An Empirical Interpolation based Fast Summation Method
for translation invariant kernels

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Abstract

The Empirical Interpolation Method (EIM) enables to represent two-variable functions in a way that makes possible the application of the Reduced Basis method, a reduced order method that efficiently approximates the solution to a class of partial differential equations. The EIM can be used to approximate translation invariant kernels to derive a multilevel Fast Multipole Method (FMM), called herein the Empirical Interpolation Fast Multipole Method (EIFMM). The approximation scheme used in EIFMM is kernel-dependent, where the basis functions are based on evaluations of the kernel itself. On some usual kernels, this scheme requires less interpolation points than a Chebychev-based procedure, and therefore uses less memory. An important feature of the EIFMM is a built-in error estimation of the interpolation error made by the low-rank approximation of the far-field behavior of the kernel: the algorithm selects the optimal number of interpolation points required to ensure a given accuracy for the result, leading to important gains for inhomogeneous kernels.

1 Introduction

We consider the following problem: compute an approximation of the sum

\[
    f(\bar{x}_i) = \sum_{j=1}^{N} \sigma_j K(\bar{x}_i, \bar{y}_j),\quad 1 \leq i \leq N,\tag{1}
\]

for a set of source points \( \bar{y}_j \), potentials \( \sigma_j \), and another set of target points \( \bar{x}_i \), in complexity \( O(N) \), with a controllable error \( \epsilon \). Some methods that only use numerical evaluations of \( K \) have been proposed, see \[1\,7\,12\]. The Fast Multipole Method (FMM) can also be used. The first FMM algorithm was proposed in \[13\] for the Laplace kernel \( K(x, y) = \frac{1}{|x - y|} \), and later extended to the oscillatory kernel \( K(x, y) = e^{ik|x-y|}/|x - y| \). FMM for general kernels have been developed leading to kernel-independent procedures,

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see [16, 20]. Among them, some procedures are based on an interpolation scheme, see [9, 10]. In [11], a kernel-independent FMM algorithm based on the Chebychev interpolation is developed and called Black-Box FMM. Since the algorithm proposed herein is in the same family as the one developed in [11], our numerical experiments contain comparisons with this method. Notice that although our procedure requires a translation-invariant kernel, the Black-Box FMM is valid for any non-oscillatory kernel.

As for any interpolation-based FMM, a scheme is needed to approximate the far-field behavior of $K(x, y)$. This is done in this work using the Empirical Interpolation Method (EIM), a procedure that represents a two-variable function in a so-called affine dependent formula and that was proposed by the Reduced Basis community in [2]. The EIM is a greedy and function-dependent procedure, that requires a precomputation step. For homogeneous kernels, the precomputation is done once and for all for a given tolerance, and can be reused for any other computation. For other kernels, this precomputation step is tree-dependent. An important feature of the EIM is a built-in error estimation, used as a stopping criterion in the greedy step. Depending on the kernel (and on the level in the tree for inhomogeneous kernels), the EIM selects an optimal number of terms that ensures a given accuracy of the approximation. To derive a FMM-compatible approximation formula based on the EIM, we use four summations over the interpolation points, instead of two summations for the Black-Box FMM. However, we will see that the M2L step, by far the most expensive one, has the same complexity as Black-Box FMM with respect to the number of interpolation points. For some considered kernels, our EIM-based approximation formula achieves the same accuracy as a Chebychev interpolation for much fewer interpolation points, leading the way towards a new efficient FMM procedure called the Empirical Interpolation Fast Multipole Method (EIFMM).

In Section 2 the EIM is recalled. In Section 3 is presented the new FMM algorithm: first is derived in Section 3.1 a four-summation formula based on the EIM that can be used in a FMM procedure, then the performance of this formula in a FMM context is evaluated in Section 3.2; a monolevel version of the EIFMM is proposed in Section 3.3 and a multilevel one in Section 3.4. In Section 4 the overall execution time is reduced using some precomputation and compression of the M2L step. Finally, some numerical experiments are presented in Section 5 and some conclusions are drawn in Section 6.

## 2 The Empirical Interpolation Method

Consider a function $K(x, y)$ defined over $\mathcal{D}_x \times \mathcal{D}_y$, assumed to be real-valued for simplicity. Fix an integer $d$. The Empirical Interpolation Method provides a way to approximate this function in the following form:

$$K(x, y) \approx (I_d K)(x, y) := \sum_{m=1}^{d} \lambda_m(x) q_m(y), \quad (2)$$
where \( \lambda_m(x) \) is such that

\[
\sum_{m=1}^{d} B_{l,m} \lambda_m(x) = K(x, y_l), \quad \forall 1 \leq l \leq d.
\]  (3)

The functions \( q_m(\cdot) \) and the matrix \( B \in \mathbb{R}^{d \times d} \), which is lower triangular with unity diagonal, are constructed in Algorithm 1, where \( \delta_d = \text{Id} - I_d \) and \( \| \cdot \|_{\mathcal{D}_y} \) is a norm on \( \mathcal{D}_y \), for instance the \( L^\infty(\mathcal{D}_y) \)- or the \( L^2(\mathcal{D}_y) \)-norm. In practice, the argmax appearing in Algorithm 1 is searched over finite subsets of \( \mathcal{D}_x \) and \( \mathcal{D}_y \), denoted respectively by \( \mathcal{D}_{x,\text{trial}} \) and \( \mathcal{D}_{y,\text{trial}} \). Note that Algorithm 1 also constructs the set of points \( \{ y_l \}_{1 \leq l \leq d} \) in \( \mathcal{D}_y \) used in (3), and a set of points \( \{ x_l \}_{1 \leq l \leq d} \) in \( \mathcal{D}_x \). The following assumption is made.

Algorithm 1 Greedy algorithm of the EIM

1. Choose \( d > 1 \)
2. Set \( k := 1 \)
3. Compute \( x_1 := \arg \max_{x \in \mathcal{D}_x} \| K(x, \cdot) \|_{\mathcal{D}_y} \)
4. Compute \( y_1 := \arg \max_{y \in \mathcal{D}_y} | K(x_1, y) | \) \[First interpolation point\]
5. Set \( q_1(\cdot) := \frac{K(x_1, \cdot)}{K(x_1, y_1)} \) \[First basis function\]
6. Set \( B_{1,1} := 1 \) \[Initialize matrix B\]
7. \textbf{while} \( k < d \) \textbf{do}
8. Compute \( x_{k+1} := \arg \max_{x \in \mathcal{D}_x} \| (\delta_k K)(x, \cdot) \|_{\mathcal{D}_y} \)
9. Compute \( y_{k+1} := \arg \max_{y \in \mathcal{D}_y} | (\delta_k K)(x_{k+1}, y) | \) \[(k + 1)-th interpolation point\]
10. Set \( q_{k+1}(\cdot) := \frac{(\delta_k K)(x_{k+1}, \cdot)}{(\delta_k K)(x_{k+1}, y_{k+1})} \) \[(k + 1)-th basis function\]
11. Set \( B_{k+1,m} := q_m(y_{k+1}) \), for all \( 1 \leq m \leq k + 1 \) \[Increment matrix B\]
12. \( k \leftarrow k + 1 \) \[Increment the size of the decomposition\]
13. \textbf{end while}

\((H)\) The dimension of \( \text{Span}(K(x, \cdot)) \) is larger than \( d \), so that the functions \( \{K(x_l, \cdot)\}_{1 \leq l \leq d} \) are linearly independent (otherwise, \( (\delta_k K)(\mu_{k+1}, x_{k+1}) = 0 \) for some \( k \) in Algorithm 1).

