Evaluation of the Integral Terms in Reproducing Kernel Methods

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Abstract

Reproducing Kernel Method (RKM) has its origins in wavelets and it is based on convolution theory. Being their continuous version, RKM is often referred as the general framework for meshless methods. In fact, since in real computation discretization is inevitable, these integrals need to be evaluated numerically, leading to the creation of Reproducing Kernel Particle Method RKPM and Moving Least Squares MLS approximation. Nevertheless, in this paper the integrals in RKM are explicitly evaluated for polynomials basis function and simple geometries in one, two and three dimensions even with conforming holes. Moreover, a general formula is provided for complicated shapes also for multiple connected domains. This is possible through a boundary formulation where domain integrals involved in RKM are transformed by Gauss Theorem in circular or flux integrals. Parallelization is readily enabled since no preliminary arrangements of nodes is needed for the moments matrix. Furthermore, using symbolic inversion, computation of shape functions in RKM is considerably speeded up.

Keywords: reproducing kernel method, Gauss Theorem, meshless, finite elements

1 Introduction

Reproducing Kernel Method (RKM) has its origins in wavelets theory (Liu et al., 1995) and (Liu et al., 1996) and its discrete counterpart resulted in the Reproducing Kernel Particle Method (RKPM) which is one of the emerging class of methods called meshless. Moreover, RKPM shares similarities with moving least squares (MLS) method and RKM is actually the general framework in which these methods can be classified (Liu et al., 1997b), even though MLS has its origins in data fitting.

Indeed, sometimes RKM is referred as a corrected SPH. In standard Smoothed Particle Hydrodynamics (SPH) (Gingold and Monaghan, 1977), (Monaghan, 1992), the function is simply approximated by an its convolution with a kernel function, which satisfies a set of properties. One of them is that the kernel is a function with compact support having dilatation parameter ρ. The function is therefore filtered conferring a smoother behavior to the approximation. SPH is one of the early meshless methods, i.e. it has the attractive feature of being based only on a distribution of nodes, or particles, thus a mesh is unnecessary.

SPH scheme though, suffers of inconsistencies at the boundaries, precisely at a distance equal to ρ (Liu et al., 1997a). SPH is not able to reproduce even the constant function, i.e. it does not realize a partition of unity (Belytschko et al., 1996). This is also the reason SPH is more suitable for unbounded domains.

In order to restore this condition, a corrected kernel must be used. It can be demonstrated that using a modified kernel (Liu et al., 1996) by the means of a moment matrix the reproducibility condition up to order n is restored. This moment matrix has entries that are essentially the kernel estimates of polynomial functions up to degree 2n. The resulting approximation is known as Reproducing Kernel Method (RKM).

Although this theory is mathematically correct, its implementation might be arduous since it is necessary to evaluate integrals. Thus, in real computations a discretization is often necessary. This discretization is based on particles associated with a measure of the domain and the integrals are replaced with summations. Whereas in RKM this matrix depends only on the domain, in RKPM it depends on the particles distribution. RKPM therefore associates the advantage of being meshless with an accuracy higher than SPH, nonetheless keeping the multi-resolution property assured by the dilatation parameter of the kernel.

Even though the starting point is different, the MLS approximation is almost identical to the RKPM. In the MLS a function is approximated by a weighted least squares procedure where the weight is actually a function and therefore called moving. The weighting function plays the same role of the kernel in the RKM, since it is a smooth

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The method states that the approximation $u$ with the introduction of corrective terms based on the calculation of the moments and the function to approximate. In order to restore consistency (or reproducibility) this kernel has to be modified reproducing kernel formulation. The 2 Reproducing Kernel Method.

Finally in sections 9 and 10 examples and conclusions are presented.

In this paper these convolution integrals are explicitly evaluated for polynomials basis function and simple geometries in one, two and three dimensions.

The kernel function is assumed to be a tensor product of single weighting functions in each dimension. Kernel functions based on radial support are currently under study by the authors.

Moreover, a general formula is provided for complicated shapes also for multiple connected domains. This is possible through a boundary formulation where domain integrals involved in RKM are transformed by Gauss Theorem in circular or flux integrals. One of the immediate consequences is the evaluation of the convolution integrals in a closed form also if the domain contains one or more rectangular (or cubic) holes. This has been achieved by defining vectorial fields from the primitives of the kernel function.

No preliminary arrangements of nodes is necessary for the construction of moments matrix, since in RKM it is an intrinsic property of the domain and the kernel function. From a practical point of view, this easily enables parallelization. Furthermore, (Zhou et al., 2005) used symbolic inversion of moments matrix and showed that computation of shape functions in RKM is considerably speeded up. The same method is used in this paper, although it has been verified by the authors that when the moment matrix exceeds the size 5x5 symbolic tools cannot provide an explicit and stable expression for the entries of the inverse.

Discretization is only necessary at a following stage with the introduction of background cells that realize a partition of unity of order $n$, for example like triangularization in finite elements, for this reason the method is therefore not truly meshfree. The same approach has been followed in the Reproducing Kernel Element Method (RKEM) (Liu et al., 2004), (Li et al., 2004), (Lu et al., 2004) and (Simkins et al., 2004) with the difference that in this work integrals are explicitly calculated.

In fact RKM can be seen in this context as a filtered version of finite element method. Conversely to finite elements, in RKM three-nodes triangular elements do not lead to a constant piecewise representation of derivatives but a much smoother approximation. Since the moment matrix is independent from the nodes arrangement, distribution of nodes can be changed (refined, rearranged and so on) without modifying the entries of the moment matrix, which can be thus retained and re-used in a subsequent calculation. This reduces run-time calculations when, for example, a refinement is needed in order to improve accuracy. This cannot be done with traditional particle methods because the moment matrix does depend on the particles distribution.

The outline of the paper is the following: in section 2 RKM and the convolution integrals are introduced, in section 3 the class of primitives of the kernel is presented, in section 4 and 5 the integrals are solved for the one-dimensional case, whereas in the following sections 6, 7 the same results are generalized to two and three dimensional domains, providing also closed forms for rectangular and cubic domains. Section 8 generalizes the principles of the previous sections to traditional finite element-like meshes, showing a link between finite elements and reproducing kernel methods. Finally in sections 9 and 10 examples and conclusions are presented.

2 Reproducing Kernel Method

The reproducing kernel formulation is based on the convolution between a kernel function (or weighting function) $w$ and the function to approximate. In order to restore consistency (or reproducibility) this kernel has to be modified with the introduction of corrective terms based on the calculation of the moments of $w(x)$ over the entire domain. The method states that the approximation $u^h(x)$ of the function $u(x)$ is given by (Liu et al., 1995) and (Liu et al., 1997b)

$$u^h(x) = p(0)^T \int_{\Omega'} p \left( \frac{x' - x}{\rho} \right) \int_{\Omega'} p \left( \frac{x' - x}{\rho} \right)^T w \left( \frac{x' - x}{\rho} \right) d\Omega' w \left( \frac{x' - x}{\rho} \right) u(x') d\Omega'$$

(1)
where \( w \) is a *weighting* function \( p(x) \) is the vector of basis functions reproduced by the kernel approximation, for example in two dimensions

\[
P(x)^T = [1 \ x \ y \ xy]
\]

(2)

In this case, only bilinear finite element shape functions can be used as \( u(x) \) because they realize a partition of unity of order one in both dimensions

\[
u(x) = \sum_{I=1}^{N} \psi_x(x-x_I)\psi_y(y-y_I)U_I
\]

(3)

where \( U_I \) are *nodal* values, \( N \) is the total number of nodes and \( \psi_x \) and \( \psi_y \) are *hat* functions having compact support of size \( \rho \) and centered in node with coordinates \( x_I \)

\[
\psi_x(x-x_I) = \begin{cases} 
1 - \frac{|x-x_I|}{\rho_x}, & \text{if } \frac{|x-x_I|}{\rho_x} \leq 1 \\
0, & \text{otherwise}
\end{cases}
\]

(4)

Thus equation (1) becomes

\[
u^h(x) = p(0)^T \left[ \int_{\Omega'} \left( \frac{x'-x}{\rho} \right) p \left( \frac{x'-x}{\rho} \right)^T w \left( \frac{x'-x}{\rho} \right) d\Omega' \right]^{-1} \int_{\Omega'} \left( \frac{x'-x}{\rho} \right) \Psi(x')^{T} d\Omega' U
\]

(5)

where

\[
\Psi(x)^T = [ \psi(x-x_1) \ \psi(x-x_2) \ldots \psi(x-x_N) ]
\]

(6)

Therefore, shape functions \( \phi(x) \) can be written as

\[
\phi(x) = p(0)^T M(x)^{-1} \Lambda(x)
\]

(7)

where \( M(x) \) is the so-called *moments matrix*

\[
M(x) = \int_{\Omega'} \left( \frac{x'-x}{\rho} \right) p \left( \frac{x'-x}{\rho} \right)^T w \left( \frac{x'-x}{\rho} \right) d\Omega'
\]

(8)

and \( \Lambda(x) \) represents a convolution between the unmodified kernel and the hat functions, also referred later in this paper as *\( \Psi-terms* *

\[
\Lambda(x) = \int_{\Omega'} \left( \frac{x'-x}{\rho} \right) w \left( \frac{x'-x}{\rho} \right) \Psi(x')^{T} d\Omega'
\]

(9)

The present work provides explicit formulas for the terms (8) and (9) and their derivatives. For regular shapes the expressions are exact, whereas for complex ones it gives a general method to evaluate them only by calculating boundary integrals (line integrals in two-dimensional problems and surface in three-dimensions) of known functions instead of full domain integrals.

