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Numerical solution of viscous flows in a network of thin tubes: asymptotics and discretization in the cross-section

Éric Canon¹, Frédéric Chardard¹, Grigory Panasenko¹, Olga Štikonienė²

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Abstract

Previously, we considered numerics for a problem on a connected 1D-graph obtained by Panasenko and Pileckas, as the limit model of nonsteady Navier-Stokes equations in a tube structure. The problem is described by nonlocal in time diffusion equations, where weakly singular convolution kernels arise. These kernels are obtained from the heat equation on the cross-sections of the tubes. Their properties and discretization are the topic of the present paper. First, the existence of asymptotic expansions for small times is proved, with explicit formula (with respect to the geometry of the cross-section) for the first five terms. Then, as direct discretization of the equations for the kernels leads to poor approximations due to lack of regularity, numerical schemes that use these asymptotics for small times are designed. Convergence theorems are proved with estimations on the order of convergence. Numerical experiments highlight the interest of this correction.

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1 Introduction

In [3] we consider a numerics for a problem set on a connected 1D-graph which consists of nonlocal in time diffusion equations on each edge of the graph, that are connected with appropriate (Kirchhoff) junctions conditions at the inner vertices of the graph. This model was obtained [14, 16] as the limit model of nonsteady Navier-Stokes equations in a tube structure, by letting the diameters of the tubes tend to zero, with appropriate scaling of the data. The aim was notably the modeling

of microfluids and flows in blood vessels. The geometry of a blood vessel network is complex, so it was important to reduce the full dimension. Suitable numerical scheme for this reduced model are developed and studied in the first part [3] of this work. In particular, the key role of a good approximation of the convolution (with respect to time) kernels in the model is highlighted in [3]. Now, the aim of the present paper is to investigate this crucial point more into detail. This is done in two main directions.

The kernels are computed by solving an auxiliary local heat equation set on some normalized cross sections of the tubes in the original full dimensional model. As these solutions are not regular at $t = 0$, we have to pay a particular attention to the approximation of the kernels for *small* times.

So our first direction is theoretical : we prove that, at least for a C^∞ -smooth domains, the associated kernel admits an asymptotic expansion at $t = 0$ at any order. It is the subject of Theorem 2. The paper by Gie-Jung and Temam [5] on boundary layers theory for the heat equation (when the diffusion coefficient tends to 0) is crucial for proving this theorem. Besides, an independent computation of such an asymptotic expansion for a disk allows us, by comparison, to identify explicitly the first five terms of this expansion, only in terms of universal constants and of the geometry of the domain. This is our first main result. A few additional properties of the kernels are also given, in particular about invertibility and coercivity of the convolution operator, following the lines in [10]. We also give asymptotic expansions (with exponential convergence) for rectangular and triangular domains. The second direction is numeric. We propose several schemes for solving the auxiliary heat equation associated with a given kernel, and show convergence of the approximate kernels associated with this schemes in the $W^{1,1}$ norm, as needed for the convergence theorem proved in [3]. This is the purpose of Theorem 3, 4 and 5. In particular, in Theorem 4, we consider schemes that uses the asymptotic expansions obtained in Theorem 2 (or Propositions 5, 6), to improve the approximation for small times, and consequently the whole approximation. Let us emphasize here that the use of a corrected scheme allows us to improve the order of $W^{1,1}$ -convergence from $1/3$ to $9/8$ theoretically (from Theorem 3 to Theorem 4), and numerically observed from $1/2$ to *ca* 0.7 (schemes of order 1) or *ca* 1.25 (schemes of order 2). Numerical experiments are provided at the end of the paper to validate and illustrate the theoretical results.

Finally, we would like to emphasize that the interest of these results about the kernels is wider than its application to the problem on the graph. The same kernels appear in other situations and other equations, such as double porosity like models, where the convolution appears in the time derivative of a parabolic equation (see for instance, [2, 1, 25, 18, 19]), or in the diffusion term of parabolic equations arising in viscoelasticity or materials with memory (see [12]). Nevertheless, to our knowledge, the results on the asymptotic expansions are new. Let us mention however that an explicit asymptotic expansion with two terms was already used in [1], for a rectangular domain.

Summary of the main result of the first part In [3] we consider a problem set on a connected graph \mathcal{B} in \mathbb{R}^d , where $d = 2$ or 3 , that we describe as follows. Let O_1, \dots, O_N be different vertices

in \mathbb{R}^d , e_1, \dots, e_M closed segments (edges) connecting these vertices. The segments only intersect at vertices. The vertices belonging to a single e_j are numbered from 1 to N_1 : O_1, \dots, O_{N_1} , $N_1 < N$; they constitute the boundary of the structure. The graph is then $\mathcal{B} = \bigcup_{j=1}^M e_j$.

A positive orientation along each edge $e_j = [O_{i_j}, O_{k_j}]$ is defined as the direction from O_{i_j} to O_{k_j} . Then for each edge e_j we denote by ∂_{e_j} the derivative in the normalized direction $\overrightarrow{O_{i_j}, O_{k_j}}$. Given an arbitrary maximal time $T > 0$, the original problem set on $\mathcal{B} \times [0, T]$ is then:

$$\begin{cases} -\partial_{e_j} (\mathcal{L}^{(\sigma_j)} \partial_{e_j} P(x, t)) (x, t) = F(x, t) & \text{for } x \in e_j, j = 1, \dots, M, \\ \sum_{e_j \ni O_i} \alpha_{i,j} \mathcal{L}^{(\sigma_j)} \partial_{e_j} P(x, t) = -\Psi_i(t) & \text{for } i = 1, \dots, N, \\ P \text{ is continuous on the graph,} \\ P(O_1, t) = 0, \end{cases} \quad (1)$$

where $\alpha_{i,j} = 1$ if the orientation of the segment e_j starting from O_i is positive, and $\alpha_{i,j} = -1$ if not. The $\mathcal{L}^{(\sigma_j)}$ are convolution operators $L^2(0, +\infty) \rightarrow H_0^1(0, +\infty)$ defined by:

$$\forall t > 0, \mathcal{L}^{(\sigma_j)} q(t) = \int_0^t K^{(\sigma_j)}(t - \tau) q(\tau) d\tau; \quad (2)$$

the kernels $K^{(\sigma_j)}$ are given by: $K^{(\sigma_j)}(t) = \int_{\sigma_j} V^{(\sigma_j)}(x, t) dx$, where each $V^{(\sigma_j)}$ solves:

$$\begin{cases} \partial_t V - \Delta V = 0 & \text{on } \Omega \times \mathbb{R}^{+*} \\ V = 0 & \text{on } \partial\Omega \times \mathbb{R}^{+*} \\ V = 1 & \text{on } \Omega \times \{0\} \\ V \text{ is continuous} & \text{on } \Omega \times \mathbb{R}^+ \cup \bar{\Omega} \times \mathbb{R}^{+*}. \end{cases} \quad (3)$$

for $\Omega = \sigma_j$, the σ_j are domains in \mathbb{R}^{d-1} corresponding to the sections of the tubes associated with the edges e_j (See [3, 16] for more details).

Last, the functions Ψ_i are given in $H_{00}^1(0, T) = \{f \in H^1(0, T); f(0) = 0\}$ and F is a given function in $H_{00}^1(0, T; L^2(\mathcal{B}))$ (with quite obvious definition of $L^2(\mathcal{B})$, see [3]), that satisfy the compatibility

condition: $\forall t \in [0, T], \sum_{i=1}^N \Psi_i(t) + \int_{\mathcal{B}} F(x, t) dx = 0$.

In [3], we consider schemes for numerically solving (1), and notably prove convergence results in terms of the error in the approximation of the kernels $K^{(\sigma_j)}$. Namely, we prove the following theorem: let

$k > 0$ be some time step such that $N_k = T/k \in \mathbb{N}$; let $t_n = kn$, $K^{(\sigma_j)} = \frac{1}{k} \int_{t_n}^{t_{n+1}} K_n^{(\sigma_j)}(s) ds$; let then $\tilde{K}_n^{(\sigma_j)}$ designate some approximation of $K_n^{(\sigma_j)}$; let the error factor in the discretization of the kernels for a given time step k be defined by:

$$\theta(k) = \max_{1 \leq j \leq M} \left\{ |K_0^{(\sigma_j)} - \tilde{K}_0^{(\sigma_j)}| + \sum_{n=1}^{N_k-1} |K_n^{(\sigma_j)} - K_{n-1}^{(\sigma_j)} - \tilde{K}_n^{(\sigma_j)} + \tilde{K}_{n-1}^{(\sigma_j)}| \right\}; \quad (4)$$

last, let $h > 0$ designates some space step, and $\mathbf{p}_{h,k} \in L^2(0, T; H^1(\mathcal{B}))$ the numerical solution as defined properly in [3]. The following convergence results hold true (Theorem 1 in [3]).

Theorem 1 *If $\theta(k) \rightarrow 0$ as $k \rightarrow 0$, then $\mathbf{p}_{h,k} \rightarrow P$ when $(h, k) \rightarrow (0, 0)$.*

Furthermore, if $F \in H^2(0, T; H^2(\mathcal{B}))$, $\Psi_1, \dots, \Psi_N \in H^2(0, T)$ and $\partial_t F$ and the $\partial_t \Psi_\ell$ vanishes at $t = 0$, there exist positive constants C_1 and C_2 such that for $\theta(k) < C_2$:

$$\begin{aligned} \|\mathbf{p}_{h,k} - P\|_{L^2([0,T], H^1(\mathcal{B}))} \leq & C_1 \left(h \left(\|P\|_{L^2([0,T], H_{dc}^2(\mathcal{B}))} + \frac{1}{C_2 - \theta(k)} \|F\|_{H^1([0,T], H_{dc}^1(\mathcal{B}))} \right) \right. \\ & \left. + k \|P\|_{H^1([0,T], H^1(\mathcal{B}))} + \|P\|_{L^2([0,T], H^1(\mathcal{B}))} \frac{\theta(k)}{C_2 - \theta(k)} \right). \end{aligned} \quad (5)$$

Remark The initial data in Equation (3) do not satisfy the Dirichlet boundary condition. It generates a singularity in V . As we need estimates for the kernels in $W^{1,1}(0, T)$, the term in $\theta(k)$ is thus the most limiting one in (5). This is the main aim of this paper: because of these singularities, we are led to use boundary layers theory to obtain accurate approximations of the kernels for small times. Those are then used to perform sufficiently accurate simulations on the graph.

Outline This paper is organized as follows.

In Section 2, we prove the first main result of this paper, Theorem 2: the existence of asymptotic expansions at any order, for infinitely smooth domains, as stated in Section 2.1. This is proven in several steps. The first step consists in proving the existence of such expansions for a primitive of a kernel. This is done using results in [5] for *well prepared* problems. As (3) is not well prepared in the sense of [5], this is done for a primitive of V which solves a well prepared heat equation. This is done in Section 2.2. In Section 2.2.1, we prove that these expansions can be differentiated term by term. In Section 2.2.2, we compute the first terms of the asymptotic expansion for a disk. This is then used in Section 2.3 to identify some universal constants and thus express the first five terms of the general asymptotic expansions in terms of the geometry of the domain and so finish the proof of Theorem 2. We end this first part with Section 2.4 by computing asymptotic expansions for rectangles and equilateral triangles, to illustrate that asymptotic expansions are of a different nature for non smooth domains.

In Section 3, additional properties of the kernel are presented. First, we propose an alternative proof for continuity, invertibility and coercivity of the \mathcal{L} operators, to those for smooth domains Ω in [20] and [21]. This is done in Section 3.1. Then, in Section 3.2, we give links with two other models: first in the case of a periodic pressure, we rediscover in links with the operator \mathcal{L} , the notion of complex admittances described by Womersley in [28]; second, we note existence of some continuous transition from the model (1) to the one considered in [15] with a different time scale.

Section 4 is devoted to the design of schemes approximating the kernels, and to convergence proofs. Error estimates are provided, with convergence rates. The Dirichlet-Laplace operator is discretized with standard finite elements, with or without Nitsche conditions. In Section 4.3, we obtain a first set of estimates for a semi-discrete scheme. In Section 4.4, full discretization is considered, in a quite general setting, and further a priori estimates are obtained. In Section 4.5 and 4.6, we prove convergence results respectively in the case of a complete discretization for the kernel, and in the case with correction for small times. In Section 4.7 we go more into detail with the link to the convergence results of [3].

Finally, Section 5 is dedicated to the presentation of numerical experiments.

2 Properties of the kernels and asymptotic expansion for small times.

2.1 General - Main result

In this section, we present a theoretical study for an arbitrary kernel. So there is no graph and a single abstract kernel. Let Ω be a domain in \mathbb{R}^2 . The kernel associated with a section Ω is defined on \mathbb{R}^+ by

$$K(t) = \int_{\Omega} V(x, t) dx, \quad (6)$$

where V is the unique solution of (3). It can be explicitly computed in terms of the eigenlements of the Dirichlet Laplace operator: let $(\lambda_k)_{k \in \mathbb{N}}$ be the eigenvalues of this operator, and $(w_k)_{i \in \mathbb{N}}$ an associated orthonormal Hilbert basis of $L^2(\Omega)$; Then

$$K(t) = \sum_{k=0}^{+\infty} a_k^2 e^{-\lambda_k t}, \quad (7)$$

where $a_k = \langle w_k, 1 \rangle$ ($\langle \cdot, \cdot \rangle$ designates the inner product in $L^2(\Omega)$). Thus, K can be extended as a continuous function on $\{t \in \mathbb{C}, \Re(t) \geq 0\}$, analytical on $\{t \in \mathbb{C}, \Re(t) > 0\}$. Besides, its derivatives satisfy:

$$\forall r \in \mathbb{N}, K^{(r)}(t) = \sum_{k=0}^{+\infty} a_k^2 (-\lambda_k)^r e^{-\lambda_k t}. \quad (8)$$

As a consequence the following proposition holds true.

Proposition 1 *K and its derivatives are monotonic and satisfy: $\lim_{+\infty} K^{(r)} = 0$ (K is totally monotonic).*

The aim of this section is to prove the following result.

Theorem 2 *Let Ω be a C^∞ -smooth simply connected domain and K be the kernel as defined above by (6). Then, there exists $(c_n)_{n \in \frac{1}{2}\mathbb{N}}$ such that:*

$$\forall n \in \mathbb{N}, \forall t \geq 0, K(t) = \sum_{r=0}^n c_{r/2} t^{r/2} + O_{t \rightarrow 0^+}(t^{(n+1)/2})$$

where

$$c_0 = S; \quad c_{1/2} = -\frac{2}{\sqrt{\pi}}L; \quad c_1 = \pi; \quad c_{3/2} = \frac{1}{6\sqrt{\pi}} \int_0^L \kappa(s)^2 ds; \quad c_2 = \frac{1}{16} \int_0^L \kappa(s)^3 ds,$$

S is the area of Ω , L is the length of $\partial\Omega$, and $\kappa : [0, L] \rightarrow \mathbb{R}$ is the curvature of $\partial\Omega$ as defined in Equation (13).

Remarks

- (i) In the case of a non simply connected domain, the coefficient c_1 becomes $(1 - k)\pi$, where k designates the number of holes. In the same spirit, the coefficients $c_{3/2}$ and c_2 have to be replaced by the sum of the corresponding terms for each hole in Ω .
- (ii) The assumption of regularity for Ω is essential. In the case of non smooth domains, the situation is possibly quite different. See the examples in Section 2.4 below.

The proof is based on the boundary layer theory for the heat equation as exposed in Gie Jung Temam [4, 5]. Also, note that there exist very similar results for the trace of $e^{t\Delta}$ conjectured in the seminal work “Can one hear the shape of drum” by Kac [9] and proved in Mac Kean Singer [11].

We first prove existence of such an asymptotic expansion for a primitive function of K . We then prove that this expansion can be differentiated term by term to obtain the existence of an asymptotic expansion. The first coefficients are then computed by comparison with the asymptotic expansion of the disk, for which we obtain an explicit expansion at any order.

2.2 General smooth domains : asymptotic expansion for $t \rightarrow 0^+$ of a primitive of K

Gie and all consider in [5] the asymptotic with respect to ε for the heat equation:

$$\begin{cases} \partial_t u^\varepsilon - \varepsilon \Delta u^\varepsilon = f \text{ in } \Omega, \\ u^\varepsilon = 0 \text{ on } \partial\Omega, \\ u^\varepsilon = u_0 \text{ at } t = 0, \end{cases} \quad (9)$$

for quite general data f and u^0 but satisfying the compatibility condition: $u_0 = 0$ on $\partial\Omega$ (what they call *well-prepared* initial condition). Obviously, our problem (3) is not well prepared, because 1 is not equal to 0, even on the boundary. So, let us introduce W defined on $\Omega \times \mathbb{R}^+$ by

$$W(x, t) = \int_0^t V(x, \tau) d\tau,$$

where V is defined in (3), so that

$$\forall t \in \mathbb{R}^+, K(t) = \partial_t \int_\Omega W(x, t) dx, \quad \int_0^t K(\tau) d\tau = \int_\Omega W(x, t) dx. \quad (10)$$

The function W satisfies

$$\begin{cases} \partial_t W - \Delta W = 1 \text{ in } \Omega, \\ W = 0 \text{ on } \partial\Omega, \\ W = 0 \text{ at } t = 0. \end{cases}$$

This is a well-prepared problem of the form (9) with $\varepsilon = 1$ and with very simple data: $f = 1$, $u_0 = 0$. Also, it is easily seen that:

Lemma 1 $\forall t \in \mathbb{R}^+, \forall x \in \Omega, W(x, t) = tu^t(x, 1)$.