It is shown in [6] that the approximation (2) can be written in the form

\[
(I_d K)(x, y) = \sum_{l,m=1}^{d} \Delta_{l,m} K(x, y_l) K(x_m, y),
\]  (4)

where \( \Delta = B^{-t} \Gamma^{-1} \), and where the matrix \( \Gamma \) is is upper triangular and constructed recursively in the loop in \( k \) of Algorithm 1 in the following way:
• $k = 1$:
  \[ \Gamma_{1,1} = K(x_1, y_1), \]

• $k \rightarrow k + 1$:
  \[ \Gamma_{k+1,k+1} = (\delta_k K)(x_{k+1}, y_{k+1}), \]
  \[ \Gamma_{m,k+1} = 0, \quad \forall 1 \leq m \leq k, \]
  \[ \Gamma_{k+1,m} = \alpha_m, \quad \forall 1 \leq m \leq k, \]

where the vector $\alpha$ is such that \[ \sum_{m=1}^{k} B_{l,m} \alpha_m = K(x_{k+1}, y_l), \] for all $1 \leq l \leq k$.

The particular form (4) is the key to the use of the EIM approximation in a fast multipole context.

We recall the interpolation property of $I_d K$; see [14, Lemma 1]:

**Property 2.1 (Interpolation property)** For all $1 \leq m \leq d$,
\[
\begin{align*}
(I)_{m}(x, y) &= K(x, y), & \forall x \in D_x, \\
(I)_{m}(x, y) &= K(x, y), & \forall y \in D_y.
\end{align*}
\]

**Remark 2.2 (Error certification)** An important aspect is that the error made by the EIM approximation over the training set $D_{x,\text{trial}} \times D_{y,\text{trial}}$, denoted $\epsilon_k$ and defined as $\epsilon_k := \max_{y \in D_y} |(\delta_k K)(x_{k+1}, y)|$, is monitored during the greedy procedure. In practice, a stopping criterion is used on $\epsilon_k$ instead of on the number of interpolation points $d$, which was used to simplify the presentation of the EIM. Hence, depending on the regularity of the function $K$, the EIM will automatically select the number of interpolation points to certify the error over $D_{x,\text{trial}} \times D_{y,\text{trial}}$.

**Remark 2.3 (Links with Adaptive Cross Approximation)** The Empirical Interpolation Method has been originally proposed in [2] to achieve a required assumption to apply the reduced basis method, a reduced order procedure to approximate the solution of a partial differential equation. It is shown in [4, Theorem 5.1] that the bivariate Adaptive Cross Approximation (ACA, see [3, 5, 19]) with full pivoting is equivalent to the EIM using the $L^\infty(D_y)$-norm. The additional ingredient contained in Equation (4) is the ability to compute the approximation not only on the training sets $D_{x,\text{trial}}$ and $D_{y,\text{trial}}$ but for all $x \in D_x$ and all $y \in D_y$. Notice that this property is also given in [4, Section 4.5].

3 The Empirical Interpolation Fast Multipole Method

The FMM algorithm is based on a low-rank approximation of the far-field behavior of the kernel. For a general presentation of the FMM algorithm, see the original article [13, Section 3].
3.1 A suitable approximation

For the simplicity of the presentation, the algorithm is described in 1D. It can be readily extended in 2D and 3D. Consider a translation invariant kernel \( K(x, y), (x, y) \in \Omega \times \Omega \), where \( \Omega = (-0.5, 0.5) \) is the complete domain on which the FMM computation is carried out. The domain \( \Omega \) is partitioned in \( 2^\kappa \) intervals, \( \kappa \in \mathbb{N}^* \), of length \( 2l_\kappa \), with \( l_\kappa := 2^{-\kappa -1} \).

Consider two intervals \( I \) and \( J \), well separated in the sense that \( \min_{(x,y) \in I \times J} |x-y| \geq 2l_\kappa \).

To anticipate the generalization to higher dimensions, \( I \) and \( J \) are called “boxes” in what follows. We denote \( c_I \) and \( c_J \) the center of the boxes \( I \) and \( J \). We recall the EIM approximation (4):

\[
K(x, y) \approx d \sum_{l,m=1}^d \Delta_{I,J}^{l,m} K(x, y_J^l) K(x_I^m, y), \quad x \in I, \ y \in J,
\]

(5)

where \( I \) and \( J \) superscripts have been added to underline the box-dependent quantities. Since the FMM requires to approximate \( K(x, y) \) in such a fashion that \( x \) and all quantities related to the box \( I \) are separated from \( y \) and all quantities related to the box \( J \), the approximation (5) is not suitable for a FMM algorithm. Define \( I_0 := \{x - c_J, x \in \hat{I}\} \) for all box \( \hat{J} \) in the partitioning of \( \Omega \) and all box \( \hat{I} \) well separated from \( \hat{J} \), and define \( J_0 \) the box of length \( 2l_\kappa \) located at the center of \( \Omega \) (notice that \( J_0 \) is not a box from the partitioning of \( \Omega \)). In our setting, \( J_0 = (-l_\kappa, l_\kappa) \) and \( I_0 = (-1 + l_\kappa, -3l_\kappa) \cup (3l_\kappa, 1 - l_\kappa) \), see Figure 1. In other words, \( J_0 \) is a source box translated to the center of the domain, \( I_0 \) is the union of possible target boxes, translated in the same fashion.

![Figure 1: Representation of the partitioning of \( \Omega \) in 1D for \( \kappa = 3 \) and of the corresponding boxes \( I_0 \) and \( J_0 \).](image)

Since \( K(x, y) = K(x - c_J, y_c J) \), with \( x - c_J \in I_0 \) and \( y - c_J \in J_0 \), it is inferred that

\[
K(x, y) \approx \sum_{l,m=1}^d \Delta_{I_0,J_0}^{l,m} K(x - c_J, y_{J_0}^l) K(x_{I_0}^m, y - c_J),
\]

(6)

where, the EIM being carried out on \( \mathcal{D}_x = I_0 \) and \( \mathcal{D}_y = J_0 \), the matrix \( \Delta_{I_0,J_0}^{l,m} \) and the sets of points \( x_{I_0}^l \) and \( y_{J_0}^l \) no longer depend on \( I \) and \( J \). Consider the first evaluation of
To derive the approximation (8), we used domains of the form

\[ \Omega = (0, 0.5)^3 \times (0, 0.5)^3 \]

which holds \( K(x - c_I, y_I^j) = K(x - c_I, y_I^j + c_J - c_I) \), where \( x - c_I \in J_0 \) and \( y_I^j + c_J - c_I \in I_0 \). It is then inferred that

\[
K(x - c_J, y_I^j) \approx \sum_{l'=1}^{d} \Delta_{l,m} \sum_{l=1}^{d} \sum_{m'=1}^{d} \Delta_{l,m'} K(x - c_I, y_{l'}^j) K(x_{m'}, y^j_I + c_J - c_I), \quad 1 \leq l \leq m, \tag{7}
\]

where a second EIM has been carried out on \( D_x = J_0 \) and \( D_y = I_0 \) (with the same number of terms \( d \) for simplicity). Notice that if the kernel is symmetric, \( \Delta_{l,m} = (\Delta_{l,0})^t \), \( x_{l,m}^l = y_{l,m}^l \) for all \( 1 \leq m \leq d \), and \( y_{m}^{I_0} = x_{m}^{J_0} \) for all \( 1 \leq m \leq d \). Injecting (7) into (6) provides a suitable approximation for the use of FMM:

\[
K(x, y) \approx \sum_{l'=1}^{d} \sum_{m'=1}^{d} \Delta_{l,m'} \sum_{l=1}^{d} \sum_{m=1}^{d} \Delta_{l,m} K(x_{l,m'}^l, y_{l,m'}^l) K(x_{m}, y - c_J). \tag{8}
\]

