Multicenter method

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In this abstract, we present a new method, called the multicenter method, that computes efficiently a long range force in a N body problem. Being kernel-independent, it is more general than the well known multipole method. The multicenter method is based upon the idea of defining a subset of sources which we call "centers" and computing a weighted contribution of these centers only. Unlike the multipole method, we have several centers and we compute a polynomial of degree 1 (the number of selected sources depends on the expected accuracy). In this abstract, we will present some of the linear algebra issues raised by the multicenter method : how the centers and the associated weights are defined. We will also present some results on the computation of the electromagnetic field lines which was one of the physical contexts for this work.

1 Define the centers

Let us define a set of n sources $\mathcal{K}$ such that the sources lie inside a ball $B_{\mathbf{c},\mathrm{r}}$ ($\mathbf{c}$ being the center and r the radius of the ball) and a set $\mathcal{T}$ of n target points distributed on a sphere $S_{\mathbf{c},\alpha r}$ with $\alpha \in \mathbb{R}$, $\alpha > 1$, α is the separation criterion between the sets $\mathcal{K}$ and $\mathcal{T}$. The number of target points should be greater than the number of source points.

The idea is to compute the matrix of the kernels between the source points and some target points far away enough from the source. More precisely, we compute the matrix $A_{\mathcal{T},\mathcal{K}}$ of the kernel between the 2 sets of points $A_{\mathcal{T},\mathcal{K}}(i,j) = k(x_{T_i}, x_{K_j})$ and evaluate its rank in order to determine the leading source points i.e. the centers. When the distance between the sets $\mathcal{K}$ and $\mathcal{T}$ increases, the rank of $A_{\mathcal{T},\mathcal{K}}$ decreases, therefore, we need fewer source points to get a good representation of the entire source set. In order to find those points, we perform a QR factorization with column pivoting of $A_{\mathcal{T},\mathcal{K}}$:

$$A_{\mathcal{T},\mathcal{K}} = Q_{\mathcal{T},\mathcal{T}} \begin{bmatrix} R_{\mathcal{K},\mathcal{K}} \\ 0_{\mathcal{T}\setminus\mathcal{K},\mathcal{K}} \end{bmatrix} \Pi^T_{\mathcal{K},\mathcal{K}} \tag{1}$$

where Q is orthogonal, R is upper triangular and Π is a permutation matrix such that :

$$|r_{1,1}| \geq |r_{2,2}| \geq \cdots \geq |r_{n_K,n_K}| \text{ and } \forall i\, |r_{i,i}| \geq ||R_{i:j,j}||_2\, j = i+1, \ldots, n_K \tag{2}$$

Let us define a low-rank threshold ϵ, the rank of $A_{\mathcal{T},\mathcal{K}}$ is given by :

$$r(\epsilon) = min(r \in \mathbb{N} : \|R_{r,r:n_K}\|_2 < \epsilon\, max(\|R_{i,i:n_K}\|_2)_{i=1,\ldots,n_K}) \tag{3}$$

The leading r columns of $A_{\mathcal{T},\mathcal{K}}\Pi_{\mathcal{K},\mathcal{K}}$ approximate $A_{\mathcal{T},\mathcal{K}}$ to an accuracy $O(\sigma_{r+1(A)})$. Let's define the matrix restricted to the leading columns r, $A_{\mathcal{T},\mathcal{C}}$: $A_{\mathcal{T},\mathcal{K}}\Pi_{\mathcal{K},\mathcal{K}} = [A_{\mathcal{T},\mathcal{C}} A_{\mathcal{T},\mathcal{K}\setminus\mathcal{C}}]$. The r first points of $\mathcal{K}$ define the r centers.

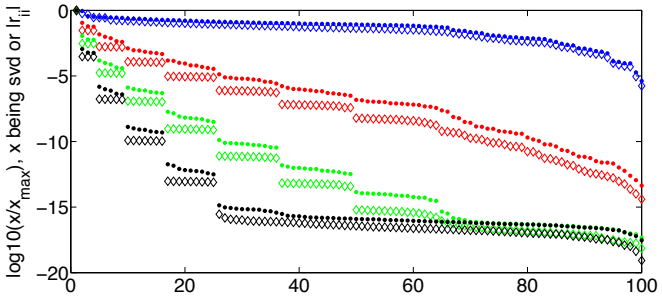

Figure 1: Singular values of $A_{\mathcal{T},\mathcal{K}}$

As a first simple example, we consider a set of source points $\mathcal{K}$ homogeneously distributed inside a ball and a set of target points $\mathcal{T}$ homogeneously distributed on a sphere such that $R_{sphere} = \alpha R_{ball}$ ($\alpha = 1, 10, 100, 1000$ for the blue lines, the red ones, the green ones and the black ones respectively). Figure (1) shows the singular values of the kernel matrix $A_{\mathcal{T},\mathcal{K}}$ (represented by ♦) as well as the values $|r_{ii}|$ resulting from the RRQR of $A_{\mathcal{T},\mathcal{K}}$ (represented by .), see equation (1).
The singular values are well separated as long as the set of points $\mathcal{T}$ is far enough from the source points set. Depending on the tolerance ϵ, we obtain either 1, 4, 9, 16... centers. The values $|r_{ii}|$ provided by (1) follow the same behaviour than the singular values except from the clustering which is not as good.

