $H_m$  and  $\beta e_1$ .

$$y = \min_y \|\beta e_1 - H_m y\| = \min_y \|g_m - R_m y\| \quad (2.5)$$

Thus, the new problem 2.5 can be solved with a simple backwards substitution. If  $g_m = [\gamma_1 \dots \gamma_{m+1}]^t$ , a  $m+1$  column vector, and  $\{R_m\}_{ij} = r_{ij}$  a  $m+1$  by  $m$  upper triangular matrix with  $r_{ii} \neq 0$  and its last row filled with zeros, each element of  $y_m = [y_1 \dots y_m]$  is given by 2.6.

$$\begin{aligned} \gamma_k &= \sum_{i=k}^m r_{ki} y_i \\ y_m &= \frac{\gamma_m}{r_{mm}} \\ y_i &= \frac{1}{r_{ii}} \left( \gamma_i - \sum_{j=i+1}^m r_{ij} \gamma_j \right) \end{aligned} \quad (2.6)$$

A simple algorithm to this end can be written as 3.

**Algorithm 3** Backwards substitution

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```

1:  $A \in \mathbb{K}^{n \times n}, \{A\}_{ij} = a_{ij}$  and  $b \in \mathbb{K}^n$ 
2: for  $k = n, n-1, \dots$  do
3:    $y_k = b_k$ 
4:   for  $j = n, n-1, \dots, k+1$  do
5:      $y_k = y_k - a_{kj}y_j$ 
6:   end for
7:    $y_k = \frac{y_k}{a_{kk}}$ 
8: end for

```

---

It can be shown that  $g_m$  also contains the residual of each iteration [7]. Since it's a  $m+1$  column vector, we have, with  $\Omega_m$  being the necessary Givens's Rotations to make  $H_m$  upper triangular 2.7.

$$\begin{aligned} \|b - Ax_m\| &= \|Q_{m+1}^t(\beta e_1 - H_m y_m)\| \\ \|\beta e_1 - H_m y_m\| &= \|\Omega_m^t(g_m - R_m y_m)\| \end{aligned} \quad (2.7)$$

Since  $y_m$  is a solution to the system, the norm in 2.7 is defined by  $\|\gamma_{m+1} - (R_m)_{m+1,1:m} y_m\|$ . But since the last row in  $R_m$  is composed by zeros, we have that  $\|b - Ax_m\| = |\gamma_{m+1}|$ , which gives a more efficient way to obtain the residuals during each iteration.

## 2.2 Inexact GMRES

The heaviest part in the code is in the matrix-vector product 1, line 4. Therefore, one approach to accelerate the iterations involves an approximation of  $Aq$ , instead of using the exact answer, as shown in 2.8.

$$\mathcal{A}q = (A + E)q \quad (2.8)$$

Where  $E$  in 2.8 is a *perturbation matrix* that changes with each iteration and will be written as  $E_k$  for iteration  $k$ .

When the inexact matrix-vector product is the one being made, the left side of 1.9 must be changed by 2.9.

$$\begin{aligned} [(A + E_1)q_1, (A + E_2)q_2, \dots, (A + E_k)q_k] &= Q_{k+1}H_k \\ (A + \mathcal{E}_k)Q_k &= Q_{k+1}H_k, \quad \mathcal{E}_k = \sum_{i=1}^k E_i q_i q_i^t \\ \mathcal{A}Q_k &= W_k \end{aligned} \quad (2.9)$$

Where  $W_m = Q_{m+1}H_m$  from this point forward.

Now the subspace spanned by the vectors of  $Q_k$  is not the Krylov's subspace  $\mathcal{K}_k(A, b)$ , but these are still orthonormal. To see what kind of subspace our new  $Q$  spans, 2.9 is looked into in 2.10.