Notice that in all the kernel evaluations in (8), the first and second variables are always separated by a distance of at least \( 2l_J \). Moreover, we did not find any obvious way to exploit the symmetry of \( I_0 \) and keep an approximation suitable for the use of the FMM.

(H2) To derive the approximation (8), we used domains of the form \( D_x = [-7a, 7a]^D \setminus [-3a, 3a]^D \) and \( D_y = [-a, a]^D \), for some \( a > 0 \), where \( D \) denotes the dimension of the space containing the particles. For the kernels considered herein, we assume that although the learning stage of the EIM has been carried out on \( D_x \times D_y \), the approximation is still valid on \( D_x \times D_y \), where \( D_x = \Omega \setminus [-3a, 3a]^D \).

In Tables 1 and 2 we check that assumption (H2) is verified for some usual kernels: we consider \( \Omega = (-0.5, 0.5)^3 \) and we carry out an EIM algorithm on \( D_x \times D_y \) as defined in (H2) for various values of \( a \) and \( d \). Then, we compute the maximum relative error made by the EIM approximation on 1000 points randomly taken in \( D_x \times D_y \) and in \( \hat{D}_x \times D_y \). For homogeneous kernels in Table 1 we see that the error over \( \hat{D}_x \times D_y \) is of the same magnitude than over \( D_x \times D_y \): the assumption (H2) is reasonable. For non-homogeneous kernels in Table 2 one can object that as \( a \) decreases (i.e. we are deeper on the tree), the difference between the error over \( D_x \times D_y \) and over \( \hat{D}_x \times D_y \) increases. However, the smaller \( a \), the smaller \( D_y \), and the more effective the EIM algorithm gets: we see in Table 2 that the same value for the error over \( \hat{D}_x \times D_y \) is obtained for all the values of \( a \), although the values of \( d \) needed are smaller as \( a \) decreases. In other words, in our tree structure, the smaller the learning set \( D_x \) is compared to the set \( \hat{D}_x \) were the EIM approximation is supposed to be valid, the fewer number of interpolation points \( d \) are needed to enforce a constant accuracy. For this reason, it is reasonable to assume that (H2) is also verified for the considered non-homogeneous kernels.

3.2 Performance of the approximation

One can object that (8) involves many summations and may result in a procedure with higher complexity than other interpolation-based FMM. However, a gain can be realized
the Chebychev approximation [11, Equation (6)] and the approximation is tested. The EIM approximation performs reasonably better than the approximation restricted to $I$ taken in the learning stage of the EIM was carried-out on $I_0 \times J_0$ (therefore, is valid for a much larger domain than $I \times J$), see Figure 4. Denote $K_{\text{Che}}$ the approximation of the kernel using the Chebychev approximation [11, Equation (6)] and $K_{\text{EIM}}$ the EIM approximation (8).

The relative error is using each approximation is respectively defined as

$$\sqrt{\frac{\sum_{(x,y)\in S_{\text{trial}}} (K_{\text{Che}}(x,y) - K(x,y))^2}{\sum_{(x,y)\in S_{\text{trial}}} (K(x,y))^2}}$$

and

$$\sqrt{\frac{\sum_{(x,y)\in S_{\text{trial}}} (K_{\text{EIM}}(x,y) - K(x,y))^2}{\sum_{(x,y)\in S_{\text{trial}}} (K(x,y))^2}}.$$

In Figure 2 are represented relative error comparisons for some kernel in 1D. The set of learning points $D_{x,\text{trial}} \times D_{y,\text{trial}}$ is different from the set of points $S_{\text{trial}}$ on which the approximation is tested. The EIM approximation performs reasonably better than

| Kernel | $a = 0.05$ | $a = 0.025$ | $a = 0.01$ |
|--------|------------|-------------|------------|
| $1/r$  | $2 \times 10^{-5}$ | $2 \times 10^{-5}$ | $2 \times 10^{-5}$ |
| $1/r^2$| $2 \times 10^{-4}$ | $2 \times 10^{-4}$ | $2 \times 10^{-4}$ |
| $1/r^3$| $1 \times 10^{-2}$ | $1 \times 10^{-2}$ | $1 \times 10^{-2}$ |

Table 1: Verification that (H2) is valid for some usual homogeneous kernels: maximum relative error made by the EIM approximation on 1000 randomly selected points, with $d = 40$.

| Kernel | $a = 0.05$, $d = 40$ | $a = 0.025$, $d = 32$ | $a = 0.01$, $d = 20$ |
|--------|---------------------|---------------------|---------------------|
| $1/\sqrt{x^2 + 1}$ | $2 \times 10^{-5}$ | $2 \times 10^{-5}$ | $2 \times 10^{-5}$ |
| $e^{-r^2}$ | $2 \times 10^{-8}$ | $2 \times 10^{-8}$ | $2 \times 10^{-8}$ |
| $e^{-2r^2/4}$ | $1 \times 10^{-4}$ | $1 \times 10^{-4}$ | $1 \times 10^{-4}$ |

Table 2: Verification that (H2) is valid for some usual non-homogeneous kernels: maximum relative error made by the EIM approximation on 1000 randomly selected points.

if the approximation is more efficient than the ones currently used, in the sense that the same levels of accuracy are achieved with fewer interpolation points. The Chebychev interpolation, used in the Black-Box FMM in [11], presents the advantages of having a uniform error distribution and is nearly optimal in the minimax sense. We will then compare the accuracy of [11, Equation (6)] to the accuracy of (8).

### 3.2.1 1D approximation

Consider two well-separated boxes $I$ and $J$ of $\Omega$ and a set of 100 couples of points taken in $I \times J$, denoted $S_{\text{trial}}$. To make a realistic comparison, we take a Chebychev approximation restricted to $I \times J$, but we take the approximation (8) such that the learning stage of the EIM was carried-out on $I_0 \times J_0$ (therefore, is valid for a much larger domain than $I \times J$), see Figure 4. Denote $K_{\text{Che}}$ the approximation of the kernel using the Chebychev approximation [11, Equation (6)] and $K_{\text{EIM}}$ the EIM approximation (8).
the Chebychev interpolation for asymptotically smooth kernels, and much better for the Helmholtz kernel. The good results for EIM with the Helmholtz kernel come from the fact that the basis function of the approximation are evaluations of the kernel itself (see (8)) therefore oscillate at the same frequency as the kernel.