Hence, we are led to consider the asymptotic with respect to ε for

$$\begin{cases} \partial_t u^\varepsilon - \varepsilon \Delta u^\varepsilon = 1 \text{ in } \Omega \times]0, T[, \\ u^\varepsilon = 0 \text{ on } \partial\Omega \times [0, T], \\ u^\varepsilon = 0 \text{ in } \Omega \text{ at } t = 0, \end{cases} \quad (11)$$

for given $T > 0$. We prove the following result.

Proposition 2 *Let Ω be a bounded C^∞ -smooth domain. Let $T > 0$. Then, there exists $(\bar{c}_n)_{n \in 1 + \frac{1}{2}\mathbb{N}}$, where $\bar{c}_1 = |\Omega|$, such that:*

$$\forall n \in \mathbb{N}, \forall t \in [0, T], \int_0^t K(\tau) d\tau = \sum_{r=2}^{2n+3} \bar{c}_{r/2} t^{r/2} + O_{t \rightarrow 0^+}(t^{n+2}).$$

Proof of Proposition 2 We prove the result when Ω is a simply connected domain of \mathbb{R}^2 . The case of a holed domain can be dealt similarly, but the boundary $\Gamma = \partial\Omega$ would have as many connected components as the number of holes plus one, and it is a bit cumbersome, though not difficult, to parameterize Γ .

In the case without hole, Γ can be parameterized by its arclength $\gamma : \mathbb{R} \rightarrow \Gamma$, $s \mapsto \gamma(s)$ in a way such that:

$$\gamma'(s) = i(n(\gamma(s))) \quad (12)$$

(we turn counter-clockwise around Ω) where $n : \Gamma \rightarrow \mathbb{R}^2$ is the normal vector to Γ and i is the vectorial rotation of angle $\pi/2$. Then, the curvature κ is defined by:

$$\kappa(s)\gamma'(s) = (n \circ \gamma)'(s). \quad (13)$$

Remark In the case of a non simply connected domain, to maintain (12) the boundaries of the holes have to be parameterized clockwise, whereas the exterior boundary is parameterized counter-clockwise.

One can also define a principal curvature coordinate system on a tubular neighborhood Ω_δ of Γ :

$$X : \begin{cases} \mathbb{R} \times]0, \delta[\rightarrow \text{Im } X = \Omega_\delta \subset \Omega \\ (s, \xi) \rightarrow \gamma(s) - \xi n(\gamma(s)) \end{cases}$$

For small enough $\delta > 0$, X is a diffeomorphism. Besides, the Jacobian matrix and its determinant are given by:

$$J(X)(s, \xi) = \begin{pmatrix} \gamma'(s)(1 - \xi\kappa(s)) & -n(\gamma(s)) \end{pmatrix}, \quad \det J(X)(s, \xi) = 1 - \xi\kappa(s).$$

We look for an asymptotic expansion for u^ε continuous solution to (3) in $\Omega \times [0, T]$. According to equations (200) in [5], u^ε can be approximated at any order $n \in \mathbb{N}$ by an asymptotic expansion of the form:

$$u_{\varepsilon, n+1/2} = \sum_{j=0}^n \left(\varepsilon^j (u^j + \theta^j) + \varepsilon^{j+\frac{1}{2}} \theta^{j+\frac{1}{2}} \right). \quad (14)$$

where u^0 is the solution to (9)_{1,3} with $\varepsilon = 0$, that is $u^0(x, t) = t$. Note that the boundary layers $\theta^{r/2}$ depend on ε . Also, it is easily seen from Equation (204) in [5] that with our constant data $u_0 = 0$ and $f = 1$, we have that for $j \neq 0$, $u^j = 0$. So for convenience, we rewrite (14) as:

$$u_{\varepsilon, n+1/2} = u^0 + \sum_{r=0}^{2n+1} \varepsilon^{r/2} \theta^{r/2}.$$

The boundary layers $\theta^{r/2}$ are defined as follows. Let us first introduce the functions $\tilde{\theta}^j$ of the variables $(s, \xi, t) \in \mathbb{R} \times \mathbb{R}^{+*} \times \mathbb{R}^{+*}$, L -periodic with respect to s , where $L = |\Gamma|$, and defined recursively for $j \in \frac{1}{2}\mathbb{N}$ by:

$$\begin{cases} \partial_t \tilde{\theta}^j - \partial_\xi^2 \tilde{\theta}^j = \tilde{f}^j \text{ in } \mathbb{R}^{+*} \times \mathbb{R}^{+*}, \\ \tilde{\theta}^j = \tilde{\theta}_0^j, \text{ at } \xi = 0, \\ \lim_{\xi \rightarrow +\infty} \tilde{\theta}^j = 0, \\ \tilde{\theta}^j = 0 \text{ at } t = 0. \end{cases} \quad (15)$$

where $\tilde{\theta}_0^0 = -u^0$, $\tilde{\theta}_0^j = 0$ for $j \neq 0$ and

$$\forall j \in \frac{1}{2}\mathbb{N}, \quad \tilde{f}^j = \sum_{k=0}^{2j-2} \xi^k \partial_s \left((k+1) \kappa^k \partial_s \tilde{\theta}^{j-1-\frac{k}{2}} \right) - \sum_{k=0}^{2j-1} \xi^k \kappa^{k+1} \partial_\xi \tilde{\theta}^{j-\frac{1}{2}-\frac{k}{2}}. \quad (16)$$

Remarks

- (i) Equations (15) and (16) come from Equations (94), (210), (211), (212) in [5]. In this reference, these equations are written for $\bar{\theta}^j$ and $\bar{f}^j(s, \xi, t)$ defined by $\bar{\theta}^j(s, \xi, t) = \tilde{\theta}^j(s, \varepsilon^{-1/2}\xi, t)$ and $\bar{f}^j(s, \xi, t) = \tilde{f}^j(s, \varepsilon^{-1/2}\xi, t)$ instead of $\tilde{\theta}^j$ and \tilde{f}^j . Note that for every $j \in \frac{1}{2}\mathbb{N}$, $\tilde{\theta}^j$ does not depend on ε , while $\bar{\theta}^j$, and thus θ^j below, do. It is important for our computations below, and thus, to prove Proposition 2, to have identified these functions $\tilde{\theta}^j$ that do not depend on ε .
- (ii) Since we chose an arclength parameterization, $g_{11} = 1$, $h_1 = h = 1 - \kappa\xi$ with the notations of [5], a lot of simplifications occurs in (94), and therefore in all the subsequent formula in [5].

Let $\sigma : \mathbb{R}^+ \rightarrow \mathbb{R}$ be a C^∞ cut-off function such that $\sigma = 1$ on $[0, \delta/3[$ and $\sigma = 0$ on $]\delta/2, +\infty[$. Then we define the C^∞ -functions θ^j on Ω by

$$\begin{aligned} \theta^j(x, t) &= \sigma(\xi) \tilde{\theta}^j(s, \varepsilon^{-1/2}\xi, t) \text{ where } (\xi, s) = X^{-1}(x) \text{ if } x \in \Omega_\delta, \\ &= 0 \text{ if } x \in \Omega \setminus \Omega_\delta. \end{aligned}$$

Our goal is to approximate $\int_\Omega u^\varepsilon dx$. So, we compute for fixed $n \in \mathbb{N}$:

$$\begin{aligned} \int_\Omega u_{\varepsilon, n+1/2} dx &= \int_\Omega u^0 dx + \sum_{r=0}^{2n+1} \varepsilon^{r/2} \int_\Omega \theta^{r/2} dx \\ &= St + \sum_{r=0}^{2n+1} \varepsilon^{r/2} \int_\Omega \theta^{r/2} dx. \end{aligned}$$

For each term, we have:

$$\int_{\Omega} \theta^{r/2} dx = \int_0^{\delta/2} \sigma(\xi) \int_0^L \bar{\theta}^{r/2}(s, \xi, t) (1 - \kappa(s)\xi) ds d\xi.$$

From Lemma 2.8 Equation (218) in [5] with $m = k = 0$ and $j + d = r/2$, we see that

$$\int_{\delta/3}^{\delta/2} \sigma(\xi) \int_0^L \bar{\theta}^{r/2}(s, \xi, t) (1 - \kappa(s)\xi) ds d\xi = O_{\varepsilon \rightarrow 0}(\exp(-C\varepsilon^{-1})) \quad (17)$$

uniformly with respect to $t \in [0, T]$, where C is a positive constant depending on n, δ and T , but not on ε . Hence, using the change of variable $\nu = \varepsilon^{-1/2}\xi$:

$$\begin{aligned} \int_{\Omega} \theta^{r/2} dx &= \int_0^{\delta/3} \int_0^L \tilde{\theta}^{r/2}(s, \varepsilon^{-1/2}\xi, t) (1 - \kappa(s)\xi) ds d\xi + O_{\varepsilon \rightarrow 0}(\exp(-C\varepsilon^{-1})) \\ &= \int_0^{\delta/3\varepsilon^{1/2}} \int_0^L \tilde{\theta}^{r/2}(s, \nu, t) (1 - \kappa(s)\nu\varepsilon^{1/2}) \varepsilon^{1/2} ds d\nu + O_{\varepsilon \rightarrow 0}(\exp(-C\varepsilon^{-1})). \end{aligned}$$

Then, reasoning as for (17), we deduce that

$$\int_{\Omega} \theta^{r/2} dx = \varepsilon^{1/2} I_{r/2}(t) - \varepsilon J_{r/2}(t) + O_{\varepsilon \rightarrow 0}(\exp(-C\varepsilon^{-1})),$$

where we have set:

$$I_{r/2}(t) = \int_0^{+\infty} \int_0^L \tilde{\theta}^{r/2}(s, \nu, t) ds d\nu, \quad J_{r/2}(t) = \int_0^{+\infty} \int_0^L \tilde{\theta}^{r/2}(s, \nu, t) \kappa(s) \nu ds d\nu. \quad (18)$$

Note that these functions, do not depend on ε .

Now we are able to finalize the proof. From Theorem 2.5 Equation (227) in [5], we know that the error in the approximation of u^ε by $u_{\varepsilon, n+1/2}$ is bounded as follows:

$$\|u_{\varepsilon, n+1/2} - u^\varepsilon\|_{L^\infty(0, T, L^2(\Omega))} \leq C\varepsilon^{n+1}.$$

With (10) and Lemma 1 we thus get:

$$\begin{aligned} \int_0^t K(\tau) d\tau &= t \int_{\Omega} u^t(x, 1) dx = St + \sum_{r=0}^{2n+1} (I_{r/2}(1) t^{(r+3)/2} - J_{r/2}(1) t^{r/2+2}) + O_{t \rightarrow 0+}(t^{n+2}). \\ &= |\Omega| t + \sum_{r=0}^{2n} (I_{r/2}(1) t^{(r+3)/2} - J_{r/2}(1) t^{r/2+2}) + O_{t \rightarrow 0+}(t^{n+2}). \end{aligned} \quad (19)$$

After rearranging, we get the announced result with

$$\begin{aligned} \bar{c}_1 &= |\Omega|, \quad \bar{c}_{3/2} = I_0(1), \\ \forall r \geq 4, \quad \bar{c}_{r/2} &= I_{(r-3)/2}(1) - J_{(r-4)/2}(1). \end{aligned} \quad (20)$$

2.2.1 Term by term differentiability - Existence of asymptotic expansions for K .

Proposition 3 *Let $m \in \mathbb{Z}$, $M \in \mathbb{N}^*$, $T > 0$. Let $H :]0, T] \rightarrow \mathbb{R}$ be a C^1 convex or concave function such that: $H(t) = \sum_{r=m}^M \alpha_r t^{r/2} + O_{t \rightarrow 0^+}(t^{(M+1)/2})$. Then*

$$H'(t) = \sum_{r=m}^{\tilde{M}-1} \frac{r}{2} \alpha_r t^{r/2-1} + O_{t \rightarrow 0^+}(t^{\tilde{M}/2-1}), \quad \text{where } \tilde{M} = \left\lfloor \frac{m+M}{2} \right\rfloor.$$

Proof Without loss of generality, H is assumed to be concave. Then, for any $t \in]0, T]$, $h > 0$,

$$H'(t) \in \left[\frac{H(t+h) - H(t)}{h}, \frac{H(t) - H(t-h)}{h} \right];$$

in particular for $h = t^n$, where $n = \frac{M-m}{4} + 1$, we get:

$$H'(t) \in \left[\frac{H(t+t^n) - H(t)}{t^n}, \frac{H(t) - H(t-t^n)}{t^n} \right]. \quad (21)$$

Now, let us compute:

$$\begin{aligned} \frac{H(t+t^n) - H(t)}{t^n} &= \sum_{r=m}^M \alpha_r t^{\frac{r}{2}-1} \frac{(1+t^{n-1})^{\frac{r}{2}} - 1}{t^{n-1}} + O_{t \rightarrow 0^+}(t^{\frac{M+1}{2}-n}) \\ &= \sum_{r=m}^M \alpha_r t^{\frac{r}{2}-1} \left(\frac{r}{2} + O_{t \rightarrow 0^+}(t^{n-1}) \right) + O_{t \rightarrow 0^+}(t^{\frac{M+1}{2}-n}) \\ &= \sum_{r=m}^M \frac{r}{2} \alpha_r t^{\frac{r}{2}-1} + O_{t \rightarrow 0^+}(t^{\frac{m}{2}-1+n-1}) + O_{t \rightarrow 0^+}(t^{\frac{M+1}{2}-n}) \\ &= \sum_{r=m}^M \alpha_r \frac{r}{2} t^{\frac{r}{2}-1} + O_{t \rightarrow 0^+}(t^{\frac{\tilde{M}}{2}-1}) = \sum_{r=m}^{\tilde{M}-1} \alpha_r \frac{r}{2} t^{\frac{r}{2}-1} + O_{t \rightarrow 0^+}(t^{\frac{\tilde{M}}{2}-1}). \end{aligned}$$

Likewise:

$$\frac{H(t) - H(t-t^n)}{t^n} = \sum_{r=m}^{\tilde{M}} a_r \frac{r}{2} t^{\frac{r}{2}-1} + O_{t \rightarrow 0^+}(t^{\frac{\tilde{M}}{2}-1})$$

Then, using (21), we conclude that H' admits the same asymptotic expansion.

Now, we are able to prove the first part of Theorem 2. Applying Proposition 3 to $H(t) = \int_0^t K(\tau) d\tau$ which is a concave function (see Proposition 1) with $m = 2$ and $M = 2n + 5$, in view of Proposition 2, the following holds true.

Corollary 1 *Let Ω be a smooth domain and K the kernel defined by (6). Then:*

$$\forall n \in \mathbb{N}, \forall t \geq 0, K(t) = \sum_{r=0}^n c_{r/2} t^{r/2} + O_{t \rightarrow 0^+}(t^{(n+1)/2}).$$

where, the coefficients $c_{r/2}$ are defined by $c_{r/2} = (r/2 + 1) \bar{c}_{r/2+1}$, the $\bar{c}_{r/2+1}$ being defined in (20).

2.2.2 Case of a disk cross-section

In this section, we consider the case when $\Omega = \{x \in \mathbb{R}^2; \|x\|_2 < 1\}$.

Proposition 4 (i) *The kernel K is given by: $K(t) = 4\pi \sum_{k=1}^{+\infty} \frac{1}{\mu_k^2} e^{-\mu_k^2 t}$ where the $(\mu_k)_{k \in \mathbb{N}^*}$ are the zeros of the 0-th Bessel function;*

$$(ii) \text{ For } t \geq 0, K(t) = \pi - 4\sqrt{\pi}t + \pi t + \frac{\sqrt{\pi}}{3}t^{3/2} + \frac{\pi t^2}{8} + o_{t \rightarrow 0^+}(t^2).$$

Proof Let J_i denote the i -th Bessel function, $i \in \mathbb{N}$; the eigenvalues λ of the Laplace-operator are known to be the square of the roots of all these Bessel functions, with associated eigenvectors of the form:

$$w_{i,\lambda}(x) = (A_i \cos i\theta + B_i \sin i\theta) J_i(\sqrt{\lambda}\rho)$$

where (ρ, θ) are the polar coordinates of x .

