Asymptotics and discretization of a weakly singular kernel: application to viscous flows in a network of thin tubes

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Abstract

Kernels obtained from the heat equation arise in several modelling contexts, like some double porosity models, or viscous flows in networks of thin tubes. These kernels are weakly singular at initial time. An accurate approximation must therefore take this singularity into account. In this paper we obtain an asymptotic expansion for small times, which we use to build a numerical scheme for approximating the kernels. Convergence of the scheme and relevance of a correction through the asymptotics are proven both analytically and numerically. Finally, we show that this approximation applies to the model on the graph studied by the authors in «Numerical solution of the viscous flows in a network of thin tubes: equations on the graph», Journal of Computational Physics, 435:110262, 2021 http://dx.doi.org/10.1016/j.jcp.2021.110262.

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Contents

1 Introduction

This work is mainly devoted to the approximation of a class of weakly singular kernels. These kernels are functions of the time variable t and are computed by solving an auxiliary heat equation set on some 2D-domain: $K(t) = \int_\Omega V(t,x)\mathrm{d}x$ where V is the solution of a heat equation. Here, weakly singular is meant in the sense of the $W^{1,1}$ norm, and more precisely means that the first derivative of the kernel is of order $-1/2 \in]-1,0[$ near $t=0$. Such kernels appear in different contexts as convolution kernels in effective equations resulting from asymptotic processes. Because of the singularity at $t=0$, one has to pay particular attention to the approximation of the kernels for *small* values of t when computing numerical solutions. So, the main purpose of the present paper is to examine this point in detail and to design accurate approximations of the kernel.

This work is originally motivated by a model obtained by Panasenko and Pileckas [23, 24] as the limit 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 in [23, 24] was notably the modeling of microfluid and flows in blood vessels. The geometry of a blood vessel network is complex, so it is essential to reduce the dimensionality. The resulting effective model is a problem set on a connected 1D-graph which consists of nonlocal in time diffusion equations on each edge, that are connected with appropriate (Kirchhoff) junctions conditions at the inner vertices. Suitable numerical schemes for this reduced model are proposed and studied in the first part [4] of our work. In particular, the key role of the approximation of the convolution (with respect to time) kernels is highlighted in [4]: the error on the kernel is the more limiting factor. In this model, one kernel is associated with each tube of the initial structure, where the corresponding heat equation is set on a normalized cross-section of the tube. So a second purpose of the present paper is to relate our results to the error estimates in [4].

Let us also mention that such kernels appear in other exciting contexts, for example: double porosity like models, with a convolution in the time derivative of a parabolic equation (see, for instance, [2, 1, 28, 25, 26]); in the diffusion term of a parabolic equation arising in viscoelasticity or materials with memory (see, for instance, [18, 11, 19]).
In this paper, we investigate the properties of the kernels in two main directions.

The first direction is theoretical: we prove that, at least for a C^∞-smooth domain, the associated kernel admits an asymptotic expansion at $t=0$ at any order. The paper by Gie, Jung and Temam [8] 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: Theorem 1. We also give asymptotic expansions (with exponential convergence) for rectangular and triangular domains.

The second direction is numerical. We propose a scheme with several variants for solving the auxiliary heat equation associated with a given kernel. Since the initial condition does not satisfy the Dirichlet boundary condition, the kernel is singular. We show convergence of the associated approximate kernels in some continuous or discrete $W^{1,1}$ norm, as needed for the convergence theorems proved in [4]. It is the subject of Theorem 2, 3 and 6. In particular, in Theorem 3, we use the asymptotic expansions obtained in Theorem 1 (or in Propositions 3, 4) to improve the kernel approximation for small times, and consequently, improve the overall approximation.
Numerical experiments are provided in the last section of the paper to validate and illustrate the theoretical results. The use of a corrected scheme improves the order of $W^{1,1}$-convergence from 1/3 to 10/9 theoretically (from Theorem 2 to Theorem 3). Numerically, we observe an improvement from 1/2 to ca. 0.7 (schemes of order 1) or ca. 1.25 (schemes of order 2), and the computational time does not change.
To our knowledge, the results on the asymptotic expansions and its use in the scheme are new. However, let us mention that an explicit two terms asymptotic approximation was already used in [1] for a rectangle, and in [9] for a disc.
Regarding the novelty of the numerical method, the discretization of the well-known heat equation has been studied intensively since the sixties [30]. As often for linear problems, the main challenge is the approximation near the boundaries, either in time or in space.
In the finite element setting, the accuracy is limited by the fact that the boundary of the domain is poorly approximated by the boundary of the mesh. Here we chose to use the Nitsche method [22], i.e. the Dirichlet boundary condition is replaced by an accurately computed penalization term. Other solutions include mesh refinement near the boundary (see e.g. [33]), isoparametric finite element [14] where the mesh is curved like the domain, adding suitable functions [21, 20] to the finite element basis like partition units or boundary elements.
Because of the incompatibility between the initial data and the boundary conditions, the solution is not smooth at initial time but the solution get smoother at later times. This smoothing effect enables to consider schemes where convergence rate is improved as the time goes on. The roughness at initial time is a limiting factor when time discretization is considered [15]. Several remedies have been considered:

- time step refinement near initial time [3, 18]
- Penalization in time such as in [5].
- subtraction of singular terms terms to get smooth data. See for example [6] in the 1D case where the smooth residual is computed

Pade approximants [31], Chebyshev polynomials [16], Laplace transform [19] have also been used. Here we develop another approach, that is, *the truncation* of the numerical solution for values of time which are smaller than a suitably chosen bound, and its replacement with the asymptotic expansion.

Another novelty lies in the error estimate. For the targeted application, we need accuracy on the *time derivative* of the solution. Semi-discretization in space [30, 12] has been proved to yield convergence for the derivative, and to the best of our knowledge, this has not been done earlier for the fully discretized problem.

Outline This paper is organized as follows.
In Section 2, we present the first main result of this paper, Theorem 1: 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. It is done using results in [8] for *well-prepared* problems. As (2) is not well-prepared in the sense of [8], this is done for a primitive of V which solves a well-prepared heat equation. It is done in Appendix A. In Section A.3, we prove that these expansions can be differentiated term by term. In Section A.1, we give an explicit formula for the case of a disk, form which the first terms of the asymptotic expansion can computed This is then used in Appendix A.4 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 1. We end this first part with Section 2.2 by computing asymptotic expansions for rectangles and equilateral triangles, to illustrate that asymptotic expansions are of a different nature for non smooth domains.
Note that in [7, 8], the authors also consider *ill-prepared* heat equation (that is with incompatible initial and Dirichlet boundary data). But in our proofs, we use many intermediate results and computations that are not explicitly presented in [7, 8] for the general case. For that reason, for the sake of clarity, we use their results in the case of well-prepared data.
Section 3 is devoted to the design of schemes approximating the kernels, and to convergence proofs. The Dirichlet-Laplace operator is discretized with standard finite elements, with or without Nitsche conditions. In Subsection 3.3, we obtain a first set of estimates for a semi-discrete scheme. In Subsection 3.4, full discretization is considered in a quite general setting, and further a priori estimates are obtained. Error estimates are provided, with convergence rates in Subsection 3.5. In Subsection 3.6, a correction for small times is proposed which leads to a better convergence rate.
Applications to the above mentioned problem on the graph are presented in Section 4. In Subsection 4.2, we relate the convergence results of Section 3 with the theorems of [4].
Finally, Section 5 is devoted to a summary of the algorithm and to the presentation of numerical experiments.

2 Asymptotic expansion of the kernel for small times

2.1 Main result : asymptotic expansion for smooth domains

Let Ω be a bounded domain in $\mathbb{R}^2$. We consider kernels of the form:

$$K(t) = \int_{\Omega} V(x,t)\mathrm{d}x, \tag{1}$$

where V is the unique solution of following heat equation:

$$\begin{cases} \partial_t V - \triangle V = 0 & \text{on } \Omega \times \mathbb{R}^{+*}, \\ V = 0 & \text{on } \partial\Omega \times \mathbb{R}^{+*}, \\ V = 1 & \text{on } \Omega \times \{0\}. \end{cases} \tag{2}$$

Let $(\lambda_k)_{k\in\mathbb{N}}$ be the eigenvalues of the Dirichlet-Laplace operator on Ω, and $(w_k)_{k\in\mathbb{N}}$ an associated orthonormal Hilbert basis of $L^2(\Omega)$. Let us consider the expansion of the initial condition with respect to this basis:

$$1 = \sum_{k=0}^{+\infty} a_k w_{k,}, \;\; a_k = \langle w_k, 1\rangle,$$

where $\langle\ ,\ \rangle$ stands for the inner product in $L^2(\Omega)$. The solution of (2) is $V(x,t) = \sum_{k=0}^{+\infty} a_k e^{-\lambda_k t} w_k(x)$, so that:

$$K(t) = \sum_{k=0}^{+\infty} a_k^2 e^{-\lambda_k t}, \;\; a_k = \langle w_k, 1\rangle. \tag{3}$$

Note that:

$$\forall \ell \in \mathbb{N},\, K^{(\ell)}(t) = \sum_{k=0}^{+\infty} a_k^2 (-\lambda_k)^{\ell} e^{-\lambda_k t}, \tag{4}$$

so that the following proposition holds true.

Proposition 1 *The kernel K and its derivatives are monotonic, non increasing if ℓ is odd, non decreasing if not, and satisfy the following relation:* $\lim\limits_{+\infty} K^{(\ell)} = 0$.

An important case is when the domain is a disk. Here, one can give an expression of K involving zeros of the 0^{th} Bessel function, which enables to give an asymptotic expansion close to zeros. More precisely, we have the following result.

Proposition 2 *Assume* $\Omega = \{x \in \mathbb{R}^2;\ \|x\|_2 < 1\}$.

(i) For $t \geq 0$*, 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) For $t \geqslant 0$, $K(t) = \pi - 4\sqrt{\pi t} + \pi t + \frac{\sqrt{\pi}}{3} t^{3/2} + \frac{\pi}{8} t^2 + o_{t\to 0^+}\left(t^2\right)$.

The proof is given in Appendix A.1. It uses an explicit expression of the Laplace transform.
We now state the first main result of this article, which generalizes this asymptotic expansion close to $t = 0^+$ for smooth domains.