### 3 The Kernel Function \( w \) and its primitives \( H_n \)

In this section are presented preliminary considerations about the kernel function \( w(x) \) and its primitives. Kernel functions could have *compact* support (for instance spline functions) or not, like gaussian function. In both cases though, it is possible to define their primitives. Their evaluation can be made once and for all for example through softwares capable of symbolic computations. Defining the variable

\[
\xi = \frac{x'-x}{\rho}
\]

(10)

the functions \( H_n \) are \( n+1 \) antiderivatives, or primitives of the kernel

\[
H_n(\xi) = \int \ldots \int w(\xi) d\xi
\]

(11)
Obviously, the following properties hold

\[ \frac{dH_n}{d\xi} = H_{n-1} \] (12a)
\[ \frac{d^{n+1}}{d\xi^{n+1}} H_n = w(\xi) \] (12b)
\[ \frac{\partial H_n}{\partial x'} = \frac{1}{\rho_x} H_{n-1}(\xi) \] (12c)
\[ \frac{\partial H_n}{\partial x} = -\frac{1}{\rho_x} H_{n-1}(\xi) \] (12d)
\[ \frac{\partial^{(n+1)}}{\partial x^{(n+1)}} H_n = -\frac{1}{\rho_x^{n+1}} (-1)^{n+1} w(\xi) \] (12e)

Moreover, it is possible to evaluate the moments of the kernel using these functions. Indeed, applying the recursive integration by parts

\[ \int \xi^k w(\xi) d\xi = \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \xi^{k-i} H_i(\xi) \] (13)

for example

\[ \int \xi^0 w(\xi) d\xi = H_0(\xi) \] (14a)
\[ \int \xi^1 w(\xi) d\xi = \xi H_0(\xi) - H_1(\xi) \] (14b)
\[ \int \xi^2 w(\xi) d\xi = \xi^2 H_0(\xi) - 2\xi H_1(\xi) - 2H_2(\xi) \] (14c)
\[ \int \xi^3 w(\xi) d\xi = \xi^3 H_0(\xi) - 3\xi^2 H_1(\xi) + 6\xi H_2(\xi) - 6H_3(\xi) \] (14d)

### 3.1 Non Compact Support Kernels

An example of kernels having non-compact support is the gaussian function

\[ w(\xi) = e^{-\frac{1}{2} \xi^2} \] (15)

The function in equation (15) is 1 for \( \xi = 0 \) and it rapidly decays to zero (even though it is not exactly zero) around \( \xi = \pm 3 \), as it can be seen from figure 1(a). Moreover, since primitives are infinite in number, in order to define \( H_n \) functions uniquely, a further condition need to be imposed. For non-compact support, the following condition is chosen

\[ \lim_{x \to -\infty} H_0(\xi) = 0 \] (16)

In this case, \( H_n \) functions are

\[ H_0(\xi) = \frac{\sqrt{2\pi}}{2} \text{erf} \left( \frac{\sqrt{2}}{2} \xi \right) + \frac{\sqrt{2\pi}}{2} \] (17)

\[ H_1(\xi) = \sqrt{\pi} \left( \frac{\sqrt{2}}{2} + \text{erf} \left( \frac{\sqrt{2}}{2} \xi \right) + \frac{e^{-1/2 \xi^2}}{\sqrt{\pi}} \right) + \frac{\sqrt{2\pi}}{2} \xi \] (18)

\[ H_2(\xi) = \sqrt{\pi} \left( \frac{\sqrt{2}}{2} \text{erf} \left( \frac{\sqrt{2}}{2} \xi \right) - 2 \left( -\frac{\sqrt{2} \xi e^{\xi^2}}{4e^{\xi^2}} + \frac{1}{\sqrt{\pi}} \text{erf} \left( \frac{\sqrt{2}}{2} \xi \right) \right) \right) + \frac{\sqrt{2\pi}}{4} \xi^2 \] (19)

where \( \text{erf} (x) \) is the error function defined as

\[ \text{erf} (x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \] (20)

These functions are plotted in figures 1. It can be observed that these functions (figures 1(b), 1(c) and 1(d) ) outside \( \xi = 3 \) have respectively constant, linear and quadratic behavior. This means that the boundary correction terms influence only a small portion of measure \( \rho \) around the boundaries of the domain, as it is also reported in (Liu et al., 1997a). This is more evident for the moment matrix entries depicted in figures 3(a), 3(b) and 3(c).
Figure 1: Non-Compact Support Kernel Functions: Gaussian Function
3.2 Compact Support Kernels

An example of compact support kernel is the \(2k^{th}\) order spline which can be rewritten using the Heaviside function \(\varphi\) as
\[
\psi(\xi) = (1 - \xi^2)^k [\varphi(\xi + 1) - \varphi(\xi - 1)]
\]
(21)

For compact support functions, the condition on the primitive has been chosen as
\[
H_0(\xi = -1) = 0
\]
(22)

Thus, naming as \(2F_1(a, b; c; z)\) the classical standard hypergeometric series
\[
H_0(\xi) = \xi 2F_1\left(\frac{1}{2}, -k; \frac{3}{2}; \xi^2\right) [\varphi(\xi + 1) - \varphi(\xi - 1)] + 2F_1\left(\frac{1}{2}, -k; \frac{3}{2}; 1\right) [\varphi(\xi + 1) + \varphi(\xi - 1)]
\]
(23)

\[
H_1(\xi) = \left[2F_1\left(\frac{1}{2}, -k; \frac{3}{2}; \xi^2\right)(\xi - 1) - \frac{1}{2(k + 1)} 2F_1\left(-\frac{1}{2}, -k - 1; \frac{3}{2}; \xi^2\right)\right] \varphi(\xi - 1) +
\]
\[+ \left[\frac{1}{2(k + 1)} 2F_1\left(-\frac{1}{2}, -k - 1; 1\right) + 2F_1\left(\frac{1}{2}, -k; \frac{3}{2}; 1\right)(\xi + 1) - \frac{1}{2(k + 1)} 2F_1\left(-\frac{1}{2}, -k - 1; 1\right)\right] \varphi(\xi + 1)
\]
(24)

This functions are drawn in figures 2 for different degree \(k\) of spline. It can be noted again the influence of the correction terms outside the support i.e. \(\xi = 1\).

4 Moments Matrix and \(\Psi\)-Terms in One Dimension

Using the \(H_n\) functions, it is immediate to evaluate the entries in the moments matrix and the convolution with the \(\psi\) terms as in equations (8) and (9). If \(\Omega\) is \(x \in [0, L]\), then the generic element \(M_{ij}\) of the moments matrix is
\[
M_{ij}(x) = \int_0^L \xi^{i+j} w(\xi)dx' = \rho_x \int_{\frac{x}{\rho_x}}^{\frac{x+1}{\rho_x}} \xi^{i+j} w(\xi) d\xi
\]
(25)

therefore, from equation (13), it follows
\[
M_{ij}(x) = \rho_x \sum_{l=0}^{i+j} (-1)^l \frac{(i+j)!}{(i+j-l)!} \xi^{i+j-l} H_l(\xi)
\]
(26)

in expanded form
\[
M_{ij}(x) = \rho_x \sum_{l=0}^{i+j} (-1)^l \frac{(i+j)!}{(i+j-l)!} \left[ \left(\frac{L-x}{\rho_x}\right)^{i+j-l} H_l\left(\frac{L-x}{\rho_x}\right) - \left(\frac{x}{\rho_x}\right)^{i+j-l} H_l\left(\frac{x}{\rho_x}\right) \right]
\]
(27)

In figures 4(a) and 4(b) correction functions are plotted for basis functions \(p^T(x) = [1 \quad x]\). Indeed correction terms are given by \(p^T(0)M(x)^{-1}\) that is
\[
p^T(0)M(x)^{-1} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} M_{11}^{-1}(x) & M_{12}^{-1}(x) \\ M_{12}^{-1}(x) & M_{22}^{-1}(x) \end{bmatrix} = \begin{bmatrix} M_{11}^{-1}(x) & M_{12}^{-1}(x) \end{bmatrix}
\]
(28)

where, using symbolic evaluation of the inverse of \(M(x)\)
\[
M_{11}^{-1}(x) = \frac{M_{22}(x)}{M_{11}(x)M_{22}(x) - M_{12}(x)^2}
\]
(29)
\[
M_{12}^{-1}(x) = -\frac{M_{12}(x)}{M_{11}(x)M_{22}(x) - M_{12}(x)^2}
\]
(30)

