Weighted Quadrature Rules for Finite Element Methods

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Abstract

We discuss the numerical integration of polynomials times non-polynomial weighting functions in two dimensions arising from multiscale finite element computations. The proposed quadrature rules are significantly more accurate than standard quadratures and are better suited to existing finite element codes than formulas computed by symbolic integration. We validate this approach by introducing the new quadrature formulas into a multiscale finite element method for the 2D reactiondiffusion equation.

Key words: Numerical integration, Finite Element Method

1 Introduction

Finite element methods are highly popular because, among other reasons, they are good and simple. Still, in its traditional form, the method fails to solve accurately some partial differential equations (PDEs) with multiscale behavior, as when the coefficients of the equations depend on small parameters. This can happen for instance if the coefficients

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are highly oscillatory (as in models for heterogeneous materials), or if a small parameter multiplies some of the terms in the equation (as in transport equations with low diffusivity).

A possible strategy to overcome the above mentioned difficulties is to use special finite element spaces instead of the usual space of piecewise polynomial functions [3-6,13-15,11,17,19]. However, for polynomial basis functions, the standard quadrature are *exact* and this property is lost if more complicated spaces are used. Hence, the use of nonpolynomial functions has its drawbacks, since standard quadratures either become innacurate or inefficient, as more integration points are necessary. This concern is not new. In seminal papers of Hughes and Brooks [8,20,21], the problem of determining good quadratures was already present, and they actually *defined upwind methods by using quadrature strategies*.

In this paper we investigate and propose several exact and approximate quadrature possibilities to integrate elementwise product of polynomials times basis functions with exponential behaviour. Such integrals appear when developing enriched methods for reaction-advection-diffusion equations [15,24], but also in other contexts [2,25,7]. Our formulas allow for a direct implementation into existing FEM codes. Due to the way many codes were developed, it can be actually simpler than implementing the results of symbolic integrations.

We organize the paper as follows. In Section 2 we present a brief review of quadrature rules in one-dimensional, and in quadrilateral elements. Next, in Section 3 we develop quadratures for triangular elements. Finally, Section 4 presents some numerical tests, Section 5 presents our conclusions.

2 One-dimensional and product rules

We are concerned with the problem of approximating weighted integrals in bounded domains. Given a weighting function, i.e., a nonnegative and nonzero real function wdefined in [a, b], a quadrature (rule) with n_{int} integration points is defined by a set of integration weights A_l and integration points $x_l \in [a, b]$ for $l = 1, \ldots, n_{int}$, such that

$$\int_{a}^{b} q(x)w(x) dx \approx \sum_{j=1}^{n_{int}} A_l q(x_l)$$
(1)

for a given function q. We say that such quadrature has degree of precision n if (1) is an equality for any polynomial q of degree less or equal to n.

Since (1) is not exact if

$$q(x) = \prod_{l=1}^{n_{int}} (x - x_l)^2,$$

the maximum degree of precision of a quadrature with n_{int} points is $2n_{int} - 1$. Thus, a quadrature with precision n must have at least (n + 1)/2 integration points [10].

One of the simplest quadratures of degree of precision n is defined by choosing distinct integration points $x_1, x_2, \ldots, x_{n+1}$ and using the weights

$$A_{l} = \prod_{\substack{i=1\\i \neq l}}^{n+1} \int_{a}^{b} \frac{(x-x_{i})}{(x_{l}-x_{i})} w(x) \, dx, \quad l = 1, \dots, n+1.$$
(2)

In particular, if the points x_l are uniformly distributed, we refer to the quadrature as a *Newton-Cotes rule*. Note that such rule has degree of precision n + 1 and uses n + 1 integration points, and that is greater than the lower bound (n + 1)/2.

An optimal alternative is to consider *Gaussian* quadratures. Let p be a polynomial of degree n_{int} , satisfying the orthogonality relation

$$\int_{a}^{b} p(x)q(x)w(x) dx = 0 \tag{3}$$

for any polynomial q of degree less than n_{int} . The roots of p are all different from each other, and a Gaussian quadrature uses them as integration points, along with the weights (2). It is not hard to show [10] that a Gaussian quadrature is *optimal*, i.e., n_{int} integration points yield a degree of precision $2n_{int} - 1$.

Although it may appear that Gaussian quadratures are always the best choice, this is not so clear when performing weighted integrals in finite element codes, since the quadrature points may change from element to element. On the other hand, in Newton-Cotes methods, it is enough to fix the quadrature points and re-calculate only the quadrature weights.

