hp Gauss-Legendre Quadrature for Layer Functions

Kleio Liotati†

Project advisor: Christos Xenophontos

Abstract. We consider the numerical approximation of integrals involving *layer* functions, which appear as components in the solution of singularly perturbed boundary value problems. The *hp* version of the Gauss-Legendre composite quadrature, from [1], is utilized in conjunction with the *Spectral Boundary Layer* mesh from [2]. We show that the error goes to zero exponentially fast, as the number of Gauss points increases, independently of the singular perturbation parameter. Numerical examples illustrating the theory are also presented.

1. Introduction.

We consider the numerical approximation of integrals

$$I^{[a,b]}[u] := \int_a^b u(x)dx, \tag{1.1}$$

where $u(x)$ is a typical *layer* function, namely

$$u(x) = f(x)e^{-\beta x/\varepsilon} \ , \ x \in [a,b] \ , \ \beta \in \mathbb{R}^+. \tag{1.2}$$

In (1.2), $\varepsilon \in (0,1]$ is a (singular perturbation) parameter that can approach 0, and $f(x)$ is a given (real) analytic function, satisfying

$$\max_{x\in[a,b]} \left| f^{(n)}(x) \right| \leq |b-a| C_f K_f^n n!, \tag{1.3}$$

for some positive constants C_f, K_f, independent of ε, and β is a given positive constant. It follows that u satisfies the bound (see, e.g. [3])

$$\max_{x\in[a,b]} \left| u^{(n)}(x) \right| \leq C_u K_u^n \max\left\{n, \varepsilon^{-1}\right\}^n,$$

where C_u, K_u are positive constants depending on u. Functions of type (1.2) arise as components in the solution of *singularly perturbed* two-point boundary value problems (SPPs) [4]. Even in two-dimensional SPPs, the solution will still contain functions of type (1.2), with x being the distance from the boundary, multiplied by a smooth function of the second variable (see, e.g. [5]). Such problems arise in a variety of contexts, from fluid and solid mechanics, to control theory and chemical reactions [6].

We study this problem from the Gauss-Legendre point-of-view: recently in [1], the *hp* Gauss-Legendre composite quadrature was studied, in the case when the integrands are either analytic functions, or functions exhibiting singularities near the endpoints of the interval. It was shown that with the proper choice of the intervals in the composite quadrature rule,

†Department of Mathematics and Statistics, University of Cyprus, PO BOX 20537, Nicosia 1678, CYPRUS (klio9965@gmail.com).

the integrals are approximated at an exponential rate, as the number of quadrature points in increased. The tools used in establishing the results in [1] stem from the *hp* theory for Finite Elements (see, e.g., [7]). We comment on how one may approximate integrals, with the integrands exhibiting layer behavior, as in (1.2), using the same tools, but the choice of the intervals is based on the *Spectral Boundary Layer* mesh [2]. For this method, we establish robust, exponential convergence as the number of quadrature points in increased.

We note that for integrals like (1.1), there holds

$$I^{[a,b]}[u] := \int_a^b u(x)dx = \int_a^{a+\xi\varepsilon} u(x)dx + \int_{a+\xi\varepsilon}^b u(x)dx, \tag{1.4}$$

for some $\xi \in \mathbb{R}^+$, and this 'separates' the interval into a *layer* region and a non-layer one. Each integral above will be approximated 'differently', as we will explain in the sequel. For now, we show in Figure 1, the graph of the function $u(x) = (x - x^2)e^{-x/\varepsilon}, x \in (0,1)$, for different ε, which shows how the area under the graph is negligible after a certain point (which depends on ε).