In the following it is supposed an equally spaced distribution of nodes over \(\Omega\) but similar arguments can be conducted for a general case. Moreover, for simplicity it is supposed that the distance between two consecutive nodes is \(\rho_x\).
Figure 2: Compact Support Kernel Functions: $2k-th$ order spline
Figure 3: Moments Matrix in One Dimension

Figure 4: Correction Factors in One Dimension for basis function $p^T(x) = [1 \ x]$
Considering that, even if the kernel has not compact support, the hat function is zero outside the support, the generic $\Psi$-term is, for internal nodes $x_i$ and for the polynomial of degree $k$

$$\Lambda_{k+1,i}(x) = \int_{x_i - \rho_x}^{x_i + \rho_x} \psi_x(x') \xi^k w(\xi) dx'$$  \hspace{1cm} (31)$$

for the first node $x_1 = 0$ is instead

$$\Lambda_{k+1,1}(x) = \int_0^{\rho_x} \psi_x(x') \xi^k w(\xi) dx'$$  \hspace{1cm} (32)$$

for the last one $x_N = L$

$$\Lambda_{k+1,n}(x) = \int_L^{L - \rho_x} \psi_x(x') \xi^k w(\xi) dx'$$  \hspace{1cm} (33)$$

Thus, equation (31) can be split in two terms

$$\Lambda_{k+1,i}(x) = \int_{x_i - \rho_x}^{x_i + \rho_x} \psi_x(x') \xi^k w(\xi) dx' = \int_{x_i - \rho_x}^{x_i} \psi_x(x') \xi^k w(\xi) dx' + \int_{x_i}^{x_i + \rho_x} \psi_x(x') \xi^k w(\xi) dx'$$  \hspace{1cm} (34)$$

The first term can be developed using integration by parts as follow

$$\int_{x_i - \rho_x}^{x_i} \psi_x(x') \xi^k w(\xi) dx' = \rho_x \int_{x_i - \rho_x}^{x_i} \psi_x \xi^k w(\xi) d\xi = \rho_x \left[ \psi_x \sum_{i=0}^{k} (-1)^i \frac{(k)!}{(k-i)!} \xi^{k-i} H_i(\xi) \right]_{x_i - \rho_x}^{x_i} + \rho_x \int_{x_i - \rho_x}^{x_i} \frac{d\psi_x}{d\xi} \xi^k w(\xi) d\xi - \rho_x \int_{x_i - \rho_x}^{x_i} \frac{d\psi_x}{d\xi} \xi^k H_i(\xi) d\xi \hspace{1cm} (35)$$

$\psi_x$ evaluated at the boundary of the support is 0, while it is 1 on the node $x_i$. The derivative can be written as

$$\frac{d\psi_x}{d\xi} = \frac{dx'}{dx} \frac{d\xi}{dx'} = \frac{1}{\rho_x} \rho_x = 1$$  \hspace{1cm} (36)$$

Therefore equation (35) becomes

$$\rho_x \sum_{i=0}^{k} (-1)^i \frac{(k)!}{(k-i)!} \left( \frac{x_i - x}{\rho_x} \right)^{k-i} H_i \left( \frac{x_i - x}{\rho_x} \right) - \rho_x \sum_{i=0}^{k} (-1)^i \frac{(k)!}{(k-i)!} \int_{x_i - \rho_x}^{x_i} \xi^{k-i} H_i(\xi) d\xi \hspace{1cm} (37)$$

Again, using the recursive integration by parts

$$\int \xi^{k-i} H_i(\xi) d\xi = \sum_{p=0}^{k-i} (-1)^p \frac{(k-i)!}{(k-i-p)!} \xi^{k-i-p} H_{i+1+p}(\xi)$$  \hspace{1cm} (38)$$

the double summation can be rewritten as

$$\sum_{i=0}^{k} (-1)^i \frac{(k)!}{(k-i)!} \sum_{p=0}^{k-i} (-1)^p \frac{(k-i)!}{(k-i-p)!} \xi^{k-i-p} H_{i+1+p}(\xi) = \sum_{i=0}^{k} (-1)^i(i+1) \frac{k!}{(k-i)!} \xi^{k-i} H_{i+1}(\xi)$$  \hspace{1cm} (39)$$

the second integral in equation (34) can be carried out similarly

$$\int_{x_i}^{x_i + \rho_x} \psi_x(x') \xi^k w(\xi) dx' = -\rho_x \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \left( \frac{x_i - x}{\rho_x} \right)^{k-i} H_i \left( \frac{x_i - x}{\rho_x} \right) + \rho_x \sum_{i=0}^{k} (-1)^i(i+1) \frac{k!}{(k-i)!} \xi^{k-i} H_{i+1}(\xi)$$  \hspace{1cm} (40)$$
Therefore, for \( I = 2, \ldots, n - 1 \)

\[
\Lambda_{k+1,I} = \rho_x \sum_{i=0}^{k} (-1)^i (i+1) \frac{k!}{(k-i)!} \left[ \left( \frac{x_I - x}{\rho_x} - 1 \right)^{k-i} H_{i+1} \left( \frac{x_I - x}{\rho_x} - 1 \right) 
- 2 \left( \frac{x_I - x}{\rho_x} \right)^{k-i} H_{i+1} \left( \frac{x_I - x}{\rho_x} + 1 \right) \right] \tag{41}
\]

and

\[
\Lambda_{k+1,1} = -\rho_x \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \frac{1}{\rho_x} \left( \frac{-x}{\rho_x} \right)^{k-i} H_i \left( \frac{-x}{\rho_x} \right) + \rho_x \left[ \sum_{i=0}^{k} (-1)^i (i+1) \frac{k!}{(k-i)!} \xi^{k-i} H_{i+1}(\xi) \right] \frac{\xi}{\rho_x} \tag{42}
\]

\[
\Lambda_{k+1,n} = \rho_x \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \left( \frac{L-x}{\rho_x} \right)^{k-i} H_i \left( \frac{L-x}{\rho_x} \right) - \rho_x \left[ \sum_{i=0}^{k} (-1)^i (i+1) \frac{k!}{(k-i)!} \xi^{k-i} H_{i+1}(\xi) \right] \frac{L-x}{\rho_x} \tag{43}
\]

for \( p^T(x) = [1 \ x] \) equations (41),(42) and (43) can be found in appendix A and are illustrated in figures 5(a) and 5(b). Shape functions in this case can be easily evaluated as

\[
\phi(x)^T = M_{11}^{-1}(x) \Lambda_1(x) + M_{12}^{-1}(x) \Lambda_2(x) \tag{44}
\]

and are depicted in figure 6

5 First Derivatives in One Dimension

Derivatives of the shape functions are always required in any Galerkin weak forms, therefore it is very important to obtain immediate formulas for the derivatives of the moments matrix and the \( \Psi \)-terms, in fact

\[
\frac{\partial \phi}{\partial x} = p(0)^T \frac{\partial M(x)}{\partial x} \Lambda(x) + p(0)^T M(x)^{-1} \frac{\partial \Lambda(x)}{\partial x} \tag{45}
\]

where

\[
\frac{\partial M(x)}{\partial x} = -M(x)^{-1} \frac{\partial M(x)}{\partial x} M(x)^{-1} \tag{46}
\]
Figure 6: Shape functions for equispaced distribution of nodes and basis functions $p^T(x) = [1 \ x]$

Hence, the calculation of $\frac{\partial M(x)}{\partial x_i}$ and $\frac{\partial \Lambda(x)}{\partial x}$ is necessary to get the derivatives of the shape functions. Regarding the moments matrix, according to equation (8)

$$\frac{\partial M_{ij}(x)}{\partial x} = \int_0^L \frac{\partial}{\partial x} (\xi^{i+j} w(\xi)) \frac{\partial \xi}{\partial x} d\xi = -\int_0^{\frac{L-x}{\rho_x}} \frac{\partial}{\partial \xi} (\xi^{i+j} w(\xi)) d\xi \tag{47}$$

then

$$\frac{\partial M_{ij}(x)}{\partial x} = \left( -\frac{x}{\rho_x} \right)^{i+j} w \left( -\frac{x}{\rho_x} \right) - \left( \frac{L-x}{\rho_x} \right)^{i+j} w \left( \frac{L-x}{\rho_x} \right) \tag{48}$$

Regarding the $\Psi$-Terms

$$\frac{\partial \Lambda_{k+1,1}(x)}{\partial x} = \int_{\frac{x-\rho_x}{\rho_x}}^{\frac{x+\rho_x}{\rho_x}} \frac{\partial}{\partial \xi} (\xi^k w(\xi)) \psi_x(x') d\xi' = \int_{\frac{x-\rho_x}{\rho_x}}^{\frac{x+\rho_x}{\rho_x}} \frac{\partial}{\partial \xi} (\xi^k w(\xi)) \psi_x(x') d\xi' +$$

$$\int_{\frac{x-\rho_x}{\rho_x}}^{\frac{x+\rho_x}{\rho_x}} \frac{\partial^i}{\partial \xi^i} \frac{\partial}{\partial x} (\xi^k w(\xi)) \psi_x(x') d\xi' \tag{49}$$

$$\frac{\partial \Lambda_{k+1}(x)}{\partial x} = \int_{\frac{x-\rho_x}{\rho_x}}^{\frac{x+\rho_x}{\rho_x}} -\frac{\partial}{\partial \xi} (\xi^k w(\xi)) \psi_x(x') d\xi + \int_{\frac{x-\rho_x}{\rho_x}}^{\frac{x+\rho_x}{\rho_x}} \frac{\partial^i}{\partial \xi^i} (\xi^k w(\xi)) \psi_x(x') d\xi \tag{50}$$

