Boundary interpolation vs boundary elements: theory and some applications

C. Gáspár
Department of Mathematics, Széchenyi István University, Hungary

Abstract

Domain and boundary type meshless methods based on the Direct Multi-Elliptic Interpolation Method are presented. The approach is equivalent to a special RBF-method but completely avoids the solution of large, full and ill-conditioned systems, thus, the computational cost is significantly reduced. The method is illustrated through the example of the usual Poisson problem. Both Dirichlet and Neumann boundary conditions are investigated. The domain version of the method results in particular solutions, while the boundary version can be applied to solve homogeneous problems. Along Neumann boundaries, either off-boundary points can be introduced or a boundary reconstruction technique based on boundary interpolation can be applied. Some further possible applications are also outlined.

Keywords: meshless methods, RBF-methods, direct multi-elliptic interpolation, quadtrees, multi-level methods.

1 Introduction

In recent years, a number of meshless (or meshfree) methods have been developed to solve various partial differential equations (PDEs). The need for the meshless methods is obvious since one of the most difficult task in finite element modelling is the proper (re)meshing. This essentially remains the case when a kind of boundary element techniques is applied, though the problem of mesh generation is often restricted to the boundary.

The meshless methods circumvent the problem of domain as well as boundary mesh generation. At present they seem to form a ’new generation’ of computational methods due to their attractive simplicity and dimension-independence. On the other hand, however, most of the popular meshless techniques suffer from a common computational disadvantage. Namely, they generally lead to large, dense
and often severely ill-conditioned matrices. Therefore they can be hardly applied to large problems, or, rather, sophisticated supplementary techniques (fast multipole evaluation [9], [2], overlapping or non-overlapping domain decomposition etc.) are needed in order to overcome these computational difficulties, which can undermine the obvious advantages of their meshless character. For instance, when the method of radial basis functions (RBF) is applied, the use of globally supported RBFs (e.g. method of multiquadrics (MQ) or thin plate splines (TPS)) exhibit excellent approximation properties, but introduce inherently dense matrices. This remains the case also in the method of fundamental solutions (MFS, see [8], [1]), the recently developed boundary knot method (BKM, see [3], [4]) and so forth.

Most of the meshless methods are based on some scattered data interpolation technique. The proper choice of the applied interpolation is of primary interest. In this paper, we intend to present the applicability of the Direct Multi-Elliptic Interpolation in constructing meshless methods. Here the interpolation function is obtained by solving a higher order auxiliary PDE supplied with the interpolation conditions as special boundary conditions, see [6], [7]. To solve this auxiliary problem, robust multi-level quadtree-based methods ([5], [10]) are used. This approach is equivalent to a special RBF-method (based on the fundamental solution of the applied PDE) but makes it possible to completely avoid the large, dense and ill-conditioned systems and reduces the memory requirement as well as the computational cost typically to $O(N \log N)$ where $N$ denotes the number of interpolation points. To derive meshless boundary methods, a boundary version of the above approach is used. The treatment of Dirichlet boundary conditions is quite straightforward, but that of Neumann conditions is not. To handle Neumann boundaries, a modified method is developed which exhibits strong similarities to the MFS, however, the large, ill-conditioned matrices are still avoided. An alternative approach based on the reconstruction of the boundary and the interpolation of boundary conditions is also presented. Finally, we outline several problems where the above methods can be successfully applied.

2 The Direct Multi-Elliptic Interpolation

First we briefly summarize the main results concerning the Direct Multi-Elliptic Interpolation. For details, see [6], [7].

Let $x_1, x_2, ..., x_N \in \mathbb{R}^2$ be arbitrary distinct points in the bounded domain $\Omega_0$ and let $f_1, f_2, ..., f_N \in \mathbb{R}$ be predefined values. The Direct Multi-Elliptic Interpolation Method defines an interpolation function $f : \Omega_0 \to \mathbb{R}$ as the solution of the following PDE:

$$L f = 0 \quad \text{in} \quad \Omega_0 \setminus \{x_1, x_2, ..., x_N\}$$

(in the sense of distributions), supplied with the interpolation conditions:

$$f(x_k) = f_k \quad (k = 1, 2, ..., N)$$

Here $L$ is a properly defined partial differential operator of order $2m$ ($m \geq 2$, integer), typically an iterated elliptic operator of the form $\prod_{j=1}^{m} (\Delta - c_j^2 I)$, where
$c_1, ..., c_m$ are scaling parameters and $I$ denotes the identity operator. The solution is sought in the Sobolev space $H_0^m(\Omega_0)$ i.e. along the boundary of $\Omega_0$, homogeneous boundary conditions are prescribed:

$$f|_{\partial\Omega_0} = 0, \quad \frac{\partial f}{\partial n}|_{\partial\Omega_0} = 0, \quad ..., \quad \frac{\partial^{m-1} f}{\partial n^{m-1}}|_{\partial\Omega_0} = 0,$$