It is easily seen that $\int_{\Omega} w_{i,\lambda} dx = 0$ for $i \neq 0$ so that only the eigenvalues of the 0-th Bessel function J_0 remains in the series expansion (7) of K :

$$K(t) = \sum_{k=1}^{+\infty} a_k^2 e^{-\mu_k^2 t}.$$

Let us consider non normalized eigenvectors associated with the $(\mu_k)_{k \in \mathbb{N}^*}$: $(J_0(\mu_k \rho))_{i \in \mathbb{N}^*}$. One can compute for $\mu > 0$:

$$\int_{\Omega} J_0(\mu \rho) dx = \frac{2\pi}{\mu} J_1(\mu),$$

$$\|J_0(\mu \rho)\|_2^2 = \pi (J_0(\mu)^2 + J_1(\mu)^2),$$

so that the normalized eigenvectors associated with the $(\mu_k)_{k \in \mathbb{N}^*}$ are the $(w_k)_{k \in \mathbb{N}^*}$ defined by: $w_k(\theta, \rho) = \frac{J_0(\mu_k \rho)}{\sqrt{\pi} |J_1(\mu_k)|}$; therefore, the $(a_k^2)_{k \in \mathbb{N}^*}$ are given by: $a_k^2 = \frac{4\pi}{\mu_k^2}$. So, Assertion (i) is proved.

Then we remark that K may be rewritten as: $K(t) = \pi(1 - F_0(t))$ where F_0 is a function introduced in [6] Equation (2.7). The Laplace transform $\mathcal{L}(K)$ of K , which obviously exists for all $s > 0$, is therefore given by $\mathcal{L}(K)(s) = \pi \left(\frac{1}{s} - \mathcal{L}(F_0)(s) \right)$. Hence (See (2.1) in [6]):

$$\mathcal{L}(K)(s) = \pi \left(\frac{1}{s} - \frac{2}{s^{3/2}} \frac{I_1(\sqrt{s})}{I_0(\sqrt{s})} \right),$$

where I_ν stands for the ν -modified Bessel function, which admits (see for instance [27] page 203) an asymptotic expansion for large s at any order. Using your favorite formal computational software, it is then easily obtained that

$$\mathcal{L}(K)(s) = Q(s^{-1/2}) + o_{s \rightarrow +\infty}(s^{-3}) \quad \text{where } Q(X) = \pi X^2 - 2\pi X^3 + \pi X^4 + \frac{\pi}{4}X^5 + \frac{\pi}{4}X^6.$$

On the other hand, we know from Corollary 1 that R_5 defined by

$$R_5(t) = K(t) - P(\sqrt{t}), \quad \text{where } P(X) = \sum_{r=0}^5 c_{r/2} X^r$$

is a C^3 function such that $R_5^{(j)}(0) = 0$ for $j \in \{0, 1, 2\}$, so that, by integration by parts,

$$\mathcal{L}(R_5)(s) = \frac{1}{s^3} \mathcal{L}(R_5^{(3)})(s) = O_{s \rightarrow +\infty}(s^{-4}),$$

and thus $\mathcal{L}(P \circ \sqrt{\cdot})(s) = Q(s^{-1/2}) + o_{s \rightarrow +\infty}(s^{-3})$. Then, using the formula $\mathcal{L}(t^{r/2})(s) = \Gamma(1 + r/2) s^{-1-r/2}$, we obtain by identification the announced result.

2.3 End of the proof of Theorem 2

We already know that $c_0 = S$. To get $c_{1/2}$, c_1 , $c_{3/2}$, c_2 we need to compute in some way $I_0(1)$, $J_0(1)$, $I_{1/2}(1)$, $J_{1/2}(1)$, $I_1(1)$, $J_1(1)$, $I_{3/2}(1)$ defined by (18).

According to [5] Equation (134), the boundary layer $\tilde{\theta}^0$ can be written as:

$$\tilde{\theta}^0(s, \xi, t) = - \int_0^t \operatorname{erfc} \left(\frac{\xi}{2\sqrt{\tau}} \right) d\tau \quad (22)$$

where $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{+\infty} e^{-y^2} dy$.

Remark Here, we use a different definition of the erfc function introduced in equation (135) of [5].

As $\tilde{\theta}^0$ does not depend on s , we get:

$$I_0(1) = L I_{0,c} \text{ where } I_{0,c} = - \int_0^{+\infty} \int_0^1 \operatorname{erfc} \left(\frac{v}{2\sqrt{\tau}} \right) d\tau dv, \quad (23)$$

$$J_0(1) = J_{0,c} \int_0^L \kappa(s) ds \text{ where } J_{0,c} = \int_0^{+\infty} \int_0^1 \operatorname{erfc} \left(\frac{v}{2\sqrt{\tau}} \right) \nu d\tau dv. \quad (24)$$

According to [5] Equations (137)-(138)-(217), the next $\tilde{\theta}^j$ are given by:

$$\tilde{\theta}^j(s, \nu, t) = \int_0^{+\infty} \int_0^t \tilde{f}^j(s, y, \tau) N(\nu, y, t, \tau) d\tau dy, \quad (25)$$

where the \tilde{f}^j are defined in (16) and

$$N(\nu, y, t, \tau) = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{t-\tau}} \left(\exp \left(-\frac{(\nu-y)^2}{4(t-\tau)} \right) - \exp \left(-\frac{(\nu+y)^2}{4(t-\tau)} \right) \right).$$

In particular,

$$\tilde{\theta}^{1/2}(s, \nu, t) = \frac{\kappa(s)}{\sqrt{\pi}} \int_0^{+\infty} \int_0^t \int_0^\tau \frac{1}{\sqrt{r}} \exp \left(-\frac{y^2}{4r} \right) N(\nu, y, t, \tau) dr d\tau dy, \quad (26)$$

so that

$$I_{1/2}(1) = I_{1/2,c} \int_0^L \kappa(s) ds \text{ and } J_{1/2,c}(1) = J_{1/2,\kappa} \int_0^L \kappa(s)^2 ds, \quad (27)$$

where

$$I_{1/2,c} = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} \int_0^{+\infty} \int_0^1 \int_0^\tau \frac{1}{\sqrt{r}} \exp \left(-\frac{y^2}{4r} \right) N(\nu, y, 1, \tau) dr d\tau dy d\nu,$$

$$J_{1/2,c} = \frac{1}{\sqrt{\pi}} \int_0^{+\infty} \nu \int_0^{+\infty} \int_0^1 \int_0^\tau \frac{1}{\sqrt{r}} \exp \left(-\frac{y^2}{4r} \right) N(\nu, y, 1, \tau) dr d\tau dy d\nu.$$

The next boundary layer $\tilde{\theta}^1$ is given by:

$$\tilde{\theta}^1(s, \nu, t) = \int_0^t \int_0^{+\infty} \left(\kappa(s) \partial_\xi \tilde{\theta}^{1/2}(s, y, t) + y \kappa(s)^2 \partial_\xi \tilde{\theta}^0(s, y, t) \right) N(\nu, y, t, \tau) d\tau dy.$$

In view of (22) and (26), $\tilde{\theta}^0$ does not depend on s and $\tilde{\theta}^{1/2}$ is equal to κ multiplied by a function which does not depend on s . Thus, $\tilde{\theta}^1$ is equal to $\kappa(s)^2$ times a function that does not depend on s , so that there are two constants $I_{1,c}$ and $J_{1,c}$ which do not depend on Ω such that

$$I_1(1) = I_{1,c} \int_0^L \kappa(s)^2 ds, \quad J_1(1) = J_{1,c} \int_0^L \kappa(s)^3 ds. \quad (28)$$

Then, according to (25) and (16)

$$\begin{aligned}\tilde{\theta}^{3/2}(s, \nu, t) &= \int_0^{+\infty} \int_0^t \left(\partial_s^2 \tilde{\theta}^{1/2}(s, y, \tau) \right) N(\nu, y, t, \tau) d\tau d\nu \\ &\quad - \int_0^{+\infty} \int_0^t \left(\kappa(s) \partial_\xi \tilde{\theta}^1(s, y, \tau) + y \kappa(s)^2 \partial_\xi \tilde{\theta}^{1/2}(s, y, \tau) + y^2 \kappa(s)^3 \partial_\xi \tilde{\theta}^0(s, y, \tau) \right) N(\nu, y, t, \tau) d\tau dy.\end{aligned}$$

As $\tilde{\theta}^1$ is equal to κ^2 multiplied by a function independent of s , as $\tilde{\theta}^{1/2}$ to κ multiplied by a function independent of s and as $\tilde{\theta}^0$ is independent of s for the fourth term, there exists some function $F_{3/2}$, independent of s such that

$$\tilde{\theta}^{3/2}(s, \nu, t) = \int_0^{+\infty} \int_0^t \partial_s^2 \tilde{\theta}^{1/2}(s, y, \tau) N(\nu, y, t, \tau) d\tau d\nu + \kappa(s)^3 F_{3/2}(\nu, t).$$

As $\partial_s \tilde{\theta}^{1/2}$ is L -periodic with respect to s , the first term vanishes when integration over $s \in [0, L]$. Therefore, there exist some constant $I_{3/2,c}$ such that

$$I_{3/2}(1) = \int_0^{+\infty} \int_0^L \tilde{\theta}^{3/2}(s, \nu, 1) ds d\nu = I_{3/2,c} \int_0^L \kappa(s)^3 ds.$$

However, this possibility to express all the coefficients via the $\int_0^L \kappa(s)^p ds$ and some universal constants stops here: when computing $J_{3/2}(1)$, because of the term $\kappa \partial_s^2 \tilde{\theta}^{1/2}$ in $\tilde{\theta}^{3/2}$ which depends on s via the factor $\kappa \kappa''$, we only obtain the existence of *two* universal constants $J_{3/2,c}$ and $J'_{3/2,c}$ such that

$$\begin{aligned}J_{3/2}(1) &= \int_0^{+\infty} \int_0^L \tilde{\theta}^{3/2}(s, \nu, 1) \kappa(s) \nu ds d\nu \\ &= J_{3/2,c} \int_0^L \kappa(s)^4 ds + J'_{3/2,c} \int_0^L \kappa'(s)^2 ds.\end{aligned}$$

Therefore, the next coefficient in the asymptotic expansion cannot be obtained only by comparison with the expansion for the disks.

Let us conclude the proof. From computations above and from the Total Curvature Theorem, we know that $\int_0^L \kappa(s) ds = 2\pi$, so we may conclude that

$$\begin{aligned}c_{1/2} &= \frac{3}{2} L I_{0,c}; & c_1 &= 4\pi (I_{1/2,c} - J_{0,c}); \\ c_{3/2} &= \frac{5}{2} (I_{1,c} - J_{1/2,c}) \int_0^L \kappa(s)^2 ds; & c_2 &= 3 (I_{3/2,c} - J_{1,c}) \int_0^L \kappa(s)^3 ds.\end{aligned}$$

As for a disk of radius 1, κ is constant equal to 1 and $L = 2\pi$. Then by comparison with the result in Proposition 4, we get the announced values for these coefficients.

Remarks

(i) In fact it is possible, although rather technical to compute explicitly, at least, $I_{0,c}$, $J_{0,c}$, $J_{1/2,c}$, $J_{1/2,c}$.

(ii) Going on further, we would get for $c_{5/2}$ an expression of the form $A \int_0^L \kappa(s)^4 ds + B \int_0^L \kappa'(s)^2 ds$.

As for a disk $\kappa' = 0$ the term A is also easily obtained by comparison with the expansion for the disk.

2.4 Non smooth domain examples

2.4.1 Case of a rectangular section

If the section Ω is the finite interval $]0, 1[$ or any rectangle $]0, a[\times]0, b[$ ($a, b \in \mathbb{R}_+^*$), the eigenfunctions and eigenvalues of the Dirichlet-Laplace operator can be computed explicitly. For $\omega =]0, 1[$, the eigenfunctions are $w_k : x \mapsto \sqrt{2} \sin(\pi k x)$ with associated eigenvalues $\pi^2 k^2$, $k \in \mathbb{N}^*$. Thus,

$$a_k = \int_0^1 w_k(x) dx = \frac{\sqrt{2}}{k\pi} (1 - (-1)^k)$$

so that the corresponding kernel K_1 is given by:

$$\forall t \geq 0, K_1(t) = 8 \sum_{k=0}^{+\infty} \frac{1}{(2k+1)^2 \pi^2} e^{-\pi^2 (2k+1)^2 t} = 4 \sum_{k=-\infty}^{+\infty} \frac{1}{(2k+1)^2 \pi^2} e^{-\pi^2 (2k+1)^2 t},$$

and that

$$\forall t > 0, K_1'(t) = -4 \sum_{k=-\infty}^{+\infty} e^{-\pi^2 (2k+1)^2 t}.$$

By applying Poisson summation formula to the function $u \mapsto 2e^{-\pi^2 (2u+1)^2 t}$, we deduce that

$$\forall t > 0, K_1'(t) = -\frac{2}{\sqrt{\pi t}} \sum_{k=-\infty}^{+\infty} \exp\left(i\pi k - \frac{k^2}{4t}\right) = -\frac{2}{\sqrt{\pi t}} - \frac{4}{\sqrt{\pi t}} \sum_{k=1}^{\infty} (-1)^k \exp\left(-\frac{k^2}{4t}\right). \quad (29)$$

Hence, for any $\varepsilon > 0$,

$$K_1'(t) = \frac{-2}{\sqrt{\pi t}} + O_{t \rightarrow 0^+} \left(e^{-1/(4+\varepsilon)t} \right).$$

By integrating, we obtain:

$$K_1(t) = 1 - 4\sqrt{\frac{t}{\pi}} + O_{t \rightarrow 0^+} \left(e^{-1/(4+\varepsilon)t} \right).$$

Remark By noting that $K_1'(t) = -4e^{-\pi^2 t} \theta(2\pi ti, 4\pi ti)$ where θ stands for the Jacobi θ -function, one could also state directly (29) by invoking the appropriate Jacobi identity. Now, for $\Omega =]0, a[\times]0, b[$, by separation of variables, one can easily deduce:

$$K(t) = abK_1(a^{-2}t)K_1(b^{-2}t).$$

Proposition 5 $\forall t \geq 0, \forall \varepsilon > 0, K(t) = ab - \frac{4(a+b)}{\sqrt{\pi}}\sqrt{t} + \frac{16}{\pi}t + O_{t \rightarrow 0^+} \left(e^{-1/(4+\varepsilon)t} \right).$

2.4.2 Case of an equilateral triangle cross-section

In this section the special case where Ω is the interior of the (equilateral) triangle with vertices $(0, 0)$, $(1, 0)$, $(1/2, \sqrt{3}/2)$. We prove the following result:

Proposition 6 (i) $\forall t > 0, K'(t) = -\frac{3}{\sqrt{\pi t}} + 4\sqrt{3} - \frac{6}{\sqrt{\pi t}} \sum_{k=1}^{+\infty} \exp\left(-\frac{3k^2}{16t}\right);$

$$(ii) \forall t \geq 0, \forall \varepsilon > 0, K(t) = \frac{\sqrt{3}}{4} - 6\sqrt{\frac{t}{\pi}} + 4\sqrt{3}t + O_{t \rightarrow 0^+} \left(\exp\left(-\frac{3}{16t + \varepsilon}\right) \right).$$

Let us state some notations, facts and preliminary results. For each fixed pair $(m, n) \in \mathbb{Z}^2$, we introduce

$$\sigma_{m,n} = ((m_j, n_j))_{1 \leq j \leq 6} = ((m, n), (m, m-n), (-n, m-n), (-n, -m), (n-m, -m), (n-m, n)),$$

$$\varepsilon_{m_j, n_j} = (-1)^{j+1} \text{ which will be called the signature of } (m_j, n_j) \text{ with respect to } (m, n),$$

$$\mathbb{I}_{m,n} = \{(m, n), (m, m-n), (-n, m-n), (-n, -m), (n-m, -m), (n-m, n)\},$$

and

$$\lambda_{m,n} = \frac{16\pi^2}{27} (m^2 + n^2 - mn). \quad (30)$$

As a consequence of the construction of the pairs eigenvalue-eigenvector for the Dirichlet–Laplace operator in Ω , we have the following symmetry properties.