![Comparison in 1D between Chebychev and EIM approximations](image)

Figure 2: Comparison in 1D between Chebychev and EIM approximations, for kernels (i) left; black: $1/r$, blue: $1/r^4$ and red: $1/\sqrt{r^2+1}$; (ii) black: $e^{-10r}/r$ and blue: $e^{-100r}/r$.

### 3.2.2 3D approximation

The approximation quality of the EIM depends strongly on the learning stage. In 3D, the sampling of $I_0 \times J_0$ can involve many points, and the line 8 of Algorithm 1 becomes very expensive, since its complexity is the product of the cardinality of $D_{x,\text{trial}}$ with the one of $D_{y,\text{trial}}$. From Remark 2.3 with $\|\cdot\|_{D_y} = \|\cdot\|_{L^\infty(D_y)}$, the set of points $x_k, y_k, 1 \leq k \leq d$, is the same as the points chosen when applying a bivariate ACA with full pivoting to the matrix $K(\hat{x}_i, \hat{y}_j), \hat{x}_i \in D_{x,\text{trial}}, \hat{y}_j \in D_{y,\text{trial}}$. In practice, to deal with large datasets, a partially pivoted version of ACA is used, see Algorithm 4.2. The complexity of this version is linear with respect to the largest number between the cardinality of $D_{x,\text{trial}}$ and the one of $D_{y,\text{trial}}$, but is suboptimal in the sense that, to certify a given error, it requires in general more interpolation points than when using fully pivoted ACA. What is done here is the use of a partially pivoted ACA, and then a fully pivoted ACA on the set of points selected by the partially pivoted ACA.

In Figure 3, the error is computed over a set of 100 points randomly taken in the whole domain $I_0 \times J_0$. In the right plot, the relative error of (8) and Chebychev approximations are represented for different kernels. One way to read this plot is to observe that for the Laplace kernel, for instance, approximately twice fewer interpolation points are needed for the approximation (8) to achieve the same accuracy as Chebychev with 6 interpolation points per dimension.
Figure 3: Comparison between Chebychev and EIM approximations for black: $1/r$, red: $1/\sqrt{r+1}$, and green: $e^{-r^2}$.

### 3.3 A monolevel multipole method

Consider a set of $N$ target points $\{\vec{x}_i\}_{1 \leq i \leq N}$, $N$ source points $\{\vec{y}_j\}_{1 \leq j \leq N}$ in $\Omega$, and $N$ potentials $\{\sigma_j\}_{1 \leq j \leq N}$, with $N \gg 1$. We look for a low complexity approximation of

$$f(\vec{x}_i) = \sum_{j=1}^{N} \sigma_j K(\vec{x}_i, \vec{y}_j), \quad 1 \leq i \leq N.$$  \hfill (9)

The set of boxes well-separated from $I$ is denoted $F(I)$, its complement in $\Omega$ is the neighborhood of $I$ and is denoted $N(I)$. The FMM aims at compressing the “far” interactions in the following fashion:

$$f_F(\vec{x}_i) = \sum_{J \in F(I)} \sum_{\vec{y}_j \in J} \sigma_j K(\vec{x}_i, \vec{y}_j), \quad \text{for all } I \text{ and all } \vec{x}_i \in I.$$  \hfill (10)

A monolevel multipole method can be directly derived from (9) to approximate $f_F(\vec{x}_i)$, see Algorithm 2. The obtained approximation of $f_F(\vec{x}_i)$ is denoted $f_{F,FMM}(\vec{x}_i)$. An approximation of $f(\vec{x}_i)$ is then given by

$$f(\vec{x}_i) \approx f_{F,FMM}(\vec{x}_i) + f_N(\vec{x}_i),$$  \hfill (11)

where the “near” interactions are defined by

$$f_N(\vec{x}_i) = \sum_{\vec{y}_j \in N(I)} \sigma_j K(\vec{x}_i, \vec{y}_j).$$  \hfill (12)

In Table 3 is given the complexity of each step of Algorithm 2. For step 3 and the computation of the near interactions to be in the same order in $N$, one must impose $(2^D)^{2^\alpha} \propto N^2(2^D)^{-\kappa}$, leading to a overall complexity of the sum of order $N^{3\frac{2}{3}}$. As classically done in the literature, the derivation of a multilevel multipole method allows to lower the complexity in $N$ of the algorithm to linear.
Algorithm 2 Monolevel EIFMM

1. Compute $W_m^I := \sum_{\bar{y}_j \in I} \sigma_j K(x_{m}^{I_0}, \bar{y}_j - c_I)$, for all box $I$ and all $1 \leq m \leq d$

2. Compute $\hat{W}_l^I := \sum_{m=1}^{d} \Delta_{l,m}^{I_0,0} W_m^I$, for all box $I$ and all $1 \leq l \leq d$

3. Compute $l_m^I := \sum_{J \in \mathcal{F}(I)} \sum_{l'=1}^{d} K(x_{l'}^{I_0}, \bar{y}_j - c_{l'}) \hat{l}_{l'}^I$, for all box $I$ and all $1 \leq m' \leq d$

4. Compute $\hat{l}_l^I := \sum_{m'=1}^{d} \Delta_{l,m}^{I_0,0} l_m^I$, for all box $I$ and all $1 \leq m' \leq d$

5. Compute $f_{\mathcal{F},FMM}(\bar{x}_i) := \sum_{l'=1}^{d} K(\bar{x}_i - c_{l'}, \bar{y}_{l'}^{I_0}) \hat{l}_{l'}^I$, for all box $I$ and all $x_i \in I$

| Step number | Complexity |
|-------------|------------|
| 1           | $dN$       |
| 2           | $d^2(2^{D})^\kappa$ |
| 3           | $d^2(2^{D})^{2\kappa}$ |
| 4           | $d^2(2^{D})^\kappa$ |
| 5           | $dN$       |
| $f_{\mathcal{F},FMM}$ | $N^2(2^{D})^{-\kappa}$ |

Table 3: Complexity of each step of Algorithm 2 and of the near interactions term.

### 3.4 A multilevel multipole method

The domain of computation $\Omega = (-0.5, 0.5)$ is now organized as a binary tree with $\kappa + 1$ levels. Level 0 is the root of the tree: there is one box equal to $\Omega$, level 1 contains the partitioning of $\Omega$ into two boxes of length $0.5$, and the following levels are obtained by partitioning each box of the previous level in the same fashion, up to level $\kappa$.

A superscript $k$ is now added to the quantities previously defined, to indicate that they depend on the level $k$. Two EIM’s are to be considered at each level, in the same fashion as in Section 3.1, except that $I_{k}^0 = (-2l_{k}, -l_{k}) \cup (2l_{k}, l_{k})$, while $J_{k}^0 = (-l_{k}, l_{k})$ is unchanged.

For symmetric kernel, this amount of precomputation can be lowered to one EIM by level, and for homogeneous and symmetric kernels (like Laplace), one EIM in total. The key to a multilevel method stands in the ability to derive recursion formulae to propagate information from the level $\kappa$ to the level 0 in the upward pass, and from the level 0 to the level $\kappa$ in the downward pass.