$$(A + E_k)q_k = \mathcal{A}_k q_k = h_{1,k}q_1 + h_{2,k}q_2 + \dots + h_{k+1,k}q_{k+1} \quad (2.10)$$

For  $k = 1$ , we have that  $q_2$  is a combination of the vectors  $\mathcal{A}_1 b$  and  $b$  (since  $q_1 = b$ ). For  $k = 2$  we see that  $q_3$  is a combination that involves  $\mathcal{A}_2 \mathcal{A}_1 b$  and so forth.

Expression 2.9 then shows that  $Q_k$  becomes a basis for a new Krylov's subspace,  $\mathcal{K}_k(A + \mathcal{E}_k, b) = \text{span}\{b, \mathcal{A}_1 b, \dots, \mathcal{A}_k \dots \mathcal{A}_1 b\}$ , made by a large perturbation in  $A$ , that gets updated in each iteration.

A new distinction should also be made between the two types of residuals appearing in the process:  $r_k$ , the exact residual of an iteration, and  $\tilde{r}_k$ , the one that will really be calculated. A detailed definition for both and a measure of how distant they are is in 2.11.

$$\begin{aligned} r_k &= r_0 - A Q_k y_k \\ &= r_0 - (Q_{k+1} H_k - [E_1 q_1, \dots, E_k q_k]) y_k \\ &= \tilde{r}_k + [E_1 q_1, \dots, E_k q_k] y_k \\ \rightarrow \delta_k &= \|r_k - \tilde{r}_k\| = \|[E_1 q_1, \dots, E_k q_k] y_k\| \end{aligned} \quad (2.11)$$

Considering  $y_k = [\eta_1^{(k)} \dots \eta_n^{(k)}]$ , upper index to clarify the iteration, an upper bound for  $\delta_k$  can be found, but before we go through 2.12.

$$\begin{aligned} \|[E_1 q_1, \dots, E_k q_k] y_k\| &= \left\| \sum_{i=1}^k E_i q_i \eta_i^{(k)} \right\| \\ \left\| \sum_{i=1}^k E_i q_i \eta_i^{(k)} \right\| &\leq \sum_{i=1}^k \|E_i\| \|q_i \eta_i^{(k)}\| \\ \left\| \sum_{i=1}^k E_i q_i \eta_i^{(k)} \right\| &\leq \sum_{i=1}^k \|E_i\| |\eta_i^{(k)}| \end{aligned} \quad (2.12)$$

Where the fact that  $q_i$  are unitary was used between the last two lines. The bound on  $\delta_k$  is then found in 2.13.

$$\delta_k = \|r_k - \tilde{r}_k\| \leq \sum_{i=1}^k \|E_i\| \|\eta_i^{(k)}\| \quad (2.13)$$

2.13 tells us that in order to keep both residuals close, either the perturbation of  $A$ , somewhat measured by  $\|E_i\|$ , or the elements of  $y_i$  should be kept small. Since we expect to use more *relaxed* approximations of  $A$  as the iterations go on, a greater tolerance in  $E_k$  could be compensated with a sufficiently small  $y_k$ .

The problem is  $y_k$  is only found after the construction of  $E_k$ , so an upper bound must be also found for its value.

Knowing  $y_k$  is the solution of the minimization of  $\|H_k y_k - e_1 \beta\|$ , we consider  $\Omega_k = G(k, k+1)G(k-1, k) \dots G(1, 2)$  where each  $G$  represents a Givens rotation as shown in 2.4, so  $\Omega_k$  is the matrix that

transforms  $H_k$  into an upper triangular matrix.

The application of  $\Omega_k$  in either side of  $H_k y_k = e_1 \beta$  gives us 2.14.

$$\begin{aligned}\Omega_k H_k y_k &= \Omega_k e_1 \beta \\ R_k y_k &= g_k \\ y_k &= R_k^{-1} g_k\end{aligned}\tag{2.14}$$

Since  $R_k$ , the transformation of a Hessenberg matrix by a series of Givens rotations, is upper triangular, then its inverse also is. Being an upper triangular matrix, the first  $i - 1$  elements of its  $i$ th line are zeros, so using Matlab index notation in 2.15

$$(R_k^{-1})_{i,1:k}(g_k)_{1:k} = (R_k^{-1})_{i,i:k}(g_k)_{i:k}\tag{2.15}$$

Using this last result in 2.14 gives 2.16.