Lemma 2 $\forall (m, n) \in \mathbb{Z}^2:$

- (i) $\forall j \in \{1, \dots, 6\}, m_j \neq 2n_j, n_j \neq 2m_j, m_j \neq -n_j, n_j \neq m_j \iff m \neq 2n, n \neq 2m, m \neq -n, n \neq m;$
- (ii) $\forall j \in \{1, \dots, 6\}, \lambda_{m_j, n_j} = \lambda_{m, n};$
- (iii) $3 \text{ divides } m + n \Rightarrow \forall j \in \{1, \dots, 6\}, 3 \text{ divides } m_j + n_j;$
- (iv) $\forall k \in \{1, \dots, 6\}, \mathbb{I}_{m, n} = \mathbb{I}_{m_k, n_k} \text{ and either all the pairs of this set have the same signature with respect to } (m, n) \text{ and } (m_k, n_k), \text{ or they all are of opposite signatures};$
- (v) $\text{the integer } m_j n_j (m_j - n_j) \text{ is independent of } j.$

As may be found in Grebenkov-Nguyen [7] and Pinski [22]:

Lemma 3 *The eigenvalues of the Dirichlet-Laplace operator in Ω are the numbers $\lambda_{m, n}$ defined by (30), satisfying the following additional conditions:*

- (i) $3 \text{ divides } m + n,$
- (ii) $m \neq 2n, n \neq 2m, m \neq -n, n \neq m.$

The associated complex eigenvectors $u_{m, n}$ are then given by

$$u_{m, n}(x_1, x_2) = \sum_{(m', n') \in \mathbb{I}_{m, n}} \varepsilon_{m', n'} \exp \left(\frac{2i\pi}{3} \left(m' x_1 + (2n' - m') \frac{x_2}{\sqrt{3}} \right) \right).$$

Remarks

- (i) As a consequence of Lemma 2 (iv) for given (m, n) and j , either $u_{m_j, n_j} = u_{m, n}$ or $u_{m_j, n_j} = -u_{m, n}$ so that the six pairs $((m_j, n_j))_{1 \leq j \leq 6}$ define (up to the sign) the same eigenvector.
- (ii) At this point, we do not yet know the normalization of these eigenvectors.

Lemma 4 *Let $(m, n) \in \mathbb{Z}^2$ satisfying Lemma 2(i)-(ii) and $mn(m - n) \neq 0$. Then $\int_{\Omega} u_{m, n}(x) dx = 0$.*

Proof of Lemma 4 Let us first compute each $A_j := \int_{\Omega} \exp \left(\frac{2i\pi}{3} \left(m_j x_1 + (2n_j - m_j) \frac{x_2}{\sqrt{3}} \right) \right) dx$.

We easily get

$$\begin{aligned} A_j &= \int_0^{\sqrt{3}/2} \left(\int_{x_2/\sqrt{3}}^{1-x_2/\sqrt{3}} \exp \left(\frac{2i\pi}{3} (m_j x_1) \right) dx_1 \right) \exp \left(\frac{2i\pi}{3} \left(m_j x_1 + (2n_j - m_j) \frac{x_2}{\sqrt{3}} \right) \right) dy \\ &= \frac{9\sqrt{3}}{8\pi^2} \frac{1}{m_j n_j (m_j - n_j)} \left(m_j - n_j + n_j \exp \left(\frac{2i\pi}{3} m_j \right) - m_j \exp \left(\frac{2i\pi}{3} n_j \right) \right) \end{aligned}$$

where $mn(m-n) \neq 0$ and point (v) in Lemma 1 have been used.

Let us now introduce the notation $I(p) = \exp\left(\frac{2i\pi}{3}p\right)$ and let $A_{m,n} = \frac{8\pi^2}{9\sqrt{3}}mn(m-n) \int_{\Omega} u_{m,n}(x)dx$.

We thus have

$$\begin{aligned} A_{m,n} &= m - n + nI(m) - mI(n) \\ &\quad - n - mI(m) + nI(m) + mI(m-n) \\ &\quad - m + mI(-n) - nI(-n) + nI(m-n) \\ &\quad + n - m + mI(-n) - nI(-m) \\ &\quad + n - mI(n-m) - nI(-m) + mI(-m) \\ &\quad + m - nI(n-m) + nI(n) - mI(n) \\ A_{m,n} &= (2n-m)(I(m) - I(-m)) \\ &\quad + (n-2m)(I(n) - I(-n)) \\ &\quad + (n+m)(I(I(m-n)) - I(I(n-m))) \end{aligned}$$

so that

$$A_{m,n} = 2i \left((2n-m) \sin\left(\frac{2\pi}{3}m\right) + (n-2m) \sin\left(\frac{2\pi}{3}n\right) + (n+m) \sin\left(\frac{2\pi}{3}(m-n)\right) \right).$$

Now, taking into account that $3 \mid (m+n)$, there exists $k \in \mathbb{Z}$ such that $m = 3k - n$. Substituting $m = 3k - n$ in $A_{m,n}$ and using oddity and 2π -periodicity of \sin we get then

$$A_{m,n} = 2i \sin\left(\frac{2\pi}{3}n\right) (3k - 3n + 3n - 6k + 3k) = 0.$$

The lemma is proved.

As shown in Pinski [22], the case where $mn(m-n) = 0$ corresponds to the case of simple eigenvalues. In this case, in view of the symmetry statements of Lemma 1, we may always chose $n = 0$ and $m = 3k$, $k \in \mathbb{N}^*$. Then according to Corollary 2 in Pinski, a possible choice of associated eigenvector to $\lambda_{3k,0}$ is $v_{3k,0}$ defined by:

$$v_{3k,0}(x) = \sin\left(\frac{4\pi k x_2}{\sqrt{3}}\right) + \sin\left(2\pi k \left(x_1 - \frac{x_2}{\sqrt{3}}\right)\right) + \sin\left(2\pi k \left(1 - x_1 - \frac{x_2}{\sqrt{3}}\right)\right).$$

With easy computations, we get the following results.

Lemma 5 $\forall k \in \mathbb{N}^*, \int_{\Omega} v_{3k,0}(x)dx = \frac{3\sqrt{3}}{4\pi k}, \int_{\Omega} v_{3k,0}(x)^2 dx = \frac{3\sqrt{3}}{8}.$

Now, we are able to prove the proposition.

Proof of Proposition 6 According to Lemmas 3, 4, 5 we get for $t \geq 0$

$$K(t) = \frac{3\sqrt{3}}{2\pi^2} \sum_{k=1}^{+\infty} \frac{1}{k^2} \exp\left(-\frac{16\pi^2}{3}k^2t\right),$$

and thus, for $t > 0$,

$$K'(t) = -8\sqrt{3} \sum_{k=1}^{+\infty} \exp\left(-\frac{16\pi^2}{3}k^2t\right) = 4\sqrt{3} - 4\sqrt{3} \sum_{k=-\infty}^{+\infty} \exp\left(-\frac{16\pi^2}{3}k^2t\right).$$

Then, with Poisson resummation formula we get

$$K'(t) = 4\sqrt{3} - \frac{3}{\sqrt{\pi t}} \sum_{k=-\infty}^{+\infty} \exp\left(-\frac{3k^2}{16} \frac{1}{t}\right) = \frac{\sqrt{3}}{4} - \frac{3}{\sqrt{\pi t}} - \frac{6}{\sqrt{\pi t}} \sum_{k=1}^{+\infty} \exp\left(-\frac{3k^2}{16} \frac{1}{t}\right).$$

Hence, we proved (i); we get (ii) by integrating (i).

Remark As in the case of a segment/rectangle, one could rewrite K' in terms of the Jacobi θ -function, by noting that $K'_1(t) = 4\sqrt{3}(1 - \theta(0, 16\pi ti/3))$.

3 Additional properties and remarks about the kernel

3.1 Coercivity

In this section, we consider a kernel $K : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ satisfying the following hypotheses.

Hypothesis 1

- $K(0) > 0$, K is a decreasing function;
- $K \in L^1(0, +\infty)$;
- K is continuous on \mathbb{R}^+ , piecewise C^1 on \mathbb{R}^{+*} .

Hypothesis 2

- $t \rightarrow t^3 K(t)$ is bounded.

Remark As it can be easily checked in Section 2, all kernels considered in the present paper satisfy these hypotheses.

Consider $\mathcal{L} : L^2(0, +\infty) \rightarrow H_0^1(0, \infty)$ defined by

$$\forall f \in L^2(0, +\infty), \forall t \in \mathbb{R}^+, \mathcal{L}(f)(t) = \int_0^t f(\tau)K(t - \tau)d\tau,$$

and for $T > 0$, $\mathcal{A} : L^2(0, T) \times L^2(0, T) \rightarrow \mathbb{R}$ defined by

$$\forall u, v \in L^2(0, T), \mathcal{A}(u, v) \mapsto \int_0^T (\mathcal{L}u)'v dt.$$

The aim of the section is to prove that \mathcal{A} is continuous and coercive. A discrete version of this proof was given in the first part of this paper [3]. Continuity and invertibility of \mathcal{L} were already proven for C^2 domains Ω with another approach, in [20] (Theorem 4.3) and [21] (Theorem 2.11); coercivity was also proven with another approach in [14], along the proof of Theorem 6.1. These results allow to prove to the well-posedness of the continuous model of [14]. In this section, we prove two results about the operator \mathcal{L} defined by (2), using only the properties of the kernel K and of its Fourier transform. The proof follows the lines of [10].

Lemma 6 *Under Hypothesis 1, \mathcal{L} is bounded, invertible with a bounded inverse.*

Proof First note that Hypothesis 1 implies that $K \in W^{1,1}(0, +\infty)$ and that $\lim_{+\infty} K = 0$. Then, as for $f \in L^2(0, +\infty)$, $\|\mathcal{L}f\|_{L^2} \leq \|K\|_{L^1}\|f\|_{L^2}$ and as for smooth functions f with compact support in $]0, +\infty[$, $(\mathcal{L}f)'(t) = K(0)f(t) + \int_0^t K'(t - \tau)f(\tau)d\tau$, we have that

$$\|(\mathcal{L}f)'\|_{L^2} \leq K(0)\|f\|_{L^2} + \|K'\|_{L^1}\|f\|_{L^2} \leq 2K(0)\|f\|_{L^2}.$$

This proves that \mathcal{L} is continuous.

Now, let $g \in H_0^1(0, \infty)$. By Paley-Wiener theorem, the Fourier transform \widehat{g} of g satisfies:

$$\eta = \sup \left\{ \|\widehat{g}\|_{L^2(\mathbb{R}-i\alpha)} + \|\widehat{g}'\|_{L^2(\mathbb{R}-i\alpha)}; \alpha \geq 0 \right\} < +\infty.$$

Let us denote, for $\Im \xi \leq 0, \xi \neq 0$:

$$\widehat{f}(\xi) = \frac{2\pi i \xi \widehat{g}(\xi)}{K(0) + \widehat{K}'(\xi)}.$$

Since $K(0) + \widehat{K}'(\xi) = \int_0^{+\infty} K'(t)(e^{-2\pi \xi i t} - 1)dt$, the real part of the denominator is positive when $\xi \neq 0, \Im \xi \leq 0$. At this point \widehat{f} is just a notation: our goal is to prove that \widehat{f} is indeed the Fourier transform of some $f \in L^2(0 + \infty)$.

Now, on one hand, as $\widehat{K'}$ is a continuous function which tends to zero when $|\xi| \rightarrow +\infty$, there exists $m_\infty > 0$ such that, for $|\xi| > 1$, $|K(0) + \widehat{K'}(\xi)| > m_\infty$.

On the other hand (note that Hypothesis 1 implies that $\lim_{t \rightarrow +\infty} tK(t) = 0$),

$$\lim_{\xi \rightarrow 0} \frac{K(0) + \widehat{K'}(\xi)}{2\pi i \xi} = \lim_{\xi \rightarrow 0} \int_0^{+\infty} K'(t) \frac{e^{-2\pi i \xi t} - 1}{2\pi i \xi} dt = - \int_0^{+\infty} tK'(t) dt = \int_0^{+\infty} K(t) dt > 0.$$

As a consequence, there exists $m_0 > 0$ such that, for $|\xi| \leq 1$, $|K(0) + \widehat{K'}(\xi)| \geq m_0 |2\pi i \xi|$.

Therefore, we have, for $\alpha \geq 0$,

$$\|\widehat{f}\|_{L^2(\mathbb{R}-i\alpha)} \leq \frac{1}{m_0} \|\widehat{g}\|_{L^2(\mathbb{R}-i\alpha)} + \frac{1}{m_\infty} \|\widehat{g'}\|_{L^2(\mathbb{R}-i\alpha)} \leq \frac{\eta}{\min\{m_0, m_\infty\}}. \quad (31)$$

Hence, f is a well-defined function of $L^2(\mathbb{R})$. According to Paley-Wiener theorem the support of f is a subset of $[0, +\infty[$. Hence, $f \in L^2(0, \infty)$ and $\widehat{g'}(\xi) = \widehat{f}(\xi) (K(0) + \widehat{K'}(\xi))$. As a consequence:

$$g'(t) = K(0)f(t) + \int_0^t f(\tau)K'(t-\tau)d\tau.$$

As $g(0) = 0$, we can conclude that $g = \mathcal{L}f$. As (31) also implies the continuity of \mathcal{L}^{-1} , this concludes the proof of the lemma.

Proposition 7 *Assume that Hypotheses 1 and 2 hold. Then, \mathcal{A} is continuous coercive.*

Proof Continuity of \mathcal{A} is a direct consequence of continuity of \mathcal{L} and Cauchy-Schwarz inequality.

Let us prove coercivity.

Let $u \in L^2(0, T)$. We extend u by zero outside $[0, T]$. By Cauchy Schwarz inequality: $\|\widehat{u}\|_\infty \leq \sqrt{T}\|u\|_{L^2}$. Therefore:

$$\int_{-1/4T}^{+1/4T} |\widehat{u}|^2 d\tau \leq \frac{1}{2} \|u\|_{L^2}^2,$$

so that, letting $\mathbb{R}_T = \mathbb{R} \setminus [-1/4T, 1/4T]$, we get

$$\int_{\mathbb{R}_T} |\widehat{u}|^2 d\tau \geq \frac{1}{2} \|u\|_{L^2}^2 \geq \int_{-1/4T}^{+1/4T} |\widehat{u}|^2 d\tau.$$

Then

$$\begin{aligned}
\mathcal{A}(u, u) &= \langle (\mathcal{L}u)', u \rangle_{L^2([0, T])} = \langle (\mathcal{L}u)', u \rangle_{L^2(\mathbb{R})} = \langle K(0)u + K' * u, u \rangle_{L^2(\mathbb{R})} \\
&= \int_{\mathbb{R}} |\widehat{u}|^2 (K(0) + \widehat{K}') d\tau = \int_{\mathbb{R}} |\widehat{u}|^2 \Re(K(0) + \widehat{K}') d\tau \\
&\geq \int_{\mathbb{R}_T} |\widehat{u}|^2 \Re(K(0) + \widehat{K}') d\tau \geq \inf_{\mathbb{R}_T} \Re(K(0) + \widehat{K}') \int_{\mathbb{R}_T} |\widehat{u}|^2 d\tau \\
&\geq \frac{1}{2} \|u\|_{L^2}^2 \inf_{\mathbb{R}_T} \Re(K(0) + \widehat{K}')
\end{aligned}$$

As $\int_0^M t^2 K'(t) dt = [t^2 K(t)]_0^M - 2 \int_0^M t K(t) dt$, we conclude that $t \mapsto t^2 K'(t)$ belongs to $L^1(0, \infty)$. Now, as in the proof of the preceding lemma,

$$K(0) + \widehat{K}'(\xi) = -2\pi i \xi \int_0^{+\infty} t K'(t) dt - 2\pi^2 \xi^2 \int_0^{+\infty} t^2 K'(t) dt + o(\xi^2)$$

As consequence: $\inf_{\mathbb{R}_T} \Re(K(0) + \widehat{K}') \geq C \min\{1, T^{-2}\} > 0$. Hence, we have proved the coercivity.

3.2 Remarks on the periodic case and on the slowly varying case

In the current paper, we deal with the transient regime of fluid motion in (networks of) thin tubes. Two other regimes have also been studied : the periodic¹ (with respect to time) case [28, 13, 24, 8, 17] and the transient slowly varying case [16]. As shown below, these two cases can be seen as limits of the transient case, so that the properties of the kernel K and its suggested approximation may be useful for these two other situations.

3.2.1 Periodic case

Let us recover the time-periodic regime by considering the initial-boundary value problem with given T -periodic pressure drop ($T > 0$). In what follows we prove that in this case the flux asymptotically approaches the time periodic regime. We give the Fourier coefficients expressing them via the Fourier transform of K (extended as zero for negative values of time).

Let $p \in L_{loc}^2(\mathbb{R})$ such that $p(t) = 0$ if $t \leq 0$ and $p(t+T) = p(t)$ if $t \geq 0$. Then, $p \in L^2(0, M)$ for any $M > 0$. Hence, $\mathcal{L}p$ (\mathcal{L} is the operator associated with K , just like in (2)) is well-defined on arbitrary large intervals. Furthermore,

$$\forall t \in \mathbb{R}^+, \forall n \in \mathbb{N}, \mathcal{L}p(t + nT) = \int_0^T \sum_{r=0}^{n-1} K(\tau + rT) p(t - \tau + T) d\tau + \int_0^t p(t - \tau) K(\tau + nT) d\tau.$$

¹Notice that the stationary Poiseuille flow [23] is a particular case of the periodic regime.