#### 3.4.1 Recursion for the upward pass: multipole to multipole (M2M)

The goal is to compute

$$W_m^{I_k} := \sum_{\bar{y}_j \in I_k} \sigma_j K(x_{m}^{I_0}, \bar{y}_j - c_{l_k}),$$

for all box $I_k$ at all level $k$ with $0 \leq k \leq \kappa$ and all $1 \leq m \leq d_k$ by recursion. The initialization of the recursion consists in computing $W_m^{I_0}$ at level $\kappa$ using (13). Then,
suppose $W_{m}^{l}$ is available at level $k$, there holds

$$W_{m}^{l-1} = \sum_{\bar{y}_{j} \in I_{k-1}} \sigma_{j} K(x_{m}^{l-1}, \bar{y}_{j} - c_{j_{k-1}}) = \sum_{J_{k} \subseteq C(I_{k-1})} \sum_{\bar{y}_{j} \in J_{k}} \sigma_{j} K(x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}}, \bar{y}_{j} - c_{j_{k}}),$$

(14)

where $C(I_{k-1})$ denotes the children boxes of $I_{k-1}$. For all $\bar{y}_{j} \in J_{k}$, $-l_{k} \leq \bar{y}_{j} - c_{j_{k}} \leq l_{k}$, i.e. $\bar{y}_{j} - c_{j_{k}} \in J_{k}$. Moreover, since $x_{m}^{l-1} \in I_{0}$, it is inferred that

$$x_{m}^{l-1} \leq -3l_{k} - 3l_{k-1} \leq x_{m}^{l-1}.$$

since for all $J_{k} \subseteq C(I_{k-1})$, $-l_{k} \leq c_{j_{k-1}} - c_{j_{k}} \leq l_{k}$ (see for instance Figure 5), it is inferred that

$$x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}} \leq -5l_{k} \leq -3l_{k} \leq 3l_{k} \leq 5l_{k} \leq x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}}.$$

From (H2), the EIM from level $k$ can then be used to write the following approximation

$$K(x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}}, \bar{y}_{j} - c_{j_{k}}) \approx \sum_{p, q = 1}^{d_{k}} \Delta_{p, q}^{l_{k}} K(x_{p}^{l-1} + c_{j_{k-1}} - c_{j_{k}}, y_{p}^{l_{k}}) W_{q}^{l_{k}}.$$

(15)

Then, injecting (15) into (14), it is inferred that

$$W_{m}^{l-1} \approx \sum_{p, q = 1}^{d_{k}} \Delta_{p, q}^{l_{k}} \sum_{J_{k} \subseteq C(I_{k-1})} K(x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}}, y_{p}^{l_{k}}) \sum_{\bar{y}_{j} \in J_{k}} \sigma_{j} K(x_{m}^{l-1} + c_{j_{k-1}} - c_{j_{k}}, \bar{y}_{j} - c_{j_{k}}).$$

(16)

which provides a recursive formula for the upward pass. In the same fashion as for the monolevel version, we then compute

$$\hat{W}_{l}^{l} := \sum_{m=1}^{d_{k}} \Delta_{l_{m}, l_{m}}^{l_{k}} \hat{W}_{m}^{l},$$

(17)

for all box $I_{k}$ at all level $k$ with $0 \leq k \leq \kappa$ and all $1 \leq l \leq d_{k}$.

3.4.2 Transfer pass: multipole to local (M2L)

We denote $\mathcal{I}(I_{k})$, the set of boxes that are the children of the boxes in the neighborhood of the parent of $I_{k}$ but are well-separated from $I_{k}$ at level $k$, and call it the interaction list of $I_{k}$, see Figure 4.
The M2L step consists in computing

\[ g_{m'}^{k} := \sum_{J^k \in \mathcal{I}(I^k)} \sum_{l=1}^{d^k} K(x_{m'}^0, y_{l}^0 + c_{J^k} - c_{I^k}) \hat{W}_{l}^{J^k}, \tag{18} \]

for all box \( I^k \) at all level \( k \) with \( 0 \leq k \leq \kappa \) and all \( 1 \leq m' \leq d^k \).

### 3.4.3 Recursion for the downward pass: local to local (L2L)

The goal is to compute

\[ l_{m'}^{k} := \sum_{J^k \in \mathcal{F}(I^k)} \sum_{l=1}^{d^k} K(x_{m'}^0, y_{l}^0 + c_{J^k} - c_{I^k}) \hat{W}_{l}^{J^k}, \tag{19} \]

for all box \( I^k \) at all level \( k \) with \( 0 \leq k \leq \kappa \) and all \( 1 \leq m' \leq d^k \) by recursion. The initialization of the recursion consists in computing \( l_{m'}^{2} \) at level 2 using (19). Then, suppose \( l_{m'}^{k} \) is available, there holds

\[ l_{m'}^{k+1} = g_{m'}^{k+1} + \sum_{J^k \in \mathcal{F}(P(I^{k+1}))} \sum_{J^{k+1} \in \mathcal{C}(J^k)} \sum_{l=1}^{d^{k+1}} K(x_{m'}^0, y_{l}^0 + c_{J^k} - c_{P(I^{k+1})}) \hat{W}_{l}^{J^{k+1}}, \]

where \( P(I^{k+1}) \) denotes the parent of \( I^{k+1} \).

It is seen on Figure 4 that

\[ -l_{k+1} \leq c_{J^{k+1}} - c_{P(I^{k+1})} \leq l_{k+1}, \]

and that

\[ c_{J^{k+1}} - c_{P(I^{k+1})} \leq -7l_{k+1} \text{ or } 7l_{k+1} \leq c_{J^{k+1}} - c_{P(I^{k+1})}. \]
Since \( x_m^{j_0+1}, y_l^{j_0+1} \in J_0^{k+1} \), it is readily verified that \( x_m^{j_0+1} + c_{j+1} - c_{P(I^{k+1})} \in J_0^k \) and 
\[ y_l^{j_0+1} + c_{j+1} - c_{P(I^{k+1})} \leq -3l_k \text{ or } 3l_k \leq y_l^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}. \]

From (H2), the EIM from level \( k \) can then be used to write the following approximation

\[
K(x_m^{j_0+1}, y_l^{j_0+1}) \approx \sum_{p', q' = 1}^{d_k} \Delta^{j_k}_{p', q'} K(x_m^{j_0+1}, y_l^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}).
\]

Then, injecting (21) into (20), it is inferred that

\[
i_{m'}^{k+1} \approx g_{m'}^{k+1} + \sum_{j_k \in P(I^{k+1})} \sum_{J_k \in C(I^{k+1})} \sum_{p', q'}^{d_k} \Delta^{j_k}_{p', q'} \sum_{l=1}^{d_k} K(x_m^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}, y_l^{j_0+1}) K(x_m^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}, y_l^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}).
\]

Consider \( K(x_m^{j_k}, y_l^{j_0+1} + c_{j+1} - c_{P(I^{k+1})}) = K(x_m^{j_k} + c_{P(I^{k+1})} - c_{j+1}, y_l^{j_0+1} + c_{j+1} - c_{j+1}). \)