Another situation in which is not clear whether optimal quadrature rules are the best choice is high-order finite elements with mass lumping ([9] and also [18, p. 443-444]). In these schemes, quadrature points and mesh nodes coincide in order to produce a diagonal mass matrix. We must constrain the integration weights A_l to be positive so that the mass matrix is positive definite.

Next we employ one-dimensional quadratures to approximate weighted integrals over quadrilateral regions. Using isoparametric maps [18], such integrals can be transformed into integrals of the form

$$\int_{-1}^{1} \int_{-1}^{1} q(x,y)w(x,y) \, dxdy \;. \tag{4}$$

We assume that the decomposition $w(x, y) = w_x(x)w_y(y)$ holds.

If f is polynomial, we write

$$f(x,y) = f_1(x)g_1(y) + \ldots + f_m(x)g_m(y) .$$
(5)

Assuming that the polynomials f_i and g_i have degree at most $2n_{int} - 1$, then the computation of

$$\int_{-1}^{1} \int_{-1}^{1} f_i(x) g_i(y) w(x, y) \, dx \, dy = \int_{-1}^{1} f_i(x) w_x(x) \, dx \int_{-1}^{1} g_i(y) w_y(y) \, dy$$

can be performed by a Gaussian quadrature with n_{int} points in each direction. Thus

$$\int_{-1}^{1} \int_{-1}^{1} f_i(x) g_i(y) w(x, y) \, dx \, dy = \sum_{j=1}^{n_{int}} A_j^x f_i(x_j) \sum_{k=1}^{n_{int}} A_k^y g_i(y_k),$$

where $A_1^x, \ldots, A_{n_{int}}^x$, and $x_1, \ldots, x_{n_{int}}$ are the weights and integration points for the one-dimensional Gaussian quadrature with respect to w_x . Similarly $A_1^y, \ldots, A_{n_{int}}^y$, and $x_1, \ldots, x_{n_{int}}$ are the weights and integration points with respect to w_y .

Adding up the integrals of each component of f, we find

$$\int_{-1}^{1} \int_{-1}^{1} f(x, y) w(x, y) \, dx dy = \sum_{i=1}^{m} \int_{-1}^{1} \int_{-1}^{1} f_i(x) g_i(x) w(x, y) \, dx dy$$
$$= \sum_{i=1}^{m} \sum_{j=1}^{n_{int}} A_j^x f_i(x_j) \sum_{k=1}^{n_{int}} A_k^y g_i(y_k)$$
$$= \sum_{j=1}^{n_{int}} \sum_{k=1}^{n_{int}} A_j^x A_k^y \sum_{i=1}^{m} f_i(x_j) g_i(y_k)$$
$$= \sum_{j=1}^{n_{int}} \sum_{k=1}^{n_{int}} A_j^x A_k^y f(x_j, y_k) .$$
(6)

The above rule is referred to as a *product rule*. From (6) it becomes clear that to propose a product rule for (4), we ought to develop one-dimensional quadratures.

Let $\hat{\phi}_1(t) = (1-t)/2$ and $\hat{\phi}_2(t) = (1+t)/2$, and consider the weights of the form

$$w_{l,-}(t) = e^{-a_x[1-\hat{\phi}_l(t)]}, \qquad w_{l,+}(t) = e^{-a_x[1+\hat{\phi}_l(t)]}, \tag{7}$$

where a_x is positive. Consider then the approximation

$$\int_{-1}^{1} f(x) w_x(x) \, dx \approx \sum_{j=1}^{n_{int}} A_j^x f(x_j),$$

where w_x is a function as in (7). Next, we present several formulas for A_j^x and x_j . To define A_j^y and y_j , it is enough to change a_x by a_y in (7). Thus the description of (6) is complete.