Introducing

$$K_T : t \mapsto \sum_{r=-\infty}^{+\infty} K(t + rT) = \frac{1}{T} \sum_{q=-\infty}^{+\infty} \hat{K}(q\omega_0) e^{iq\omega_0 t} \quad (32)$$

where $\omega_0 = \frac{2\pi}{T}$ (the second equality is Poisson summation formula), we get:

$$\mathcal{L}p(t + nT) - \int_0^T K_T(\tau) p(t - \tau + T) d\tau = \int_0^T \sum_{r=n}^{+\infty} K(\tau + rT) p(t - \tau + T) d\tau + \int_0^t p(t - \tau) K(\tau + nT) d\tau. \quad (33)$$

Now, in view of (8), the sequence of functions $t \rightarrow K(t + rT)$ converges exponentially to zero in $W^{1,1}(0, T)$, as $r \rightarrow +\infty$. Hence using (33) and its derivative with respect to t together with Young's inequality, we see that the sequence $t \mapsto \mathcal{L}p(t + nT)$ converges to Φ_T in $H^1(0, T)$, when $n \rightarrow +\infty$, where:

$$\Phi_T : t \mapsto \int_0^T K_T(\tau) p(t - \tau) d\tau.$$

Let us denote by $c_q(f) = \frac{1}{T} \int_0^T f(\tau) e^{-i\omega_0 q \tau} d\tau$, $q \in \mathbb{Z}$, the Fourier coefficients of $f \in L^2(0, T)$. On one hand, we have that: $c_q(\Phi_T) = T c_q(K_T) c_q(p)$. On the other hand, by comparing (32) with

$$K_T(t) = \sum_{q=-\infty}^{+\infty} c_q(K_T) e^{i\omega_0 q t},$$

we get that

$$\forall q \in \mathbb{Z}, c_q(K_T) = \frac{1}{T} \hat{K}(\omega_0 q) = \frac{1}{T} \int_0^T K(t) e^{-i\omega_0 q t} dt.$$

Hence, the coefficients $(T c_q(K_T))_{q \in \mathbb{Z}} = (\hat{K}(\omega_0 T))_{q \in \mathbb{Z}}$ are the complex admittances as described by Womersley in [28].

3.2.2 Slowly varying case

Assume that p is a slowly varying function. What follows shows that the flux $\Phi = \mathcal{L}p$ is also slowly varying. More precisely, let $P : \mathbb{R} \rightarrow \mathbb{R}$ be a fixed smooth function such that $P = 0$ on $] -\infty, 0[$ and $p(t) = P(\varepsilon t)$. Then:

$$\Phi(t\varepsilon^{-1}) = \int_0^{t\varepsilon^{-1}} K(s) P(t - \varepsilon s) ds.$$

Using the Taylor expansion of P at t , we get:

$$\Phi(t\varepsilon^{-1}) = \sum_{j=0}^J \varepsilon^j \frac{P^{(j)}(t)}{j!} (-1)^j \int_0^{+\infty} K(s) s^j ds + O(\varepsilon^{J+1})$$

Now, let $(V^{(-n)})$ be defined by $V^{(0)} = V$, where V is the solution of (3), and

$$\forall n \in \mathbb{N}, V^{(-n-1)}(x, t) = - \int_t^{+\infty} V^{(-n)}(x, s) ds.$$

Then, integrating by parts n times, we obtain:

$$\forall x \in \Omega, \int_0^{+\infty} V^{(-n)}(x, t) dt = \frac{(-1)^n}{n!} \int_0^{+\infty} t^n V(x, t) dt = -V^{(-n-1)}(0).$$

Since V solves the homogeneous heat equation, so that $V^{(-n+1)} = \Delta V^{(-n)}$. Hence:

$$\frac{(-1)^j}{j!} \int_0^\infty K(s) s^j ds = \frac{(-1)^j}{j!} \int_\Omega \int_0^\infty V(x, t) t^j dt dx = - \int_\Omega \Delta^{-j-1} 1 dx$$

where Δ stands for the Dirichlet-Laplace operator.

So, we recover the asymptotic expansion used in [15] (equations (3.3) page 136).

4 Approximation of the operator relating the pressure drop to the flux

This section is devoted to the approximation of the operators $\mathcal{L}^{(\sigma_j)}$ defined in (2). All along this section we consider t in a fixed bounded interval $[0, T]$, $T > 0$, and C is an arbitrary positive constant (which does not depend on the parameters of discretization, h and k) so the value of C can change from one line to the other.

The kernel K is assumed to satisfy:

(i) $\forall t \in [0, T], 0 \leq K(0) - K(t) \leq Ct^{1/2}.$

Note that for C^∞ -smooth domains Ω , Theorem 2 implies that this assumption is fulfilled, while Propositions 5 and 6 imply that it is also true in the rectangular and triangular cases.

4.1 Finite space elements

Let $(S_h)_{h>0}$ denote a family of space of discretization, $(T_h)_{h>0}$ the associated family of approximations of $-\Delta^{-1}$, the opposite of the inverse of Dirichlet-Laplace operator, such that: $T_h : L^2(\Omega) \rightarrow S_h \subset L^2(\Omega)$. For each T_h we assume that:

(ii) T_h is self-adjoint, positive semidefinite on $L^2(\Omega)$ and positive definite on S_h ;

(iii) there exists $r \geq 2$ such that:

$$\forall s \in [2, r], \forall f \in H^{s-2}(\Omega), \|(T_h + \Delta^{-1})f\|_{L^2} \leq Ch^s \|f\|_{H^{s-2}}.$$

Example of finite element methods satisfying these conditions are described in Thomee's book [26] (most notably, \mathbb{P}^{r-1} -elements over quasi-uniform triangulations with boundary conditions dealt with Nitsche method when $r > 2$).

4.2 Approximation of the initial condition

Consider \mathbb{P}^k -elements on a given triangulation \mathcal{T}_h . Let U be a function which is affine on each triangle, equal to 1 at the vertices inside Ω , and equal to 0 at the vertices on $\partial\Omega$. Then: $\int_{\Omega} \mathbb{I}_{\{0 \leq U < 1\}} dx = O(h)$,

that is $\int_{\Omega} (\mathbf{1} - U)^2 dx = O(h)$, $\|\mathbf{1} - U\|_{L^2} = O(h^{1/2})$.

As discrete initial condition for our schemes, we use V_h^0 , the orthogonal projection of $\mathbf{1}$ on S_h . Since V_h^0 and $\mathbf{1} - V_h^0$ are orthogonal, we have:

$$\int_{\Omega} (\mathbf{1} - V_h^0) dx = \int_{\Omega} (\mathbf{1} - V_h^0)^2 dx \leq \int_{\Omega} (\mathbf{1} - U)^2 dx,$$

so that

$$\int_{\Omega} (\mathbf{1} - V_h^0) dx = \int_{\Omega} (\mathbf{1} - V_h^0)^2 dx = O(h). \quad (34)$$

Note that if Nitsche method is used, then $V_h^0 = \mathbf{1} \in S_h$.

4.3 Space discretization

In this section we present semi-discretization (with respect to the space variable) for (3). We then introduce the associated approximate kernel K_h , and obtain a priori estimates for it. Note that from (34), $K_h(0) - K(0) = O(h)$. Let $A_h = T_h^{-1}$. We consider the following semi-discretization:

$$V_h(t) = e^{-tA_h} V_h^0.$$

As $\mathbf{1} \in L^2(\Omega)$, according to Theorems 3.4 and 3.5 (with $s = 0$) p.46 in [26], with (i)-(iii), we have, for C^∞ -smooth Ω (weaker regularity could be enough):

$$\|(V - V_h)(t)\|_{L^2} \leq Ch^r t^{-\frac{r}{2}}, \quad \|\partial_t(V - V_h)(t)\|_{L^2} \leq Ch^r t^{-\frac{r}{2}-1}. \quad (35)$$

Let us introduce the approximate kernel K_h by letting

$$K_h(t) = \int_{\Omega} V_h(x, t) dx.$$

We prove the following estimates.

Proposition 8 *Assume that assumption (i)-(iii) hold. Then:*

$$|K - K_h|(t) \leq Ch^r t^{-r/2};$$

$$\int_0^T |K'(t) - K'_h(t)| dt \leq Ch^{\frac{r}{r+1}}.$$

Proof The first estimate is obtained by integrating (35)₁ over Ω . Let us prove the second one. Let $\lambda_{h,1}, \dots, \lambda_{h,N_h}$ denote the eigenvalues of A_h arranged in ascending order, and $w_{h,1}, \dots, w_{h,N_h}$ denote the corresponding eigenfunctions, normalized with respect to the L^2 norm. As T_h is self-adjoint, we choose an orthonormal system of eigenfunctions. Let $a_{h,j} = \langle w_{h,j}, V_h^0 \rangle = \langle w_{h,j}, \mathbf{1} \rangle$ (the last equality holds because V_h^0 is the orthogonal projection of $\mathbf{1}$). Then:

$$K_h(t) = \sum_{j=1}^{N_h} a_{h,j}^2 e^{-\lambda_{h,j}t}. \quad (36)$$

As K_h and $-K'_h$ are positive and decreasing, using also the second inequality in (35) we have

$$\begin{aligned} \forall \tau \in [0, T], \quad \int_0^T |K'_h - K'| (t) dt &= \int_0^\tau |K'_h - K'| (t) dt + \int_\tau^T \left| \int_\Omega \partial_t (V_h - V)(x, t) dx \right| dt \\ &\leq - \int_0^\tau (K'_h(t) + K'(t)) dt + Ch^r \int_\tau^T t^{-r/2-1} dt \\ &\leq K_h(0) - K_h(\tau) + K(0) - K(\tau) + Ch^r \tau^{-r/2}. \end{aligned}$$

As V_h^0 is the orthogonal projection of $V(., 0)$, $K_h(0) = \|V_h^0\|_{L^2}^2 \leq \|V(., 0)\|_{L^2}^2 = K(0)$ so that

$$K_h(0) - K_h(\tau) + K(0) - K(\tau) = 2K(0) - 2K(\tau) + K(\tau) - K_h(\tau) \leq 2(K(0) - K(\tau)) + |K - K_h|(\tau).$$

Using assumption (i) and the first estimate, we conclude that for all $\tau \in [0, T]$:

$$\int_0^T |K'_h(t) - K'(t)| dt \leq C\tau^{1/2} + Ch^r \tau^{-r/2}.$$

Choosing $\tau = h^{\frac{2r}{r+1}}$, we get the announced result.

4.4 Full discretization

Let $k > 0$ be a time step such that $N_k := T/k$ is integer, and let for all $n \in \mathbb{N}$, $t_n = nk$, $t_{n+1/2} = (t_n + t_{n+1})/2$.

In this section, we consider a family of schemes for (3) associated to the former semi-discretizations, that may be of order 1 or 2 with respect to time. We then introduce the associated approximate kernels, and get a priori estimates relating the approximate kernels corresponding to the fully discrete schemes to the ones corresponding to the semi-discrete schemes. These estimates are used in the next section to prove convergence in the $W^{1,1}$ norm for these approximate kernels.

4.4.1 General setting

We consider full discretizations of the form:

$$V_{h,k}^n = F_n(-kA_h) V_h^0, \quad (37)$$

where F_n are functions satisfying the following properties: there exist three constants $\xi_0 > 0$, $\rho \in \{1, 2\}$, $\varepsilon \in]0, 1[$ and two functions f and $c :]-\xi_0, 0] \rightarrow \mathbb{R}$ such that

$$\begin{aligned} F_n(\xi) &= c(\xi)f(\xi)^n + O_{n \rightarrow +\infty}(\varepsilon^n) && \text{uniformly in }]-\xi_0, 0], \\ |f(\xi)| &\leq 1 && \text{in }]-\xi_0, 0], \\ F_n(\xi) &= O_{n \rightarrow +\infty}(\varepsilon^n) && \text{uniformly in }]-\infty, -\xi_0], \\ f(\xi) &= e^\xi + O_{\xi \rightarrow 0}(\xi^{\rho+1}), && c(\xi) = 1 + O_{\xi \rightarrow 0}(\xi^\rho). \end{aligned} \quad (38)$$

The first three equations are stability conditions, the two equations on the fourth line express consistency of order ρ of the method.

For instance, by choosing $\xi_0 = 1$, $\rho = 1$, $\varepsilon = 1/2$, $f(\xi) = (1 - \xi)^{-1}$, $c = 1$, and $F_n(\xi) = (1 - \xi)^{-n}$, we get the implicit Euler method.

The second order Backward Difference Formula (BDF2) initialized with the Implicit Euler method:

$$\begin{cases} F_0 = 1, F_1(\xi) = (1 - \xi)^{-1}, \\ \forall n \geq 2, (3 - 2\xi)F_{n+2}(\xi) = 4F_{n+1}(\xi) - F_n(\xi), \end{cases}$$

may also be written in this form (38) with $\xi_0 = 2/5$, $\rho = 2$ and $\varepsilon = 2/3$, and with

$$F_n(\xi) = c(\xi)f(\xi)^n + d(\xi)g(\xi)^n,$$

where for $\xi \in]-\xi_0, 0]$:

$$f(\xi) = \frac{2 + \sqrt{1 + 2\xi}}{3 - 2\xi}, \quad g(\xi) = \frac{2 - \sqrt{1 + 2\xi}}{3 - 2\xi},$$

$$c(\xi) = \frac{F_1(\xi) - g(\xi)F_0(\xi)}{f(\xi) - g(\xi)}, \quad d(\xi) = \frac{F_1(\xi) - f(\xi)F_0(\xi)}{g(\xi) - f(\xi)}.$$

It is then easily seen that $|d(\xi)g(\xi)^n| \leq C \left(\frac{2}{3}\right)^n$. The verification of the third condition in (38), which is not trivial, is postponed to the Appendix.

4.4.2 A priori estimates for the discrete kernel

According to Theorem 7.2 p.117 in [26], for one-step schemes, and C^∞ -smooth (weaker regularity could be enough) domains:

$$\|V_{h,k}^n - V_h(t_n)\|_{L^2} \leq Ck^\rho t_n^{-\rho} \|V_h^0\|_{L^2}. \quad (39)$$

This is not enough, we need an error estimate on the time derivative of V . From (38), there exist $\xi_0 > 0$, $\rho \in \{1, 2\}$ and $\varepsilon \in]0, 1[$ such that:

$$\forall \xi \in]-\xi_0, 0], \quad |e^\xi - f(\xi)| \leq C|\xi|^{\rho+1}, \quad (40)$$

$$\forall \xi \in]-\xi_0, 0], \quad |f(\xi)| \leq e^{\xi/2}. \quad (41)$$

Besides, one may always choose ε sufficiently large to satisfy

$$\forall \xi \in]-\infty, -\xi_0], \quad e^\xi \leq \varepsilon. \quad (42)$$

Let us prove the following estimate relating the time derivatives for the full discrete scheme and the semi-discrete scheme.

Lemma 7 *Assume that the hypotheses of Section 4.4.1 hold; assume that*

$$\frac{t_n}{k} \geq -\frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h}),$$

then:

$$\left\| \frac{1}{k} (V_{h,k}^{n+1} - V_{h,k}^n) - \partial_t V_h(t_{n+1/2}) \right\|_{L^2} \leq Ck^\rho t_n^{-\rho-1}.$$

Remark For quasi-uniform triangulations, $\lambda_{h,N_h} = O(h^{-2})$. Hence, the time interval where the bound is not valid is small.

Proof We use the notations of Section 4.3. Then

$$V_{h,k}^{n+1} - V_{h,k}^n - k\partial_t V_h(t_{n+1/2}) = \sum_{j=1}^{N_h} a_{h,j} \left(F_{n+1}(-k\lambda_{h,j}) - F_n(-k\lambda_{h,j}) + k\lambda_{h,j} e^{-(n+\frac{1}{2})k\lambda_{h,j}} \right) w_{h,j} \quad (43)$$

We have to discuss the contribution of each term in the sum, according to whether $-k\lambda_{h,j} \in]-\xi_0, 0[$ or not.