Since \( J_k \in P(I^{k+1}) \) and \( J_k \) is the parent of \( J_k^{k+1} \), it is seen on Figure 5 that

\[-l_{k+1} \leq c_{j+1} - c_{j+1} \leq l_{k+1},\]

and that

\[c_{P(I^{k+1})} - c_{j+1} \leq -7l_{k+1} \text{ or } 7l_{k+1} \leq c_{P(I^{k+1})} - c_{j+1}.\]

Since \( x_m^{j_k}, y_l^{j_0+1} \in J_0^{k+1}, J_k \in P(I^{k+1}) \), and \( J_k \) is the parent of \( J_k^{k+1} \), it is readily verified that \( y_l^{j_0+1} + c_{j+1} - c_{j+1} \in J_0^k \) and

\[x_m^{j_0+1} + c_{P(I^{k+1})} - c_{j+1} \leq -3 \times 2^{k-1} \text{ or } 3 \times 2^{k-1} \leq x_m^{j_0+1} + c_{P(I^{k+1})} - c_{j+1}.\]
Once again, from (H2), the EIM from level $k$ can then be used to write the following approximation

$$K(x_{q'}^{l_k}, y_l^{j_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k} + c_{j_k+1} - c_{j_k}) \approx \sum_{u,v=1}^{d_k} \Delta_{l_k}^{I_{u,v}} K(x_{q'}^{l_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k} + c_{j_k+1} - c_{j_k}).$$

(23)

Injection (23) into (22), making use of the formula (17) to express $\hat{l}$, which provides a recursive formula for the upward pass. In the same fashion as for the monolevel version, we then compute

$$l_{m'}^{k+1} \approx g_{m'}^{k+1} + \sum_{j_k \in \mathcal{P}(P(j_k+1))} \sum_{u,v=1}^{d_k} \Delta_{l_k}^{I_{u,v}} \sum_{l=1}^{d_k} K(x_{q'}^{l_k}, y_l^{j_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k} + c_{j_k+1} - c_{j_k}) \sum_{m=1}^{d_k} \Delta_{l_m}^{I_{m'}^{k+1}} W_m^{k+1}. \quad (24)$$

Making use of $K(x_{q'}^{l_k}, y_l^{j_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k}) = K(x_{q'}^{l_k}, y_l^{j_k} + c_{j_k+1} - c_{j_k}, y_l^{j_k})$ and $K(x_{q'}^{l_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k})$, and reorganizing some terms, there holds

$$l_{m'}^{k+1} \approx g_{m'}^{k+1} + \sum_{p',q'=1}^{d_k} \Delta_{l_k}^{I_{p',q'}} K(x_{m'}^{l_k} + c_{P(j_k+1)}, y_l^{j_k}) \sum_{j_k \in \mathcal{P}(P(j_k+1))} \sum_{u,v=1}^{d_k} \Delta_{l_k}^{I_{u,v}} \sum_{l=1}^{d_k} K(x_{q'}^{l_k}, y_l^{j_k} + c_{P(j_k+1)} - c_{j_k}, y_l^{j_k}) \sum_{m=1}^{d_k} \Delta_{l_m}^{I_{m'}^{k+1}} W_m^{k+1}, \quad (25)$$

which provides a recursive formula for the upward pass. In the same fashion as for the monolevel version, we then compute

$$\hat{H}_{l'}^{\kappa} := \sum_{m'=1}^{d_{l'}} \Delta_{l',m'}^{I_{l'}} H_{l'}^{m'}, \quad (26)$$

for all box $I_{l'}^{\kappa}$ at level $\kappa$ and all $1 \leq l' \leq d_{l'}$.  

3.4.4 Algorithm and complexity

Using the recursion formulae derived above, the multilevel procedure is detailed in Algorithm 3.
The EIFMM is an interpolation-based FMM with the following characteristics:

1. Any translation invariant kernel can be considered. Depending on the number of terms in the EIM approximation in the precomputation stage, we can directly deduce the performance of the EIFMM: if the convergence of the EIM is very fast, the EIFMM will be very effective, and conversely.
2. Any number of interpolation points can be used at each level of the tree, not only an integer number per dimension.
3. The interpolation scheme is kernel dependent, unlike for instance the Chebychev interpolation. The procedure should capture any irregularity of the kernel better.
Table 4: Complexity of each step of Algorithm 3 (for the most expensive level) and of the near interactions term; \( n_I \) denotes the maximum number of elements in the interaction list of a box (4 in 1D, 40 in 2D and 316 in 3D).

than a fixed basis interpolation procedure, since the basis functions of the EIM are based on evaluations of the kernel itself.

- The learning procedure of the EIM is done directly in the right space: for a 3D procedure, a low-rank approximation of the kernel is searched directly in 3D.
- The greedy procedure enables to chose the optimal number of interpolation to certify the error on the training set. For inhomogeneous kernels, the number of interpolation points is optimized at each level of the tree.
- For homogeneous kernels, one EIM is done once and for all. For other kernels, the EIM procedures to be carried out depend on the tree (size of the boxes, depth).

4 Optimizing the overall complexity

4.1 Precomputations for the M2M and L2L steps

Recall that when using an EIM approximation, there holds \( \Delta = B^{-t} \Gamma^{-1} \), where the matrices \( B \) and \( \Gamma \) are triangular and constructed in a precomputation step. In practice, the condition number of the matrix \( \Gamma \) worsens as the EIM approximation gets more accurate. It is well known in linear algebra that when a matrix \( \Gamma \) is ill-conditioned, solving the linear system \( \Gamma x = b \) for some \( b \in \mathbb{R}^d \) provides a result much less polluted by numerical errors than first inverting the matrix \( \Gamma \) and then computing the matrix vector product \( \Gamma^{-1}b \). Since the matrices \( \Gamma \) and \( B \) are triangular, computing \( \Delta h = y \) by first solving \( \Gamma x = b \) and then solving \( B^t y = x \) is of the same complexity \( d^2 \) as the direct matrix-vector product.
Consider step 2 in Algorithm 3 at level $k$:

$$W_m^{j_k} = \sum_{\rho,q=1}^{d^{k+1}} \Delta_{\rho,q}^{j_k+1} \sum_{j^{k+1} \in I_C(\rho,q) \cap (j^{k+1})} K(x_m^\rho + c_{j^k} - c_{j^{k+1}}, y_p^q) W_q^{j^{k+1}}.$$  

We see that $W_m^{j_k} = \sum_{j^{k+1} \in I_C(\rho,q)} K_I(j_k,j^{k+1}) \Delta_{\rho,q}^{j_k+1} W_q^{j^{k+1}}$, where $K_m^{j_k,j^{k+1}} = K(x_m^\rho + c_{j^k} - c_{j^{k+1}}, y_p^q)$, $1 \leq m \leq d^k$, $1 \leq p \leq d^{k+1}$. The matrix $K_{M2M}^{I_k,j^{k+1}} := K_I(j_k,j^{k+1}) \Delta_{\rho,q}^{j_k+1} W_q^{j^{k+1}}$ can be precomputed as $(K_I(j_k,j^{k+1}) \Delta_{\rho,q}^{j_k+1} W_q^{j^{k+1}})^T$, where each matrix-vector product for each column of $(K_I(j_k,j^{k+1}) W_q^{j^{k+1}})^T$ is computed solving linear systems involving $B$ and $\Gamma$ matrices to preserve numerical accuracy, as explained in the previous paragraph. Notice that $K_{M2M}^{I_k,j^{k+1}}$ only depends on the relative position and $I_k$ and $j^{k+1}$. Since $j^{k+1}$ is a child of $I_k$, there are actually only $2^D$ different operators $K_{M2M}^{I_k,j^{k+1}}$, where $D$ denotes the dimension of the space containing the particles. We denote them $K_{M2M}^i$, $1 \leq i \leq 2^D$, and step 2 in Algorithm 3 at level $k$ is reduced to

$$W_m^{j_k} = \sum_{i=1}^{2^D} K_{M2M}^i W_q^{j^{k+1}}, \tag{27}$$

where $j^{k+1}$ denotes the $i$th child of $I_k$. This step if now of complexity $d^2 2^D (2^D)^k$ at level $k$, and the leading order of step 2 in Algorithm 3 is $d^2 2^D (2^D)^{k-1} = d^2 (2^D)^{k}$.