2.1 A nine-point Newton-Cotes Rule

We consider here a quadrature of Newton–Cotes type using nine integration points for the domain $\hat{K} = [-1, 1] \times [-1, 1]$. Such rule has degree of precision two with respect to each variable. The integration points are the tensor product of the Newton-Cotes onedimension coordinates -1/3, 0, and 1/3. Using the notation as in (6), we have *nint* = 3, and

 $x_1 = y_1 = -1/3,$ $x_2 = y_2 = 0,$ $x_3 = y_3 = 1/3.$

The weights in this case are given in Table 1, where

$$\begin{aligned} a_1 &= 6\frac{12 - a_x(7 - 2a_x) - (12 + a_x(5 + a_x))e^{-a_x}}{a_x^3}, \\ b_1 &= 6e^{-a_x}\frac{12 - (5 - a_x)a_x - (12 + a_x(7 + 2a_x))e^{-a_x}}{a_x^3}, \\ a_2 &= 8\frac{(18 + 9a_x + 2a_x^2)e^{-a_x} - 18 + a_x(9 - 2a_x)}{a_x^3}, \\ b_2 &= 8e^{-a_x}\frac{(18 + 9a_x + 2a_x^2)e^{-a_x} - 18 + a_x(9 - 2a_x)}{a_x^3}, \\ a_3 &= 6\frac{12 - a_x(5 - a_x) - (12 + a_x(7 + 2a_x))e^{-a_x}}{a_x^3}, \\ b_3 &= 6e^{-a_x}\frac{12 - a_x(7 - 2a_x) - (12 + a_x(5 + a_x))e^{-a_x}}{a_x^3}. \end{aligned}$$

Replacing a_x by a_y in the equations above yields the definition of A_i^y .

Table 1

Weights for one-dimensional quadrature using a three-point Newton Cotes rule. The table on the left consider $w_x = w_{l,-}$, and the table on the right assume $w_x = w_{l,+}$.

	A_1^x	A_2^x	A_3^x		A_1^x	A_2^x	A_3^x
l = 1	a_1	a_2	a_3	l = 1	b_1	b_2	b_3
l = 2	a_3	a_2	a_1	l = 2	b_3	b_2	b_1

2.2 A four-point Gaussian Rule

We now seek x_1, x_2, A_1^x, A_2^x such that

$$\int_{-1}^{1} p(x)w_x(x) \, dx = A_1^x p(x_1) + A_2^x p(x_2),$$

for all polynomials p with degree at most three with respect to each variable, where w_x is as in (7). The weights and points are given in Table 2, where

$$a_{1} = \frac{1 - e^{-a_{x}}}{a_{x}} - \frac{c_{3}}{a_{x}\sqrt{c_{4}}}, \quad a_{2} = \frac{1 - e^{-a_{x}}}{a_{x}} + \frac{c_{3}}{a_{x}\sqrt{c_{4}}}, \quad a_{3} = -\frac{c_{1} + \sqrt{c_{4}}}{a_{x}c_{2}},$$

$$a_{4} = -\frac{c_{1} - \sqrt{c_{4}}}{a_{x}c_{2}}, \quad b_{1} = e^{-a_{x}}\frac{1 - e^{-a_{x}}}{a_{x}} + \frac{c_{3}e^{-a_{x}}}{a_{x}\sqrt{c_{4}}}, \quad b_{2} = e^{-a_{x}}\frac{1 - e^{-a_{x}}}{a_{x}} - \frac{c_{3}e^{-a_{x}}}{a_{x}\sqrt{c_{4}}},$$

$$b_{3} = \frac{c_{1} - \sqrt{c_{4}}}{a_{x}c_{2}}, \quad b_{4} = \frac{c_{1} + \sqrt{c_{4}}}{a_{x}c_{2}},$$

$$c_{1} = (4 + a_{x})e^{-2a_{x}} - 2(4 + a_{x}^{2})e^{-a_{x}} + 4 - a_{x}, \quad c_{2} = (2 + a_{x}^{2})e^{-a_{x}} - 1 - e^{-2a_{x}},$$

$$c_{3} = (6 - a_{x}^{3})e^{-2a_{x}} - 2e^{-3a_{x}} - (6 + a_{x}^{3})e^{-a_{x}} + 2,$$

$$c_{4} = 8e^{-4a_{x}} - 4(8 + 3a_{x}^{2} - a_{x}^{3})e^{-3a_{x}} + 8 + (12(4 + 2a_{x}^{2} + a_{x}^{4}) + a_{x}^{6})e^{-2a_{x}} - 4(8 + 3a_{x}^{2} + a_{x}^{3})e^{-a_{x}}.$$

Finally, the definition of A_l^y and y_k is complete when a_x is replaced by a_y in the equations

Table 2

Weights for one-dimensional quadrature using a two-point Gaussian rule. The table on the left consider $w_x = w_{l,-}$, and the table on the right assume $w_x = w_{l,+}$.