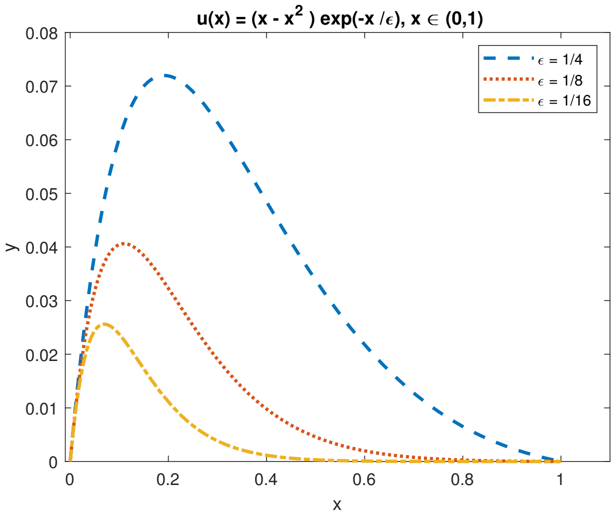

Figure 1. *A typical layer function.*

We close this section with some notation: with $I \subset \mathbb{R}$ a bounded open interval with boundary ∂I and measure $|I|$, we will denote by $C^k(I)$ the space of continuous functions on I with continuous derivatives up to order k. We will use the usual Sobolev spaces $W^{k,q}(I)$ of functions on I with $0, 1, 2, ..., k$ generalized derivatives in $L^q(I)$. The norm of the space $L^\infty(I)$ of essentially bounded functions is denoted by $\|\cdot\|_{L^\infty(I)}$. When $q = \infty$ and k is an integer, we equip the Sobolev space $W^{k,\infty}(I)$ with the norm

$$\|v\|_{W^{k,\infty}(I)} = \max_{0\leq j\leq k} \left\| v^{(j)} \right\|_{L^\infty(I)},$$

with $v^{(j)}$ denoting the j^{th} derivative of v. When $k \geq 0$ is not an integer, the fractional-order space $W^{k,\infty}(I)$ is defined via the K-method of interpolation [8]. The letter C, with or without decorations, will be used to denote a generic positive constant independent of ε and u, and possibly having different values at each occurance.

2. *hp* Gauss-Legendre quadrature.

In [1] the hp version of the Gauss-Legendre (G-L) quadrature was presented, in which the interval is subdivided into N subintervals, and a G-L quadrature is used on each subinterval. To describe the material from [1], let $\Lambda = [a,b], N \in \mathbb{N}$ and define the quadrature nodes $\{x_k\}_{k=1}^N$ and weights $\{w_k\}_{k=1}^N$ by

$$x_k = \frac{b-a}{2}\xi_k + \frac{b+a}{2}\ ,\ w_k = \frac{b-a}{2}\omega_k,$$

where $\{\xi_k, \omega_k\}_{k=1}^N$ are the standard G-L nodes and weights with respect to the interval $[-1,1]$ (see, e.g. [9]). Then, the N point G-L quadrature rule $I_N^{[a,b]}[u]$ for the approximation of $I^{[a,b]}[u]$, is defined as

$$I_N^{[a,b]}[u] := \sum_{k=1}^N w_k u(x_k). \tag{2.1}$$

The hp version of the G-L composite quadrature is defined as follows: we begin with an arbitrary partition $\mathcal{M} = \{\Lambda_m\}_{m=1}^M$ of $\Lambda = [a,b]$ into M open subintervals $\Lambda_m = (x_{m-1}, x_m)$ of length $h_m = x_m - x_{m-1}$. To each subinterval Λ_m we associate $p_m + 1$ quadrature points and set $\overrightarrow{p} = \{p_1, \ldots, p_M\}$ the vector of quadrature nodes. Then, the hp quadrature rule for a given continuous function u on $[a,b]$ is defined as

$$I_{hp}^{[a,b]}[u] = \sum_{m=1}^M I_{p_m}^{[x_{m-1},x_m]}[u] = \sum_{m=1}^M \sum_{k=1}^{p_m} w_{m,k} u(x_{m,k}), \tag{2.2}$$

where $\{x_{m,k}, w_{m,k}\}_{k=1}^{p_m}$ are the shifted G-L quadrature nodes and weights for the interval Λ_m. The following result was established in [1].

Proposition 2.1. *Let $\mathcal{M}$ be an arbitrary partition of $[a,b]$ and let $u \in C([a,b])$ be given, satisfying $u|_{\Lambda_m} \in W^{s_{0,m}+1,\infty}(\Lambda_m)$ for some $s_{0,m} \geq 0$. Then*

$$\left| I^{[a,b]}[u] - I_{hp}^{[a,b]}[u] \right| \leq C \sum_{m=1}^M \left(\frac{h_m}{2}\right)^{s_m+2} \left[\frac{\Gamma(2p_m+2-s_m)}{(2p_m+1)\Gamma(2p_m+2+s_m)}\right]^{1/2} \|u\|_{W^{s_m+1,\infty}(\Lambda_m)},$$

for any $s_m = 0, \ldots, \min\{2p_m+1, s_{0,m}\}$, where Γ is the usual Gamma function and $C > 0$ is a constant independent of h_m, p_m and s_m.