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

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

where

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

Here, S *designates the area of* Ω*,* L *the length of* $\partial\Omega$*, and* $\kappa : [0, L] \to \mathbb{R}$ *is the curvature of* $\partial\Omega$ *as defined in Equation* (33) *page 34.*

The proof of this theorem is rather long and is given in Appendix A. It is based on the boundary layer theory for the heat equation as exposed in Gie Jung Temam [7, 8], which enables to compute an asymptotic expansion of the primitive in time of V. The proof relies on a change of variable close to the boundary of the domain. Instead of standard cartesian variables, the distance to the boundary and the arclength parameter of the projection on the boundary are used.

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. This will become clear in the proof.

(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 2.2.

(iii) Note that there exist similar results for the trace of $e^{t\Delta}$ conjectured in the seminal work "Can one hear the shape of drum" by Kac [13] and proved in Mac Kean Singer [17].

2.2 Non smooth domain examples

We end this part by computing asymptotic expansions for rectangular and equilateral triangle domains, which are non smooth domains, for which the asymptotic expansions take a different form.

2.2.1 Case of a rectangular domain

If the open set 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,

$$a_k = \int_0^1 w_k(x)\mathrm{d}x = \frac{\sqrt{2}}{k\pi}\left(1-(-1)^k\right)$$

so that the corresponding kernel K_1 is given by:

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

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

$$\forall t > 0,\ K_1'(t) = -\frac{2}{\sqrt{\pi t}}\sum_{k=-\infty}^{+\infty}\exp\left(i\pi k - \frac{k^2}{4t}\right) = -\frac{2}{\sqrt{\pi t}} - \frac{4}{\sqrt{\pi t}}\sum_{k=1}^{\infty}(-1)^k\exp\left(-\frac{k^2}{4t}\right). \qquad (5)$$

Hence, for any $\varepsilon > 0$,

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

By integrating, we obtain:

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

Remark By noting that $K_1'(t) = -4e^{-\pi^2 t}\,\theta\left(2\pi t i, 4\pi t i\right)$ where θ stands for the Jacobi θ-function, one could also state directly (5) 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 3 $\forall t \geqslant 0, \forall \varepsilon > 0,\ K(t) = ab - \frac{4\left(a+b\right)}{\sqrt{\pi}}\sqrt{t} + \frac{16}{\pi}t + O_{t\to 0^+}\left(e^{-1/(4+\varepsilon)t}\right).$

2.2.2 Case of an equilateral triangular domain

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

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

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

3 Accurate approximations of the kernels

The kernels K as defined above are approximated by using a discretization of (1)-(2), or by combining this discretization with the asymptotics obtained in Theorem 1. In the latter case, better convergence rates are obtained and observed, as illustrated by the numerical simulations of Section 5.
All along this section, we will assume that :

$$\textbf{(H}_1\textbf{)} \qquad \forall t \in \mathbb{R}^+,\ 0 \le K(0) - K(t) \le Ct^{1/2}.$$

We know from Theorem 1 that this assumption holds for C^∞-smooth domains Ω, and from Propositions 3 and 4 that it also holds true for rectangular and triangular domains.

The plan of the section is as follows. We first set some notations and state facts about finite space elements and about the discretization of the initial condition. This is the aim of Subsections 3.1 and 3.2. We then present a semi-discrete version of (2), define a corresponding approximate kernel K_h and prove estimates on the error for the approximation $K \simeq K_h$ in the $W^{1,1}(0,T)$-norm for any $T > 0$. This is done in Subsection 3.3, Proposition 5. Subsection 3.4 is devoted to the full discretization of (2). We introduce there a general framework for the time discretization, which includes Implicit Euler method and the second order Backward Difference Formula (BDF2) that we use in the numerical simulation. Then, we define a corresponding approximate kernel $K_{h,k}$ and prove estimates for the error on the approximation $K_h \simeq K_{h,k}$ in the $W^{1,1}$-norm away from $t = 0$: Proposition 6. In the last two Subsections 3.5 and 3.6 using the preceding results, we prove convergence in $W^{1,1}(0,T)$, with rates of convergence, both for schemes without corrections for small times (Theorem 2) and for schemes using the asymptotic for small times (Theorem 3). As a matter of fact, in this last case, the estimate is with some discrete $W^{1,1}$-norm.
All along this section C designates any arbitrary positive constant (which does not depend on the parameters of discretization h and k) so the value of C may change from one line to the other, although the same generic letter C is used.

3.1 Finite space elements

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

H$_2$ T_h is self-adjoint, positive semidefinite on $L^2(\Omega)$ and positive definite on S_h;

H$_3$ 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 Thomée's book [30] (most notably, $\mathbb{P}^{r-1}$-elements over quasi-uniform triangulations, with boundary conditions dealt with Nitsche method when $r > 2$).

3.2 Approximation of the initial condition

In Equation (2), the approximation V_h^0 of $V^0 := 1$ is defined as the L^2-orthogonal projection of V^0 on S_h . When Nitsche method is used $V_h^0 = V^0 = 1$. When considering $\mathbb{P}^k$-elements on a given triangulation $\mathcal{T}_h$ satisfying the homogeneous Dirichlet condition ($S_h \subset H_0^1(\Omega)$), $V^0 \notin S_h$. In that case the following error estimate holds for V_h^0:

$$\|V^0 - V_h^0\|_{L^2} = O(h^{1/2}). \tag{6}$$

Indeed, consider $U \in S_h$ such that U is affine on each triangle of $\mathcal{T}_h$, constant equal to 1 at the vertices inside Ω, and equal to 0 at the vertices on $\partial\Omega$. Then: $\displaystyle\int_\Omega \mathbb{I}_{\{0 \leq U < 1\}}(x)\,\mathrm{d}x = O(h)$, so that $\displaystyle\int_\Omega (1-U)^2(x)\mathrm{d}x = O(h)$, $\|1 - U\|_{L^2} = O(h^{1/2})$. But as V_h^0 is the best approximation of 1 in the L^2-norm:

$$\int_\Omega (1 - V_h^0)^2(x)\,\mathrm{d}x \leq \int_\Omega (1-U)^2(x)\,\mathrm{d}x$$

so that, using that V_0^h and $1 - V_0^h$ are orthogonal:

$$\int_\Omega \left(1 - V_h^0\right)(x)\,\mathrm{d}x = \int_\Omega (1 - V_h^0)^2(x)\,\mathrm{d}x = O(h) \tag{7}$$

which is the announced result.

3.3 Space discretization

In this section we present a semi-discretization (with respect to the space variable) for (2), and show a priori estimates in $W^{1,1}(0,T)$ for the associated approximate kernel K_h. Let us introduce the following semi-discrete approximation of V:

$$V_h(t) = e^{-tA_h} V_h^0, \quad A_h = T_h^{-1}. \tag{8}$$

As $V^0 \in L^2(\Omega)$, according to Theorem 3.4 p.46 in [30], with the assumptions (H$_2$)-(H$_3$), we have, for C^∞-smooth Ω (weaker regularity could be enough):

$$\| (V - V_h)(t) \|_{L^2} \leq C h^r t^{-\frac{r}{2}}, \quad \|\partial_t (V - V_h)(t) \|_{L^2} \leq C h^r t^{-\frac{r}{2}-1}. \tag{9}$$

Let us define K_h by letting

$$K_h(t) = \int_\Omega V_h(x,t)\mathrm{d}x. \tag{10}$$

From (9) we get the following estimates.

Proposition 5 *Assume that assumptions (H$_1$)-(H$_3$) hold. Then, for any $t, T \in \mathbb{R}^{+*}$, $\tau \in]0,T]$:*

$$|K - K_h|(t) \leq C h^r t^{-r/2},$$

$$\int_\tau^T |K_h' - K'|(t)\mathrm{d}t \leq C h^r \tau^{-r/2},$$

$$\int_0^T |K' - K_h'|(t)\mathrm{d}t \leq C h^{\frac{r}{r+1}},$$

where C does not depend on k, h and S_h.

Remark With (7) and the third inequality, we have an estimate in the $W^{1,1}$-norm: $\|K - K_h\|_{W^{1,1}(0,T)}$.
Proof The first estimate is obtained by integrating $(9)_1$ over Ω. Let us prove the second one. Let $\lambda_{h,1}, \ldots, \lambda_{h,N_h}$ denote the eigenvalues of A_h arranged in ascending order, and $w_{h,1}, \ldots, w_{h,N_h}$ 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 $a_{h,j} = \langle w_{h,j}, V_h^0 \rangle = \langle w_{h,j}, 1 \rangle$ (the last equality holds because V_h^0 is the orthogonal projection of 1), then:

$$V_h^0 = \sum_{j=1}^{N_h} a_{h,j} w_{h,j}, \tag{11}$$

$$V_h(t) = \sum_{j=1}^{N_h} a_{h,j} e^{-\lambda_{h,j} t} w_{h,j}, \tag{12}$$

$$K_h(t) = \sum_{j=1}^{N_h} a_{h,j}^2 e^{-\lambda_{h,j} t}. \tag{13}$$

Let $T \in \mathbb{R}^{+*}$. Using the second inequality in (9) we get;

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

This is the second inequality of the proposition. As $-K'$ and $-K_h'$ are nonnegative and decreasing, then:

$$\begin{aligned}
\forall \tau \in]0,T], \ \int_0^T |K_h' - K'|(t)\mathrm{d}t &= \int_0^\tau |K_h' - K'|(t)\mathrm{d}t + \int_\tau^T |K_h' - K'|(t)\mathrm{d}t \\
&\leq -\int_0^\tau \left(K_h'(t) + K'(t)\right)\mathrm{d}t + Ch^r \tau^{-r/2} \\
&\leq K_h(0) - K_h(\tau) + K(0) - K(\tau) + Ch^r \tau^{-r/2}.
\end{aligned}$$

As V_h^0 is the orthogonal projection of V^0,

$$K_h(0) = \left\| V_h^0 \right\|_{L^2}^2 \leq \| V_0 \|_{L^2}^2 = K(0) \tag{14}$$

so that

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

Using assumption (H_1) and the first estimate, we conclude that for all $\tau \in [0,T]$:

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

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

3.4 Full discretization

Let $k > 0$ be a time step, and let for all $n \in \mathbb{N}$, $t_n = nk$, $t_{n+1/2} = \left(t_n + t_{n+1}\right)/2$.
In this section, we consider a family of schemes for (2), associated to semi-discretizations (8), 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.