	A_1^x	A_2^x	x_1	x_2		A_1^x	A_2^x	x_1	x_2
l = 1	a_1	a_2	a_3	a_4	l = 1	b_1	b_2	b_3	b_4
l = 2	a_2	a_1	b_3	b_4	l = 2	b_2	b_1	a_3	a_4

above.

2.3 A numerical example

For the sake of illustration, we plot the point locations as we vary a_x and a_y . We choose the weight as $w(x, y) = w_{1,-}(x)w_{1,-}(y)$. Hence, $w(\cdot, \cdot)$ has an exponential behaviour in $[-1, 1] \times [-1, 1]$, with $w(1, 1) = e^{-a_x - a_y}$, and w(-1, -1) = 1. So, for large values of a_x , the quadrature points should cluster around the axis x = -1. Similarly, as a_y increases, the quadrature points cluster around the axis y = -1.

In Figure 1, we fix $a_x = 10$, and plot the Gaussian points for $a_y = 1$, $a_y = 10$, $a_y = 100$. We also plot the points of the Newton–Cotes quadrature, which does not depend neither on a_x , nor on a_y , staying over the diagonal y = x.

The Gaussian points were employed in [24] to compute the finite element matrices of a hybrid finite element method for advection-diffusion problems with outflow boundary layers.



Fig. 1. Quadrature point locations, always with $a_x = 10$. The diamonds correspond to $a_y = 1$, crosses to $a_y = 10$, and squares to $a_y = 100$. The circles correspond to the Newton Cotes points, which remain fixed.

3 Quadratures in triangular regions

Optimal quadratures for triangles rely on two-dimensional orthogonal polynomials [23,26] or on the solution of non-linear systems [26, Sec 3.8]. Similarly to quadrilaterals, integrals in arbitrary triangles can be reduced by a linear transformation to integrals in the triangle with vertices (0,0), (0,1) and (1,0). However, the limits of integration in

$$\int_0^1 \int_0^{1-x} f(x,y) w(x,y) \, dy dx \ , \ w(x,y) = w_x(x) w_y(y) \ . \tag{8}$$

prevent the direct use of product rules. An alternative is to use the change of variables

$$x = \frac{1 + \bar{x}}{2}$$
, $y = \frac{1 - \bar{x}}{2} \frac{1 + \bar{y}}{2}$,

which transforms (8) into the following integral [12] (see also [22,27]):

$$\int_{-1}^{1} \int_{-1}^{1} f\left(\frac{1+\bar{x}}{2}, \frac{1-\bar{x}}{2}\frac{1+\bar{y}}{2}\right) w\left(\frac{1+\bar{x}}{2}, \frac{1-\bar{x}}{2}\frac{1+\bar{y}}{2}\right) \frac{1-\bar{x}}{8} d\bar{y}d\bar{x}.$$

We consider next integrals of the form

$$I = \int_0^1 \int_0^{1-x} f(x)g(y)e^{-ax-by} \, dy dx,$$

where a and b are postive numbers. Using the above transformation, we find that

$$I = \int_{-1}^{1} f\left((1+\bar{x})/2\right) \frac{1-\bar{x}}{8} e^{-a(1+\bar{x})/2} G(\bar{x}) d\bar{x},$$

where

$$G(\bar{x}) = \int_{-1}^{1} g\left((1-\bar{x})(1+\bar{y})/4\right) e^{-b(1-\bar{x})(1+\bar{y})/4} \, d\bar{y}.$$

Consider now a one-dimensional quadrature as

$$\int_{-1}^{1} q(\bar{x}) e^{-a(1+\bar{x})/2} d\bar{x} \approx \sum_{j=1}^{n_{int}} A_j(a) q\Big(x_j(a)\Big),$$

where both the weights A_l and the quadrature points x_l might depend on a. For instance, consider the quadratures developed in Section 2, noting that $(1+\bar{x})/2 = 1 - \hat{\phi}_1(\bar{x})$. Then

$$I \approx \sum_{j=1}^{n_{int}} A_j(a) f([1+x_j(a)]/2) \frac{1-x_j(a)}{8} G(x_j(a)).$$

Note that the above quadrature is not exact even if f and g are polynomials since G is not a polynomial, but rather a polynomial times a exponential.