(3)

Due to the embedding theorems, $H_0^m(\Omega_0)$ consists of continuous functions, and the pointwise conditions of (2) do not make the problem ill-posed.

Problem (1)-(3) can be reformulated in a variational form, for which existence, uniqueness and approximation theorems have been proved. The interpolation function has the minimal norm among the functions of $H_0^m(\Omega_0)$ satisfying the interpolation conditions (2) with respect to a special norm which is equivalent to the original norm of $H_0^m(\Omega_0)$.

**Remark:** Along $\partial \Omega_0$, any other regular boundary condition can be prescribed, which causes only minor changes in the theory. Moreover, if $m > 2$, not only the values of $f$, but its derivatives (up to the $(m-2)$th order) can also be prescribed, and the Direct Multi-Elliptic Interpolation problem still remains well-posed (Hermite-type interpolation).

The connection between the Direct Multi-Elliptic Interpolation and the RBF-methods is clearly shown by a representation theorem, which states that the interpolation function $f$ is uniquely represented in the form:

$$f(x) = w(x) + \sum_{j=1}^{N} \beta_j \Phi(x - x_j),$$

(4)

where $w$ is a function satisfying $Lv = 0$ everywhere in $\Omega_0$ (including the interpolation points), and $\Phi$ is the fundamental solution of $L$.

If the function $\Phi$ is a sufficiently rapidly decreasing function, which is often the case, the domain $\Omega_0$ can be chosen to be the whole plane $\mathbb{R}^2$, and the regular term $w$ of the representation vanishes. In this case, the representation (4) is simply an RBF-interpolation formula based on the fundamental solution of the operator $L$ as an RBF. Consequently, the theory of the Direct Multi-Elliptic Interpolation immediately guarantees the applicability of this RBF-method. However, unlike the classical RBF-methods, one need not generate and solve any system of equations in order to determine the a priori unknown coefficients $\beta_1, \beta_2, ..., \beta_N$. Once the Direct Multi-Elliptic Interpolation function has been determined, these coefficients can be computed by the numerical implementation of the formula

$$Lf = \sum_{j=1}^{N} \beta_j \delta_{x_j},$$

(5)

which is a straightforward consequence of (4). Here $\delta_{x_j}$ denotes the Dirac distribution concentrated to the point $x_j$. It should be pointed out, however, that, in practice, one almost never needs the values of $\beta_j$. Instead, it is the interpolation functions that is in fact important.
When implementing the Direct Multi-Elliptic Interpolation, the higher order PDE (1)-(2) has to be solved. At first glance, this task seems much more complicated than the original interpolation problem. Exploiting the fact, however, that the domain $\Omega_0$ can be defined in a practically arbitrary way, especially robust techniques like the multi-level quadtree-(QT-)based methods can (and should) be applied [5]. These methods are based on finite volume schemes defined on a non-uniform cell system which has local refinements at the interpolation points. Since the whole procedure including the QT-cell generation as well as the multi-level solution algorithm is completely controlled by the interpolation points only, in this sense, the method can be considered a meshfree technique.

The simplest multi-elliptic interpolation method is based on the biharmonic operator: $L := \Delta \Delta$ (biharmonic interpolation). A more general choice is: $L := (\Delta - c^2 I)^2$ (bi-Helmholtz interpolation), where $c$ is a scaling constant. Unlike the biharmonic interpolation, now the corresponding fundamental solution is rapidly decreasing, i.e. ’almost compactly supported’. The size of the ’essential support’ can be controlled by the scaling parameter $c$. Table 1 lists a few multi-elliptic operators and their fundamental solutions in 2D ($K_0$ and $K_1$ denote the usual modified Bessel functions). Note that the fundamental solutions have even simpler form in 3D.