3.4.1 General setting - Schemes and approximate kernels without correction

In the numerical experiments of Section 5, we use two different time integrators: the Implicit Euler method and the second order Backward Difference Formula (BDF2). In order to propose a single proof of convergence for both as well as for other suitable schemes, we set the time integrator in an abstract framework. So we consider the full discretization:

$$V_{h,k}^n = G_n(-kA_h)\, V_h^0, \tag{15}$$

with abstract functions $G_n : \mathbb{R} \to \mathbb{R}$ such that: there exist three constants $\xi_0 > 0$, $\rho \in \{1,2\}$, $\varepsilon \in]0,1[$ and two continuous functions f and $c : [-\xi_0, 0] \to \mathbb{R}$ satisfying

$$\begin{cases} \forall \xi \in [-\xi_0, 0[,\ |G_n(\xi) - c(\xi) f(\xi)^n| \leq C\varepsilon^n; \\ \forall \xi \in [-\xi_0, 0[,\ |f(\xi)| < 1; \\ \forall \xi \in]-\infty, -\xi_0],\ |G_n(\xi)| \leq C\varepsilon^n; \\ f(\xi) = e^\xi + O_{\xi\to 0}(\xi^{\rho+1}); \\ c(\xi) = 1 + O_{\xi \to 0}(\xi^\rho). \end{cases} \tag{16}$$

The second and the third points are stability conditions, the other ones express consistency of order ρ.

Remarks The Implicit Euler method ($V_{h,k}^{n+1} - V_{h,k}^n = -kA_h V_{h,k}^{n+1}$ for $n \geq 0$) satisfies these conditions with $\xi_0 = 1$, $\rho = 1$, $\varepsilon = 1/2$, $f(\xi) = (1-\xi)^{-1}$, $c = 1$, $G_n(\xi) = (1-\xi)^{-n}$.
The second order Backward Difference Formula (BDF2) initialized with the Implicit Euler method

$$\begin{cases} V_{h,k}^1 - V_{h,k}^0 = -kA_h V_{h,k} \\ \forall n \geq 0,\ \ 3V_{h,k}^{n+2} + 2kA_h V_{h,k}^{n+2} = 4V_{h,k}^n - V_{h,k} \end{cases} \tag{17}$$

can also be put in this form (See Appendix C.1 for details).

The uncorrected approximate kernel $K_{h,k}$ based on such a discretization is then defined as the continuous function on $\mathbb{R}^+$, affine on each $[t_n, t_{n+1}]$, determined by:

$$\forall n \in \{0, ..., N_k\},\ K_{h,k}(t_n) = \int_\Omega V_{h,k}^n(x)\mathrm{d}x. \tag{18}$$

As V_h^0 is the orthogonal projection of 1 on S_h, similarly to (12) and (13), we have:

$$V_{h,k}^n = \sum_{j=1}^{N_h} a_{h,j} G_n(-k\lambda_{h,j}) w_{h,j}, \quad K_{h,k}(t_n) = \sum_{j=1}^{N_h} a_{h,j}^2 G_n(-k\lambda_{h,j}). \tag{19}$$

3.4.2 A priori estimates for the full discrete kernel away from $t = 0$

We have the following estimates, relating the full discrete kernel $K_{h,k}$ and the semi-discrete kernel K_h. The proof is given in Appendix C.2.

Proposition 6 *Let $T > 0$ be number such that T/k is an integer and $T > \dfrac{2k}{\ln(1/\varepsilon)} \ln(1 + k\lambda_{h,N_h})$. Under the assumptions (H_1)-(H_3) and the assumptions of Section 3.4.1, for any t and t_n that are larger than $\dfrac{2k}{\ln(1/\varepsilon)} \ln(1 + k\lambda_{h,N_h})$, the following inequalities hold:*

$$
\begin{aligned}
&|\left(K'_{h,k} - K'_h\right)(t_{n+1/2})| \le Ck^\rho t_n^{-1-\rho}, \\
&|K_{h,k}(t) - K_h(t)| \le Ckt^{-1}, \\
&\int_t^T |K'_{h,k}(\tau) - K'_h(\tau)| \mathrm{d}\tau \le Ckt^{-1} \text{ if } t \le T,
\end{aligned}
$$

where C does not depend on k, h and S_h.

3.5 Convergence of the uncorrected scheme

This section is devoted to one step schemes only. We prove convergence in $W^{1,1}(0, T)$, for any $T > 0$, of the approximate kernel $K_{h,k}$, under the additional assumption on the time discretization:

$$\forall n \in \mathbb{N},\ \forall \xi \le 0, \quad G_n(\xi) = f(\xi)^n \ge 0. \tag{20}$$

This applies in particular to the Implicit Euler method.
Remarks

(i) With (20) we also assume that in (16), f is defined on all $\mathbb{R}^-$.

(ii) The assumption of non negativity is not a big restriction. Indeed, consider a one step scheme corresponding to $G_n(x) = f(x)^n$ and satisfying hypotheses (16), but not (20). Then the scheme defined by $\tilde{G}_n(x) = G_n(x/2)^2 = f(x/2)^{2n}$ satisfies both (16) and (20), since $f(x)^2 \ge 0$. This corresponds to taking a one step scheme over two half-time steps: $u_{n+1/2} = f(-kA_h/2)u_n$, $u_{n+1} = f(-kA_h/2)u_{n+1/2} = f(-kA_h/2)^2 u_n$.

(iii) Such a procedure would not work for BDF2 since it is a multi-step scheme. Hence, the result of this paragraph does not apply, unless it is corrected for small times as done in the next section.

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

Theorem 2 *Assume that assumptions (H_1)-(H_3), (16) and (20) hold, then for any $T > 0$ and sufficiently small k such that T/k is an integer:*

$$\int_0^T |K'_{h,k}(t) - K'(t)|\mathrm{d}t \le Ck^{\frac{\mu}{2}},$$

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 (20) yields that $K_{h,k}$ is decreasing and positive. Indeed:

$$\forall n \in \mathbb{N},\, K_{h,k}(t_n) = \sum_{j=1}^{N_h} a_{h,j}^2 f(-k\lambda_{h,j})^n;$$

but, from (16), $0 \leqslant f(\xi) < 1$ for $\xi \in [-\xi_0, 0[$ while for $\xi \le -\xi_0$, $0 \leqslant f(\xi) \le C^{1/n}\varepsilon$ for all n; thus, as for n large enough, $C^{1/n}\varepsilon < 1$, we have that $0 \leqslant f(\xi) < 1$ for all $\xi \in \mathbb{R}^{-*}$. This implies that the sequence $(K_{h,k}(t_n))$ is decreasing and positive, and therefore that the function $K_{h,k}$, too as a continuous, piecewise affine interpolation of it.
Then, arguing as in the proof of Proposition 5, we get:

$$\begin{aligned}\forall \tau \in [0,T],\ \int_0^\tau |K'_{h,k} - K'_h|(t)\mathrm{d}t &\le K_{h,k}(0) - K_{h,k}(\tau) + K_h(0) - K_h(\tau)\\ &\le (K_{h,k}(0) - K_h(0)) + |K_h(\tau) - K_{h,k}(\tau)|\\ &+ 2(K_h(0) - K(0)) + 2(K(0) - K(\tau)) + 2(K(\tau) - K_h(\tau)).\end{aligned}$$

The first term on the right is equal to 0 (see (13)); from the second inequality of Proposition 6, if $\tau \ge \frac{2}{\ln 1/\varepsilon}\ln(1 + k\lambda_{h,N_h})$, the second term is bounded by $Ck\tau^{-1}$; the third one is non positive (see (14)); from hypothesis (H_1) the fourth one is bounded by $C\tau^{1/2}$; from Proposition 5 the last term is bounded by $Ch^r\tau^{-r/2}$. We then get

$$\int_0^\tau |K'_{h,k}(t) - K'_h(t)|\mathrm{d}t \le C\left(k\tau^{-1} + \tau^{1/2} + h^r\tau^{-r/2}\right).$$

Now take $\tau = k^\mu$ with k sufficiently small to have $\tau \ge k\frac{2}{\ln 1/\varepsilon}\ln(1+k\lambda_{h,N_h})$. Together with the third inequality of Proposition 6, and then the third one of Proposition 5 this proves the first estimate.

3.6 Convergence with correction for small times

In this section, we assume that the asymptotic expansion of K obtained in Section 2 (Theorem 1) holds. It is the case when Ω is C^∞-smooth and simply connected. However, a weaker regularity may be enough. This expansion is used for small times in order to improve the convergence rate.
Using the first five terms of the expansion, that are known from Theorem 1, we define the corrected approximate kernel $K_{h,k,\tau}$ by:

$$K_{h,k,\tau}(t) = \begin{cases} K_{h,k}(t) & \text{if } t \geq \tau \\ K_{h,k}(\tau) + \left[S - 2L\sqrt{\dfrac{s}{\pi}} + \pi s + \dfrac{s^{3/2}}{6\sqrt{\pi}} \displaystyle\int_0^L \kappa(s)^2 \mathrm{d}s + \dfrac{s^2}{16} \int_0^L \kappa(s)^3 \mathrm{d}s \right]_\tau^t & \text{if } t < \tau \end{cases}, \quad (21)$$

so that:

$$\int_0^\tau \left| K'_{h,k,\tau} - K' \right| (t) \mathrm{d}t \leq C \int_0^\tau t^{m-1} \mathrm{d}t \leq C\tau^m, \text{ where } m = 5/2. \quad (22)$$

Remark The value of m can be increased if more terms are known. Since $K'_{h,k}$ is a piecewise constant approximation of the singular function K', this approximation cannot be superlinear in $L^1(0,T)$. However we can prove an accurate approximation for a discrete integral on $[\tau, T]$ for τ not too small. So the estimate in Theorem 3 differs from the estimate in Theorem 2.

Theorem 3 *Assume that assumptions (H_1)-(H_3) and (16) hold, then for any $T > 0$ and sufficiently small k, such that T/k is an integer, we have*

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

where $m = 5/2$, $\mu = \min\left\{ \dfrac{\rho}{m+\rho}, \gamma \dfrac{2r}{2m+r} \right\}$, $h = k^\gamma$ *and* $\tau = k \left\lfloor k^{\mu-1} \right\rfloor$.