Now, given $x_j(a)$ let $b_j = b(1 - x_j(a))/2$. Thus

$$G(x_j(a)) = \int_{-1}^{1} g([1 - x_j(a)](1 + \bar{y})/4) e^{-b_j[1 - \hat{\phi}_1(\bar{y})]} d\bar{y}$$
$$\approx \sum_{k=1}^{n_{int}} A_k(b_j) g([1 - x_j(a)][1 + y_k(b_j)]/4).$$

The final quadrature reads as

$$I \approx \sum_{j=1}^{n_{int}} A_j(a) f\left([1+x_j(a)]/2\right) \frac{1-x_j(a)}{8} \sum_{k=1}^{n_{int}} A_k(b_j) g\left([1-x_j(a)][1+y_k(b_j)]/4\right).$$

Next, we present rules of Newton–Cotes and Gaussian types. These are genuinely two dimensional quadratures, not based on product rules.

3.1 A three-point Newton-Cotes Rule

One can select (d+2)(d+1)/2 integration points that integrate (8) exactly if f is a polynomial of degree at most d [26, Sc. 3.2], i.e.,

$$\int_0^1 \int_0^{1-x} f(x,y) w(x,y) \, dy \, dx = \sum_{k=1}^{(d+2)(d+1)/2} A_k f(\mathbf{p}_k).$$

Each integration weight A_k (k = 1, ..., (d + 2)(d + 1)/2) can be found by integrating the Lagrange interpolation polynomial associated to the point $\mathbf{p}_k = (x_k, y_k)$, similarly to (2). For instance, if d = 1, we can choose the points

$$\mathbf{p}_1 = (1/2, 1/2), \, \mathbf{p}_2 = (0, 1/2), \, \mathbf{p}_3 = (1/2, 0),$$
(9)

whose barycentric coordinates are invariant to affine transformations that map a triangle into itself [16]. In particular, when $w(x, y) = e^{-a(x+y)}$ we have $A_k = a_k/a^3$, where

$$a_1 = 4(1 - e^{-a}) - a(1 + (3 + a)e^{-a}),$$

$$a_2 = a(1 + e^{-a}) - 2(1 - e^{-a}).$$

If $w(x,y) = e^{-ax-by}$ with $a \neq b$, $A_k = b_k/(a^2(a-b)b^2)$ and

$$b_1 = e^{-a}(2+a)b^2 - a^2(2+b)e^{-b} - (a(b-2)-2b)(a-b),$$

$$b_2 = (a-2)(a-b)^2 + (2+b-a)a^2e^{-b} - (a^2-a(b-4)-2b)be^{-a},$$

$$b_3 = (b-2)(b-a)^2 + (2+a-b)b^2e^{-a} - (b^2-b(a-4)-2a)ae^{-b}.$$

3.2 A six-point Newton-Cotes Rule

If d = 2, the points are

$$\mathbf{p}_1 = (1/3, 1/3), \ \mathbf{p}_2 = (1/3, 2/3), \ \mathbf{p}_3 = (2/3, 1/3), \mathbf{p}_4 = (1/2, 1/2), \ \mathbf{p}_5 = (0, 1/2), \quad \mathbf{p}_6 = (1/2, 0),$$
(10)

where again the barycentric coordinates are invariant to affine transformations within triangles [16]. These points are also found in [23, Tab 5].

When $w(x, y) = e^{-a(x+y)}$ we have $A_i = a_i/a^4$, where

$$a_{1} = 9((3 + (3 + a)^{2})e^{-a} - 3 - (3 - a)^{2})$$

$$a_{2} = 3((24 + 9a - a^{3}/2)e^{-a} - 3(8 - 5a + a^{2}))$$

$$a_{3} = a_{2}$$

$$a_{4} = 2(80 - 32a + 10(1 - a)^{2} - (89 + 41a + (1 - a)^{3})e^{-a})$$

$$a_{5} = 2(18 - 10a + 2a^{2} - ((4 + a)^{2} + 2)e^{-a})$$

$$a_{6} = a_{5}$$

If $w(x,y) = e^{-ax-by}$ with $a \neq b$, $A_i = b_i/(a^3(a-b)b^3)$ and

$$b_1 = 9((4 + (a - 3)a)b^3 - (4 + (b - 3)b)a^3 - b^3(a + 4)e^{-a} + a^3(4 + b)e^{-b})$$

$$b_{2} = 3((b-a)^{3}(4a(3-2b)b+8b^{2}+a^{2}(1-b)(4-3b)) + b^{3}(a^{2}(8+a(5+a))+a(4+a)(3-2a)b-(8-a^{2})b^{2})e^{-a} + a^{3}(ab^{2}(13+4b)-2b^{2}(8+b(5+b))+a^{2}(4-b(3+2b)))e^{-b})$$