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2 Define the weights

As seen before, the rank of $A_{\mathcal{T},\mathcal{K}}$ allows to define a subset of the source points : the centers. Once the centers are defined, the correlation between them and the other source points are defined by a "barycentric matrix". In order to minimize the error, the barycentric $B_{\mathcal{C},\mathcal{K}}$ matrix is defined as follows :

$$A_{\mathcal{T},\mathcal{K}}\Pi_{\mathcal{K},\mathcal{K}} = \begin{bmatrix} Q_{\mathcal{T},\mathcal{C}} & Q_{\mathcal{T},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix} \begin{bmatrix} R_{\mathcal{C},\mathcal{C}} & R_{\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \\ 0_{\mathcal{K}\setminus\mathcal{C},\mathcal{C}} & R_{\mathcal{K}\setminus\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix} \tag{4}$$

$$\approx \begin{bmatrix} Q_{\mathcal{T},\mathcal{C}}R_{\mathcal{C},\mathcal{C}} & Q_{\mathcal{T},\mathcal{C}}R_{\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix} \tag{5}$$

$$= Q_{\mathcal{T},\mathcal{C}}R_{\mathcal{C},\mathcal{C}} \begin{bmatrix} I_{\mathcal{C},\mathcal{C}} & R_{\mathcal{C},\mathcal{C}}^{-1}R_{\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix} \tag{6}$$

$$= A_{\mathcal{T},\mathcal{C}}B_{\mathcal{C},\mathcal{K}} \tag{7}$$

where $B_{\mathcal{C},\mathcal{K}} = \begin{bmatrix} I_{\mathcal{C},\mathcal{C}} & \widehat{R}_{\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix} \equiv \begin{bmatrix} I_{\mathcal{C},\mathcal{C}} & R_{\mathcal{C},\mathcal{C}}^{-1}R_{\mathcal{C},\mathcal{K}\setminus\mathcal{C}} \end{bmatrix}$

By summing up the row entries of $B_{\mathcal{C},\mathcal{K}}$, we obtain the weight associated to each center. If the matrix $A_{\mathcal{T},\mathcal{K}}$ were full rank, then there would be as many centers as source points in set $\mathcal{K}$ and the barycentric matrix $B_{\mathcal{C},\mathcal{K}}$ would be the identity matrix. To compute the resulting long-range force at one point P far away from the sources, we only need to compute the sum of the weighted interactions between P and the centers.

3 Results

In this section, we compare 3 methods : the multipole method, the multicenter method and the direct method which consists in taking into account the contributions of each source. Unlike the multipole and the multicenter methods, the direct method does not do any approximation and, therefore, constitues our reference.

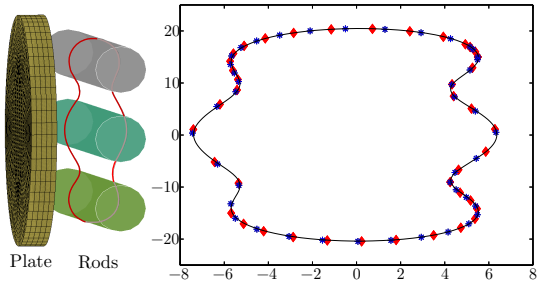

Figure 2: Direct method: −, multipole method: ♦, multicenter method: ∗

Let's consider a conductor formed by 3 rods and a plate. An electric current circulates into the 3 tubes which induces a current in the plate. An electromagnetic field is generated around the 3 tubes. We want to visualize a magnetic field line close to the rods. To do that, we need to solve the magnetic field line equations which requires to compute the magnetic field $\vec{B}$. $\vec{B}$ is the sum of the contributions of each source point which can be computed either directly or by an approximation method (FMM or multicenter). Figure (2) shows one of the magnetic field lines generated around the rods on the left hand side. On the right hand side, only the magnetic field line is represented, the results given by the three methods are placed on top of each other. Both multipole and multicenter methods ensure a relatively good accuracy, the results are comparable to those obtained with the direct method.

For the next problem, we want to study the interaction between two sets of points instead of one set of points and one point only. It is of importance when it comes to build the BEM-FEM system to solve for the electromagnetic fields for example. The BEM system is dense and solved through an iterative method such as GMRES or PCG, therefore using either the FMM or the multicenter method can be useful to accelerate the assembly of the matrix as well as the operations for the matrix-vector product.

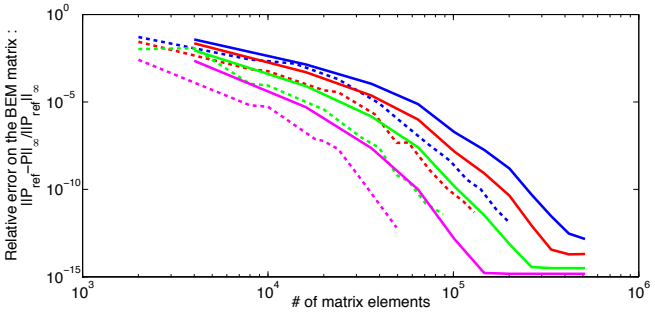

Figure 3: Multicenter versus FMM

Here, we consider 2 cubes of 1000 points each. We want to compute the kernel matrix between those cubes with both methods and compare their cost in terms of matrix-vector product. Figure (3) shows the relative error induced on the kernel matrix against the number of entries in the matrix for different separations (12, 20, 50, 200 for the blues lines, the red ones, the green ones and the pink ones respectively). The dashed lines correspond to the multicenter method whereas the solid lines represent the FMM. For a given distance between the cubes, the multicenter method requires less entries than the FMM to reach the same accuracy on the kernel matrix therefore the low rank representation obtained is better and the operation for the matrix-vector multiply will be more efficient.

In order to improve the efficiency of the matrix-vector product, following the example of the FMM, we intend to add the multilevel aspect to the multicenter method. Work is in progress.