For $0 \leq \xi \leq \xi_0$, from (38) we have that

$$F_{n+1}(-\xi) - F_n(-\xi) + \xi e^{-(n+\frac{1}{2})\xi} = c(-\xi)f(-\xi)^n (f(-\xi) - 1) + \xi e^{-(n+\frac{1}{2})\xi} + O(\varepsilon^n). \quad (44)$$

Using the identity $a^n - b^n = (a - b) \sum_{r=0}^{n-1} a^r b^{n-r-1}$,

$$f(-\xi)^n - e^{-n\xi} = (f(-\xi) - e^{-\xi}) \sum_{r=0}^{n-1} f(-\xi)^r e^{-(n-1-r)\xi}$$

so that, with (40) and 41:

$$|f(-\xi)^n - e^{-n\xi}| \leq C\xi^{\rho+1} n e^{-\frac{n}{2}\xi}.$$

Also, with the last two assumptions in (38) and Taylor expansion for $e^{-\xi} - 1 + \xi e^{-\xi/2}$ and $\rho \leq 2$, one easily gets:

$$|c(-\xi)(f(-\xi) - 1) + \xi e^{-\frac{1}{2}\xi}| \leq C\xi^{\rho+1},$$

while from the fourth point in (38), we have

$$|f(-\xi) - 1| \leq \xi.$$

Hence

$$\begin{aligned} & \left| c(-\xi)f(-\xi)^n (f(-\xi) - 1) + \xi e^{-(n+\frac{1}{2})\xi} \right| \\ &= \left| (c(-\xi)(f(-\xi) - 1) + \xi e^{-\xi/2}) e^{-n\xi} + c(-\xi)(f(-\xi) - 1)(f(-\xi)^n - e^{-n\xi}) \right| \\ &\leq C\xi^{\rho+1} e^{-n\xi} + C\xi^{\rho+2} n e^{-\frac{n}{2}\xi}. \end{aligned} \quad (45)$$

Since the functions $x \mapsto x^{\rho+1}e^{-x}$ and $x \mapsto x^{\rho+2}e^{-x/2}$ are bounded on \mathbb{R}^+ , we can conclude that for $0 \leq \xi \leq \xi_0$:

$$\begin{aligned} \left| c(-\xi)f(-\xi)^n (f(-\xi) - 1) + \xi e^{-(n+\frac{1}{2})\xi} \right| &\leq C\xi^{\rho+1} e^{-n\xi} + C\xi^{\rho+2} n e^{-\frac{n}{2}\xi} \\ &\leq \frac{C}{n^{\rho+1}} = C \frac{k^{\rho+1}}{t_n^{\rho+1}}. \end{aligned}$$

For $\xi \geq \xi_0$, using the third assumption in (38) and (42), we get:

$$\left| F_{n+1}(-\xi) - F_n(-\xi) + \xi e^{-(n+\frac{1}{2})\xi} \right| \leq C\varepsilon^n (1 + \xi).$$

But, as we assume that $n \geq 2 \frac{\ln(1+\xi)}{\ln \varepsilon^{-1}}$, $(1+\xi)\varepsilon^{n/2} \leq 1$, this implies

$$\left| F_{n+1}(-\xi) - F_n(-\xi) + \xi e^{-(n+\frac{1}{2})\xi} \right| \leq C\varepsilon^{n/2} = \frac{C}{n^{\rho+1}} (n^{\rho+1}\varepsilon^{n/2}) \leq \frac{C}{n^{\rho+1}} = C \frac{k^{\rho+1}}{t_n^{\rho+1}}. \quad (46)$$

From (43), (44), (45), (46) and $\varepsilon^n \leq 1/n^{\rho+1}$ we conclude that

$$\|V_{h,k}^{n+1} - V_{h,k}^n - \partial_t V_h(t_{n+1/2})\|_{L^2} \leq k^{\rho+1} t_n^{-\rho-1} C \left(\sum_{j=1}^{N_h} a_{h,j}^2 \right)^{1/2} \leq k^{\rho+1} t_n^{-\rho-1} C \|V_h^0\|_{L^2}.$$

□

Let us now introduce an approximation of the kernel based on a full discrete approximation of the form (37)-(38) of V . So let $K_{h,k}$ be the continuous function on $[0, T]$, affine on each $[t_n, t_{n+1}]$, defined by:

$$\forall n \in \{0, \dots, N_k\}, K_{h,k}(t_n) = \int_{\Omega} V_{h,k}^n(x) dx. \quad (47)$$

As V_0^h is the orthogonal projection of $\mathbf{1}$ on S_h , similarly to (36), we also have

$$K_{h,k}(t_n) = \sum_{j=1}^{N_h} a_{j,h}^2 F_n(-k\lambda_{j,h}).$$

Proposition 9 *Assume that the hypotheses of Section 4.4.1 hold. Then*

$$\begin{aligned} |K_{h,k}(t_n) - K_h(t_n)| &\leq Ck^{\rho} t_n^{-\rho}; \\ |K'_{h,k}(t_{n+1/2}) - K'_h(t_{n+1/2})| &\leq Ck^{\rho} t_n^{-1-\rho} \text{ if } \frac{t_n}{k} \geq -\frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h}); \\ |K_{h,k}(t) - K_h(t)| &\leq Ckt^{-1} \text{ if } \frac{t}{k} \geq -\frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h}); \\ \int_t^T |K'_{h,k}(\tau) - K'_h(\tau)| d\tau &\leq Ckt^{-1} \text{ if } \frac{t}{k} \geq -\frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h}). \end{aligned}$$

Proof The first assertion is obtained by integrating (39) over Ω , the second one by integrating the estimate of Lemma 7.

Let us prove the third one. From (36), it is easily seen that $-K'_h$ is nonnegative and K_h is convex and nonnegative. Thus:

$$0 \leq -K'_h(t) \leq \frac{K_h(0) - K_h(t)}{t} \leq \frac{K_h(0)}{t} \leq \frac{K(0)}{t}.$$

Then, using the concavity of K'_h , we get:

$$0 \leq K''_h(t) \leq \frac{K'_h(t) - K'_h(t/2)}{t/2} \leq \frac{-K'_h(t/2)}{t/2} \leq 4K(0)t^{-2}. \quad (48)$$

Now, on each $]t_n, t_{n+1}[$, using the second inequality of the proposition with $\rho = 1$ for the first term, the mean value theorem and (48) for the second one, for $t_n \geq -2k \ln(1 + k\lambda_{h,N_h})/\ln \varepsilon$ we have:

$$\begin{aligned} |(K'_{h,k} - K'_h)(t)| &= |K'_{h,k}(t_{n+1/2}) - K'_h(t)| \leq |(K'_{h,k} - K'_h)(t_{n+1/2})| + |K'_h(t) - K'_h(t_{n+1/2})| \\ &\leq Ckt^{-2} + Ckt^{-2}. \end{aligned} \quad (49)$$

But from the third assumption of (38) and (47) $\lim_{+\infty} K'_{h,k} = 0$ and from (36), $\lim_{+\infty} K'_h = 0$, so that, by integration from t to $+\infty$, we get:

$$|K_{h,k}(t) - K_h(t)| \leq Ckt^{-1}.$$

The fourth inequality follows by integrating (49) on $[t, T]$.

4.5 Convergence of the uncorrected scheme

In this section, we prove convergence in $W^{1,1}(0, T)$ of the approximate kernel, when suitable first or second order in time schemes are used to solve problem (3) numerically.

Let us make the additional assumption on the time discretization:

$$\forall n \in \mathbb{N}, \forall \xi \leq 0, \quad F_n(\xi) = f(\xi)^n \geq 0. \quad (50)$$

The implicit Euler method and the second order method defined by

$$f(\xi) = \left(1 - \left(1 - \frac{\sqrt{6}}{3}\right)\xi\right)^{-3} \left(1 + \left(\frac{\sqrt{6}}{2} - 1\right)\xi\right)^2$$

satisfy this condition.

Let us describe how to construct a scheme satisfying (50). Consider a one step scheme corresponding to $F_n(x) = f(x)^n$ and satisfying hypotheses (38), but not (50). Then the scheme defined by $\tilde{F}_n(x) = F_n(x/2)^2 = f(x/2)^{2n}$ satisfies both (38) and (50), since $f(x)^2 \geq 0$. This corresponds to taking a one step scheme over two half-time steps: $u_{n+1/2} = f(-kA_h/2)u_n$, $u_{n+1} = f(-kA_h/2)u_{n+1/2} = f(-kA_h/2)^2 u_n$.

Remark Note that such a procedure would not work for BDF2 since it is a multi-step scheme. Hence, the result of this paragraph does not apply to BDF2 unless it is corrected for small times as it is shown in the next section.

Now we are able to prove the following convergence theorem for the approximate kernel.

Theorem 3 Assume that assumptions (i)-(iv), (38) and (50) hold, then for sufficiently small k ,

$$\int_0^T |K'_{h,k}(t) - K'(t)| dt \leq C k^{\frac{\mu}{2}},$$

where $h = k^\gamma$ and $\mu = \min \left\{ \frac{2}{3}, \gamma \frac{2r}{r+1} \right\}$.

Remark Hence, for sufficiently large γ , the method is of order 1/3 in time.

Proof Assumption (50) yields that $K_{h,k}$ is decreasing and positive: indeed, from (38), $|f(\xi)| \leq 1$ for $\xi \in [-\xi_0, 0]$ while for $\xi \leq -\xi_0$, $F_n(\xi) = O(\varepsilon^n) \Rightarrow |f(\xi)| \leq C^{1/n} \varepsilon < 1$ for n large enough, so that for all n :

$$K_{h,k}(t_n) = \sum_{j=1}^{N_h} a_{j,h}^2 f(-k\lambda_{j,h})^n \geq 0 \text{ and } K'_{h,k}(t_{n+1/2}) = \frac{1}{k} \sum_{j=1}^{N_h} a_{j,h}^2 f(-k\lambda_{j,h})^n (f(-k\lambda_{j,h}) - 1) \leq 0.$$

Thus, reasoning as in the proof of Proposition (8), we get:

$$\begin{aligned} \int_0^\tau |K'_{h,k}(t) - K'_h(t)| dt &\leq K_{h,k}(0) - K_{h,k}(\tau) + K_h(0) - K_h(\tau) \\ &\leq K_{h,k}(0) - K_h(0) + |K_h(\tau) - K_{h,k}(\tau)| \\ &\quad + 2(K_h(0) - K(0)) + 2(K(0) - K(\tau)) + 2(K(\tau) - K_h(\tau)). \end{aligned}$$

The first term on the right is 0; from the third inequality of Proposition 9, for $\tau \geq -k \frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h})$, the second term is bounded by $Ck\tau^{-1}$; the third one is non positive; from hypothesis (i) the fourth one is bounded by $C\tau^{\frac{1}{2}}$; from Proposition 8 the last term is bounded by $Ch^r \tau^{-\frac{r}{2}}$. We thus get

$$\int_0^\tau |K'_{h,k}(t) - K'_h(t)| dt \leq C (k\tau^{-1} + \tau^{1/2} + h^r \tau^{r/2}).$$

Now take $\tau = k^\mu$, and k sufficiently small, then $\tau \geq -k \frac{2}{\ln \varepsilon} \ln(1 + k\lambda_{h,N_h})$. Together with the fourth inequality of Proposition (9), this proves the announced result.

4.6 Convergence with correction for small times

In this section, we also assume that the asymptotic expansion for the corresponding kernel obtained in Section 2 (Theorem 2) holds for K . This is case when Ω is C^∞ -smooth and simply connected, but

weaker regularity may be enough. These expansions are used for small times in order to improve the convergence rate.

For $\rho \in \{1, 2\}$, summing up the second inequality in Proposition 9, for $\tau \geq -\frac{2k}{\ln \varepsilon} \ln(1 + \lambda_{h, N_h})$, we get:

$$k \sum_{\tau \leq t_n < T} |K'_{h,k}(t_{n+1/2}) - K'_h(t_{n+1/2})| \leq k \sum_{\tau \leq t_n < T} Ck^\rho t_n^{-\rho-1} \leq Ck^\rho \int_{\tau}^{+\infty} t^{-\rho-1} dt \leq Ck^\rho \tau^{-\rho};$$

Let us define:

$$K_{h,k,\tau}(t) = \begin{cases} K_{h,k}(t) & \text{if } t \geq \tau \\ K_{h,k}(\tau) + \left[S - 2L\sqrt{\frac{s}{\pi}} + \pi s + \frac{s^{3/2}}{6\sqrt{\pi}} \int_0^L \kappa(s)^2 ds + \frac{s^2}{16} \int_0^L \kappa(s)^3 ds \right]_{\tau}^t & \text{if } t < \tau \end{cases}.$$

Then, for $m = 5/2$:

$$\int_0^{\tau} |K'_{h,k,\tau}(t) - K'(t)| dt \leq C \int_0^{\tau} t^{m-1} dt \leq C\tau^m.$$

Theorem 4 Assume that assumptions (i)-(iv) and (38) hold, then for sufficiently small k ,

$$\int_0^{\tau} |K'_{h,k,\tau}(t) - K'(t)| dt + k \sum_{\tau \leq t_n < T} |K'_{h,k,\tau}(t_{n+1/2}) - K'(t_{n+1/2})| \leq Ck^{m\mu}$$

where $\mu = \min \left\{ \frac{\rho}{m + \rho}, \gamma \frac{2r}{2m + r} \right\}$ and $\tau = k^\mu$.

The proof is the same as in the previous section.

Remarks

- (i) Hence, if γ is chosen sufficiently large, for $\rho = 2$, the method is of order $10/9 > 1$ in time.
- (ii) In particular, this theorem can be applied to the corrected implicit Euler and BDF2 schemes.

4.7 Link with $\theta(k)$

Let us take $\tilde{K}_n = \frac{1}{k} \int_{t_n}^{t_{n+1}} K_{h,k,\tau}(t) dt$ for the uncorrected scheme and $\tilde{K}_n = \frac{1}{k} \int_{t_n}^{t_{n+1}} K_{h,k}(t) dt$ for the corrected scheme. In the first part [3] of this article, we introduced $K_n = \frac{1}{k} \int_{t_n}^{t_{n+1}} K(s) ds$ and

$$\theta(k) = |K_0 - \tilde{K}_0| + \sum_{0 < nk < T} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}|.$$

We also have

$$K_n - K_{n-1} = k \int_{-1}^1 K'(k(n+t))(1-|t|)dt = k \int_0^1 (K'(k(n+t)) + K'(k(n-t)))(1-t)dt. \quad (51)$$

Theorem 5 *Under the assumptions of Theorem 3 or those of Theorem 4, we have:*

$$\theta(k) \leq Ck^{m\mu}$$

with $m = 1/2$ (e.g. Implicit Euler without correction) or $m = 5/2$ (e.g. Implicit Euler and BDF2 with correction).

Proof Let's first deal with the corrected scheme. First, as for (51), when $t_n < \tau$:

$$\begin{aligned} \sum_{0 < nk < \tau} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| &\leq \sum_{0 < nk < \tau} \int_{t_{n-1}}^{t_{n+1}} |(K'(t) - K'_{h,k,\tau}(t))(1 - \frac{1}{k}|t - t_n|)| dt \\ &\leq 2 \int_0^\tau |K'_{h,k,\tau}(t) - K'(t)| dt. \end{aligned}$$

Then, for $t_n \geq \tau$,

$$\begin{aligned} \left| \tilde{K}_n - \tilde{K}_{n-1} - kK'(t_n) \right| &= k \left| \frac{1}{2} (K'_{h,k}(t_{n-1/2}) + K'_{h,k}(t_{n+1/2})) - K'(t_n) \right| \\ &\leq k \left| \frac{1}{2} (K'_{h,k}(t_{n-1/2}) + K'_{h,k}(t_{n+1/2})) - \frac{1}{2} (K'(t_{n-1/2}) + K'(t_{n+1/2})) \right| \\ &\quad + k \left| \frac{1}{2} (K'(t_{n-1/2}) + K'(t_{n+1/2})) - K'(t_n) \right|. \end{aligned}$$

As,

$$\left| \frac{1}{2} (K'(t_{n-1/2}) + K'(t_{n+1/2})) - K'(t_n) \right| \leq k^2 \sup_{[(n-1)k, (n+1)k]} |K^{(3)}| \leq Ck^2 t_n^{-5/2},$$

we thus get

$$\left| \tilde{K}_n - \tilde{K}_{n-1} - kK'(t_n) \right| \leq \frac{1}{2} |K'_{h,k}(t_{n-1/2}) - K'(t_{n-1/2}) + K'_{h,k}(t_{n+1/2}) - K'(t_{n+1/2})| + Ck^3 t_n^{-5/2}.$$

Similarly, $|K'(k(n+t)) + K'(k(n-t)) - 2K'(t_n)| \leq Ck^2 \sup_{[(n-1)k, (n+1)k]} |K^{(3)}|$, so that

$$|K_n - K_{n-1} - kK'(t_n)| \leq Ck^3 t_n^{-5/2}.$$

Hence

$$\begin{aligned}
& \sum_{0 \leq nk < T} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| \\
& \leq 2 \int_0^\tau |K'_{h,k,\tau}(t) - K'(t)| dt + C \sum_{\tau \leq nk < T} k^3 t_n^{-5/2} \\
& \quad + \frac{k}{2} \sum_{\tau \leq nk < T} |K'_{h,k,\tau}(t_{n-1/2}) - K'(t_{n-1/2})| + |K'_{h,k,\tau}(t_{n+1/2}) - K'(t_{n+1/2})|
\end{aligned}$$

With Theorem 4, and $\sum_{\tau \leq nk < T} k^3 t_n^{-5/2} \leq Ck^2 \tau^{-3/2}$, this proves the result.