Using integration by parts, the first term in equation (50) is

$$[-\psi_x^k w(\xi)]_{\frac{x+\rho_x}{\rho_x}}^{\frac{x-\rho_x}{\rho_x}} \left( \frac{x-\rho_x}{\rho_x} \right)^{i+j} w \left( \frac{x-\rho_x}{\rho_x} \right) + \left[ \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \xi^{k-i} H_i(\xi) \right]_{\frac{x+\rho_x}{\rho_x}}^{\frac{x-\rho_x}{\rho_x}} \tag{51}$$

while the second one

$$[-\psi_x^k w(\xi)]_{\frac{x+\rho_x}{\rho_x}}^{\frac{x-\rho_x}{\rho_x}} \left( \frac{x-\rho_x}{\rho_x} \right)^{i+j} w \left( \frac{x-\rho_x}{\rho_x} \right) - \left[ \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!} \xi^{k-i} H_i(\xi) \right]_{\frac{x+\rho_x}{\rho_x}}^{\frac{x-\rho_x}{\rho_x}} \tag{52}$$
Figure 7: First Derivative of Moments Matrix in One Dimension

Figure 8: First Derivative of Correction Factors in One Dimension for basis function $p^T(x) = [1 \ x]$
It can be also noted that derivatives can be obtained from equations (121) to (122) using properties (12), namely changing sign, dividing by $\rho_x$ and subtracting 1 to the order of primitive $H$. The same applies also to the derivatives of the moments matrix. Similarly to subsection 4, in expanded form derivatives are in appendix A. From equation (44), derivatives of shape functions can be calculated as

$$\frac{\partial \phi^T}{\partial x} = \frac{\partial M_{11}^{-1}}{\partial x} \Lambda_1(x) + \frac{\partial M_{12}^{-1}}{\partial x} \Lambda_2(x) + M_{11}^{-1}(x) \frac{\partial \Lambda_1}{\partial x}(x) + M_{12}^{-1}(x) \frac{\partial \Lambda_2}{\partial x}(x)$$

and are reported in figure 10.

Figure 9: First Derivative of $\Psi$-terms in One Dimension

Figure 10: First Derivative of Shape functions for equispaced distribution of nodes and basis functions $p^T(x) = [1 \ x]$
6 Moments Matrix and $\Psi$-Terms in Higher Dimensions

In this section a generalization to two-dimensional and three-dimensional domains is showed.

6.1 Two-Dimensional Domains

A tensor product kernel of the type

$$w \left( \frac{x'-x}{\rho} \right) = w \left( \frac{x'-x}{\rho_x} \right) w \left( \frac{y'-y}{\rho_y} \right)$$

is used in the following section. Therefore, recalling equation (8), the generic entry is

$$M_{ij}(x,y) = \int_{\Omega'} \xi^i \eta^j w(\xi) w(\eta) dx' dy'$$

where

$$\eta = \frac{y'-y}{\rho_y}$$

Using Gauss' Theorem, the integral (55) can be written as

$$M_{ij}(x,y) = \oint_{\partial \Omega'} F_{ij}(x,y) \cdot d\mathbf{n}$$

where $d\mathbf{n}$ is the infinitesimal normal vector and $F_{ij}$ a vectorial field resulting from

$$\nabla \cdot F_{ij}(x,y) = \frac{\partial F_{ij}}{\partial x'} + \frac{\partial F_{ij}}{\partial y'} = \xi^i \eta^j w(\xi) w(\eta)$$

The following equations satisfy equation (58). No boundary conditions are required to solve them, so the solution can be made by simple indefinite integrations by separation of variables.

$$\begin{cases} 
\frac{\partial F_{ij}}{\partial x'} = \frac{1}{2} \xi^i \eta^j w(\xi) w(\eta) \\
\frac{\partial F_{ij}}{\partial y'} = \frac{1}{2} \xi^i \eta^j w(\xi) w(\eta)
\end{cases}$$

Thus

$$F_{ij}^{x'}(x,y) = \int \frac{1}{2} \xi^i \eta^j w(\xi) w(\eta) dx' = \frac{\rho_x}{2} \left[ \sum_{p=0}^{i} (-1)^p \frac{j!}{(i-p)!} \xi^{i-p} H_p(\xi) \right] \eta^j w(\eta)$$

$$F_{ij}^{y'}(x,y) = \int \frac{1}{2} \xi^i \eta^j w(\xi) w(\eta) dy' = \frac{\rho_y}{2} \xi^i w(\xi) \left[ \sum_{m=0}^{j} (-1)^m \frac{j!}{(j-m)!} \eta^{j-m} H_m(\eta) \right]$$

6.2 Three-Dimensional Domains

Analogously to the previous section, a tensor product kernel of the type

$$w \left( \frac{x'-x}{\rho} \right) = w \left( \frac{x'-x}{\rho_x} \right) w \left( \frac{y'-y}{\rho_y} \right) w \left( \frac{z'-z}{\rho_z} \right)$$

and the generic entry is

$$M_{ijk}(x,y,z) = \iiint_{\Omega'} \xi^i \eta^j \zeta^k w(\xi) w(\eta) w(\zeta) dx' dy' dz'$$

where

$$\zeta = \frac{z'-z}{\rho_z}$$
Using Gauss’ Theorem,

$$\mathbf{M}_{ij}(x, y, z) = \iiint_{\partial V} \mathbf{F}^{ijk}(x, y, z) \cdot d\mathbf{A}$$  \hspace{1cm} (65)$$

where \(d\mathbf{A}\) is the infinitesimal superficial normal vector and \(\mathbf{F}^{ijk}\) a vectorial field resulting from

$$\nabla \cdot \mathbf{F}^{ijk}(x, y, z) = \frac{\partial F^{ijk}_{x'}}{\partial x'} + \frac{\partial F^{ijk}_{y'}}{\partial y'} + \frac{\partial F^{ijk}_{z'}}{\partial z'} = \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta)$$  \hspace{1cm} (66)$$

The equations (59) become

$$\begin{align*}
\frac{\partial F^{ijk}_{x'}}{\partial x'} &= \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta) \\
\frac{\partial F^{ijk}_{y'}}{\partial y'} &= \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta) \\
\frac{\partial F^{ijk}_{z'}}{\partial z'} &= \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta)
\end{align*}$$

Therefore,

\begin{align*}
F^{ijk}_{x'}(x, y, z) &= \int \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta) dx' = \frac{\rho_x}{3} \sum_{p=0}^{i} (-1)^{i-p} \frac{j!}{(i-p)!} \xi^{i-p} H_p(\xi) \\
F^{ijk}_{y'}(x, y, z) &= \int \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta) dy' = \frac{\rho_y}{3} \xi^i w(\xi) \sum_{m=0}^{j} (-1)^{j-m} \frac{m!}{(j-m)!} \eta^{j-m} H_m(\eta) \\
F^{ijk}_{z'}(x, y, z) &= \int \frac{1}{3} \xi^i \eta^j \zeta^k \nu(\xi) \nu(\eta) \nu(\zeta) dz' = \frac{\rho_z}{3} \xi^i w(\xi) \sum_{l=0}^{k} (-1)^{k-l} \frac{k!}{(k-l)!} \zeta^{k-l} H_l(\xi)
\end{align*}$$

\hspace{1cm} (67)$$

\hspace{1cm} (68)$$

\hspace{1cm} (69)$$

\hspace{1cm} (70)$$

7 First Derivatives in Higher Dimensions

Starting from equation (57), derivatives can be evaluated as

\begin{align*}
\frac{\partial \mathbf{M}_{ij}(x, y)}{\partial x} &= \oint_{\partial V} \frac{\partial \mathbf{F}_{ij}}{\partial x} \cdot d\mathbf{n} = -\frac{1}{\rho_x} \oint_{\partial V} \frac{\partial \mathbf{F}_{ij}}{\partial \xi} \cdot d\mathbf{n} \\
\frac{\partial \mathbf{M}_{ij}(x, y)}{\partial y} &= \oint_{\partial V} \frac{\partial \mathbf{F}_{ij}}{\partial y} \cdot d\mathbf{n} = -\frac{1}{\rho_y} \oint_{\partial V} \frac{\partial \mathbf{F}_{ij}}{\partial \eta} \cdot d\mathbf{n}
\end{align*}$$