Using the above theorem, it was shown in [1] that the error tends to 0 exponentially fast for functions u that have a point singularity, provided the partition $\mathcal{M}$ is geometrically refined towards the point causing the singularity and the quadrature nodes vector $\overrightarrow{p}$ is increasing linearly (see [1] for details).

For layer functions, we believe the best choice is the *Spectral Boundary Layer* mesh/partition, defined below.

Definition 2.2. *Let $p \in \mathbb{N}, \varepsilon \in (0,1], \kappa \in \mathbb{R}_+$ be given. We define the Spectral Boundary Layer mesh/partition on $I = [a,b]$ as*

$$\mathcal{M}_{SBL}(\kappa, p) = \begin{cases} [a,b] & , \quad \kappa p \varepsilon > 1/2 \\ [a, a+\kappa p \varepsilon, b] & , \quad \kappa p \varepsilon \leq 1/2 \end{cases}.$$

Strictly speaking, it is not a hp but rather a p version, since the number of subintervals is not increasing – only p is. Nevertheless, we use this terminology to be consistent with the literature [2].

Using the above mesh, in conjunction with the composite G-L rule and increasing the number of quadrature nodes p, yields extremely accurate results (as shown in Theorem 2.3 below). In practice, we take $\kappa = 1$ and we simply divide the interval $[a,b]$ into $[a, a+p\varepsilon], [a+p\varepsilon, b]$ and we use as our approximation to (1.1),

$$I^{[a,a+p\varepsilon]}[u] \approx I_{hp}^{[a,a+p\varepsilon]}[u] + u(a+p\varepsilon) = \sum_{k=0}^{p} \ell_k u(\chi_k) + u(a+p\varepsilon),$$

where $\{\ell_k, \chi_k\}$ are the shifted G-L nodes and weights for the interval $[a, a+p\varepsilon]$.

Theorem 2.3. *The approximation of (1.1) by the hp G-L quadrature rule on the* Spectral Boundary Layer *mesh/partition satisfies*

$$\left| I^{[a,b]}[u] - I_{hp}^{[a,b]}[u] \right| \leq C\varepsilon e^{-\sigma p},$$

with $C, \sigma \in \mathbb{R}^+$ independent of ε, u and p.

Proof. We note that in the case $\kappa p \varepsilon > 1/2$, the function (1.2) is analytic and the results of [1] for analytic functions apply.

Thus, we will concentrate on the case where $\kappa p \varepsilon \leq 1/2$. In this case, we have two sub-intervals $\Lambda_1 := (a, a+\kappa p\varepsilon)$ and $\Lambda_2 := (a+\kappa p \varepsilon, b)$. In the second one, we will simply approximate the integral by the value of the integrand at $\kappa p \varepsilon$, as seen below:

$$\begin{aligned} I^{[a,b]}[u] &= I^{[a,a+\kappa p\varepsilon]}[u] + I^{[a+\kappa p\varepsilon,b]}[u] \leq I^{[a,a+\kappa p\varepsilon]}[u] + u(a+\kappa p\varepsilon) \\ &\leq I^{[a,a+\kappa p\varepsilon]}[u] + f(a+\kappa p\varepsilon) e^{-\kappa p} \\ &\leq I^{[a,a+\kappa p\varepsilon]}[u] + C\varepsilon e^{-\kappa p}, \end{aligned} \tag{2.3}$$

since by (1.3), we have

$$|f(a+\kappa p\varepsilon)| \leq Cp\varepsilon.$$

For $I^{[a,a+\kappa p\varepsilon]}[u]$ we will use the G-L quadrature rule with p nodes, viz.

$$I_{hp}^{[a,a+\kappa p\varepsilon]}[u] = \sum_{k=1}^{p} w_k u(x_k).$$

Proposition 2.1, then gives

(2.4)

$$\left| I^{[a,a+\kappa p\varepsilon]}[u] - I_{hp}^{[a,a+\kappa p\varepsilon]}[u] \right| \leq C \left(\frac{\kappa p \varepsilon}{2} \right)^{s+2} \left[\frac{(2p+1-s)!}{(2p+1)(2p+1+s)!} \right]^{1/2} \|u\|_{W^{s+1,\infty}([a,a+\kappa p\varepsilon])}.$$