$$\begin{aligned}|\eta_i^{(k)}| &= \|(R_k^{-1})_{i,i:k}(g_k)_{i:k}\| \\ |\eta_i^{(k)}| &\leq \|e_k R_k^{-1}\| \|(g_k)_{i:k}\| \\ |\eta_i^{(k)}| &\leq \|e_k R_k^{-1}\| \|(g_k)_{i:k}\|\end{aligned}\tag{2.16}$$

Since  $\|e_k R_k^{-1}\| \leq \|R_k^{-1}\| = \sigma_k(H_k)^{-1}$  and  $\|(g_k)_{i:k}\| \leq \|\tilde{r}_{i-1}\|$  [8], the bound is given by 2.17.

$$\|\eta_i^{(k)}\| \leq \frac{1}{\sigma_k(H_k)} \|\tilde{r}_{i-1}\|\tag{2.17}$$

Putting 2.17 in 2.13 gives the results in 2.18. Setting  $\delta_k \leq \epsilon$  and determining a bound for each  $\|E_i\|$  gets us 2.19.

$$\delta_k \leq \sum_{i=1}^k \frac{\|E_i\|}{\sigma_k(H_k)} \|\tilde{r}_{i-1}\|\tag{2.18}$$

$$\|E_i\| \leq \frac{\sigma_k(H_k) \epsilon}{k \|\tilde{r}_{i-1}\|}\tag{2.19}$$

Since  $H_k$  is also one of the matrices being constructed throughout the method, a workaround is necessary to apply find these bounds in a practical situation. Either using an estimation of  $\sigma_k(H_k)$  with the singular values of  $A$  or grouping all uncalculated terms in a  $\ell_k$  that will be estimated empirically [8], obtaining 2.20.

$$\|E_i\| \leq \ell_k \frac{1}{\|\tilde{r}_{i-1}\|} \epsilon\tag{2.20}$$

It should be noted [8] that some of the initial bounds found aren't really sharp, mainly 2.12 and 2.17, and further empirical analysis of these bounds could show a better theoretical bound can be found for both. A plot of these bounds for the cavity problem that will be studied is shown later. It should also be noted that  $\tilde{r}_i$ , after the Givens's Rotations, is also found in the  $i + 1$ 'th element of  $g_m$  in 2.14. The demonstration follow the same proof as for  $g_m$  in 2.5, given that  $y_m$  is a solution

to a linear system that involves an upper triangular matrix.

The remaining theory in this report explains the basics of Hierarchical Matrices, the structure that will be used to compress the matrices  $A$  that appear in the discretization of integral operators, since these usually appear in large dimensions, but also to construct each  $E_k$ . As it will be explained later, at each iteration a  $E_k$  will be indirectly constructed during the inexact product  $\mathcal{A}_k q$ , mainly using the residues that appear during this structure's construction, in the iterations of the *ACAMethod*.

## Chapter 3

# Hierarchical Matrices and ACA Method

### 3.1 Low-rank Matrices

In reality, most matrices are large, so storing each element is not efficient, or even possible. If  $A \in \mathbb{C}^{n \times m}$  has a rank  $k$  such that  $k \leq m$  and  $k(n+m) < n * m$  ( $A$  is low-rank),  $A$  can be written in outer product form, as a product between the matrices  $U \in \mathbb{C}^{n \times k}$  and  $V \in \mathbb{C}^{m \times k}$ , which can be seen in 3.1, where  $u_i, v_i$  are the column vectors of  $U$  and  $V$ .

$$A = UV^H = \sum_{i=1}^k u_i v_i^* \quad (3.1)$$

Therefore, storing  $k(n+m)$  elements to write  $A$ , and not  $n \times m$ . A matrix  $A$  that can be represented as 3.1 is an element of  $\mathbb{C}_k^{n \times m}$ .