### 3 Meshless formulations

Now we derive meshless methods based on the Direct Multi-Elliptic Interpolation through the model problem:

$$\Delta u = f \quad \text{in } \Omega, \quad u|_{\Gamma_1} = u_1, \quad \frac{\partial u}{\partial n}|_{\Gamma_2} = v_2,$$

(6)

where $\Gamma_1$, $\Gamma_2$ form a non-overlapping decomposition of the boundary $\partial \Omega$ allowing $\Gamma_1$ or $\Gamma_2$ to be empty. To discretize the problem, let us define interpolation points in the domain $(x_1, x_2, ..., x_N)$, and also on the boundaries $\Gamma_1 (x_1', x_2', ..., x_{N_1}')$ and $\Gamma_2 (x_1'', x_2'', ..., x_{N_2}'')$. 
\[ \Gamma_2 \left( x''_1, x''_2, \ldots, x''_{N_2} \right) \]. Using the idea of particular solutions, the solution of (6) is expressed as a sum of a particular (inhomogeneous) solution and a homogeneous solution: \( u = u_0 + w \), where:

\[ \Delta u_0 = f \quad \text{in} \ \Omega_0 \supset \Omega \] (7)

without specifying any boundary conditions, and:

\[ \Delta w = 0 \quad \text{in} \ \Omega, \quad w|_{\Gamma_1} = u_1 - u_0|_{\Gamma_1}, \quad \frac{\partial w}{\partial n}|_{\Gamma_2} = v_2 - \frac{\partial u_0}{\partial n}|_{\Gamma_2} \] (8)

### 3.1 Domain problems

Equation (7) is usually solved by applying the dual reciprocity principle, where first the function \( f \) is to be interpolated. Using the Direct Multi-Elliptic Interpolation instead of a traditional RBF-method, a direct multi-elliptic e.g. biharmonic interpolation has to be performed:

\[ \Delta^2 f = 0 \quad \text{in} \ \Omega_0 \setminus \{ x_1, x_2, \ldots, x_N \} \] (9)

where the values \( f(x_k) \) are prescribed at the interpolation points. Once the values of the interpolation function have been computed at each QT-cell center, the particular solution \( u_0 \) is obtained by solving (7) using the same QT-cell system in \( \Omega_0 \). Thus, the solution of the inhomogeneous problem is converted to a biharmonic plus a Poisson problem (both of them are solved by multi-level techniques). Note that the algorithm mimics the evaluation of a Newtonian potential, however, in a meshless way.

### 3.2 Boundary problems

For the homogeneous problem (8), two different approaches are presented.

#### 3.2.1 Solution by direct boundary interpolation

The solution of (8) is directly approximated by an interpolation technique based on the boundary points only. The idea is similar to the MFS (though the MFS uses some fictitious points outside of \( \Omega \) due to the singularities of the potentials generated by point sources) and also to the BKM (which uses nonsingular RBFs, therefore avoids the introduction of fictitious points). Using the philosophy of the Direct Multi-Elliptic Interpolation, the homogeneous solution \( w \) is approximated by a Laplace-Helmholtz interpolation function \( \tilde{w} \):

\[ \Delta(\Delta - c^2I)\tilde{w} = 0 \quad \text{in} \ \Omega_0 \setminus \{ x'_1, \ldots, x'_{N_1}, x''_1, \ldots, x''_{N_2} \} \] (10)

Since the Bessel function \( K_0 \) is a rapidly decreasing function, the fundamental solution of the Laplace-Helmholtz-operator \( \Delta(\Delta - c^2I) \) approximates the harmonic fundamental solution far from the origin (but is still continuous at the origin). This implies that the interpolation function \( \tilde{w} \) is (nearly) harmonic far from the boundary points i.e. inside of \( \Omega \), apart from a narrow vicinity of the boundary.
The key issue is the proper choice of the scaling parameter $c$. If $c$ is too large, weak singularities are generating at the interpolation points, which destroys the approximation of the interpolation along the boundary. If $c$ is too small, the approximation along the boundary is fairly good, but $\tilde{w}$ is far from being harmonic inside of $\Omega$. The correct analysis is lengthy, therefore omitted here. As a rule of thumb, the value of $1/c$ (the size of the ‘essential support’ of $K_0(rc)$) should not be below the characteristic distance of the neighboring boundary points.