Let us now consider the case of an uncorrected scheme. We have, in the same way:

$$\sum_{0 < nk < T} |K_n - K_{n-1} - \tilde{K}_n - \tilde{K}_{n-1}| \leq 2 \int_0^T |K'_{h,k}(t) - K'(t)| dt \leq Ck^{m\mu}.$$

Now, one needs to bound $|K_0 - \tilde{K}_0|$:

$$|K_0 - \tilde{K}_0| \leq |K_{N_k-1} - \tilde{K}_{N_k-1}| + \sum_{0 < nk < T} |K_n - K_{n-1} - \tilde{K}_n - \tilde{K}_{n-1}|,$$

so that from the error estimate of the trapezoid formula error:

$$|K_{N_k-1} - \tilde{K}_{N_k-1}| \leq k^2 \sup_{[T/2, T]} |K''| + \frac{1}{2} |K_{h,k}(T - k) - K(T - k)| + \frac{1}{2} |K_{h,k}(T) - K(T)|$$

Hence, (39) and (47) yields:

$$|K_{N_k-1} - \tilde{K}_{N_k-1}| \leq Ck^2 + CT^{-\rho} k^\rho + CT^{-\rho/2} h^r.$$

All these terms can be bounded by $Ck^{m\mu}$ for sufficiently small k . This completes the proof of theorem. \square

We conclude this section, by proving that the conditions on the discrete kernels for convergence and stability of the schemes in [3] are satisfied by the discrete kernels presented in this paper.

Proposition 10 *If the hypotheses of Theorem 3 are satisfied (e.g. Implicit Euler without correction), then $(\frac{1}{k} \int_{t_n}^{t_{n+1}} K_{h,k}(t) dt)_n$ and $(K_{h,k}(t_n))_n$ satisfy Lemma 4 of [3].*

Remark Using proposition 2 of [3], this proves that the scheme presented in equations (1.8-11) and (3.26) of [3] with $W = 1$ is unconditionally stable.

Proof

$$U_n := \frac{K_{h,k}(t_n) - 2K_{h,k}(t_{n+1}) + K_{h,k}(t_{n+2})}{k^2} = \sum_{j=1}^{N_h} a_{j,h}^2 f(-k\lambda_{j,h})^n (f(-k\lambda_{j,h}) - 1)^2 \geq 0.$$

Besides $U_{n+1} - U_n = \sum_{j=1}^{N_h} a_{j,h}^2 f(-k\lambda_{j,h})^n (f(-k\lambda_{j,h}) - 1)^3 \leq 0$. Hence $(U_n)_n$ is nonnegative and decreasing.

For sufficiently small k ,

$$\int_{T/2}^{3T/4} K'_{h,k}(t + T/4) - K'_{h,k}(t) dt > E := \frac{1}{2} \int_{T/2}^{3T/4} K'(t + T/4) - K'(T) dt.$$

Hence, there exists $t_{n+1/2} \in [T/2, 3T/4]$ such that $(T/4)|K'_{h,k}(t_{n+1/2} + T/4) - K'_{h,k}(t_{n+1/2})| > E$.

Hence, there exists $t_p > T/2$ such that $(T/2)U_{p-1} \geq \frac{E}{T/2}$. We conclude that, as (U_n) is decreasing,

for $t_n \leq \frac{T}{2}$, $U_n \geq 4\frac{E}{T^2}$ and $\frac{U_n + U_{n+1}}{2} \geq 4\frac{E}{T^2}$. This concludes the proof.

For the scheme presented in [3], Section 3.4.2, we prove the following result.

Proposition 11 *If the hypotheses of Theorem 3 are satisfied (e.g. Implicit Euler without correction), and if we take $\tilde{K}_n = K_{h,k}(t_n)$ or $\tilde{K}_n = K_{h,k}(t_{n+1})$, then the conclusions of Theorem 5 also hold.*

Proof

$$\begin{aligned} & \sum_{0 < t_n < T} |K_{h,k}(t_n) - K_{h,k}(t_{n-1}) - \int_{t_n}^{t_{n+1}} K_{h,k}(t) dt + \int_{t_{n-1}}^{t_n} K_{h,k}(t) dt| \\ &= \sum_{0 < t_n < T} \left| \frac{K_{h,k}(t_{n-1}) - 2K_{h,k}(t_n) + K_{h,k}(t_{n+1}))}{2} \right| \\ &= \sum_{0 < t_n < T} \frac{K_{h,k}(t_{n-1}) - 2K_{h,k}(t_n) + K_{h,k}(t_{n+1}))}{2} \\ &= \frac{K_{h,k}(0) - K_{h,k}(k)}{2} - \frac{K_{h,k}(T-k) - K_{h,k}(T)}{2} \\ &\leq \frac{K_{h,k}(0) - K_{h,k}(k)}{2} \leq \frac{1}{2} \int_0^k |K'_{h,k}(t) - K'(t)| dt + \frac{1}{2} \int_0^k |K'(t)| dt \\ &\leq Ck^{\mu/2} + Ck^{1/2}. \end{aligned}$$

Using Theorem 5, we get the announced result.

5 Numerical results

In this section, we test the schemes designed in the previous sections. As it was predicted above theoretically, we observe convergence. We also compare the theoretically predicted convergence rate with the one obtained in numerical experiments. This *experimental* convergence rate is better than predicted by Theorem 5.

Figure 1 presents the graph of function V for small values of time. One can observe that the leading term of the deviation to $\mathbf{1}$ essentially depends on the distance to the boundary of the domain. It motivates the application of the boundary layer theory.

Analysing 2 and 3, one can observe the following three regimes of behavior of the error of approximation of the time derivative of the kernel K :

- the initialization regime for small times the multistep BDF2 scheme, when the hypotheses of Lemma 7 are not satisfied;
- the discretization error regime, when the results of the previous section are applicable;
- the rounding error regime, when the rounding errors dominate and the error fluctuations become important.

The numerical results show that when the time discretization error dominates then the error of approximation of the time derivative of K is:

- proportional to $kt^{-3/2}$ for the implicit Euler scheme (with a factor of proportionality of about 0.37);
- proportional to $k^2t^{-5/2}$ for the BDF2 scheme (with a factor of proportionality of about $\simeq 0.58$).

Note that these convergence rates are better than those predicted by the estimates of Lemma 7. Similar observations can be done for the regime when the discretization in space error is dominant, although in this case the experimental convergence rate is more equivocal and closer to the theoretically predicted one.

Last, we compare the numerically computed convergence rate with the one theoretically predicted by the estimate of Theorem 5. The results of this comparison are presented in the tables below. In order to test the accuracy of the schemes we run the tests for domains Ω for which the exact kernels are known, namely:

- the equilateral triangle with the length of the side equal to 2;

- square with the side of the length 1;
- the disc of radius 1.

The error is given both in L^1 -norm and $\dot{W}^{1,1}$ semi-norm in the following senses:

$$\|f\|_{L_k^1} = \sum_{0 \leq t_n < T} k \frac{|f(t_n) + f(t_{n+1})|}{2}, \quad \|f\|_{\dot{W}_k^{1,1}} = \sum_{0 \leq t_n < T} |f(t_{n+1}) - f(t_n)|.$$

For the uncorrected scheme we observe an error of order 1/2 in time and 1 in space (both for Implicit Euler/ \mathbb{P}^1 , BDF2/ \mathbb{P}^2) which is better than the theoretical 1/3 in time and 2/3 and 3/4 in space. For the schemes with correction for small times, the observed orders in space and time are (the first one is computed for \mathbb{P}^1 elements in space, the second one for \mathbb{P}^2 elements):

- $\simeq 0.84$ and $\simeq 1.23$ for Implicit Euler/ \mathbb{P}^1 (theoretical 3/4, 6/5),
- $\simeq 1.47$ and $\simeq 2.36$ for BDF2/ \mathbb{P}^2 (theoretical 10/9, 15/8).

The first series of four tables uses the \mathbb{P}^1 -elements for the space discretization and the BDF2 method for the time discretization for triangular and squared domain. We give the accuracy results both with respect to the space discretization (first tables) and with respect to the time discretization (second tables), but focus our attention on the order in time. As mentioned above, although order 1/3 was proven, the order 1/2 is actually observed. We investigate further for the disk geometry, in Tables 5 and 6.

Table 1: accuracy with respect to space discretization, case of an equilateral triangle with side 2, Nitsche, BDF2.

h	k	L_k^1 -error	order	$\dot{W}_k^{1,1}$ -error	order
1e+00	5e-05	1.8175e-02	-	5.8193e-01	-
4e-01	5e-05	9.1221e-03	0.752	2.7825e-01	0.805
2e-01	5e-05	3.7106e-03	1.298	1.3868e-01	1.005
1e-01	5e-05	1.0619e-03	1.805	6.5145e-02	1.090
4e-02	5e-05	1.8547e-04	1.904	2.5610e-02	1.019
2e-02	5e-05	4.7558e-05	1.963	1.8005e-02	0.508
1e-02	5e-05	1.2097e-05	1.975	1.5205e-02	0.244
4e-03	5e-05	2.1411e-06	1.890	1.4530e-02	0.050

Table 2: accuracy with respect to time discretization, case of an equilateral triangle with side 2, Nitsche, BDF2.

h	k	L_k^1 -error	order	$\dot{W}_k^{1,1}$ -error	order
4e-03	1e-01	3.2533e-02	-	6.7891e-01	-
4e-03	5e-02	1.3683e-02	1.250	4.7059e-01	0.529
4e-03	2e-02	3.8177e-03	1.393	2.9155e-01	0.523
4e-03	1e-02	1.4100e-03	1.437	2.0521e-01	0.507
4e-03	5e-03	5.1521e-04	1.452	1.4490e-01	0.502
4e-03	2e-03	1.3384e-04	1.471	9.1594e-02	0.501
4e-03	1e-03	4.7590e-05	1.492	6.4761e-02	0.500
4e-03	5e-04	1.6955e-05	1.489	4.5794e-02	0.500
4e-03	2e-04	5.1646e-06	1.297	2.8972e-02	0.500
4e-03	1e-04	2.8542e-06	0.856	2.0503e-02	0.499
4e-03	5e-05	2.1411e-06	0.415	1.4530e-02	0.497

Table 3: accuracy with respect to space discretization, case of a square with side 1, Nitsche, BDF2.

h	k	L_k^1 -error	order	$\dot{W}_k^{1,1}$ -error	order
1e-01	1e-04	5.4807e-03	-	2.9615e-01	-
5e-02	1e-04	1.8170e-03	1.593	1.3815e-01	1.100
2e-02	1e-04	5.3235e-04	1.340	6.3231e-02	0.853
1e-02	1e-04	1.5954e-04	1.738	3.0414e-02	1.056
5e-03	1e-04	2.7544e-05	2.534	1.4971e-02	1.023
2e-03	1e-04	6.8637e-06	1.516	1.3868e-02	0.084
1e-03	1e-04	2.3534e-06	1.544	1.3686e-02	0.019
5e-04	1e-04	1.1414e-06	1.044	1.3654e-02	0.003

Table 4: accuracy with respect to time discretization, case of a square with side 1, Nitsche, BDF2.

h	k	L_k^1 -error	order	$\dot{W}_k^{1,1}$ -error	order
5e-04	1e-01	1.9611e-02	-	4.5902e-01	-
5e-04	5e-02	9.1157e-03	1.105	3.2094e-01	0.516
5e-04	2e-02	2.6101e-03	1.365	1.9619e-01	0.537
5e-04	1e-02	9.5608e-04	1.449	1.3721e-01	0.516
5e-04	5e-03	3.4703e-04	1.462	9.6689e-02	0.505
5e-04	2e-03	9.0114e-05	1.472	6.1075e-02	0.501
5e-04	1e-03	3.2243e-05	1.483	4.3175e-02	0.500
5e-04	5e-04	1.1443e-05	1.494	3.0527e-02	0.500
5e-04	2e-04	2.9076e-06	1.495	1.9307e-02	0.500
5e-04	1e-04	1.1414e-06	1.349	1.3654e-02	0.500

The next table (Table 5) presents accuracy results for the disk, with \mathbb{P}^1 finite elements and Nitsche boundary conditions in space, and implicit Euler method. We compare in the same table, the results without correction for small times on the left side of the table, and the results with corrections on the right side. Note that, as predicted in the previous section, the results are much better for the scheme with correction. Indeed, the results are even much better with order 1 in time with correction than with order 2 in time without correction. The last table (Table 6) shows the same comparisons for the second order schemes (\mathbb{P}^1 plus BDF2).

Table 5 : disk, \mathbb{P}^1 + Nitsche, Implicit Euler method.

h/π	k	$\ K_{h,k} - K\ $				$\ K_{h,k,\tau} - K\ $			
		L_k^1		$\dot{W}_k^{1,1}$		L_k^1		$\dot{W}_k^{1,1}$	
2^{-2}	$0.1 \cdot 2^{-18}$	7.7569e-03		5.1079e-01		6.8658e-03		1.2161e-02	
2^{-3}	$0.1 \cdot 2^{-18}$	4.2895e-03	0.85	3.1177e-01	0.71	3.9197e-03	0.81	2.1384e-02	-0.81
2^{-4}	$0.1 \cdot 2^{-18}$	1.2743e-03	1.75	1.6544e-01	0.91	1.0254e-03	1.93	1.0026e-02	1.09
2^{-5}	$0.1 \cdot 2^{-18}$	3.4323e-04	1.89	9.0047e-02	0.88	2.5132e-04	2.03	3.9360e-03	1.35
2^{-6}	$0.1 \cdot 2^{-18}$	9.0154e-05	1.93	4.4007e-02	1.03	6.7331e-05	1.90	1.4194e-03	1.47
2^{-7}	$0.1 \cdot 2^{-18}$	2.2885e-05	1.98	2.1364e-02	1.04	1.7637e-05	1.93	4.7988e-04	1.56
2^{-8}	$0.1 \cdot 2^{-18}$	5.7614e-06	1.99	1.1607e-02	0.88	4.4413e-06	1.99	1.6490e-04	1.54
2^{-9}	$0.1 \cdot 2^{-18}$	1.2969e-06	2.15	5.6007e-03	1.05	1.0189e-06	2.12	5.3222e-05	1.63
2^{-10}	$0.1 \cdot 2^{-18}$	2.0038e-07	2.69	2.1013e-03	1.41	1.5362e-07	2.73	1.3127e-05	2.02
2^{-10}	$0.1 \cdot 2^{-1}$	2.2640e-02		2.4466e-01		3.1890e-02		6.0248e-02	
2^{-10}	$0.1 \cdot 2^{-2}$	1.1223e-02	1.01	1.8981e-01	0.37	1.2882e-02	1.31	2.9966e-02	1.01
2^{-10}	$0.1 \cdot 2^{-3}$	5.7809e-03	0.96	1.4570e-01	0.38	5.9278e-03	1.12	2.1383e-02	0.49
2^{-10}	$0.1 \cdot 2^{-4}$	3.0129e-03	0.94	1.0962e-01	0.41	2.7347e-03	1.12	1.0704e-02	1.00
2^{-10}	$0.1 \cdot 2^{-5}$	1.5670e-03	0.94	8.1023e-02	0.44	1.3314e-03	1.04	5.9707e-03	0.84
2^{-10}	$0.1 \cdot 2^{-6}$	8.0942e-04	0.95	5.9083e-02	0.46	6.6861e-04	0.99	3.5482e-03	0.75
2^{-10}	$0.1 \cdot 2^{-7}$	4.1492e-04	0.96	4.2647e-02	0.47	3.4173e-04	0.97	2.2000e-03	0.69
2^{-10}	$0.1 \cdot 2^{-8}$	2.1125e-04	0.97	3.0535e-02	0.48	1.7427e-04	0.97	1.3054e-03	0.75
2^{-10}	$0.1 \cdot 2^{-9}$	1.0691e-04	0.98	2.1702e-02	0.49	8.9098e-05	0.97	7.8028e-04	0.74
2^{-10}	$0.1 \cdot 2^{-10}$	5.3800e-05	0.99	1.5300e-02	0.50	4.5376e-05	0.97	4.5670e-04	0.77
2^{-10}	$0.1 \cdot 2^{-11}$	2.6900e-05	1.00	1.0671e-02	0.52	2.2994e-05	0.98	2.6285e-04	0.80
2^{-10}	$0.1 \cdot 2^{-12}$	1.3324e-05	1.01	7.3285e-03	0.54	1.1564e-05	0.99	1.4874e-04	0.82
2^{-10}	$0.1 \cdot 2^{-13}$	6.4901e-06	1.04	4.9239e-03	0.57	5.7282e-06	1.01	8.1169e-05	0.87
2^{-10}	$0.1 \cdot 2^{-14}$	3.0571e-06	1.09	3.2245e-03	0.61	2.7538e-06	1.06	4.1283e-05	0.98
2^{-10}	$0.1 \cdot 2^{-15}$	1.3347e-06	1.20	2.0923e-03	0.62	1.2386e-06	1.15	1.7482e-05	1.24
2^{-10}	$0.1 \cdot 2^{-16}$	4.7146e-07	1.50	1.4611e-03	0.52	4.6622e-07	1.41	2.9301e-06	2.58
2^{-10}	$0.1 \cdot 2^{-17}$	1.7834e-07	1.40	1.5866e-03	-0.12	1.4477e-07	1.69	6.9816e-06	-1.25
2^{-10}	$0.1 \cdot 2^{-18}$	2.0038e-07	-0.17	2.1013e-03	-0.41	1.5362e-07	-0.09	1.3127e-05	-0.91