The representation in 3.1 also facilitates other operations with  $A$ , like matrix-vector products  $Ab$  that are always present in methods like GMRES [4] and different kinds of norms, like  $\|A\|_F, \|A\|_2$  [4].

However, even full rank matrices can be approximated by matrices with lower rank. A theorem [4] establishes that the closest matrix from  $\mathbb{C}_k^{n \times m}$  of a matrix from  $\mathbb{C}^{n \times m}$  can be obtained from the SVD  $A = U\Sigma V^H$ , where  $\Sigma$  contains the singular values  $\sigma_1 \geq \sigma_2 \dots \sigma_m \geq 0$  and  $U, V$  are unitary. If  $A_k$  is the approximation obtained after taking the first  $k$  elements of  $\Sigma$  (creating the matrix  $\Sigma_k$ ), the error between  $A$  and  $A_k$  is 3.2.

$$\|A - A_k\| = \left\| U\Sigma V^H - U'\Sigma_k V_H \right\| = \|\Sigma - \Sigma_k\| \quad (3.2)$$

If the spectral norm,  $\|\cdot\|_2$  is used instead, the error in 3.2 is given by  $\sigma_{k+1}$ . For Frobenius's norm,  $\|\cdot\|_F$ , the error becomes  $\sum_{l=k+1}^n \sigma_l^2$ .

Instead of approximating large matrices entirely, it's better to think in approximations made to each of their blocks. Blocks that appear after the discretization of elliptic operators also have the possibility of being approximated by matrices that decay exponentially with  $k$ ,  $S_k$ , as in 3.3.

$$\|A - S_k\|_2 < q^k \|A\|_2 \quad (3.3)$$

That way, the rank and the precision are related in a logarithmic manner, and the rank required by a certain  $\epsilon$  is 3.4.

$$k(\epsilon) = \min\{k \in \mathbb{N} : \sigma_{k+1} < \epsilon \sigma_1\} \quad (3.4)$$

## 3.2 ACA Method(Adaptative Cross Approximation)

As shown in the last section, the SVD methods gives us an approximation of  $A$  given a certain  $\epsilon$ , through the relation in 3.2. Nevertheless, this is an expensive method, where the complexity becomes too heavy for some calculations.

The algorithm for the method is in 4, where  $a_{ij}$  are the elements of a matrix  $A \in \mathbb{R}^{n \times m}$ . The main objective is to approximate  $A$  as  $A = S_k + R_k$ ,  $S_k = \sum_{l=1}^k u_l v_l^t$  and  $R_k$  is the residual.

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### Algorithm 4 ACA Method

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```

1:  $k = 1$  et  $\mathbf{Z} = \emptyset$ 
2: repeat
3:   TFind  $i_k$ 
4:    $\hat{v}_k = a_{i_k, 1:m}$ 
5:   for  $l = 1, \dots, k-1$  do
6:      $\hat{v}_k = \hat{v}_k - (u_l)_{i_k} v_l$ 
7:   end for
8:    $Z = Z \cup \{i_k\}$ 
9:   if  $\hat{v}_k$  doesn't disappear then
10:     $j_k = \operatorname{argmax}_j |(\hat{v}_k)_j|$  ;  $v_k = (\hat{v}_k)_{j_k}^{-1} \hat{v}_k$ 
11:     $u_k = a_{1:n, j_k}$ 
12:    for  $l = 1, \dots, k-1$  do
13:       $u_k = u_k - (v_l)_{j_k} u_l$ 
14:    end for
15:     $k = k + 1$ 
16:   end if
17: until  $\|u_k\| \|v_k\| \leq \epsilon$ 

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Considering  $I, J \in \mathbb{N}$  the index set of a given matrix and  $\mathbf{T}_{I \times J}$  the cluster block tree that contains an admissible partition  $P$  of  $I \times J$  in its leaves,  $\mathfrak{L}(\mathbf{T}_{I \times J})$ . The set of hierarchical matrices in  $\mathbf{T}_{I \times J}$  rank  $k$  for each block  $A_b$  defined in 3.5.