Proof Summing up the first inequality in Proposition 6, for $\tau \geq \dfrac{2k}{\ln 1/\varepsilon} \ln(1 + \lambda_{h,N_h})$,we get:

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

Similarly, using the second estimate of Proposition 5:

$$k \sum_{\tau \leq t_n < T} \left| K'_h - K' \right| (t_{n+1/2}) \leq C \int_\tau^T \left| K'_h - K' \right| (t) \mathrm{d}t \leq Ch^r \tau^{-r/2}.$$

Then, using inequality (22) and $\tau + k \leq 2\tau$, we get

$$\int_0^{\tau+k} \left|K'_{h,k,\tau}(t) - K'(t)\right| \mathrm{d}t + k \sum_{\tau \leq t_n < T} \left|K'_{h,k,\tau}(t_{n+1/2}) - K'(t_{n+1/2})\right| \leq C\left(\tau^m + Ch^r\tau^{-r/2} + Ck^\rho\tau^{-\rho}\right),$$

and we conclude as in the proof of Theorem 2.

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 applies to the corrected Implicit Euler and BDF2 schemes.

(iii) Implementing the correction is straightforward and does not change the computational time.

4 Application : numerical solution of viscous flows on a graph

4.1 Description of the problem on the graph

In [4] we consider a problem set on a connected graph $\mathcal{B}$ in $\mathbb{R}^d$, where $d = 2$ or 3, that we briefly describe as follows.
Let $O_1, \dots O_N$ be 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 $\mathcal{B} = \bigcup_{j=1}^{M} e_j$ and is assumed to be connected. A positive orientation is defined along each edge $e_j = [O_{i_j}, O_{k_j}]$ 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 problem set on $\mathcal{B}\times[0,T]$ is:

$$\begin{cases} -\partial_{e_j}\left(\mathcal{L}^{(\sigma_j)}\partial_{e_j}P(x,t)\right)(x,t) = F(x,t) & \text{for } x \in e_j,\ j = 1,\dots,M, \\ \displaystyle\sum_{e_j \ni O_i} \alpha_{i,j}\mathcal{L}^{(\sigma_j)}\partial_{e_j}P(x,t) = -\Psi_i(t) & \text{for } i = 1,\dots,N, \\ P \text{ is continuous on the graph,} & \\ P(O_1,t) = 0, & \end{cases} \tag{23}$$

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 functions Ψ_i are given in $H^1_{00}(0,T) = \left\{f \in H^1(0,T);\ f(0) = 0\right\}$ and F is a given function in $H^1_{00}(0,T;L^2(\mathcal{B}))$ (with quite obvious definition of $L^2(\mathcal{B})$, see [4]), that satisfy the compatibility

condition: $\forall t \in [0,T],\ \sum_{i=1}^{N} \Psi_i(t) + \int_{\mathcal{B}} F(x,t)\mathrm{d}x = 0$. In real life applications, the function F is usually equal to zero, but the possibility of a more general F was kept in order to construct test cases with known exact solution to compare with approximate solutions in numerical experiments.
Last, the $\mathcal{L}^{(\sigma_j)}$ are convolution operators $L^2(0,+\infty) \to H^1_0(0,+\infty)$ defined by:

$$\forall t > 0,\ \mathcal{L}^{(\sigma_j)} q(t) = \int_0^t K^{(\sigma_j)}(t-\tau) q(\tau)\mathrm{d}\tau, \tag{24}$$

where the kernels $K^{(\sigma_j)}$ are given by (1)-(2) with $\Omega = \sigma_j$.
This problem comes from Navier-Stokes equations on a network of thin tubes, after letting the diameter of the tubes tend to zero, with specific scaling of the data. The domains σ_j are scaled original cross-sections of the tubes while the operators $\mathcal{L}^{(\sigma_j)}$ relate the flux and the pressure drop in the original $3D$-structure. See [4, 24] for more detail and bibliography.
In [4], we considered schemes to solve numerically (23). We proved the two theorems cited below. Let $k > 0$ be some time step such that $N_k = T/k \in \mathbb{N}$, $t_n = kn$, $K^{(\sigma_j)} = \frac{1}{k}\int_{t_n}^{t_{n+1}} K_n^{(\sigma_j)}(t)\mathrm{d}t$; let $\tilde{K}_n^{(\sigma_j)}$ designate some approximation of $K_n^{(\sigma_j)}$. Let us recall the error factor associated with the approximation:

$$\theta(k) = \max_{1\le j\le M} \left\{ |K_0^{(\sigma_j)} - \tilde{K}_0^{(\sigma_j)}| + \sum_{n=1}^{N_k-1} |K_n^{(\sigma_j)} - K_{n-1}^{(\sigma_j)} - \tilde{K}_n^{(\sigma_j)} + \tilde{K}_{n-1}^{(\sigma_j)}| \right\}. \tag{25}$$

Last, let $h > 0$ be some space step, and $\mathbf{p}_{h,k} \in L^2(0,T;H^1(\mathcal{B}))$ be the numerical solution of (23), piecewise constant with respect to time, $\mathbb{P}^1$ with respect to space (defined properly in [4] by Equations (3.18)-(3.19)). The following convergence results are proven in [4] (Theorem 1 page 16 and Theorem 2 page 20).

Theorem 4 *If $\theta(k) \to 0$ as $k \to 0$, then $\mathbf{p}_{h,k} \to P$ when $(h,k) \to (0,0)$.*
Furthermore, if $F \in H^2(0,T;H^2(\mathcal{B}))$, $\Psi_1,\ldots,\Psi_N \in H^2(0,T)$, if $F, \partial_t F$, the Ψ_ℓ and the $\partial_t\Psi_\ell$ vanish at $t = 0$, there exists a positive constant C depending on F and on the Ψ_ℓ such that for k small enough:

$$\|\mathbf{p}_{h,k} - P\|_{L^2([0,T],H^1(\mathcal{B}))} \le C\left(h + k + \theta(k)\right).$$

Theorem 5 *Let $\tilde{p}_{h,k}$ be the interpolant ($\mathbb{P}^1$ in space, $\mathbb{P}^0$ in time) of the exact solution P of (23): Assume that P is a C^4 function on each edge of the graph; assume that $\theta(k) \to 0$ as $k \to 0$. Let $\beta(k)$ be defined by $\beta(k) = k^2$ if $\partial_t P(.,0)$ is constant, $\beta(k) = k^2\sqrt{\log(T/k)}$ otherwise.*
Then, there exists a positive constant C, depending on P, such that for k small enough:

$$\|\mathbf{p}_{h,k} - \tilde{p}_{h,k}\|_{L^2(0,T,H^1(\mathrm{B}))} \le C\left(\beta(k) + h^2 + \theta(k)\right).$$

4.2 Link with $\theta(k)$

To make the link with Theorems 4 and 5, it is sufficient to consider the case of a single kernel. The sequence (K_n) is defined by $K_n = \dfrac{1}{k}\displaystyle\int_{t_n}^{t_{n+1}} K(t)\mathrm{d}t$. Consider the approximations:

$$\begin{cases} \tilde{K}_n = \dfrac{1}{k}\displaystyle\int_{t_n}^{t_{n+1}} K_{h,k,\tau}(t)\mathrm{d}t \ \text{ for the corrected scheme,} \\ \tilde{K}_n = \dfrac{1}{k}\displaystyle\int_{t_n}^{t_{n+1}} K_{h,k}(t)\mathrm{d}t \ \text{ for the uncorrected scheme.} \end{cases}$$

and

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

Theorem 6 *Under the assumptions of Theorem 2 or those of Theorem 3, 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).

The proof, more technical than difficult, is given in Appendix D.
To end this section, we prove that the conditions on the discrete kernels for convergence and stability of the schemes in [4] are satisfied by the discrete kernels presented in this paper.

Proposition 7 *If the hypotheses of Theorem 2 are satisfied (e.g. Implicit Euler without correction), then $\left(\dfrac{1}{k}\displaystyle\int_{t_n}^{t_{n+1}} K_{h,k}(t)\,dt\right)_n$ and $(K_{h,k}(t_n))_n$ satisfy Lemma 4 of [4].*

Remark Using Proposition 2 of [4], this proves that the scheme presented in equations (1.8-11) and (3.26) of [4] with $W = 1$ is unconditionally stable.

Proof Define

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

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

Because of Theorem 2, we have for k sufficiently small,

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

Hence, there exists $t_{n+1/2} \in [T/2, 3T/4]$ such that $(T/4)|K'_{h,k}(t_{n+1/2}+T/4) - K'_{h,k}(t_{n+1/2})| > E$. But $K'_{h,k}(t_{n+1/2}+T/4) - K'_{h,k}(t_{n+1/2}) = \dfrac{K_{h,k}(t_{n+1+\frac{T}{4k}}) - K_{h,k}(t_{n+\frac{T}{4k}})}{k} - \dfrac{K_{h,k}(t_{n+1}) - K_{h,k}(t_n)}{k} = k\displaystyle\sum_{p=n}^{n+\frac{T}{4k}-1} U_p$. Hence, there exists $t_p > T/2$ such that $(T/4)U_p \geq |K'_{h,k}(t_{n+1/2}+T/4) - K'_{h,k}(t_{n+1/2})| > \dfrac{4}{T}E$.

We conclude that, as (U_n) is decreasing, for $t_n \leq \dfrac{T}{2}$, $U_n \geq 4\dfrac{E}{T^2}$ and $\dfrac{U_n + U_{n+1}}{2} \geq 4\dfrac{E}{T^2}$. This concludes the proof.

For the scheme presented in [4], Section 3.4.2, we prove the following result.

Proposition 8 *If the hypotheses of Theorem 2 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 6 also hold.*

Proof

$$\sum_{0<t_n<T} |K_{h,k}(t_n) - K_{h,k}(t_{n-1}) - \int_{t_n}^{t_{n+1}} K_{h,k}(t)\mathrm{d}t + \int_{t_{n-1}}^{t_n} K_{h,k}(t)\mathrm{d}t|$$
$$= \sum_{0<t_n<T} |\frac{K_{h,k}(t_{n-1}) - 2K_{h,k}(t_n) + K_{h,k}(t_{n+1})}{2}|$$

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

Using Theorem 6, we get the announced result.