Table 6 : disk, \mathbb{P}^2 + Nitsche, BDF2.

h/π	k	$\ K_{h,k} - K\ $				$\ K_{h,k,\tau} - K\ $			
		L_k^1		$\dot{W}_k^{1,1}$		L_k^1		$\dot{W}_k^{1,1}$	
2^{-2}	$0.1 \cdot 2^{-18}$	5.0127e-03		4.4303e-01		9.2845e-05		6.4401e-03	
2^{-3}	$0.1 \cdot 2^{-18}$	8.9903e-04	2.48	2.3810e-01	0.90	3.9114e-04	-2.07	8.4831e-03	-0.40
2^{-4}	$0.1 \cdot 2^{-18}$	1.3434e-04	2.74	1.2124e-01	0.97	1.9698e-05	4.31	6.9236e-04	3.61
2^{-5}	$0.1 \cdot 2^{-18}$	1.8159e-05	2.89	6.0173e-02	1.01	9.5696e-07	4.36	4.8201e-05	3.84
2^{-6}	$0.1 \cdot 2^{-18}$	2.3337e-06	2.96	3.0067e-02	1.00	1.6260e-07	2.56	5.9797e-06	3.01
2^{-7}	$0.1 \cdot 2^{-18}$	2.7912e-07	3.06	1.5179e-02	0.99	1.4163e-08	3.52	1.5222e-06	1.97
2^{-8}	$0.1 \cdot 2^{-18}$	4.5899e-08	2.60	7.6611e-03	0.99	1.3268e-08	0.09	3.4836e-07	2.13
2^{-9}	$0.1 \cdot 2^{-18}$	1.3353e-08	1.78	4.1620e-03	0.88	9.1745e-09	0.53	1.2214e-07	1.51
2^{-10}	$0.1 \cdot 2^{-18}$	4.1871e-09	1.67	1.9915e-03	1.06	3.5450e-09	1.37	5.4059e-08	1.18
2^{-10}	$0.1 \cdot 2^{-1}$	1.4334e-02		3.3695e-01		1.4334e-02		3.3695e-01	
2^{-10}	$0.1 \cdot 2^{-2}$	5.3433e-03	1.42	2.4956e-01	0.43	8.5621e-03	0.74	1.2090e-01	1.48
2^{-10}	$0.1 \cdot 2^{-3}$	1.9827e-03	1.43	1.7890e-01	0.48	1.6564e-03	2.37	3.0048e-02	2.01
2^{-10}	$0.1 \cdot 2^{-4}$	7.3156e-04	1.44	1.2717e-01	0.49	2.5419e-04	2.70	4.2445e-03	2.82
2^{-10}	$0.1 \cdot 2^{-5}$	2.6748e-04	1.45	9.0104e-02	0.50	6.9242e-05	1.88	1.4501e-03	1.55
2^{-10}	$0.1 \cdot 2^{-6}$	9.6946e-05	1.46	6.3756e-02	0.50	2.0807e-05	1.73	5.8135e-04	1.32
2^{-10}	$0.1 \cdot 2^{-7}$	3.4894e-05	1.47	4.5091e-02	0.50	6.1545e-06	1.76	2.2248e-04	1.39
2^{-10}	$0.1 \cdot 2^{-8}$	1.2496e-05	1.48	3.1885e-02	0.50	1.8497e-06	1.73	8.8581e-05	1.33
2^{-10}	$0.1 \cdot 2^{-9}$	4.4598e-06	1.49	2.2546e-02	0.50	5.5914e-07	1.73	3.5762e-05	1.31
2^{-10}	$0.1 \cdot 2^{-10}$	1.5890e-06	1.49	1.5942e-02	0.50	1.6937e-07	1.72	1.4267e-05	1.33
2^{-10}	$0.1 \cdot 2^{-11}$	5.6655e-07	1.49	1.1273e-02	0.50	5.2919e-08	1.68	5.7136e-06	1.32
2^{-10}	$0.1 \cdot 2^{-12}$	2.0320e-07	1.48	7.9714e-03	0.50	1.8155e-08	1.54	2.2811e-06	1.32
2^{-10}	$0.1 \cdot 2^{-13}$	7.4262e-08	1.45	5.6404e-03	0.50	7.8791e-09	1.20	9.3660e-07	1.28
2^{-10}	$0.1 \cdot 2^{-14}$	2.8545e-08	1.38	4.0048e-03	0.49	4.8191e-09	0.71	3.9281e-07	1.25
2^{-10}	$0.1 \cdot 2^{-15}$	1.2337e-08	1.21	2.8858e-03	0.47	3.9132e-09	0.30	1.7526e-07	1.16
2^{-10}	$0.1 \cdot 2^{-16}$	6.5853e-09	0.91	2.1831e-03	0.40	3.6361e-09	0.11	7.6785e-08	1.19
2^{-10}	$0.1 \cdot 2^{-17}$	4.6041e-09	0.52	1.9025e-03	0.20	3.5638e-09	0.03	5.1164e-08	0.59
2^{-10}	$0.1 \cdot 2^{-18}$	4.1871e-09	0.14	1.9915e-03	-0.07	3.5450e-09	0.01	5.4059e-08	-0.08

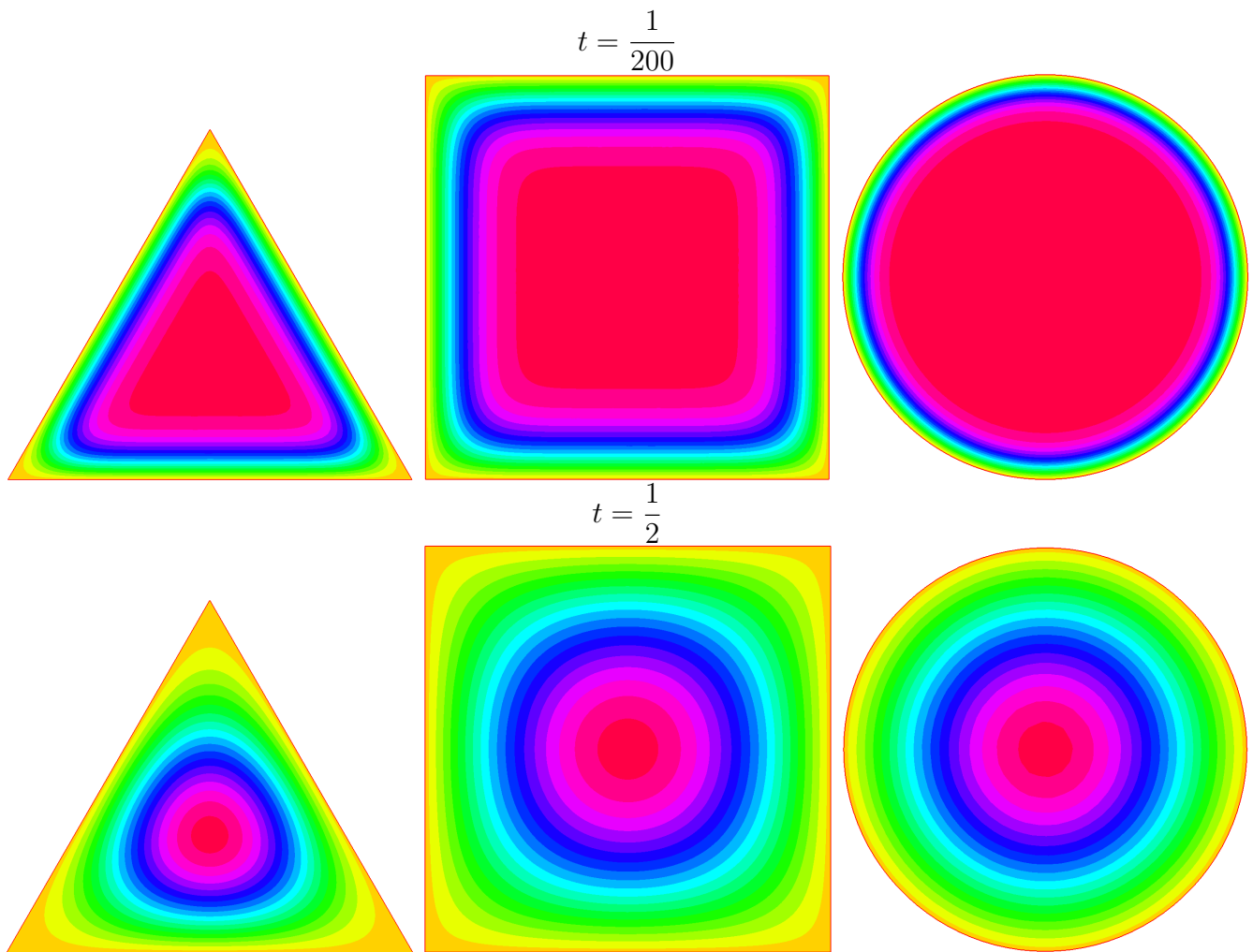


Figure 1: Solution to (3) with Dirichlet boundary equations at time $t = 1/200$ and $t = 1/2$ for three different domains. (The triangle is shown at a scale twice smaller than the square and the disc)

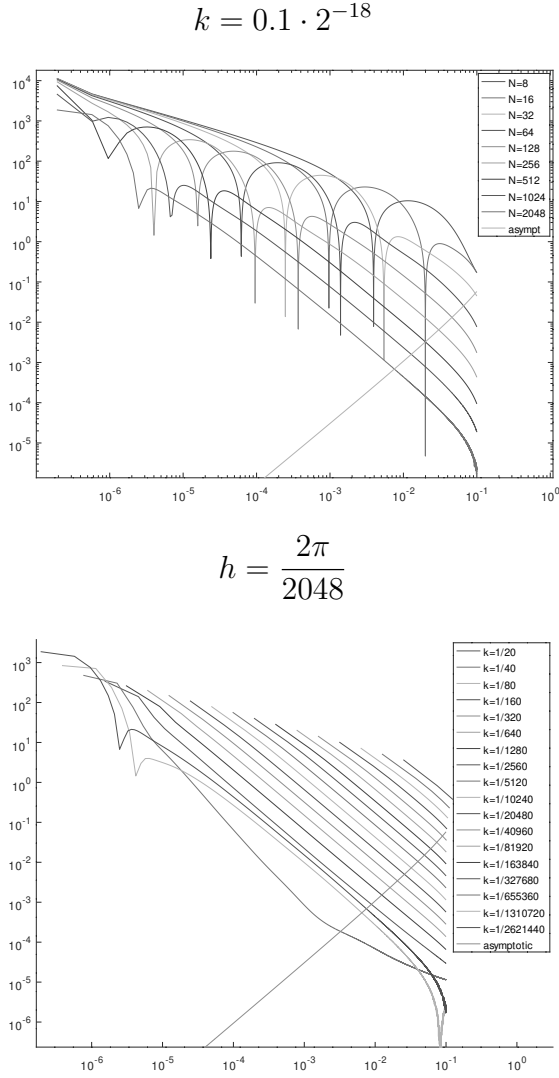
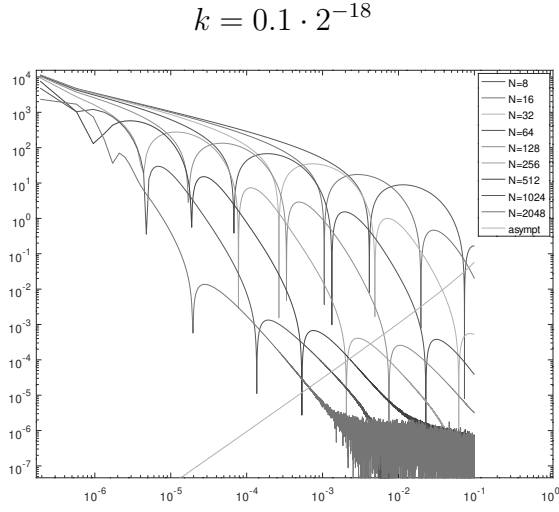


Figure 2: Case of the disc discretized with \mathbb{P}^1 -elements in space and Implicit-Euler in time. $\left| \frac{K_{h,k}(t_{n+1}) - K_{h,k}(t_n)}{k} - \frac{K(t_{n+1}) - K(t_n)}{k} \right|$ as a function of $t_{n+1/2}$ for various values of the space step $h = \frac{2\pi}{N}$ (top, $k = 0.1 \cdot 2^{-18}$) and the time step k (bottom, $h = \frac{2\pi}{2048}$). We also present the error for the asymptotic expansion.



$$h = \frac{2\pi}{2048}$$

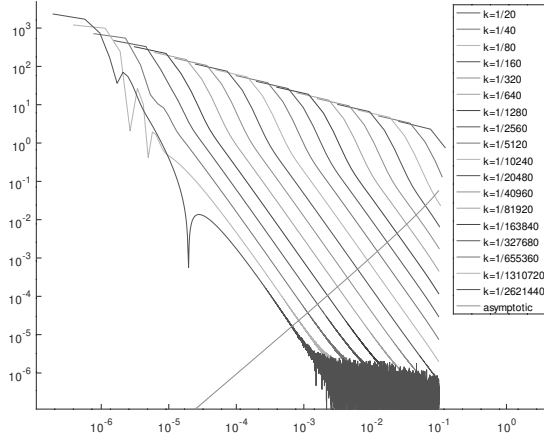


Figure 3: Case of the disc discretized with \mathbb{P}^2 -elements in space and BDF2 in time. $\left| \frac{K_{h,k}(t_{n+1}) - K_{h,k}(t_n)}{k} - \frac{K(t_{n+1}) - K(t_n)}{k} \right|$ as a function of $t_{n+1/2}$ for various values of the space step $h = \frac{2\pi}{N}$ (top, $k = 0.1 \cdot 2^{-18}$) and the time step k (bottom, $h = \frac{2\pi}{2048}$). We also represent the error made for the asymptotic expansion.

Appendix

Proof of the condition $F_n(\xi) = O_{n \rightarrow +\infty}(\varepsilon^n)$ uniformly in $] -\infty, -\xi_0]$, for the BDF2 Scheme.

We have $\begin{pmatrix} F_{n+1}(\xi) \\ F_{n+2}(\xi) \end{pmatrix} = A(\xi) \begin{pmatrix} F_n(\xi) \\ F_{n+1}(\xi) \end{pmatrix}$ where $A(\xi) = \begin{pmatrix} 0 & 1 \\ \frac{-1}{3-2\xi} & \frac{4}{3-2\xi} \end{pmatrix}$. Let us also denote $A(-\infty) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$.

One can check directly that the spectral radius $\rho(\xi)$ of $A(\xi)$ is bounded by $\frac{10 + \sqrt{5}}{19} \approx 0.644 < 2/3 = \varepsilon$ on $[-\infty, -\xi_0]$. Besides, $\lim_{n \rightarrow +\infty} \|A(\xi)^n\|^{1/n} = \rho(\xi)$. Now, if we take an algebra norm,

$$\|(A(\xi))^{2^{n+1}}\|^{2^{-n-1}} \leq (\|A(\xi)^{2^n}\|^2)^{2^{-n-1}} \leq \|A(\xi)^{2^n}\|^{2^{-n}}.$$

Hence $(\xi \rightarrow \|A(\xi)^{2^n}\|^{2^{-n}})_n$ is a sequence of continuous functions decreasing and converging to $\rho(\xi)$ on $[-\infty, -\xi_0]$. By Dini theorem, this sequence converges uniformly. Hence, there exists $m > 0$, such that: $\|A(\xi)^{2^m}\|^{2^{-m}} \leq \varepsilon$, and therefore $\|A(\xi)^{2^m}\| \leq \varepsilon^{2^m}$, uniformly in $[-\infty, -\xi_0]$. It yields $A(\xi)^n = O(\varepsilon^n)$ and then $F_n(\xi) = O(\varepsilon^n)$ uniformly with respect to ξ .

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