The same optimization is done for step 5 in Algorithm 3 reducing the complexity of this step to the order $d^2 (2^D)^{k}$.

### 4.2 Optimization of the M2L step

It is well known that the M2L step is the most expensive one. Numerous efforts have been made to reduce the execution time of this step without degrading the accuracy of the overall result, see in particular [17]. We use the optimization denoted SArcmp in [17]. It consists of a bivariate ACA applied to the collection of all the M2L operators at each level, followed by a truncated SVD. The bivariate ACA and truncated SVD is then applied for each M2L operator at each level to increase further the compression. The procedure is detailed for symmetric kernels for completeness of the presentation.

Consider a level $k$ and the collection of all the M2L operators at this level. Consider a level $k$, a box $I_k$ of the tree at this level $k$, and a box $J_k$ in the interaction list of $I_k$. The vector $\delta := c_{I_k} - c_{J_k}$ only depends on the relative position of the boxes $I_k$ and $J_k$.

Therefore, there are only $n_I = 7D - 3D$ different M2L matrices $K_{i,j}^k := K(x_i^k, y_j^k + \delta)$ per level (we recall that $D$ denotes the dimension of the space containing the particles), see [18]. We suppose that EIM algorithms have been carried-out for a certain error bound $\epsilon$, leading to the choice of $d_k$ interpolation points. The M2L matrices are organized in one large matrix as follows $K_{\text{fat}} := \{K_{\delta_1}, K_{\delta_2}, \ldots, K_{\delta_{d_k}}\}$, where $K_{\text{fat}} \in \mathbb{R}^{d_k \times n_I d_k}$. Two rectangular matrices $U, V$ are computed by a bivariate ACA such that $\|UV\|_F \leq \epsilon \|K_{\text{fat}}\|_F$. 

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where \(| \cdot |_F\) denotes the Frobenius norm. Then, two QR decompositions are computed, such that \(U = Q_U R_U\) and \((V)^t = Q_V R_V\), and a SVD is computed on \(R_U (R_V)^t\). Denote \(s_i, 1 \leq i \leq d_k\), the singular values of \(R_U (R_V)^t\) in decreasing order, and \(U, V\) the unitary matrices such that \(R_U^t (R_V)^t = U \text{diag}(s) V\). The two following filters are applied: (i) keep the first \(j\) singular values such that \(s_j / s_0 \leq \epsilon \leq s_{j-1} / s_0\), (ii) keep the first \(j\) singular values such that \(\sum_{i=1}^{j} s_i / \sum_{i=1}^{d_k} s_i \geq 1 - \epsilon \geq \sum_{i=1}^{j-1} s_i / \sum_{i=1}^{d_k} s_i\). We denote \(U_{r_k}\) and \(V_{r_k}\) the first \(r_k\) columns of respectively \(U\) and \(V\). Following [11], we can show that the M2L step can be reduced to size \(r_k \times r_k\) (instead of size \(d_k \times d_k\)) matrix-vector products involving the matrices \(C^\delta := U_{r_k}^T K^\delta U_{r_k}\), plus low complexity pre- and post-processing steps.

Then, the same compression is applied locally for each compressed M2L operator \(C^\delta\). This time, the bivariate ACA is applied on each \(C^\delta\), producing the rectangular matrices \(U\) and \(V\). The QR decompositions, SVD and filters are applied in the same fashion, selecting the singular values \(s_k\). The rectangular matrices \(U_{s_k}\) and \(V_{s_k}\) are constructed, and a diagonal matrix \(S_{s_k}\), whose diagonal entries are the square roots of the selected singular values, is constructed. Then, we construct \(U_{s_k} = Q_U U_{s_k} S_{s_k} \in \mathbb{R}^{r_k \times s_k}\) and \(V_{s_k} = S V_{s_k} Q_V^t \in \mathbb{R}^{s_k \times r_k}\), so that \(C^\delta\) is approximated by \(U_{s_k} V_{s_k}\). Thus, size \(r_k \times r_k\) matrix-vector products involving the matrices \(C^\delta\) are replaced by two \(r_k \times s_k\) matrix-vector products involving the matrices \(U_{s_k}\) and \(V_{s_k}\).

5 Numerical experiments in 3D

5.1 Some elements on the implementation

The EIFMM has been implemented in C++, using the open source library scalfmm, see [8]. From [21], scalfmm is one of the fastest opensource library for FMM computations. We will mainly compare our implementation of the EIFMM to the Chebychev interpolation-based implementation in scalfmm, which follows the Black-Box FMM [11]. In our code, the EIM precomputation and the SArcmp precomputation steps are performed in C++ using BLAS and LAPACK, and store in binary files. These precomputations are then read by the modified scalfmm library, using also BLAS for the basis linear algebra operations.

5.2 Test-cases

We consider sets of points included in \(\Omega = (-0.5, 0.5)^3\), randomly taken following (i) a uniform law in \(\Omega\), (ii) a uniform law on the sphere of radius 0.5 and (iii) a modification of the set (ii) in an ellipsoid, see Figure 6.

When comparing runtimes, we have to make sure that the Black-Box FMM is used in an optimal way. There are two parameters to choose: the number of interpolation points per dimension and the accuracy \(\epsilon_c\) of the compression. First, we chose 3 interpolation points per dimension and compute the relative error with \(\epsilon_c = 10^{-15}\). Then, if this relative error is smaller than the desired one, we search by dichotomy the largest value
of the $\epsilon_c$ so that the relative error is smaller or equal to the desired one. Otherwise, we increase the number of interpolation points per dimension by one and repeat the process. That way, the runtimes comparison is fair in the sense that Block-Box FMM is not artificially slowed down by a too large number of interpolation points together with a too large value for $\epsilon_c$. Notice that this trick is necessary since we do not know in advance how the Chebyshev interpolation will perform in practice for a new kernel, while for the EIFMM, the error estimate automatically selects the right number of interpolation points.

5.3 Performance for the Laplace kernel

5.3.1 Accuracy and memory

We first check the results of Figure 3 by plotting the relative error with respect to the number of interpolation points used by the approximation formula of the far-field behavior of the kernel. We consider the FMM summation (1) with only 1% of the $\sigma_j$ having nonzero values, to compute the reference values with reasonable execution times. The EIFMM achieves better accuracy with fewer interpolation points. The M2L operators are not compressed (in the Black-Box implementation in scalfmm, a compression is actually carried-out, but we set its accuracy to $10^{-15}$).