$$b_{3} = 3((b-a)^{3}(a(12-7b)b+4b^{2}+a^{2}(8-b(8-3b))) + b^{3}(2a^{2}(8+a(5+a))-a^{2}(13+4a)b-(4-a(3+2a))b^{2})e^{-a} + a^{3}(ab(4+b)(-3+2b)+a^{2}(8-b^{2})-b^{2}(8+b(5+b)))e^{-b})$$

$$b_4 = -4((b-a)^3(a(21-13b)b+12b^2+a^2(12-b(13-5b))) + b^3(a^2(15+2a(5+a)) + (1-a)a(15+4a)b - (12-a-2a^2)b^2)e^{-a} + a^3(a(-1+b)b(15+4b) + a^2(12-b-2b^2) - b^2(15+2b(5+b)))e^{-b})$$

$$b_5 = 4((a-b)^2(4b^2 + 3a(1-b)b + a^2(2+(b-2)b)) + b^3(a(5+a) - (4+a)b)e^{-a} + a^3(b-2a)e^{-b})$$

$$b_6 = 4((a-b)^2(a(3-2b)b+2b^2+a^2(4-(3-b)b)) + (a-2b)b^3e^{-a} + a^3(b(5+b)-a(4+b))e^{-b})$$

3.3 Gaussian Rules

Gaussian quadratures for triangular domains are derived from common roots of twodimensional orthogonal polynomials [26, Sc. 3.7]. While generalizing the Jacob polynomials to two dimensions, Appell and Kampel of Fériet [1, Chap. VI,Note V] observed that the resulting polynomials where orthogonal at reference triangle with with respect to the weighting function w(x, y) = 1 (see also [26]). Moan [23] presented orthogonal polynomials of degree ≤ 4 (with respect to w(x, y) = 1) and found roots for polynomials of degree 1 to 3.

The formula for degree one [26, (3.8-1)] results easily from the system

$$\int_0^1 \int_0^{1-x} f(x,y)w(x,y) \, dy \, dx = A_1 f(x_1,y_1),$$

for any weight w, where f(x, y) = 1, x, y, and A_1, x_1, y_1 are the unknowns. Making f = 1 yields A_1 , and then x_1 and y_1 follow from simple substitutions. Thus

$$A_{1} = \int_{0}^{1} \int_{0}^{1-x} w(x, y) \, dy dx,$$

$$x_{1} = \frac{1}{A_{1}} \int_{0}^{1} \int_{0}^{1-x} xw(x, y) \, dy dx,$$

$$y_{1} = \frac{1}{A_{1}} \int_{0}^{1} \int_{0}^{1-x} yw(x, y) \, dy dx.$$

For $w(x, y) = e^{-ax-by}$ it follows for a = b that

$$A_1 = \frac{1 - (1 + a)e^{-a}}{a^2}, \quad x_1 = y_1 = \frac{1 - (1 + a + a^2/2)e^{-a}}{a(1 - (1 + a)e^{-a})},$$

and for $a \neq b$ that

$$\begin{aligned} A_1 &= \frac{b(1-e^{-a}) - a(1-e^{-b})}{a(b-a)b}, \\ x_1 &= \frac{(a-b)^2 + b((a-b)(1+a) + a)e^{-a} - a^2e^{-b}}{a(b-a)(b(1-e^{-a}) - a(1-e^{-b}))}, \\ y_1 &= \frac{(a-b)^2 - a((a-b)(1+b) - b)e^{-b} - b^2e^{-a}}{b(b-a)(b(1-e^{-a}) - a(1-e^{-b}))}. \end{aligned}$$

4 Application: a multiscale finite element

Let $\Omega \subset \mathbb{R}^2$ be an open bounded domain with polygonal boundary $\partial \Omega$. The linear reaction-diffusion problem consists of finding a function $u = u(\mathbf{x})$ such that

$$-\varepsilon \Delta u + \sigma u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial \Omega, \tag{11}$$

where the reactive and diffusive parameters σ and ε are positive constants. We assume that the source $f = f(\mathbf{x})$ is a given linear function. The weak formulation related to (11) states that $u \in H_0^1(\Omega)$ satisfies

$$\varepsilon \int_{\Omega} \nabla u \cdot \nabla v \, d\mathbf{x} + \sigma \int_{\Omega} u \, v \, d\mathbf{x} = \int_{\Omega} f \, v \, d\mathbf{x} \quad \forall v \in H_0^1(\Omega), \tag{12}$$

where $H_0^1(\Omega)$ is the space of functions in $L^2(\Omega)$ that vanish in $\partial\Omega$, and with weak derivatives in $L^2(\Omega)$.