5 Numerics

5.1 Summary of the algorithm

Let us first recapitulate the whole algorithm.

- Choose γ a parameter linking the time step and the space step, Ω the open set for which the kernel is to be computed, $m = 5/2$ the degree at which the asymptotic expansion is known, $\rho \in \{1, 2\}$ the time degree of the method, $r - 1$ the finite element degree of the method and k the time step. Compute $\mu = \min\left\{\frac{\rho}{m+\rho}, \gamma\frac{2r}{2m+r}\right\}$, $h = k^\gamma$.
- Compute $\mathcal{T}_h$ a triangulation of Ω of step h.
- Take the finite element space S_h of the $\mathbb{P}^{r-1}$-elements on $\mathcal{T}_h$.
- Take $T_h : L^2(\Omega) \to S_h$ such that (Nitsche method)
$$\forall v_h \in S_h, \quad \int_\Omega u_h v_h = \int_\Omega \langle \nabla v_h, \nabla T_h u\rangle + \int_{\partial\Omega} -v\partial_n T_h u - T_h u \partial_n v + \frac{C}{h} v_h T_h u,$$
where ∂_n denotes the normal derivative and C is a sufficiently large constant.
- Let V_0^h be the orthogonal projection of 1 over S_h, and $A_h = (T_h)^{-1}_{|S_h}$.
-
  - If $\rho = 1$, compute $V_{h,k}^{n+1} - V_{h,k}^n = -kA_h V_{h,k}^{n+1}$ (Implicit Euler) for $n \geq 0$
  - If $\rho = 2$, compute $\begin{cases} V_{h,k}^1 - V_{h,k}^0 = -kA_h V_{h,k} \\ 3V_{h,k}^{n+2} + 2kA_h V_{h,k}^{n+2} = 4V_{h,k}^n - V_{h,k} \end{cases}$ (BDF2 initialized with implicit Euler) for $n \geq 0$.
- Define $K_{h,k}$ the continuous function, affine on each $[nk, (n+1)k]$ such that $K_{h,k}(nk) = \int_\Omega V_{h,k}^n$, the uncorrected kernel approximation (convergent if $\rho = 1$).
- Compute $\tau = k^{m\mu}$. Define and return the corrected kernel approximation.:
$$K_{h,k,\tau}(t) = \begin{cases} K_{h,k}(t) & \text{if } t \geq \tau \\ K_{h,k}(\tau) + \left[S - 2L\sqrt{\frac{s}{\pi}} + \pi s + \frac{s^{3/2}}{6\sqrt{\pi}}\int_0^L \kappa(s)^2 \mathrm{d}s + \frac{s^2}{16}\int_0^L \kappa(s)^3 \mathrm{d}s\right]_\tau^t & \text{if } t < \tau. \end{cases}$$
- Return $\frac{K_{h,k}(nk) + K_{h,k}((n+1)k)}{2}$ as an approximation of $\frac{1}{k}\int_{nk}^{(n+1)k} K(t)\mathrm{d}t$.

If $r = 1$ and the domain is polygonal, one may replace S_h by the finite elements which vanish on the boundary.

5.2 Results

In this section, we test the schemes designed in the previous sections. As it was predicted above, 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 6.
Figure 1 presents the graph of function V for small values of time. One can observe the boundary layer: the leading term of the deviation to $\mathbf{1}$ essentially depends on the distance to the boundary of the domain, as shown theoretically for smooth domains (Equation (43)).
Analysing Figures 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 for the multistep BDF2 scheme, when the hypotheses of Lemma 6 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, 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 6. 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 6. 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:

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

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 that 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 (Tables 1 and 2) and squared domain (Tables 3 and 4). We give the accuracy results both with respect to the space discretization (Tables 1 and 3) and with respect to the time discretization (Tables 2 and 4), 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^1_k-error	order	$\dot{W}^{1,1}_k$-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

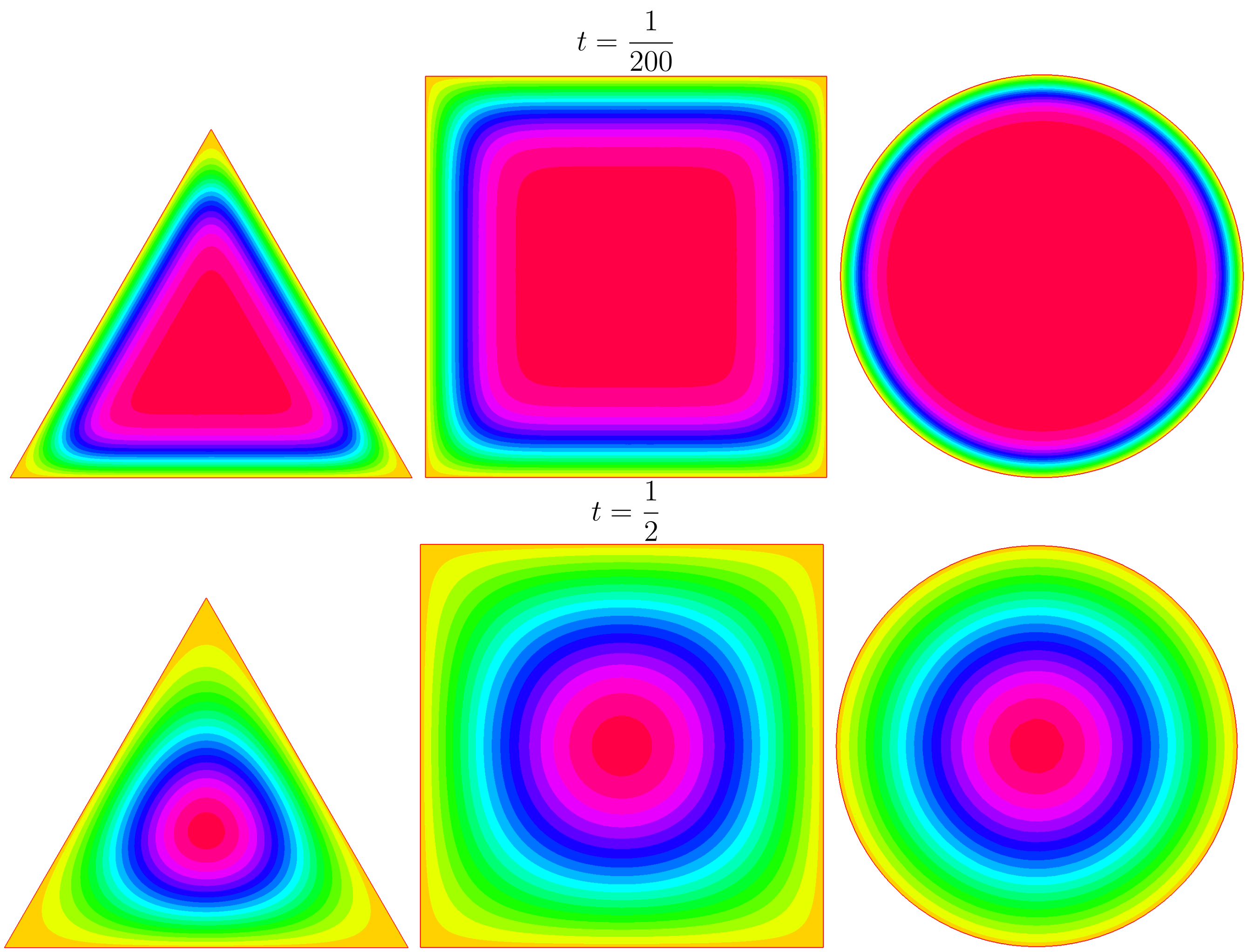
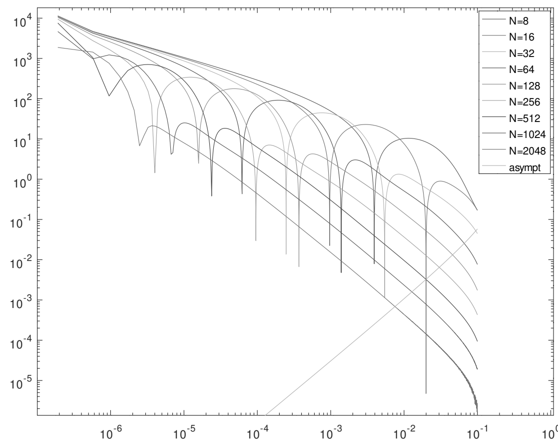


Figure 1: Solution to (2) with Dirichlet boundary equations at time $t = 1/200$ and $t = 1/2$ for three different domains. (The triangle is shown at a scale twice smaller than the square and the disc)

$$k = 0.1 \cdot 2^{-18}$$



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

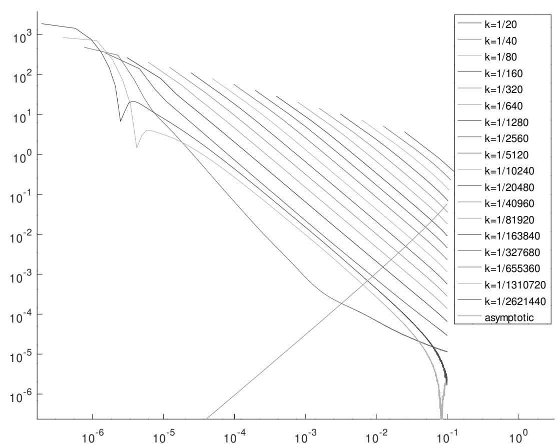
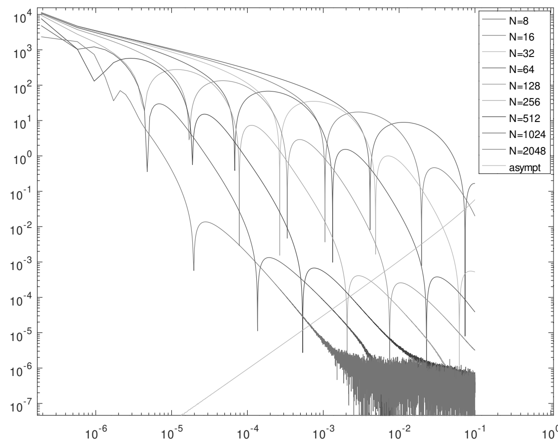