The implementation of the Direct Multi-Elliptic Interpolation Method depends on the type of the boundary conditions.

**Dirichlet boundary conditions:** Along $\Gamma_1$, Eq. (10) is supplied with
\[
\tilde{w}(x'_k) = (u_1 - u_0)(x'_k), \quad k = 1, \ldots, N_1, 
\]
i.e. the homogeneous solution is directly approximated by the Laplace-Helmholtz-interpolation.

The method is illustrated through the following simple example. Let $\Omega_0$ be the unit square and consider the Laplace equation in a circle $\Omega \subset \Omega_0$ supplied with Dirichlet boundary condition. The exact solution is $u(x, y) = \frac{1}{2} - x + 2y$. Only 64 boundary nodes are used. Figure 1 shows two approximate solutions obtained by the Direct Multi-Elliptic Interpolation with two different scaling parameters. When $c = 500$ (case (a)), singularities are generated at the boundary interpolation points. The relative error measured in the discrete $L_2$-norm is $4.03\%$. When $c = 20$ (case (b)), no boundary singularities occur, but the inner approximation is poor (relative error: $12.64\%$). Setting $c := 180$, however, the relative error is reduced to $0.23\%$.

**Neumann boundary conditions:** Along Neumann boundaries, the above idea fails even if a higher order direct multi-elliptic interpolation is applied (based on e.g. the operator $\Delta(\Delta - c^2 I)^2$). Now the following strategy can be applied. Define new points $\bar{x}_1''$, $\ldots$, $\bar{x}_{N_2}''$ outside of $\Omega$ in the outward normal direction from $x_1''$, $\ldots$, $x_{N_2}''$ (off-boundary points), and solve (10) supplied with Dirichlet boundary conditions.
Figure 2: Solutions of the model problem by boundary multi-elliptic interpolation using off-boundary points. Mixed boundary conditions.

at the points $\bar{x}_1'', ..., \bar{x}_{N_2}''$ in such a way that the Neumann condition at the points $x_1'', ..., x_{N_2}''$ is enforced. This can be carried out by the iteration:

$$
\tilde{w}(\bar{x}_k'')_{improved} = \tilde{w}(\bar{x}_k'') + \omega \cdot \left( \frac{\partial \tilde{w}}{\partial n} - v_2 + \frac{\partial u_0}{\partial n} \right)(x_k''), \quad k = 1, ..., N_2
$$

(12)

with some relaxation parameter $\omega$. This iteration can obviously be incorporated in the multi-level solution procedure.

The procedure mimics the MFS based on the fictitious points $\bar{x}_1'', ..., \bar{x}_{N_2}''$ but the solution of dense, ill-conditioned systems is still avoided.

An example is shown in Figure 2. The model problem is again the Laplace equation defined on the same subdomain $\Omega$. The exact solution is $u(x, y) = \frac{1}{2} - x + 2y$. Here mixed boundary conditions are defined. Along the upper (resp. lower) half-circle, Dirichlet (resp. Neumann) boundary condition is given. The scaling parameter is $c = 180$, the distance between the Neumann points and the corresponding outer off-boundary points is $0.1$. The approximate solution exhibits extreme variations in the vicinity of the off-boundary points, but remains quite exact in the domain $\Omega$. This phenomenon is very similar to the behaviour of the MFS. The relative error measured in the discrete $L_2$-norm is $0.21\%$.

### 3.2.2 Solution by boundary reconstruction

Unlike the previous method, our first goal now is to reconstruct the boundary i.e. to find all the QT-cells lying along the boundary. Next, the boundary conditions have to be extended to these cells by boundary interpolation. Finally, in the rest of the QT-cell system, the original boundary problem (8) is to be solved using the same QT-based multi-level method. That is, in the last step, no direct multi-elliptic interpolation is performed. Note that the above reconstruction of the boundary does not mean the (re)construction of any boundary mesh structure.