To approximate (12) using finite elements, we discretize Ω by a conforming and regular partition using triangular elements K and select the finite dimensional subspace $V_h(\Omega) \subset$ $H_0^1(\Omega)$ of continuous linear piecewise polynomials. We thus approximate u by $u_h \in V_h(\Omega)$ such that

$$\varepsilon \int_{\Omega} \nabla u_h \cdot \nabla v_h \, d\mathbf{x} + \sigma \int_{\Omega} u_h \, v_h \, d\mathbf{x} = \int_{\Omega} f \, v_h \, d\mathbf{x} \quad \forall v_h \in V_h(\Omega).$$
(13)

The classical Galerkin method just described is inadequate to approach problem (12) accurately as long as $\varepsilon \ll \sigma h_K^2$, where h_K denotes the characteristic length of element K. Actually, non-physical spurious oscillations characterize such numerical solutions due to the lack of stability. Such issue is treated in [15] by replacing the trial linear finite element space $V_h(\Omega)$ by the enriched space $V_h(\Omega) \oplus E_h(\Omega)$. Such space is generated by the multi-scale functions $\lambda(\mathbf{x})$, given by the formula

$$\lambda(\mathbf{x}) := \frac{\sinh(\alpha_{\mathbf{K}} \,\psi(\mathbf{x}))}{\sinh(\alpha_{\mathbf{K}})},\tag{14}$$

where the coefficient $\alpha_K \sim h_K(\sigma/\varepsilon)^{1/2}$ is the Peclet number, and $\psi(\mathbf{x})$ are piecewise linear shape functions. Thus, the resolution of problem (13) using the trial space $E_h(\Omega) \oplus V_h(\Omega)$ requires the accurate computation of

$$\int_{K} \lambda(\mathbf{x}) \, \psi(\mathbf{x}) \, \mathbf{d}\mathbf{x}, \qquad \int_{\mathbf{K}} \nabla \lambda(\mathbf{x}) \, \nabla \psi(\mathbf{x}) \, \mathbf{d}\mathbf{x}.$$

The integrals above can be actually written as combinations of polynomials times exponential functions of the form presented in previous sections.

4.1 A numerical validation

Let the domain Ω be the unit square, which we discretize by a non-uniform mesh of 400 elements.



Fig. 2. Description of the domain discretization and boundary conditions.

Such mesh as well as the imposed boundary conditions are depicted in Figure 2 (actually to impose continuity over the boundary, and get the solution in $H_0^1(\Omega)$ a transition element is used). Concerning the reaction-diffusion problem (11), we set $\sigma = 1$ and let ε takes the values $\varepsilon = 10^{-5}$ and $\varepsilon = 10^{-6}$. The three-point Newton-Cotes rule (see Section 3.1) allows us to conserve all desirable properties of the multi-scale method unlike the classical one-point Gauss which lead to a loss of accuracy similar to the one observed through the Galerkin method, see Figure 3.



Fig. 3. Solutions by standard one-point Gauss integration and the new exponential-adaptative integration formula ($\sigma = 1$ and $\varepsilon = 10^{-6}$).

Next, we use MAPLE to obtain an analytical expression for the exact integrals as it comes out from the software. Adopting such formula carelessly results in rounding errors, and spurious oscillations show up. This issue is avoided selecting the new numerical integration as it can be seen on Figure 4, where we plot solution's profiles at y = 1/2.



Fig. 4. Profile of solutions at y = 1/2, using numerical and analytical integration adopting $\sigma = 1$ and $\varepsilon = 10^{-5}$ (top) and $\varepsilon = 10^{-6}$ (below).

5 Conclusions

Multiscale finite element methods lead to integrals that cannot be handled with standard Gaussian quadratures. On the other hand, it is not always trivial to insert symbolic manipulation of such integrals into existing finite element codes. We address this issue with weighted quadratures, which combine the accuracy of symbolic integrals and the algorithmic structure of classical integration rules.

The quadrature formulas presented herein are specific to exponential shape functions. Nevertheless, the methodology is readly extendable to other applications.

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