Figure 2: Case of the disc discretized with $\mathbb{P}^1$-elements in space and Implicit-Euler in time. $\left|\dfrac{K_{h,k}(t_{n+1}) - K_{h,k}(t_n)}{k} - \dfrac{K(t_{n+1}) - K(t_n)}{k}\right|$ as a function of $t_{n+1/2}$ for various values of the space step $h = \dfrac{2\pi}{N}$ (top, $k = 0.1 \cdot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

$k = 0.1 \cdot 2^{-18}$



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

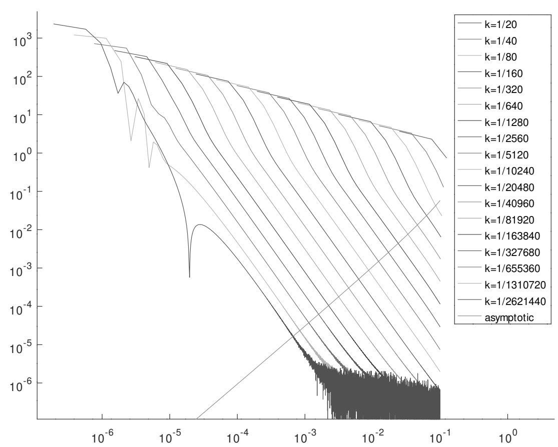


Figure 3: Case of the disc discretized with $\mathbb{P}^2$-elements in space and BDF2 in time. $\left|\dfrac{K_{h,k}(t_{n+1}) - K_{h,k}(t_n)}{k} - \dfrac{K(t_{n+1}) - K(t_n)}{k}\right|$ as a function of $t_{n+1/2}$ for various values of the space step $h = \dfrac{2\pi}{N}$ (top, $k = 0.1 \cdot 2^{-18}$)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

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

h	k	L^1_k-error	order	$\dot{W}^{1,1}_k$-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^1_k-error	order	$\dot{W}^{1,1}_k$-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^1_k-error	order	$\dot{W}^{1,1}_k$-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: disc, $\mathbb{P}^1$, Nitsche, Implicit Euler method.

		$\|K_{h,k} - K\|$				$\|K_{h,k,\tau} - K\|$			
h/π	k	L^1_k		$\dot{W}^{1,1}_k$		L^1_k		$\dot{W}^{1,1}_k$	
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: disc, $\mathbb{P}^2$, Nitsche, BDF2.

		$\|K_{h,k}-K\|$				$\|K_{h,k,\tau}-K\|$			
h/π	k	L^1_k		$\dot{W}^{1,1}_k$		L^1_k		$\dot{W}^{1,1}_k$	
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

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A Asymptotic expansion of the kernel: proof of Theorem 1

The proof of Theorem 1 page 7 is rather long and thus is decomposed into several steps. First, in section A.1, we consider the case where Ω is a disk of radius 1 and obtain the explicit asymptotic expansion of Proposition 2 page 7. Subsection A.2 is devoted to obtaining the asymptotic expansions for a primitive of K: Proposition 9. As already mentioned, here we use computations and results in [7, 8] for well-prepared data. Along the proof, all the needed results and equations are explicitly mentioned with the numbering of [8]. Subsection A.3 is devoted to the justification of the term by term differentiation of the obtained expansion: Proposition 10. The first five coefficients of the expansions are then characterized in terms of geometric data of the domain (area, length, curvature) and of several *universal constants*: see Subsection A.4, Proposition 11. From this, we deduce by comparison the universal constants for the first five terms of the general asymptotic expansion and thereby conclude the proof of Theorem 1.

A.1 Kernel in the case of a disk - Proof of Proposition 2

Let us prove Proposition 2 page 7.

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

$$w_{j,\lambda}(x) = (A_j \cos j\theta + B_j \sin j\theta)\, J_j(\sqrt{\lambda}\rho)$$

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

It is easily seen that $\displaystyle\int_\Omega w_{j,\lambda} \mathrm{d}x = 0$ for $j \neq 0$ so that only the eigenvalues of the 0-th Bessel function J_0 remains in the series expansion (3):

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

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

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

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

so that the normalized eigenvectors associated with the $(\mu_k)_{k\in\mathbb{N}^*}$ are the $(w_k)_{k\in\mathbb{N}^*}$ defined by:

$$w_k(x) = \frac{J_0(\mu_k\rho)}{\sqrt{\pi}\,|J_1(\mu_k)|}.$$

Hence: $a_k = \displaystyle\int_\Omega w_k \mathrm{d}x = \frac{2\sqrt{\pi}}{\mu_k}$. Assertion (i) is proved.

Now we remark that, using Equations (2.1)-(2.7) in [9], the Laplace transform $\mathsf{L}(K)$ of K, which obviously exists for all $s > 0$, is given by:

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

where I_ν stands for the ν-modified Bessel function of the first kind. As each function $z \to z^{1/2}e^{-z}I_\nu(z)$ admits (see for instance [32] page 203) an asymptotic expansion for large z at any order, one can compute:

$$\mathsf{L}(K)(s) = Q(s^{-1/2}) + o_{s\to+\infty}\left(s^{-3}\right) \quad \text{where } Q(X) = \pi X^2 - 2\pi X^3 + \pi X^4 + \frac{\pi}{4}X^5 + \frac{\pi}{4}X^6. \tag{26}$$

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

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

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

$$\mathsf{L}(R_5)(s) = \frac{1}{s^3}\mathsf{L}\left(R_5^{(3)}\right)(s) = O_{s\to+\infty}\left(s^{-4}\right),$$

and thus,

$$\mathsf{L}(K)(s) = \mathsf{L}(R_5)(s) + \mathsf{L}(P\circ\surd)(s) = \mathsf{L}(P\circ\surd)(s) + o_{s\to+\infty}\left(s^{-3}\right). \tag{27}$$

Comparing (26) and (27) we have that

$$\mathsf{L}(P\circ\surd)(s) = Q(s^{-1/2}) + o_{s\to+\infty}\left(s^{-3}\right).$$

Then, using the formula $\mathsf{L}(t^{r/2})(s) = \Gamma(1 + r/2)\, s^{-1-r/2}$, we get

$$\begin{aligned}
\mathsf{L}(P\circ\surd)(s) &= \frac{c_0}{\sqrt{s}} + c_{1/2}\frac{\sqrt{\pi}}{2}\frac{1}{s^{3/2}} + c_1\frac{1}{s^2} + c_{3/2}\frac{3\sqrt{\pi}}{4}\frac{1}{s^{5/2}} + c_2\frac{2}{s^3} \\
&= \pi\frac{1}{\sqrt{s}} - 2\pi\frac{1}{s^{3/2}} + \pi\frac{1}{s^2} + \frac{\pi}{4}\frac{1}{s^{5/2}} + \frac{\pi}{4}\frac{1}{s^3} + o_{s\to+\infty}\left(s^{-3}\right).
\end{aligned}$$

This proves Proposition 2.

A.2 Existence of the asymptotic expansions for a primitive of K

We consider a general simply connected smooth domain Ω as in Section 2. First note that V defined by (2) is not solution to a well-prepared problem in the sense of [7, 8] because the initial condition does not satisfy the boundary condition.

Let us introduce W defined on $\Omega \times \mathbb{R}^+$ by

$$W(x,t) = \int_0^t V(x,s)\mathrm{d}s,$$

so that

$$\forall t \in \mathbb{R}^+,\ K(t) = \partial_t \int_\Omega W(x,t)\mathrm{d}x \text{ and } \int_0^t K(s)\mathrm{d}s = \int_\Omega W(x,t)\mathrm{d}x. \tag{28}$$

This W satisfies the following problem with compatible initial and boundary data:

$$\begin{cases} \partial_t W - \Delta W = 1 \text{ in } \Omega, \\ W = 0 \ \text{ on } \partial\Omega, \\ W = 0 \ \text{ at } t = 0, \end{cases} \tag{29}$$

and in view of (28), asymptotic for W when $t \to 0$ will provides asymptotic for primitives of K when $t \to 0$.

The problem addressed in [7, 8] is the asymptotic with respect to ε for :

$$\begin{cases} \partial_t u^\varepsilon - \varepsilon\Delta u^\varepsilon = f \text{ in } \Omega, \\ u^\varepsilon = 0 \ \text{ on } \partial\Omega, \\ u^\varepsilon = u_0 \ \text{ at } t = 0, \end{cases} \tag{30}$$

where, in the *well-prepared* case, $u_0 = 0$ on $\partial\Omega$. We are interested here in this problem with the very simple data: $f = 1$, $u_0 = 0$:

$$\begin{cases} \partial_t u^\varepsilon - \varepsilon\Delta u^\varepsilon = 1 \text{ in } \Omega, \\ u^\varepsilon = 0 \ \text{ on } \partial\Omega, \\ u^\varepsilon = 0 \ \text{ at } t = 0. \end{cases} \tag{31}$$

Obviously, it is equivalent to look for asymptotics for (29) when $t \to 0$ or for (31) when $\varepsilon \to 0$. Indeed, let $w^\varepsilon(x,t) = \varepsilon u^\varepsilon(x, t/\varepsilon)$; it is easily checked that w^ε solves (29). Hence,

$$\forall \varepsilon > 0, \forall t \in \mathbb{R}^+, \forall x \in \Omega,\ W(x,t) = w^\varepsilon(x,t) = \varepsilon u^\varepsilon(x, t/\varepsilon).$$

With $\varepsilon = t$ we get the following expression for W, from which we will deduce the asymptotic expansion for W.