We first estimate the norm appearing above:

$$\|u\|_{W^{s+1,\infty}([a,a+\kappa p\varepsilon])} = \max_{0\le j\le s+1} \left\|u^{(j)}\right\|_{L^\infty([a,a+\kappa p\varepsilon])},$$

and using Leibniz's rule we find

$$\begin{aligned} |u^{(j)}(x)| &= \left|\frac{d^j}{dx^j}\left(f(x)e^{-\alpha(x)/\varepsilon}\right)\right| \le \sum_{k=0}^{j} \frac{j!}{(j-k)!k!}|f^{(k)}(x)||(e^{-x/\varepsilon})^{(j-k)}| \\ &\le C\sum_{k=0}^{j} \frac{j!}{(j-k)!k!}|f^{(k)}(x)|\varepsilon^{k-j}. \end{aligned}$$

Hence we have

$$\left\|u^{(j)}\right\|_{L^\infty([a,a+\kappa p\varepsilon])} \le C\sum_{k=0}^{j}\varepsilon^{k-j}\frac{j!}{(j-k)!k!}\max_{x\in\Lambda_1}\left|f^{(k)}(x)\right|,$$

and by (1.3) we get, after summing,

$$\left\|u^{(j)}\right\|_{L^\infty([a,a+\kappa p\varepsilon])} \le C\varepsilon^{-j}\sum_{k=0}^{j}\frac{j!}{(j-k)!}C_f K^k \le C\varepsilon^{-j}C_f e^{1/K}K^j\Gamma(j+1),$$

where $\Gamma(\cdot)$ is the usual *Gamma* function [10]. Therefore,

$$\|u\|_{W^{s+1,\infty}([a,a+\kappa p\varepsilon])} \le \max_{0\le j\le s+1}\left\|u^{(j)}\right\|_{L^\infty([a,a+\kappa p\varepsilon])} \le C\varepsilon^{-(s+1)}K^{s+1}(s+2)!, \tag{2.5}$$

and thus combining (2.4) and (2.5), we obtain the following expression for the error between the exact integral and its approximation on the interval $[a, a+\kappa p\varepsilon]$:

$$\begin{aligned} \left|I^{[a,a+\kappa p\varepsilon]}[u] - I_{hp}^{[a,a+\kappa p\varepsilon]}[u]\right| &\le C\left(\frac{\kappa p\varepsilon}{2}\right)^{s+2}\left[\frac{(2p+1-s)!}{(2p+1)(2p+1+s)!}\right]^{1/2}\varepsilon^{-(s+1)}K^{(s+1)}(s+2)! \\ &\le C\varepsilon\left(\frac{\kappa p}{2}\right)^{s+2}K^{(s+1)}(s+2)!\left[\frac{(2p+1-s)!}{(2p+1)(2p+1+s)!}\right]^{1/2}. \end{aligned}$$

Aiming for convergence as $p\to\infty$, for all $\varepsilon > 0$, we continue by choosing $s = \lambda(2p+1), \lambda \in (0,1)$ to be selected shortly, which gives

$$\left|I^{[a,a+\kappa p\varepsilon]}[u] - I_{hp}^{[a,a+\kappa p\varepsilon]}[u]\right| \le C\varepsilon\left(\frac{\kappa p}{2}\right)^{\lambda(2p+1)+2}K^{\lambda(2p+1)+1}\frac{(\lambda(2p+1)+2)!}{(2p+1)^{1/2}}\left[\frac{(2p+1-\lambda(2p+1))!}{(2p+1+\lambda(2p+1))!}\right]^{1/2}.$$

Stirling's formula (see, e.g., [2, Lemma 3.6]) allows us to handle the factorials:

$$\left[\frac{(2p+1-\lambda(2p+1))!}{(2p+1+\lambda(2p+1))!}\right]^{1/2} \le C\left[\frac{(1-\lambda)^{1-\lambda}}{(1+\lambda)^{1+\lambda}}\right]^{p+1/2}(2p+1)^{-\lambda(2p+1)}e^{\lambda(2p+1)},$$

$$\frac{(\lambda(2p+1)+2)!}{(2p+1)^{1/2}} \leq C(\lambda(2p+1)+2)^{(\lambda(2p+1)+2)}e^{-(\lambda(2p+1)+2)} \leq C(2\lambda p+3)^{2\lambda p+3}e^{-\lambda(2p+1)}.$$