Figure 7 shows the number of interpolation points per dimension required by EIFMM and Black-Box FMM to ensure given levels of accuracy of the FMM summation. With the EIFMM, the multipole and local expansions (respectively the vectors $W_m$ and $l_m'$ in Algorithm 3) require less memory than the Black-Box FMM, see Table 6.

5.3.2 Runtimes

In this section, we compare runtimes of the FMM summation using the Black-Box FMM and the EIFMM. The computation are carried out in sequential, on a laptop with 4GB of RAM and a Intel Core i5 CPU at 2.76 GHz. The reported runtimes do not contain
Figure 7: Comparison of the accuracy of the Black-Box FMM (solid lines) and the EIFMM (dashed lines) on the sets of points following the repartition represented in Figure 6; black: $10^6$ random point, blue and red: 992,046 points respectively on a sphere and an ellipsoid.

| Relative accuracy | $3 \times 10^{-4}$ | $4 \times 10^{-5}$ | $5 \times 10^{-6}$ | $7.5 \times 10^{-7}$ |
|-------------------|------------------|------------------|------------------|------------------|
| Black-Box FMM     | 27               | 64               | 125              | 216              |
| EIFMM             | 27               | 46               | 77               | 122              |

Table 5: Number of interpolation points required for both FMM algorithms to produce results of the same accuracy.

the times required to build the tree, nor the EIM, M2L compression, M2M and L2L precomputations. For the EIFMM, we use the SArcmp compression for the M2L operators, as described in Section 4.2. For the Black-Box FMM, we use a so-called symmetric M2L compression, based on local SVD for each M2L operator. The symmetric M2L compression exploit the symmetry of the Chebychev nodes to express the M2L step as matrix-matrix products, and even if the complexity of this step is not improved, runtimes are drastically improved due to better reuse of memory cache by the processor. Proposed in [17], the symmetric compression is currently the most efficient compression strategy for the Black-Box FMM applied to the Laplace kernel.

First, since the approximation [8] used in EIFMM has four summations instead of two for Black-Box FMM, the steps 3 and 6 in Algorithm 3 for EIFMM are not present in Black-Box FMM. Moreover, we notice in our numerical experiences that step 1 in Algorithm 3 for EIFMM is slower than the corresponding step in Black-Box FMM. Hence, there is a competition between these facts and the complexity reduction enabled by the smaller number of interpolation points for the EIFMM.

In Figure 8 are represented execution time with respect to the relative error on the FMM summation for the Laplace kernel, for the symmetric Black-Box FMM, the
| Relative accuracy | $3 \times 10^{-4}$ | $4 \times 10^{-5}$ | $5 \times 10^{-6}$ | $7.5 \times 10^{-7}$ |
|-------------------|-------------------|-------------------|-------------------|-------------------|
| EIFMM memory savings | 0% | 28% | 38% | 43% |

Table 6: Memory saving in the storage of the multipole and local expansions induced by the use of EIFMM, with respect to the Black-Box FMM, for some relative accuracy on the FMM summation. These quantities are not measured, they represent the theoretical gain induced by the fewer interpolation points needed by EIFMM.

EIFMM and the fastest algorithm available in scalfmm. This last algorithm is dedicated to the Laplace kernel, explaining why it performs better than the other two. The test-case corresponds to $10^6$ random points taken in the unity cube, organized in a 6-level tree, see Figure 6, left picture. Although memory savings are reported with EIFMM, the execution times are similar for EIFMM and Black-Box FMM.

![Figure 8](image)

Figure 8: Execution time with respect to the relative error on the FMM summation for the Laplace kernel; black: symmetric Black-Box FMM, blue: EIFMM, red: fastest spherical algorithm available in scalfmm.

### 5.4 Performance for some inhomogeneous kernels

The advantages of the EIFMM mainly apply to inhomogeneous kernels, for which the error estimation allows the selection of an optimal number of interpolation points at each level of the tree by the EIM.

The three test-cases presented in Figure 6 are considered: $10^6$ random points in the unity cube with a 6-level tree (denoted "cube"), 992,046 points at the surface of a sphere and an ellipsoid, with respectively 8-level and 9-level trees (denoted respectively "sphere" and "ellipsoid").

Figures 9, 10 and 11 present execution times with respect to the relative error on the FMM summation, respectively for the kernels $\cos \frac{2\pi r}{r}$, $e^{-r^2}$ and $\sqrt{r^2 + 1}$, for the three
test-cases cube, sphere and ellipsoid. In these figures, missing data correspond to cases requiring more memory than available with our computer. Due to the memory savings enabled by the use of EIFMM, these cases are only computable by EIFMM: our computer does not have enough memory for Black-Box FMM to be used. For the three kernels, and especially the last two, the EIFMM is much faster than the Black-Box FMM, because the error estimation and the greedy procedure in EIFMM allows the selection of an optimal number of interpolation points at each level of the tree. For instance, for the kernel $e^{-r^2}$ on the ellipsoid and a relative error of $10^{-6}$, the Black-Box FMM needs 6 interpolation points per dimension (i.e. 216 interpolation points), whereas the EIFMM needs respectively 167, 74, 36, 21, 13, 10, 9, and 4 points at levels 2 to 9 of the tree. As we go deeper in the tree, the interpolation problems become easier, and the EIM selects fewer points to produce an interpolation of the same quality.

Figure 9: Execution time with respect to the relative error on the FMM summation for the kernel $\cos 20r/r$, black: symmetric Black-Box FMM, blue: EIFMM. From to to bottom and left to right: cube, sphere and ellipsoid test-cases.

Remark 5.1 In EIFMM, the kernel has to be evaluated on the fly in steps 1 and 7.
of Algorithm 3, whereas in the Black-Box FMM, Chebychev polynomials are evaluated at these steps. As a consequence, the performance of the EIFMM is affected by the time required to evaluate the kernel itself: that is why the gains for the kernel $\cos 20r$ in Figure 9 and less important than for kernels $e^{-r^2}$ and $\sqrt{r^2 + 1}$ in Figures 10 and 11.

6 Conclusion and outlook

This work introduces a new Fast Multipole Method (FMM) using a low-rank approximation of the kernel based on the Empirical Interpolation Method, called the Empirical Interpolation Fast Multipole Method (EIFMM). The proposed multilevel algorithm is implemented in scalfmm, a FMM library written in C++. Precomputation steps and the compression of M2L operators, also programmed in C++, enable good performance: on the Laplace kernel, the execution times are equivalent to the one measured using
Figure 11: Execution time with respect to the relative error on the FMM summation for the kernel \( \sqrt{r^2 + 1} \), black: symmetric Black-Box FMM, blue: EIFMM. From top to bottom and left to right: cube, sphere and ellipsoid test-cases.

the Black-Box FMM with the best available compression routine for the M2L operators. The important feature of the EIFMM is a built-in error estimation of the interpolation error made by the low-rank approximation of the far-field behavior of the kernel. As a consequence, the algorithm automatically selects the optimal number of interpolation points required to ensure a given accuracy for the result, leading to important gains for inhomogeneous kernels, for which the difficulty of the approximation varies from one level of the tree to another.

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