The first step can be simply performed by solving the Laplace equation $\Delta z = 0$ supplied with Dirichlet boundary condition which is identically equal to 1. Along the boundary of the larger domain $\Omega_0$, zero Dirichlet boundary condition is imposed.
This auxiliary problem can be solved by a direct Laplace-Helmholtz interpolation discussed earlier, and we obtain the following algorithm:

- Perform a Laplace-Helmholtz interpolation method for the auxiliary Laplace equation i.e. solve:

\[
\Delta(\Delta - c^2 I)z = 0 \quad \text{in} \quad \Omega_0 \setminus \{x'_1, ..., x'_N_1, x''_1, ..., x''_{N_2}\}
\]

\[z(x'_k), z(x''_j) = 1, \quad k = 1, ..., N_1, \quad j = 1, ..., N_2, \quad z|_{\partial \Omega_0} = 0\]  

(13)

- With a given tolerance parameter \(\epsilon > 0\), find the QT-cells where \(z\) is not less than \(1 - \epsilon\). These cells are accepted as inner cells, the remaining cells are considered outer cells. Now find all the cells that have a neighboring cell of opposite type (boundary cells).

- By performing a direct multi-elliptic interpolation based on the boundary points, extend the boundary conditions to each boundary cell (including also the normal vectors along Neumann boundaries).

- Using the same QT-cell system, solve (8) directly.

In this way, the homogeneous Neumann condition can be treated much simpler than previously. If the homogeneous problem has the form:

\[
\Delta w = 0 \quad \text{in} \quad \Omega, \quad w|_{\Gamma_1} = w_1, \quad \frac{\partial w}{\partial n}|_{\Gamma_2} = 0,
\]

then it is sufficient to solve the more general elliptic equation

\[
\text{div } \sigma \text{ grad } w = 0 \quad \text{in} \quad \Omega_0, \quad w|_{\Gamma_1} = w_1, \quad w|_{\partial \Omega_0} = 0,
\]

(15)

where \(\sigma\) is identically 1 inside \(\Omega\) (i.e. in the inner cells) and zero outside (i.e. in the outer cells). The QT-based multi-level technique can be easily extended to that type of problems as can be seen in [5].

4 Further applications

In the previous section, the idea of Direct Multi-Elliptic Interpolation for constructing meshless methods was restricted to the Poisson problems. Now we outline some more fields of applications.

Modified Helmholtz equation. The meshless solution of the PDE

\[
(\Delta - k^2 I)u = f
\]

(16)

is expressed again as a sum of a particular (inhomogeneous) and a homogeneous solution (with modified boundary conditions): \(u = u_0 + w\). The particular solution is created in the same way as earlier. The construction of the homogeneous solution is now based on the multi-elliptic operator \((\Delta - k^2 I)(\Delta - c^2 I)\) (instead of the operator \(\Delta(\Delta - c^2 I)\)).
Time-dependent diffusion problems:

$$\frac{\partial u}{\partial t} - D \Delta u = f$$ \hspace{1cm} (17)

A time discretization of implicit type leads to a Helmholtz-type problem of the form

$$(I - \tau D \Delta)u^{(n+1)} = u^{(n)} + \tau f^{(n+1)}$$ \hspace{1cm} (18)

in each time step (where \(\tau\) denotes the time increment), which can now be treated in the same way as in the previous example.

More general elliptic equations. In principle, the equation

$$\text{div } \sigma \text{ grad } u = f$$ \hspace{1cm} (19)

is equivalent to the form:

$$\sigma \Delta u = f - \text{grad } \sigma \cdot \text{grad } u$$ \hspace{1cm} (20)

and the previously discussed meshless Poisson solver can be applied iteratively. However, is \(\text{grad } \sigma\) has extremely large values (which is often the case), this approach may be inconvenient. Instead of this, it is worth reconstructing the boundary and applying the QT-based multi-level scheme directly to (19) as discussed in Subsection 3.2.2. Note that the values of the function of \(\sigma\) has also to be interpolation.

Biharmonic problems:

$$\Delta \Delta u = f, \quad u|_\Gamma = u_0, \quad \frac{\partial u}{\partial n}|_\Gamma = v_0,$$ \hspace{1cm} (21)

The particular solution can be constructed exactly in the same way as in the case of Poisson problem. To obtain a homogeneous solution, the boundary interpolation based on the sixth-order operator \(L := \Delta \Delta (\Delta - c^2 I)\) can be applied. Note that, using the stream function approach, the 2D Stokes flow equations lead to the same problem.

Acknowledgement

This research was party supported by the Hungarian National Research Fund (OTKA) under the projects T034652 and T043258.

References