Lemma 1 *The solution to (29) is given by:* $\forall t \in \mathbb{R}^+$, $\forall x \in \Omega$, $W(x,t) = tu^t(x,1)$, *where for any* $\varepsilon > 0$, u^ε *is the solution to (31).*

So, in order to get an asymptotic expansion for W when $t \to 0$, it is sufficient to obtain an asymptotic expansion for u^ε when $\varepsilon \to 0$, and this is exactly what we are doing in the sequel : this is the first step of the proof of Theorem 1:

Proposition 9 *Let Ω be a bounded $C^\infty-$smooth domain. Let $T > 0$. Then, there exists $(\bar{c}_j)_{j \in 1+\frac{1}{2}\mathbb{N}}$, where $\bar{c}_1 = |\Omega|$, such that:*

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

Proof 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 $\Gamma = \partial\Omega$ then has 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 $\gamma : \mathbb{R} \to \Gamma$, $s \mapsto \gamma(s)$ in such a way that:

$$\gamma'(s) = i(\mathbf{n}(\gamma(s))) \tag{32}$$

where $\mathbf{n} : \Gamma \to \mathbb{R}^2$ is the inward-pointing normal vector to Γ and i is the vector rotation of angle $\pi/2$. Then, the curvature κ is defined by:

$$\kappa(s)\gamma''(s) = \mathbf{n} \circ \gamma(s). \tag{33}$$

Remark In the case of a non simply connected domain, to maintain (32) 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:

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

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

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

We look for an asymptotic expansion for u^ε continuous solution of (2) in $\Omega \times [0,T]$. According to [8], u^ε can be approximated at any order $n \in \mathbb{N}$ by an asymptotic expansion of the form (equations (200) in [8]):

$$u^\varepsilon \simeq u_{\varepsilon,n+1/2} = \sum_{j=0}^{n} \left(\varepsilon^j(u^j + \theta^j) + \varepsilon^{j+1/2}\theta^{j+1/2}\right), \tag{34}$$

where the error in the approximation is bounded as follows (Theorem 2.5 Equation (227) in [8]):

$$\|u_{\varepsilon,n+1/2} - u^{\varepsilon}\|_{L^\infty(0,T,L^2(\Omega))} \le C\varepsilon^{n+1}. \tag{35}$$

Here u^0 is the solution to $(30)_{1,3}$ with $\varepsilon = 0$, that is $u^0(x,t) = t$. Also, from Equation (204) in [8], as here $u_0 = 0$ and $f = 1$ are constant, one can easily see that for $j \neq 0$, $u^j = 0$. So for convenience, we rewrite (34) 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 in [8] from functions $\bar{\theta}^{r/2}$ that solve one dimensional heat equations on a half line : equations (211)-(212)-(210)-(94). Note that the functions $\bar{\theta}^{r/2}$, and thus the functions $\theta^{r/2}$ do depend on ε. In order to carry on our computations to prove Proposition 9, we need to make explicit every dependence with respect to ε. For that purpose, we 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 $L = |\Gamma|$, defined recursively for $j \in \dfrac{1}{2}\mathbb{N}$ by:

$$\begin{cases} \partial_t\tilde{\theta}^j - \partial_\xi^2\tilde{\theta}^j = \widetilde{f}^j \text{ in } \mathbb{R}^{+*}\times\mathbb{R}^{+*}, \\ \tilde{\theta}^j = \tilde{\theta}^j_0, \text{ at } \xi = 0, \\ \lim\limits_{\xi\to+\infty} \tilde{\theta}^j = 0, \\ \tilde{\theta}^j = 0 \text{ at } t = 0. \end{cases} \tag{36}$$

where $\tilde{\theta}^0_0 = -u^0$, $\tilde{\theta}^j_0 = 0$ for $j \neq 0$ and,

$$\forall j \in \frac{1}{2}\mathbb{N},\ \ \widetilde{f}^j = \sum_{k=0}^{2j-2} \xi^k \partial_s\left((k+1)\kappa^k\partial_s\widetilde{\theta}^{j-1-\frac{k}{2}}\right) - \sum_{k=0}^{2j-1}\xi^k\kappa^{k+1}\partial_\xi\widetilde{\theta}^{j-\frac{1}{2}-\frac{k}{2}}. \tag{37}$$

Note that the functions $\widetilde{\theta}^j$ do not depend on ε.
These equations (36) and (37) are easily deduced from Equations (94), (210), (211), (212) in [8], with the correspondence: $\bar{\theta}^j(s,\xi,t) = \widetilde{\theta}^j(s,\varepsilon^{-1/2}\xi,t)$ and $\bar{f}^j(s,\xi,t) = \widetilde{f}^j(s,\varepsilon^{-1/2}\xi,t)$. With our choice of arclength parametrization above we have that $g_{11} = 1$ and $h_1 = h = 1-\kappa\xi$ in the notations of [8]. This was used to in (94) and (210) to make (37) explicit.
Now, following the lines in [8], we define the boundary layers θ^j from the $\widetilde{\theta}^j$.
Let $\sigma : \mathbb{R}^+ \to \mathbb{R}$ 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 $C^\infty-$functions θ^j on Ω by

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

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

$$\begin{aligned}\int_\Omega u_{\varepsilon,n+1/2}\mathrm{d}x &= \int_\Omega u^0 \mathrm{d}x + \sum_{r=0}^{2n+1} \varepsilon^{r/2} \int_\Omega \theta^{r/2}\mathrm{d}x \\ &= |\Omega|\, t + \sum_{r=0}^{2n+1} \varepsilon^{r/2} \int_\Omega \theta^{r/2}\mathrm{d}x.\end{aligned}$$

For each term, we have that

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

From Equation (218) of Lemma 2.8 in [8] with $m = k = 0$ and $j + d = r/2$, we see that

$$\int_{\delta/3}^{\delta/2} \sigma(\xi) \int_0^L \bar{\theta}^{r/2}(s,\xi,t)(1-\kappa(s)\xi)\mathrm{d}s\mathrm{d}\xi = O_{\varepsilon\to 0}(\exp(-C\varepsilon^{-1})) \tag{38}$$

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 $\nu = \varepsilon^{-1/2}\xi$:

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

Then, reasoning as for (38), we deduce that

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

where:

$$I_{r/2}(t) = \int_0^{+\infty} \int_0^L \widetilde{\theta}^{r/2}(s,\nu,t)\mathrm{d}s\mathrm{d}\nu, \quad J_{r/2}(t) = \int_0^{+\infty} \int_0^L \widetilde{\theta}^{r/2}(s,\nu,t)\kappa(s)\nu\mathrm{d}s\mathrm{d}\nu, \tag{39}$$

and therefore that

$$\int_\Omega u_{\varepsilon,n+1/2}\mathrm{d}x = |\Omega|\, t + \sum_{r=0}^{2n+1} \varepsilon^{(r+1)/2} I_{r/2}(t) - \sum_{r=0}^{2n+1} \varepsilon^{(r+2)/2} J_{r/2}(t) + O_{\varepsilon\to 0}(\exp(-C\varepsilon^{-1})).$$

Note that the functions $I_{r/2}$ and $J_{r/2}$ are independent of ε.

Now we are able to end the proof of Proposition 9. With (28), Lemma 1 and the error estimate (35) we get:

$$\begin{aligned}\int_0^t K(\tau)\mathrm{d}\tau &= t\int_\Omega u^t(x,1)\mathrm{d}x = t\int_\Omega u_{t,n+1/2}(x,1)\mathrm{d}x + O_{t\to 0^+}(t^{n+2}) \\ &= t\left(|\Omega| + \sum_{r=0}^{2n+1} t^{(r+1)/2} I_{r/2}(1) - \sum_{r=0}^{2n+1} t^{(r+2)/2} J_{r/2}(1)\right) + O_{t\to 0^+}(t^{n+2}) \\ &= |\Omega|\, t + \sum_{r=0}^{2n} t^{(r+3)/2} I_{r/2}(1) - \sum_{r=0}^{2n-1} t^{(r+4)/2} J_{r/2}(1) + O_{t\to 0^+}(t^{n+2}) \\ &= |\Omega|\, t + I_0(1)t^{3/2} + \sum_{r=4}^{2n+3}\left(t^{r/2} I_{(r-3)/2}(1) - t^{r/2} J_{(r-4)/2}(1)\right) + O_{t\to 0^+}(t^{n+2}).\end{aligned} \tag{40}$$

This is the announced result with:

$$\begin{aligned}&\bar{c}_1 = |\Omega|\,,\ \bar{c}_{3/2} = I_0(1), \\ &\forall r \geqslant 4,\ \bar{c}_{r/2} = I_{(r-3)/2}(1) - J_{(r-4)/2}(1).\end{aligned} \tag{41}$$

A.3 Term by term differentiability - Existence of the asymptotic expansions for K

Proposition 10 *Let $m \in \mathbb{Z}$, $M \in \mathbb{N}^*$, $T > 0$. Let $H :]0,T] \to \mathbb{R}$ be a C^1 convex or concave function such that: $H(t) = \sum_{r=m}^{M} \alpha_r t^{r/2} + O_{t\to 0^+}(t^{(M+1)/2})$. Then*

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

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

$$\frac{H(t+h) - H(t)}{h} \leqslant H'(t) \leqslant \frac{H(t) - H(t-h)}{h};$$

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

$$\frac{H(t+t^n) - H(t)}{t^n} \leqslant H'(t) \leqslant \frac{H(t) - H(t-t^n)}{t^n}. \tag{42}$$

Now, let us compute:

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

Likewise:

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

Then, using (42), we conclude that H' admits the same asymptotic expansion.

Now, we are able to prove the first part of Theorem 1. Applying Proposition 10 to $H(t) = \int_0^t K(\tau)\mathrm{d}\tau$ which is a concave function (see Proposition 1) with $m = 2$ and $M = 2n+5$, in view of Proposition 9, the following holds true.

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

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

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 (41).

The next step in proving Theorem 1 is to express the coefficients $c_{r/2}$ for $r = 1...4$ in terms of the geometry of Ω, namely in terms of powers of the curvature κ, and of some universal constants, that do not depend on Ω. This is done in the next subsection.

A.4 Characterization of the first five coefficients of Theorem 1

We already know that $c_0 = |\Omega|$. 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 (39).

Proposition 11 *The first coefficients in the asymptotic expansion in Corollary 1 are such that* $c_0 = |\Omega|$*, and:*

$$c_{1/2} = L\, a_{1/2}; \qquad c_1 = a_1 \int_0^L \kappa(s)\mathrm{d}s = 2\pi a_1;$$
$$c_{3/2} = a_{3/2} \int_0^L \kappa(s)^2\mathrm{d}s; \quad c_2 = a_2 \int_0^L \kappa(s)^3\mathrm{d}s.$$

where $a_{1/2}$*,* a_1*,* $a_{3/2}$*,* a_2 *do not depend on* Ω*.*

Remark The second equality for c_1 holds by application of the Hopf's Umlaufsatz (see [29] pp.36-37 and 62), a particular case of Gauss-Bonnet theorem, which yields $\int_0^L \kappa(s)\mathrm{d}s = 2\pi$.