\hspace{1cm} (71)$$

\hspace{1cm} (72)$$

In a more compact form

$$\nabla_x \mathbf{M}_{ij}(x, y) = \mathbf{R} \oint_{\partial V} \nabla_\xi \mathbf{F}_{ij} \cdot d\mathbf{n}$$

\hspace{1cm} (73)$$

with

$$\mathbf{R} = \begin{bmatrix}
-\frac{1}{\rho_x} & 0 \\
0 & -\frac{1}{\rho_y}
\end{bmatrix}$$

\hspace{1cm} (74)$$

and \(\nabla_x\) and \(\nabla_\xi\) mean respectively gradient with respect to variables \(x = (x, y)\) and \(\xi = (\xi, \eta)\). Therefore

$$\nabla_\xi \mathbf{F}_{ij} = \begin{bmatrix}
\frac{\partial F^{ij}_{x'}}{\partial \xi} & \frac{\partial F^{ij}_{y'}}{\partial \xi} \\
\frac{\partial F^{ij}_{x'}}{\partial \eta} & \frac{\partial F^{ij}_{y'}}{\partial \eta}
\end{bmatrix}$$

\hspace{1cm} (75)$$

where

$$\frac{\partial F^{ij}_{x'}}{\partial \xi} = \frac{1}{2} \xi^i \eta^j \nu(\xi) \nu(\eta)$$

\hspace{1cm} (76)$$
where

\[ \frac{\partial F_{ij}^x}{\partial \xi} = \frac{1}{2\rho_x} \left( i \xi^{i-1} w(\xi) + \xi^i \frac{\partial w}{\partial \xi} \right) \left[ \sum_{m=0}^{j} (-1)^m \frac{\eta^{j-m} H_m(\eta)}{(j-m)!} \right] \]  \quad (77)

\[ \frac{\partial F_{ij}^y}{\partial \eta} = \frac{1}{2\rho_y} \sum_{p=0}^{i} (-1)^{j-p} \frac{\eta^{j-p} H_p(\xi)}{(i-p)!} \left[ j \eta^{j-1} w(\eta) + \eta^i \frac{\partial w}{\partial \eta} \right] \]  \quad (78)

\[ \frac{\partial F_{ij}^z}{\partial \eta} = \frac{1}{2} \xi^i \eta^j w(\xi)w(\eta) \]  \quad (79)

Formula (73) applies of course also to three-dimensional domains, with the due modifications

\[ \nabla_x M_{ijk}(x, y, z) = R \oint_{\partial \Omega'} \nabla_\xi F_{ijk} \cdot dA \]  \quad (80)

where

\[ R = \begin{bmatrix} -\frac{1}{\rho_x} & 0 & 0 \\ 0 & -\frac{1}{\rho_y} & 0 \\ 0 & 0 & -\frac{1}{\rho_z} \end{bmatrix} \]  \quad (81)

8 \quad \Psi\text{-Terms for Triangular Background Meshes}

Very often a two dimensional domain of a complicated shape can be easily approximated with a triangular mesh. This choice, from a FE point of view does not automatically imply the best choice for the resulting approximation, which is linear piecewise. Strain (and stress) fields are in this case constant piecewise which is not the most accurate solution. With this method, though, even if a triangular mesh is used, shape functions are smooth. If bilinear elements are used in the discretization, for example as in equation (3), \( \Psi \text{-terms} \) are immediately derived as tensor product from equation (121) and (122).

In order to give a general criterion, the generalization of the formula for the integration by parts need to be considered

\[ \int_{\hat{\Omega}'} u \nabla \cdot \mathbf{v} = \oint_{\partial \hat{\Omega}'} u \mathbf{v} \cdot d\mathbf{n} - \int_{\hat{\Omega}'} \nabla u \cdot \mathbf{v} d\hat{\Omega}' \]  \quad (82)

where \( u \) and \( v \) are generic scalar and vectorial functions. For a generic triangular 3 nodes element \( \hat{\Omega}' \) with coordinates \( x_i = (x_i, y_i) \), \( x_j = (x_j, y_j) \) and \( x_k = (x_k, y_k) \), FE shape function for the \( i \)-th node is

\[ \psi_i(x, y) = \frac{1}{A} [(y_k y_j - x_k y_j) + (y_j - y_k)x + (x_k - x_j)y] \]  \quad (83)

where \( A \) is the area of the element. Applying equation (82) leads to

\[ \int_{\hat{\Omega}'} \psi_i(x', y') \xi^m \eta^p w(\xi)w(\eta) d\hat{\Omega}' = \oint_{\partial \hat{\Omega}'} \psi_i(x', y') F_{im} \cdot d\mathbf{n} - \int_{\hat{\Omega}'} \nabla \psi_i(x', y') \cdot F_{im} d\hat{\Omega}' \]  \quad (84)

Assuming an anti-clockwise order \( (i, j, k) \), first term is zero on the part of the boundary from node \( j \) to node \( k \), while \( \psi_i \) evaluated on the remaining two parts is a linear function which ranges from 0 to 1. From node \( i \) to \( j \), the boundary can be parameterized as

\[ \begin{align*}
  x' &= (1 - t)x_i + tx_j \\
  y' &= (1 - t)y_i + ty_j
\end{align*} \quad t \in [0, 1] \]  \quad (85)

with

\[ d\mathbf{n} = \begin{bmatrix} y_j - y_i \\ -(x_j - x_i) \end{bmatrix} \]  \quad (86)

The parameterization is analogous for segment orientated from \( k \) to \( i \).

\[ \oint_{\partial \hat{\Omega}'} \psi_i(x', y') F_{im} \cdot d\mathbf{n} = \int_0^1 (1 - t)[F_{ik}^y(t)(y_j - y_i) - F_{ik}^x(t)(x_j - x_i)] + t[F_{ik}^x(t)(y_i - y_k) - F_{ik}^y(t)(x_i - x_k)] dt \]  \quad (87)

Even though an explicit form could not be obtained, this integral is quite simply to evaluate numerically, because the domain of integration is one-dimensional between 0 and 1. Good results can be obtained even with a simple
It should be noted that these terms simplify for the adjacent elements. The remaining term in equation (84) is simplified because \( \nabla \psi_i \) is constant and it is given by the opposite to the normal to vector \( \mathbf{a} = x_k - x_j \) where \( d_{kj} = |x_k - x_j| \)

\[
\nabla \psi_i = \frac{1}{d_{kj}} \left[ -\frac{(y_k - y_j)}{x_k - x_j} \right] 
\]

therefore

\[
\nabla \psi_i \cdot \int_{\partial \Omega} \mathbf{F}^{ml} d\Omega' = \nabla \psi_i \cdot \int_{\partial \Omega} \mathbf{G}^{ml} \cdot d\mathbf{n}
\]

where \( \mathbf{F}^{ml} \) is defined as the divergence of a matrix \( \mathbf{G}^{ml} \)

\[
\mathbf{F}^{ml} = \nabla \cdot \mathbf{G}^{ml}
\]

thus

\[
F_{x'}^{ml} = \frac{\partial G_{x'x'}^{ml}}{\partial x'} + \frac{\partial G_{x'y'}^{ml}}{\partial y'}
\]

\[
F_{y'}^{ml} = \frac{\partial G_{y'x'}^{ml}}{\partial x'} + \frac{\partial G_{y'y'}^{ml}}{\partial y'}
\]

Similarly to the previous section, the differential equations for \( \mathbf{G}^{ml} \) can be written as

\[
\frac{\partial G_{x'x'}^{ml}}{\partial x'} = \frac{1}{2} F_{x'}^{ml} = \frac{\rho_x}{4} \sum_{p=0}^{m} (-1)^p \frac{m!}{(m-p)!} \xi^{m-p} H_m(\xi) \eta^l w(\eta) \]

\[
\frac{\partial G_{x'y'}^{ml}}{\partial y'} = \frac{1}{2} F_{y'}^{ml} = \frac{\rho_y}{4} \xi^l \eta^q w(\xi) \sum_{q=0}^{l} (-1)^q \frac{l!}{(l-q)!} \eta^{l-q} H_q(\eta) \]

\[
\frac{\partial G_{y'x'}^{ml}}{\partial x'} = \frac{1}{2} F_{x'}^{ml} = \frac{\rho_x}{4} \xi^l \eta^q w(\xi) \sum_{q=0}^{l} (-1)^q \frac{l!}{(l-q)!} \eta^{l-q} H_q(\eta) \]

\[
\frac{\partial G_{y'y'}^{ml}}{\partial y'} = \frac{1}{2} F_{y'}^{ml} = \frac{\rho_y}{4} \xi^l \eta^q w(\xi) \sum_{q=0}^{l} (-1)^q \frac{l!}{(l-q)!} \eta^{l-q} H_q(\eta) \]