Hence,

$$\left|I^{[a,a+\kappa p\varepsilon]}[u] - I_{hp}^{[a,a+\kappa p\varepsilon]}[u]\right| \leq C\varepsilon(\kappa K)^{2\lambda p}\left[\frac{(1-\lambda)^{1-\lambda}}{(1+\lambda)^{1+\lambda}}\right]^{p+1/2}\left(\frac{p}{2}\right)^{2\lambda p+3}(2p+1)^{-(2\lambda p+1)}(2\lambda p+3)^{2\lambda p+3}$$

$$\begin{aligned} &\leq C\varepsilon(\kappa K)^{2\lambda p}\left[\frac{(1-\lambda)^{1-\lambda}}{(1+\lambda)^{1+\lambda}}\right]^{p+1/2}\left(\frac{p}{2}\right)^{2\lambda p+3}(2p+1)^{-(2\lambda p+1)}(2\lambda p+3)^{2\lambda p+3} \\ &\leq Cp^3\varepsilon(\kappa K)^{2p}, \end{aligned}$$

since there exists $\lambda \in (0,1)$ such that (see [1])

$$\left[\frac{(1-\lambda)^{1-\lambda}}{(1+\lambda)^{1+\lambda}}\right]^{p+1/2}\left(\frac{p}{2}\right)^{2\lambda p+3}(2p+1)^{-(2\lambda p+1)}(2\lambda p+3)^{2\lambda p+3} \leq Cp^3.$$

Choosing $\kappa < 1/K \in (0,1)$ in the definition of the mesh, we obtain

$$\left|I^{[a,a+\kappa p\varepsilon]}[u] - I_{hp}^{[a,a+\kappa p\varepsilon]}[u]\right| \leq C\varepsilon e^{-\gamma p},$$

where $\gamma = |\ln q|, q = 1/K < 1$, and we have absorbed the powers of p into the exponential. Combining the above with (2.3), we get the desired result. ■

3. Numerical computations. In this section we show the results of numerical computations for the integral (1.1), for two different choices of the function $f(x), x \in (0,1)$. We will be measuring the error

$$Error = 100 \times \varepsilon\frac{|I[u] - I_{hp}[u]|}{|I[u]|},$$

where $I_{hp}[u]$ denotes the approximation. (We omitted the superscripts.) The factor of ε is used to test the results of Theorem 2.3. We will be plotting the above *Error* versus the number of Gauss points, in a semi-log scale. The resulting lines will verify the exponential convergence.

Example 1 : The integral we wish to approximate is

$$I^{[0,1]}[u] := 1 + \int_0^1(-x^2+x)e^{-x/\varepsilon}dx,$$

with exact value[1]

$$I^{[0,1]}[u] = (2\varepsilon^3+\varepsilon^2)e^{-1/\varepsilon} - 2\varepsilon^3 + \varepsilon^2 + 1.$$

[1]We want the answer to be different from 0.

We show in Figure 2 the results for the G-L quadrature on the SBL mesh/partition, for various value of ε – other values gave similar results and smaller ones gave results beyond machine precision. Since the semi-log plot results in straight lines coinciding, we deduce that the method converges uniformly, at an exponential rate.