$$\mathfrak{H}(\mathbf{T}_{I \times J}, k) = \{A \in \mathbb{C}^{I \times J} : \operatorname{rank} A_b \leq k, \forall b \in P\} \quad (3.5)$$

In practise, 4 works with  $\epsilon$  given by the user during the assembling of the Hierarchical Matrix, and the compression acts in each of the admissible blocks that will then be represented as low rank matrices, shown in 3.1. We also store each one of the residuals obtained in the outer loop of 4.

After giving a tolerance  $\sigma$  for an inexact product, the algorithm has, for each admissible block of the cluster tree, use the right amount of columns of the outer product representation of the block as to reach the desired tolerance, what can be inferred by the list of residuals of the ACA Method.

So, the different perturbations  $E_k$  used in 2.9, are the matrices that when added to  $A$ , leave each admissible block with the right amount  $k'$  of columns in 3.1 so the product of the admissible block  $B_k$  and  $q$  be approximated by the tolerance  $\sigma$ . Calling this approximation of each block  $B_k$  as  $\tilde{B}_k$ , we have 3.6.

$$\frac{\|B_k q - \tilde{B}_k q\|}{\|B_k q\|} \leq \sigma, \quad \tilde{B}_k = \sum_{i=1}^{k'} u_i v_i^* \quad (3.6)$$

## Chapter 4

### First results

(Not results in the cluster, left to remake them after finishing the discussions we had about residuals) (I thought about changing the beginning of this chapter as a whole small chapter about BEM)

(Also, I thought about using the graphs with the bounds of each expression in the article, but I'm not sure if we put them here or with the Inexact theory chapter above)

Before using the inexact product in more complex problems, simpler examples are used to validate the approach and fix minor parameters in the scheme.

The two first tests evaluate the speedup in the product of a Hierarchical Matrix and a vector and an execution of the Inexact GMRES with few iterations, using the operators obtained through 2nd type Equations of Laplace and Helmholtz 4.1, where the last one is a scattering problem, where  $\Delta$  is the Laplace operator and everything is supposed to be solved in two dimensions. The last test will use a cavity problem to test the speedup of the algorithm in a situation with more iterations.

$$\begin{aligned}\Delta u &= 0 \\ \Delta u + k^2 u &= 0\end{aligned}\tag{4.1}$$

Reformulating both equations as a Boundary Integral Equation, the simple *direct* formulation is used to write the solution as 4.2, where  $\Gamma$  is boundary of the domain,  $S$  and  $D$  are the single and double layer operators, defined as 4.3, and  $G(x, y)$  is the fundamental solution of the desired PDE.

$$-\frac{u(x)}{2} + D[u](x) = S[\partial_\nu u](x), \quad x \in \Gamma\tag{4.2}$$

$$\begin{aligned}S[\sigma](x) &= \int_{\Gamma} G(x, y) \sigma(y) ds(y) \\ D[\sigma](x) &= \int_{\Gamma} \frac{\partial G}{\partial \nu_y}(x, y) \sigma(y) ds(y)\end{aligned}\tag{4.3}$$

For the first two examples, a unit circle around the origin is used as the boundary to generate the operators, with the mesh being created with the *Inti* library [3].

For the last test, the mesh is made from a cavity *.geo* file available in [1]. A view of the figure can be seen in 4.1. The incident wave' angle is chosen to be  $\frac{\pi}{4}$  rad.