Integrating, it can be obtained

\[
G_{x'x'}^{ml} = \frac{\rho_x}{4} \sum_{p=0}^{m} (-1)^p (p+1) \frac{m!}{(m-p)!} \xi^{m-p} H_{m+1}(\xi) \eta^l w(\eta) \]

\[
G_{x'y'}^{ml} = \frac{\rho_x \rho_y}{4} \sum_{p=0}^{m} (-1)^p \frac{m!}{(m-p)!} \xi^{m-p} H_m(\xi) \sum_{q=0}^{l} (-1)^q \frac{l!}{(l-q)!} \eta^{l-q} H_q(\eta) \]

\[
G_{y'x'}^{ml} = \frac{\rho_x \rho_y}{4} \sum_{p=0}^{m} (-1)^p \frac{m!}{(m-p)!} \xi^{m-p} H_m(\xi) \sum_{q=0}^{l} (-1)^q \frac{l!}{(l-q)!} \eta^{l-q} H_q(\eta) \]

\[
G_{y'y'}^{ml} = \frac{\rho_y}{4} \xi^l \eta^q w(\xi) \sum_{q=0}^{l} (-1)^q (q+1) \frac{l!}{(l-q)!} \eta^{l-q} H_{q+1}(\eta) \]

It should be noted that \( G_{x'y'}^{ml} = G_{y'x'}^{ml} \), thus matrix \( \mathbf{G}^{ml} \) is symmetric. Therefore, the equations for \( \mathbf{G}^{ml} \) can be written also as

\[
\nabla \cdot (\nabla \cdot \mathbf{G}^{ml}) = \xi^m \eta^l w(\xi) w(\eta)
\]

that is

\[
\frac{1}{\rho_x^2} \frac{\partial^2 G_{x'x'}^{ml}}{\partial \xi^2} + \frac{2}{\rho_x \rho_y} \frac{\partial^2 G_{x'y'}^{ml}}{\partial \xi \partial \eta} + \frac{1}{\rho_y^2} \frac{\partial^2 G_{y'y'}^{ml}}{\partial \eta^2} = \xi^m \eta^l w(\xi) w(\eta)
\]
The integrals in formula (105) are well known and have been determined in equation (13). Therefore,

\begin{align}
\frac{\partial^2 G_{\eta^2}}{\partial \xi^2} &= \frac{\rho^2}{4} \xi^m \eta \xi^m \eta w(\xi) w(\eta) \\
\frac{\partial^2 G_{\eta^2}}{\partial \xi \partial \eta} &= \frac{\rho^2 \rho_\xi}{4} \xi^m \eta \xi^m \eta w(\xi) w(\eta) \\
\frac{\partial^2 G_{\eta^2}}{\partial \eta^2} &= \frac{\rho^2}{4} \xi^m \eta \xi^m \eta w(\xi) w(\eta)
\end{align}

Integrating these equations it is thus possible to obtain again equations from (97) to (100).

9 Numerical Examples

In this section integral terms are computed for simple domains. However, the formulation is easily applicable to complicated domains whenever a parametrization of the boundary is provided. Nevertheless, moments for rectangular domains with one or more holes can be explicitly calculated.

9.1 Rectangular Domain

A rectangular domain \( \Omega = \{ (x, y) \in [0, L_x] \times [0, L_y] \} \) is considered for the evaluation of moments. Conversely to classical particle methods, no arrangement of nodes is required, as mentioned before in section 1. Indeed, moments depend only on boundary \( \partial \Omega \). Moreover, it could be anticipated that \( M_{ij}(x, y) \) is a tensor product of (26) evaluated in both dimensions. Recalling equation (57), generic entry is given by

\[ M_{ij}(x, y) = \oint_{\partial \Omega} \mathbf{F}^{ij}(x, y) \cdot d\mathbf{n} = -\int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} F^{ij}_{xy}(\xi, \frac{-y}{\rho_y}) \rho_x \xi d\xi + \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} F^{ij}_{xy}(\xi, \frac{-x}{\rho_x}, \eta) \rho_y \eta d\eta + \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} F^{ij}_{xy}(\xi, \frac{-x}{\rho_x}, \eta) \rho_y \eta d\eta \]

Thus

\[ M_{ij}(x, y) = \frac{\rho_x \rho_y}{2} \sum_{m=0}^{j} (-1)^m \frac{j!}{(j-m)!} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \xi^i w(\xi) d\xi + \frac{\rho_x \rho_y}{2} \sum_{i=0}^{j} (-1)^i \frac{i!}{(i-p)!} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \eta^i w(\eta) d\eta + \frac{\rho_x \rho_y}{2} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \xi^i w(\xi) d\xi + \frac{\rho_x \rho_y}{2} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \eta^i w(\eta) d\eta \]

The integrals in formula (105) are well known and have been determined in equation (13). Therefore,

\[ M_{ij}(x, y) = \rho_x \rho_y \left[ \sum_{i=0}^{j} (-1)^i \frac{i!}{(i-p)!} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \xi^i w(\xi) d\xi \right]^{\frac{\pi}{p_x}}_{\frac{\pi}{p_y}} \left[ \sum_{m=0}^{j} (-1)^m \frac{(j)!}{(j-m)!} \int_{\frac{\pi}{p_x}}^{\frac{\pi}{p_y}} \eta^i w(\eta) d\eta \right]^{\frac{\pi}{p_x}}_{\frac{\pi}{p_y}} \]

These moments can be seen in figures 11 and 12 for \( i, j = 0, 1, 2 \). Derivatives can be promptly obtained both from equation (106) (using properties (12) ) or by integration using (71) and (72). The quickest way is the former one

\[ \frac{\partial M_{ij}(x, y)}{\partial x} = -\rho_x \left[ \xi^i w(\xi) \right]^{\frac{\pi}{p_x}}_{\frac{\pi}{p_y}} \left[ \sum_{m=0}^{j} (-1)^m \frac{(j)!}{(j-m)!} \eta^i w(\eta) d\eta \right]^{\frac{\pi}{p_x}}_{\frac{\pi}{p_y}} \]
Figure 11: Moments Matrix for Rectangular Domain
\[ \frac{\partial M_{ij}(x, y)}{\partial y} = \frac{\partial M_{ij}}{\partial \eta} \frac{\partial \eta}{\partial y} = -\rho_x \left[ \sum_{p=0}^{i} (-1)^p \frac{(i)!}{(i-p)!} \xi^{i-p} H_p(\xi) \right] \frac{L_y}{\rho_y^2} \left[ \eta^2 w(\eta) \right] \frac{L_z - y}{\rho_z^2} \]

Using tensor product, it is straightforward to compute \( \Psi \)-terms and their derivatives using equations (41), (42), (43), (51) and (52).

### 9.2 Rectangular Domain with Holes

If the domain under consideration has one or more holes, the circular integral needs to be carried out on two or more boundaries, according to equation (57). Domains can be seen as a difference among separated domains.

If the holes are rectangular, this is immediate, since equations (106) can be directly applied.

\[ M_{ij}(x, y) = \int_{\partial \Omega} \Phi^{ij}(x, y) \cdot \mathbf{d}n = \int_{\partial \Omega_{\text{ext}}} \Phi^{ij}(x, y) \cdot \mathbf{d}n - \int_{\partial \Omega_{\text{hole}}} \Phi^{ij}(x, y) \cdot \mathbf{d}n \]

If \( n_i \) is the number of holes, one just needs to subtract to equation (106) all the terms related to the holes \( \partial \Omega_i^{\text{hole}} \), \( i = 1, \ldots, n_h \).

The same applies also to derivatives. As an example, for a rectangular domain with a rectangular hole \( \Omega_{\text{hole}} = \{(x, y) \in [lx_1, lx_2] \times [ly_1, ly_2]\} \), moments are (figures 17(a), 17(c), 17(e) and 17(g))

\[ M_{ij}(x) = \rho_x \rho_y \left[ \sum_{p=0}^{i} (-1)^p \frac{(i)!}{(i-p)!} \xi^{i-p} H_p(\xi) \right] \frac{L_y - y}{\rho_y^2} \left[ \sum_{m=0}^{j} (-1)^m \frac{(j)!}{(j-m)!} \eta^{j-m} H_m(\xi) \right] \frac{L_z - z}{\rho_z^2} \]

\[ - \rho_x \rho_y \left[ \sum_{p=0}^{i} (-1)^p \frac{(i)!}{(i-p)!} \xi^{i-p} H_p(\xi) \right] \frac{L_y - y}{\rho_y^2} \left[ \sum_{m=0}^{j} (-1)^m \frac{(j)!}{(j-m)!} \eta^{j-m} H_m(\xi) \right] \frac{L_z - z}{\rho_z^2} \]

if \( lx_1 = 0 \) and \( ly_1 = 0 \) or \( lx_2 = L_x \) and \( ly_2 = L_y \) the domain turns to be L-shaped (figures 17(b), 17(d), 17(f) and 17(h)).