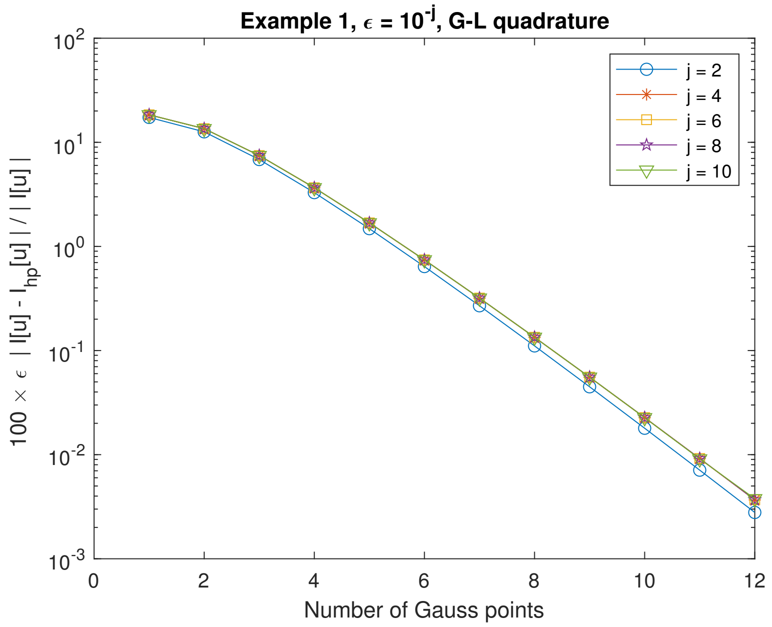

Figure 2. *Example 1: Convergence of the G-L quadrature rule.*

Example 2: Next, we consider the integral

$$I^{[0,1]}[u] := \frac{\ln(3)}{2} + \int_0^1 \frac{4xe^{-x/\varepsilon}}{2x+1} dx,$$

whose exact value involves special functions (and in particular the *exponential integral function* [10]). So, we will use as the exact value the answer that MATLAB© gives with the **integral** command. We repeat the experiment, showing the results in Figure 3, for the same values of ε. The conclusions are the same as in Example 1.

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REFERENCES

[1] M. Zhang, X. Mao and L. Yi, *Exponential convergence of the hp-version of the composite Gauss-Legendre quadrature for integrals with endpoint singularities*, Applied Num. Math., 170 (2021), pp. 340–352.

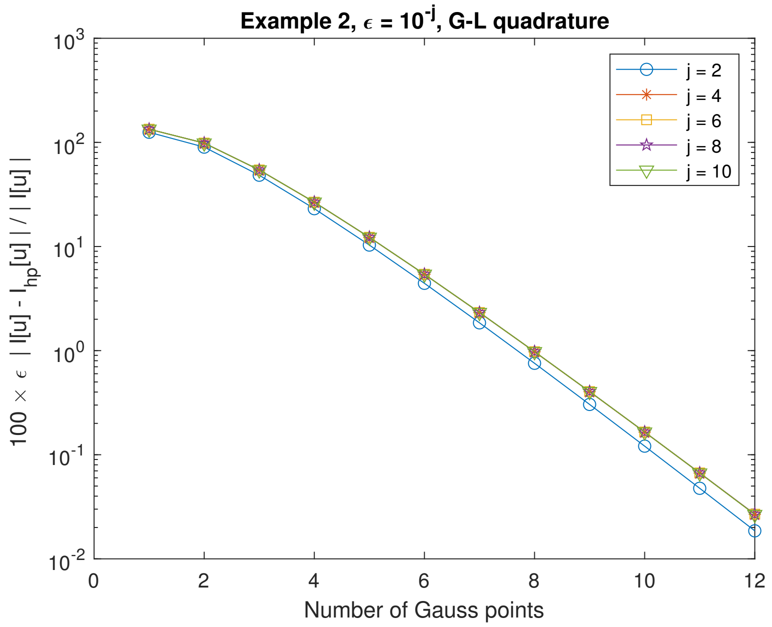

Figure 3. *Example 2: Convergence of the G-L quadrature rule.*

[2] J. M. Melenk, C. Xenophontos and L. Oberbroeckling, *Robust exponential convergence of hp-FEM for singularly perturbed systems of reaction-diffusion equations with multiple scales*, IMA J. Num. Anal., 33 (2013), pp. 609–628.

[3] J. M. Melenk, *hp Finite Element Methods for Singular Perturbations*, Lecture Notes in Mathematics 1796, Springer-Verlag, 2002.

[4] T. Linss, *Layer-adapted meshes for reaction-convection-diffusion problems*, Lecture Notes in Mathematics 1985, Springer-Verlag, 2010.

[5] C. Xenophontos, *The hp finite element method for singularly perturbed problems*, Ph.D. Dissertation, University of Maryland, Baltimore Co, USA, 1996.

[6] H.-G. Roos, M. Stynes, and L. Tobiska, *Robust numerical methods for singularly perturbed differential equations. Convection-diffusion-reaction and flow problems.* Volume 24 of Springer Series in Computational Mathematics, Springer-Verlag, 2008.

[7] C. Schwab, *p- and hp-Finite Element Methods*, Oxford Science Publications, 1998.

[8] L. Tartar, *An Introduction to Sobolev Spaces and Interpolation*, Springer, ISBN 978-3-540-71482-8, 2007.

[9] M. B. Allen III and E. L. Isaacson, *Numerical Analysis for Applied Science*, Wiley & Sons, 1998.

[10] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Applied Mathematics Series. Vol. 55, Dover Publications, 1964.