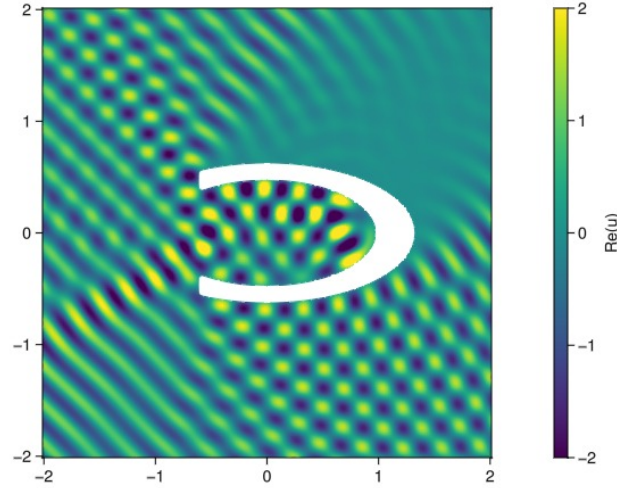


Figure 4.1: Geometry used in the test.

A good way to infer the maximum acceleration possible for the inexact products would be using only admissible rank 1 blocks and measuring its execution time. Although such thing would not happen in a practical situation, it gives a maximum bound for the speed up we should expect. For doing that, the product tolerance is changed to *Infinity*, and the product will be realised with only rank-1 blocks, since it's programmed to get the first approximation lower than its given tolerance.

## 4.1 Laplace's results

Setting our product tolerance to *Infinity* and using only rank-1 blocks in the product, we got a () speedup.

All results are contained in 4.2, showing the evolution of the residual with the product tolerance aswell as the speedup to each of these values.

## 4.2 Helmholtz's results

For a maximum speedup bound in the product, the infinity tolerance brought a () speedup.

For the unitary circle boundary the results can be seen in 4.3.

For the cavity, 4.4.

An evolution of the number of iterations in face of the different tolerances passed to the algorithm is in 4.5.

To start assessing the maximum gain possible, we start by initiating the product tolerance as infitine and seeing the result. Choosing an infinite tolerance grants us the all admissible block used in the products will have rank 1.



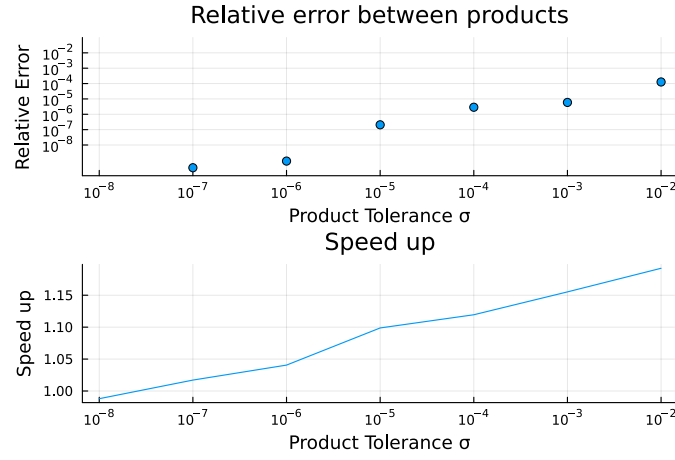
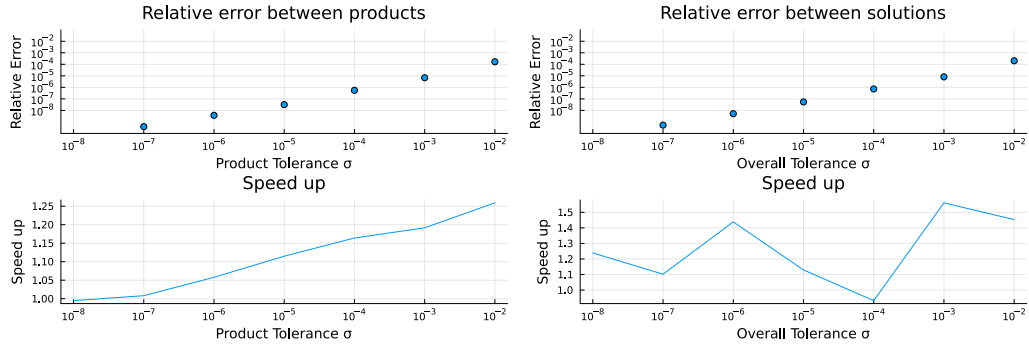


Figure 4.2: Speedup and residual evolution for the product between a 8000x8000 HMatrix and a vector.