### 9.3 Cubic Domain

It is straightforward to generalize equations (106) to three-dimensional domains like cubes. Considering a cubic domain defined as \( \Omega = \{(x, y, z) \in [0, L_x] \times [0, L_y] \times [0, L_z]\} \), moments can be readily evaluated as

\[ M_{ijk}(x, y, z) = \rho_x \rho_y \rho_z \left[ \sum_{p=0}^{i} (-1)^p \frac{(i)!}{(i-p)!} \xi^{i-p} H_p(\xi) \right] \frac{L_y - y}{\rho_y^2} \left[ \sum_{m=0}^{j} (-1)^m \frac{(j)!}{(j-m)!} \eta^{j-m} H_m(\xi) \right] \frac{L_z - z}{\rho_z^2} \]

\[ \left( \sum_{l=0}^{k} (-1)^l \frac{(k)!}{(k-l)!} \zeta^{k-l} H_l(\xi) \right) \frac{L_x - x}{\rho_x^2} \]
Figure 13: Partial Derivative of the Moments Matrix for Rectangular Domain
Analogously equations (107), (108) and (110) can be extended in the same manner.

9.4 Rectangular Domain with Elliptical Hole

In figures 19 are shown examples of moments for a domain with an elliptical hole of parametric equation

$$\begin{align*}
    x' &= x_c + a \cos(\theta) \\
    y' &= y_c + b \sin(\theta)
\end{align*} \quad \theta \in [0, 2\pi] \quad (112)$$

where \((x_c, y_c)\) are the coordinates of the center and \(a\) and \(b\) are the semi-axis. The term to be subtracted from equation (105) is

$$\int_{\partial \Omega'} F_{x'ij}(x, y) dy' - F_{y'ij}(x, y) dx' = \int_0^{2\pi} F_{x'ij}(\frac{x_c + a \cos(\theta) - x}{\rho_x}, \frac{y_c + b \sin(\theta) - y}{\rho_y}) b \cos(\theta) d\theta +
$$

$$F_{y'ij}(\frac{x_c + a \cos(\theta) - x}{\rho_x}, \frac{y_c + b \sin(\theta) - y}{\rho_y}) a \sin(\theta) d\theta \quad (113)$$

In this case no analytical solution can be obtained, thus a numerical integration is needed. Though, a simple trapezoidal integration can produce satisfactory results without having too many integration points as illustrated in figures 18(a), 18(b), 18(c) and 18(d)).

9.5 Shape Functions for a Rectangular Domain

In this subsection shape functions are evaluated for a rectangular domain for two different background meshes. In fact, as in equation (1), \(u(x')\) is given by a distribution of nodes able to reproduce all functions in the basis. For example, three-nodes element, can reproduce basis function \(p^{T}(x, y) = [1 \ x \ y]\) whereas basis function \(p^{B}(x, y) = [1 \ x \ y \ xy]\) are reproduced by four-nodes bilinear element.

9.5.1 Background 4 Nodes Bilinear Elements

In figures 21 are illustrated shape functions and their derivatives for a rectangular domain, with an equispaced distribution of nodes as in figure 20(a). Bilinear element can only be used as background cells, as in equation (3). Furthermore, using symbolic inversion as in (Zhou et al., 2005), the entries of \(M(x, y)\) can be explicitly expressed in terms of the entries of \(M(x, y)\) and thus without the need of numerical routines for the inversion. Figure 21(a) shows an internal node, which is reasonably far from the boundaries and thus unaffected from the correction terms, in fact these terms are equal to \(\frac{1}{\rho}\) for every point at a distance \(\rho\) from \(\partial \Omega\). On the other hand, in figure 21(b) it is shown a point near the left corner, which indeed needs a correction. In fact, recalling equation (44) and (121), if
Figure 15: Partial Derivative of the Moments Matrix for Rectangular Domain
the generic $I$-th interior node located at $x_I$ is considered and for a point $x$ far from the boundaries

$$
\begin{align*}
\phi_I(x) &= M^{-1}_{11}(x)\Lambda_{1,I}(x) + M^{-1}_{12}(x)\Lambda_{2,I}(x) + 0\Lambda_{2,I}(x) = \frac{1}{\rho_x}\Lambda_{1,I}(x) = \\
\frac{\rho_x}{\rho_x} &H_1\left(\frac{x_I-x}{\rho_x} - 1\right) - 2H_1\left(\frac{x_I-x}{\rho_x}\right) + H_1\left(\frac{x_I-x}{\rho_x} + 1\right)\\
&= H_1\left(\frac{x_I-x}{\rho_x} - 1\right) - 2H_1\left(\frac{x_I-x}{\rho_x}\right) + H_1\left(\frac{x_I-x}{\rho_x} + 1\right)
\end{align*}
$$

This suggests the possibility to evaluate the correction terms only in points within a strip of measure $\rho$ around the boundaries and thus save computational time and storage memory.

### 9.5.2 Background 3 Nodes Linear Element

In this case, classical triangular elements are used, as in figure 20(b). In order to evaluate shape functions, $\Psi$-terms are calculated according to section 8 and are shown in figures 23(a), 23(b) and 23(c) while shape function is instead illustrated in figure 23(d). At this point, numerical integration is necessary since the line integrals have not explicit expression. Trapezoidal integration has been used and different number of integration points have been tried. In order to keep the reproduction error low, the number of integration points needs to be further increased.

### 9.6 Reproduction Error

As mentioned before, the term reproducing means that the shape functions are able to reproduce exactly all the polynomials in the basis functions $p(x)$. These are also known as consistency properties and they are imposed by construction, which means that the introduction of the correction terms is based on the assumption that these conditions are met.

$$
\phi(x)^T P = p(x)^T \quad (115)
$$

where

$$
P = \begin{bmatrix} 
    p(x_1)^T \\
    p(x_2)^T \\
    \vdots \\
    p(x_N)^T 
\end{bmatrix} \quad (116)
$$

For all the other functions not included in $p(x)$, the shape functions reproduce them with an error, since RKM can be seen also as a moving weighted least squares procedure. Therefore, if the shape functions are correctly evaluated, they should theoretically satisfy equation (115) exactly, but practically a very small error always exists even in case of correct calculation. This means that the error is only due to computer approximation and not generated by the method itself. Thus, the following error can be defined

$$
e(x) = \phi(x)^T P - p(x)^T \quad (117)
$$
Figure 17: Moments Matrix for Domains with Holes
Figure 18: Moments for a Rectangular Domain with an Elliptical Hole with different number of integration points

and for the derivative

$$e_d(x) = \frac{\partial \phi}{\partial x}(x)^T P - \frac{\partial P^T}{\partial x}(x) = \frac{\partial e}{\partial x}(x)$$

(118)

The first condition of equation (115) is the well known partition of unity, which means that

$$\sum_{I=1}^{N} \phi_I(x) = 1$$

(119)

whereas for the derivatives is the partition of nullity

$$\sum_{I=1}^{N} \frac{\partial \phi_I}{\partial x}(x) = 0$$

(120)

For example, for the shape functions and their derivatives evaluated in section 4 and 5 for the one-dimensional case, figures 24 and 25 show that, being at most $10^{-10}$, the error is absolutely negligible and mostly concentrated randomly at the boundaries. Likewise, for the two-dimensional example in subsection 9.5, the errors on the reproducing conditions are illustrated in figures 26, 27 and 28. As it can be seen, the biggest error, due only to the computer approximation, is on the partition of nullity (figure 27(a)) and it is of order of magnitude of $10^{-9}$, then it can be considered absolutely insignificant. In figures 29 are depicted reproduction errors for a triangular mesh. Differently from the example in subsection 9.5.1, these error contain the errors related with the trapezoidal integration involved in the circular integrals. Even it is larger than the case with 4 nodes element, it is still relatively little.

10 Conclusions

In this paper integral terms in Reproducing Kernel Methods have been evaluated in the case of polynomial basis function and tensor product weight function. This result has been obtained through the definition of the primitives
Figure 19: Moments for a Rectangular Domain with an Elliptical Hole
of the kernel up to the \((n + 1)\)-th order in a scaled variable. These functions are readily available with the use of a software capable of symbolic calculation. In this way, integral terms in RKM in one dimension can be explicited in a complete form, allowing a much easier implementation. The generalization to two and three dimensions is possible with the definition of a vectorial field and the Gauss’ Theorem. The domain integrals are therefore recasted as boundary integrals, more simple to evaluate. In case of simple geometries, such as rectangular and cubic domains, the expression can be obtained analytically. Moreover, the boundary integrals consent the application of these formulas also to multiple connected regions. The main outcome of this formulation is a faster and parallelized calculation of shape functions as they can directly programmed.

A One-dimensional \(\Psi\)-Terms in Expanded Form

As mentioned in section 4, for basis functions \(p^T(x) = [1 \ x]\) \(\Psi\)-Terms are

\[
\Lambda_{1,1}(x) = \rho_x \left[ H_1 \left( \frac{x_1 - x}{\rho_x} - 1 \right) - 2H_1 \left( \frac{x_1 - x}{\rho_x} \right) + H_1 \left( \frac{x_1 - x}{\rho_x} + 1 \right) \right] \tag{121a}
\]

\[
\Lambda_{1,1}(x) = -\rho_x H_0 \left( \frac{x}{\rho_x} \right) + \rho_x \left[ H_1 \left( \frac{x}{\rho_x} + 1 \right) - H_1 \left( \frac{x}{\rho_x} \right) \right] \tag{121b}
\]

\[
\Lambda_{1,N}(x) = \rho_x H_0 \left( \frac{L - x}{\rho_x} \right) - \rho_x \left[ H_1 \left( \frac{L - x}{\rho_x} \right) - H_1 \left( \frac{L - x}{\rho_x} - 1 \right) \right] \tag{121c}
\]
Figure 22: Derivatives of Shape functions in two different nodes
Figure 23: $\Psi$-terms and Shape Function for triangular mesh

(a) $\Lambda_{1,I}(x,y)$  \hspace{1cm} (b) $\Lambda_{2,I}(x,y)$

(c) $\Lambda_{3,I}(x,y)$  \hspace{1cm} (d) $\phi_I(x,y)$

Figure 24: Reproducing Error for Shape Functions with basis $p^T(x) = [1 \ x]$
Figure 25: Reproducing Error for the Derivatives of Shape Functions with basis $p^T(x) = [1 \ x]$

Figure 26: Reproducing Error for Shape Functions with basis $p^T(x) = [1 \ x \ y \ xy]$
Figure 27: Reproducing Error for $x$ Partial Derivative of Shape Functions with basis $\mathbf{p}^T(x) = [1\ x\ xy]$
Figure 28: Reproducing Error for $y$ Partial Derivative of Shape Functions with basis $p^T(x) = [1 \ x \ xy]$
Figure 29: Reproducing Error for Shape Functions with basis $p^T(x) = [1 \ x \ y]$ and Triangular Mesh

and

\[
\Lambda_{2,1}(x) = \rho_x \left[ \left( \frac{x_1 - x}{\rho_x} - 1 \right) H_1 \left( \frac{x_1 - x}{\rho_x} - 1 \right) - 2H_2 \left( \frac{x_1 - x}{\rho_x} - 1 \right) - 2\rho_x \left[ \left( \frac{x_1 - x}{\rho_x} \right) H_1 \left( \frac{x_1 - x}{\rho_x} \right) \right] \right]
- 2H_2 \left[ \left( \frac{x_1 - x}{\rho_x} + 1 \right) H_1 \left( \frac{x_1 - x}{\rho_x} + 1 \right) - 2H_2 \left( \frac{x_1 - x}{\rho_x} + 1 \right) \right].
\] (122a)

\[
\Lambda_{2,1}(x) = -\rho_x \left[ \left( \frac{-x}{\rho_x} \right) H_0 \left( \frac{-x}{\rho_x} \right) - H_1 \left( \frac{-x}{\rho_x} \right) \right] + \rho_x \left[ \left( \frac{-x}{\rho_x} + 1 \right) H_1 \left( \frac{-x}{\rho_x} + 1 \right) - 2H_2 \left( \frac{-x}{\rho_x} + 1 \right) \right]
+ \rho_x \left[ \left( \frac{-x}{\rho_x} \right) H_1 \left( \frac{-x}{\rho_x} \right) - 2H_2 \left( \frac{-x}{\rho_x} \right) \right].
\] (122b)

\[
\Lambda_{2,N}(x) = \rho_x \left[ \left( \frac{L-x}{\rho_x} \right) H_0 \left( \frac{L-x}{\rho_x} \right) - H_1 \left( \frac{L-x}{\rho_x} \right) \right] - \rho_x \left[ \left( \frac{L-x}{\rho_x} \right) H_1 \left( \frac{L-x}{\rho_x} \right) - 2H_2 \left( \frac{L-x}{\rho_x} \right) \right]
+ \rho_x \left[ \left( \frac{L-x}{\rho_x} - 1 \right) H_1 \left( \frac{L-x}{\rho_x} - 1 \right) - 2H_2 \left( \frac{L-x}{\rho_x} - 1 \right) \right].
\] (122c)

First order derivatives are:

\[
\frac{\partial \Lambda_{1,1}}{\partial x}(x) = -H_0 \left( \frac{x_1 - x}{\rho_x} - 1 \right) + 2H_0 \left( \frac{x_1 - x}{\rho_x} + 1 \right)
- H_0 \left( \frac{x_1 - x}{\rho_x} + 1 \right).
\] (123a)

\[
\frac{\partial \Lambda_{1,1}}{\partial x}(x) = w \left( \frac{-x}{\rho_x} \right) - \left[ H_0 \left( \frac{-x}{\rho_x} + 1 \right) - H_0 \left( \frac{-x}{\rho_x} \right) \right).
\] (123b)

\[
\frac{\partial \Lambda_{1,N}}{\partial x}(x) = w \left( \frac{L-x}{\rho_x} \right) + \left[ H_0 \left( \frac{L-x}{\rho_x} \right) - H_0 \left( \frac{L-x}{\rho_x} - 1 \right) \right]
\] (123c)
\[\frac{\partial \mathbf{A}_{2,1}}{\partial x}(x) = -\left[ \left( \frac{x_1 - x}{\rho_x} - 1 \right) H_0 \left( \frac{x_1 - x}{\rho_x} - 1 \right) - H_1 \left( \frac{x_1 - x}{\rho_x} - 1 \right) \right] + 2 \left[ \left( \frac{x_1 - x}{\rho_x} \right) H_0 \left( \frac{x_1 - x}{\rho_x} \right) \right] - H_1 \left( \frac{x_1 - x}{\rho_x} \right) - H_1 \left( \frac{x_1 - x}{\rho_x} + 1 \right) \right] \]

\[\frac{\partial \mathbf{A}_{2,1}}{\partial x}(x) = \left[ \left( \frac{1 - x}{\rho_x} \right) w \left( \frac{1 - x}{\rho_x} \right) - \left[ \left( \frac{1 - x}{\rho_x} + 1 \right) H_0 \left( \frac{1 - x}{\rho_x} + 1 \right) - H_1 \left( \frac{1 - x}{\rho_x} + 1 \right) \right] + \left[ \left( \frac{1 - x}{\rho_x} H_0 \left( \frac{1 - x}{\rho_x} \right) - H_1 \left( \frac{1 - x}{\rho_x} \right) \right) \right] \]

\[\frac{\partial \mathbf{A}_{2,N}}{\partial x}(x) = -\left[ \left( \frac{L_x - x}{\rho_x} \right) w \left( \frac{L_x - x}{\rho_x} \right) + \left[ \left( \frac{L_x - x}{\rho_x} H_0 \left( \frac{L_x - x}{\rho_x} \right) - H_1 \left( \frac{L_x - x}{\rho_x} \right) \right] - \left( \frac{L_x - x}{\rho_x} - 1 \right) H_0 \left( \frac{L_x - x}{\rho_x} - 1 \right) - H_1 \left( \frac{L_x - x}{\rho_x} - 1 \right) \right] \]

\[\text{B Vectorial Field } F^{kl} \text{ in expanded form} \]

The following equations are the explicit forms for vector \( F^{kl} \) with \( k, l = 0, 1 \). These are the required fields for the evaluation of the moments matrix for basis function \( \mathbf{p}^T(x) = [1 \ x \ y] \) and for \( \Psi \)-terms for boundary nodes.

\[\mathbf{F}^{00}(x, y) = \left[ \frac{\partial}{\partial x} H_0(\xi) w(\eta) \right] \]

\[\mathbf{F}^{10}(x, y) = \left[ \frac{\partial}{\partial x} (\xi H_0(\xi) - H_1(\xi)) w(\eta) \right] \]

\[\mathbf{F}^{01}(x, y) = \left[ \frac{\partial}{\partial y} H_0(\xi) \eta w(\eta) \right] \]

\[\mathbf{F}^{11}(x, y) = \left[ \frac{\partial}{\partial y} (\xi H_0(\xi) - H_1(\xi)) \eta w(\eta) \right] \]

\[\mathbf{F}^{20}(x, y) = \left[ \frac{\partial}{\partial y} (\xi^2 H_0(\xi) - 2\xi H_1(\xi) - 2H_2(\xi)) w(\eta) \right] \]

\[\mathbf{F}^{02}(x, y) = \left[ \frac{\partial}{\partial y} w(\xi) \left( \eta^2 H_0(\eta) - 2\eta H_1(\eta) - 2H_2(\eta) \right) \right] \]

\[\text{C Matrix } G^{ml} \text{ in expanded form} \]

The following equations are the explicit forms for matrix \( G^{kl} \) with \( k, l = 0, 1 \). These are the required fields for the evaluation of the \( \Psi \)-terms for basis function \( \mathbf{p}^T(x) = [1 \ x \ y \ xy] \)

\[\mathbf{G}^{00}(x, y) = \left[ \frac{\partial}{\partial x} H_1(\xi) w(\eta) \right] \]

\[\mathbf{G}^{10}(x, y) = \left[ \frac{\partial}{\partial x} (\xi H_1(\xi) - 2H_2(\xi)) w(\eta) \right] \]

\[\mathbf{G}^{01}(x, y) = \left[ \frac{\partial}{\partial y} H_1(\xi) \eta w(\eta) \right] \]

\[\mathbf{G}^{11}(x, y) = \left[ \frac{\partial}{\partial y} (\xi H_1(\xi) - 2H_2(\xi)) \eta w(\eta) \right] \]
References