(a) Results for the product of a 70000x 70000 HMatrix and a vector. (b) Results for an initial application of the Inexact GMRES algorithm.

Figure 4.3: Results for the application of the Inexact GMRES algorithm with a 70000x70000 HMatrix.

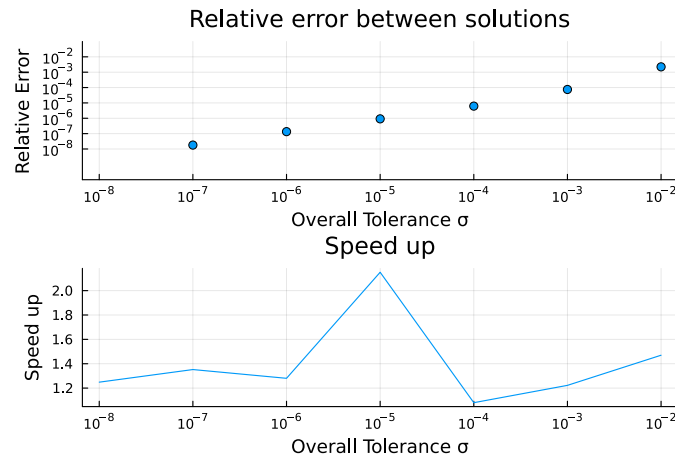


Figure 4.4: Speedup witnessed in the application of the Inexact GMRES in a 50000x50000 matrix.

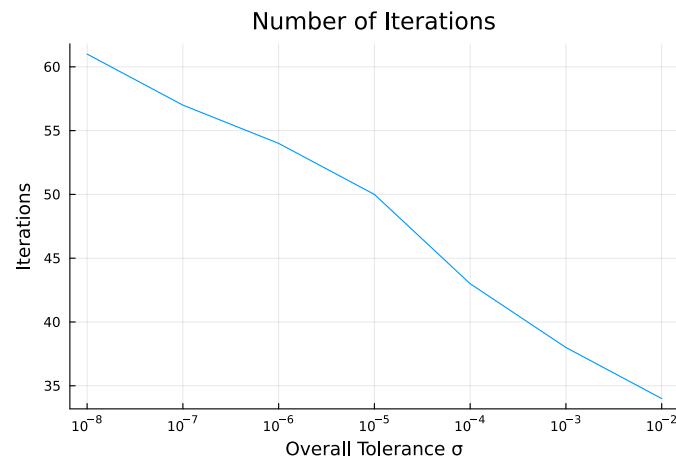


Figure 4.5: Evolution of the quantity of iterations needed for convergence and overall tolerance passed as an argument.

# Bibliography

- [1] Dépôt github. <https://github.com/DuduGuima/InexactGMRES.git>.
- [2] Hmatrices.jl. <https://github.com/IntegralEquations/HMatrices.jl>.
- [3] Inti.jl. <https://github.com/IntegralEquations/Inti.jl>.
- [4] Mario Bebendorf. *Hierarchical matrices*. Springer, 2008.
- [5] Marc Bonnet. *Lecture notes on numerical linear algebra*. ENSTA Paris - POEMS Group, 2021.
- [6] Eric Darve and Mary Wootters. *Numerical linear algebra with Julia*. SIAM, 2021.
- [7] Yousef Saad. *Iterative methods for sparse linear systems*. SIAM, 2003.
- [8] Valeria Simoncini and Daniel B Szyld. Theory of inexact krylov subspace methods and applications to scientific computing. *SIAM Journal on Scientific Computing*, 25(2):454–477, 2003.
- [9] Lloyd N Trefethen, David Bau III, and Ricardo D Fierro. Numerical linear algebra. *SIAM Review*, 40(3):735–738, 1998.