Proof According to [8] Equation (134), the boundary layer $\tilde{\theta}^0$ can be written as:

$$\tilde{\theta}^0(s,\xi,t) = -\int_0^t \operatorname{erfc}\left(\frac{\xi}{2\sqrt{\tau}}\right)\mathrm{d}\tau \tag{43}$$

where $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^{+\infty} e^{-y^2}\mathrm{d}y$ (Note that we use a different definition of the erfc function introduced in equation (135) of [8]).
As $\tilde{\theta}^0$ does not depend on s, we get:

$$I_0(1) = L\, I_{0,c} \text{ where } I_{0,c} = -\int_0^{+\infty}\int_0^1 \operatorname{erfc}\left(\frac{v}{2\sqrt{\tau}}\right)\mathrm{d}\tau\mathrm{d}v, \tag{44}$$

$$J_0(1) = J_{0,c}\int_0^L \kappa(s)\mathrm{d}s \;\text{ where } J_{0,c} = \int_0^{+\infty}\int_0^1 \operatorname{erfc}\left(\frac{v}{2\sqrt{\tau}}\right)\nu\mathrm{d}\tau\mathrm{d}v. \tag{45}$$

According to [8] Equations (137)-(138)-(217), the next $\tilde{\theta}^j$ are given by:

$$\tilde{\theta}^j(s,\nu,t) = \int_0^{+\infty}\int_0^t \tilde{f}^j(s,y,\tau)N(\nu,y,t,\tau)\mathrm{d}\tau\mathrm{d}y, \tag{46}$$

where the $\tilde{f}^j$ are defined in (37) 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,

$$\tilde{\theta}^{1/2}(s,\nu,t) = \frac{\kappa(s)}{\sqrt{\pi}}\int_0^{+\infty}\int_0^t\int_0^\tau \frac{1}{\sqrt{r}}\exp\left(-\frac{y^2}{4r}\right)N(\nu,y,t,\tau)\mathrm{d}r\mathrm{d}\tau\mathrm{d}y, \tag{47}$$

so that

$$I_{1/2}(1) = I_{1/2,c} \int_0^L \kappa(s)\mathrm{d}s \text{ and } J_{1/2,c}(1) = J_{1/2,\kappa} \int_0^L \kappa(s)^2\mathrm{d}s, \tag{48}$$

where

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

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

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

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

In view of (43) and (47), $\tilde{\theta}^0$ 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

$$\begin{cases} I_1(1) = \displaystyle\int_0^{+\infty} \int_0^L \widetilde{\theta}^1(s, \nu, 1)\mathrm{d}s\mathrm{d}\nu = I_{1,c} \int_0^L \kappa(s)^2\mathrm{d}s, \\ J_1(1) = \displaystyle\int_0^{+\infty} \int_0^L \widetilde{\theta}^{r/2}(s, \nu, 1)\kappa(s)\nu\mathrm{d}s\mathrm{d}\nu = J_{1,c} \int_0^L \kappa(s)^3\mathrm{d}s. \end{cases}$$

Then, according to (46) and (37)

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

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

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

As $\partial_s \tilde{\theta}^{1/2}$ is L-periodic with respect to s, the first term vanishes when integrating over $s \in [0, L]$. Therefore, there exists another constant $I_{3/2,c}$ not depending on Ω, such that

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

so we may conclude that

$$c_{1/2} = \frac{3}{2} L\ I_{0,c}; \qquad c_1 = 4\pi \left(I_{1/2,c} - J_{0,c}\right) \int_0^L \kappa(s) \mathrm{d}s;$$
$$c_{3/2} = \frac{5}{2} \left(I_{1,c} - J_{1/2,c}\right) \int_0^L \kappa(s)^2 \mathrm{d}s; \quad c_2 = 3 \left(I_{3/2,c} - J_{1,c}\right) \int_0^L \kappa(s)^3 \mathrm{d}s.$$

This is the announced result.

Remark The possibility to express each coefficient via a $\int_0^L \kappa(s)^p \mathrm{d}s$ and a unique universal constant ends here: if computing $J_{3/2}(1)$, because of the term $\kappa \partial_s{}^2 \widetilde{\theta}^{1/2}$ in $\kappa\widetilde{\theta}^{3/2}$ which depends on s via the factor $\kappa\kappa''$, we can only obtain the existence of *two* universal constants $J_{3/2,c}$ and $J'_{3/2,c}$ such that

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

To prove Theorem 1, it remains to determine the coefficients $a_{1/2}$, a_1, $a_{3/2}$, a_2. It is possible, although rather technical to compute explicitly, at least the integrals $I_{0,c}$, $J_{0,c}$, $J_{1/2,c}$, $J_{1/2,c}$. However, as we are able to compute explicitly the coefficients of the expansion for a disk, we determine these four constants by comparison with the asymptotics for a disk of radius 1.

As for the disk, $\kappa = 1$, we get:

$$-4\sqrt{\pi} = 2\pi\ a_{1/2}; \quad \pi = 2\pi\ a_1; \quad \frac{\sqrt{\pi}}{3} = 2\pi\ a_{3/2}; \quad \frac{\pi}{8} = 2\pi\ a_2.$$

This concludes the proof of Theorem 1.

B Triangular case : proof of Proposition 4 page 9

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

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

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

and

$$\lambda_{m,n} = \frac{16\pi^2}{27}\left(m^2+n^2-mn\right). \tag{49}$$

We have the following symmetry properties (see [10, 27]):

Lemma 2 $\forall (m,n) \in \mathbb{Z}^2, \forall j \in \{1,\dots,6\}$*:*

(i) $m_j \neq 2n_j$, $n_j \neq 2m_j$ $m_j \neq -n_j, n_j \neq m_j \iff m \neq 2n$, $n \neq 2m$, $m \neq -n$, $n \neq m$*;*

(ii) $\lambda_{m_j,n_j} = \lambda_{m,n}$*;*

(iii) 3 *divides* $m+n \Rightarrow \forall j \in \{1,..,6\}$, 3 *divides* $m_j + n_j$*;*

(iv) $\mathbb{I}_{m,n} = \mathbb{I}_{m_j,n_j}$*. Besides, either all the pairs of this set have the same sign with respect to* (m,n) *and* (m_j,n_j)*, or the signs of every pair with respect to* (m,n) *and* (m_j,n_j) *are opposite;*

(v) $m_j n_j (m_j - n_j) = mn(m-n)$.

As may be found in Grebenkov-Nguyen [10] and Pinski [27]:

Lemma 3 *The eigenvalues of the Dirichlet-Laplace operator in* Ω *are the numbers* $\lambda_{m,n}$ *defined by (49), satisfying the following additional conditions:*

(i) 3 *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 $((m_j,n_j))_{1\leqslant j\leqslant 6}$ 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 3(i)-(ii) and* $mn\,(m-n) \neq 0$*. Then* $\displaystyle\int_\Omega u_{m,n}(x)\mathrm{d}x = 0$.

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

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

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 $A_{m,n} = \frac{8\pi^2}{9\sqrt{3}}mn\,(m-n)\int_\Omega u_{m,n}(x)\mathrm{d}x$.
We thus have

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

$$\begin{aligned} A_{m,n} = \; & (2n-m)\left(I\left(m\right) - I\left(-m\right)\right) \\ & + (n-2m)\left(I\left(n\right) - I\left(-n\right)\right) \\ & + (n+m)\left(I(m-n) - I(n-m)\right) \end{aligned}$$

so that

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

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 $2\pi-$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 [27], 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 $\forall k \in \mathbb{N}^*$, $\int_\Omega v_{3k,0}(x)\mathrm{d}x = \frac{3\sqrt{3}}{4\pi k}$, $\int_\Omega v_{3k,0}(x)^2\mathrm{d}x = \frac{3\sqrt{3}}{8}$.

Now, we are able to prove the proposition.

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

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

and thus, for $t > 0$,

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

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 $K'(t) = 4\sqrt{3}\,(1 - \theta\,(0, 16\pi t i/3))$.

C Proofs regarding time discretization

C.1 Conditions (16) page 13 for the second order Backward Difference Formula (BDF2)

The BDF2 scheme (17) can be put in the abstract form by defining $(G_n)_n$ with the following linear difference difference equation of order 2:

$$\begin{cases} G_0 = 1,\, G_1(\xi) = (1-\xi)^{-1}, \\ \forall n \geq 0,\, (3-2\xi)G_{n+2}(\xi) = 4G_{n+1}(\xi) - G_n(\xi), \end{cases} \tag{50}$$

For small enough ξ if may be rewritten as :

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

where

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

$$c(\xi) = \frac{G_1(\xi) - g(\xi)G_0(\xi)}{f(\xi) - g(\xi)}, \quad d(\xi) = \frac{G_1(\xi) - f(\xi)G_0(\xi)}{g(\xi) - f(\xi)}.$$

Then, with $\xi_0 = 2/5$, $\rho = 2$ and $\varepsilon = 2/3$, it is not too difficult to see that

$$\forall \xi \in]-\xi_0, 0], \quad |d(\xi)g(\xi)^n| \leq C\left(\frac{2}{3}\right)^n, |f(\xi)| \leq 1,$$

and that

$$c(\xi) = 1 + \frac{3}{4}\xi^2 + O_{\xi\to 0}(\xi^3), f(\xi) = 1 + \xi + \frac{1}{2}\xi^2 + \frac{1}{2}\xi^3 + O_{\xi\to 0}(\xi^4),$$

so that all conditions in (16) are satisfied, except for $G_n(\xi) = O_{n\to+\infty}(\varepsilon^n)$ uniformly in $]-\infty, -\xi_0]$. Let us check this condition in detail.

We have $\begin{pmatrix} G_{n+1}(\xi) \\ G_{n+2}(\xi) \end{pmatrix} = A(\xi)\begin{pmatrix} G_n(\xi) \\ G_{n+1}(\xi) \end{pmatrix}$ where $A(\xi) = \begin{pmatrix} 0 & 1 \\ \dfrac{-1}{3-2\xi} & \dfrac{4}{3-2\xi} \end{pmatrix}$. 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 $\dfrac{10+\sqrt{5}}{19} \approx 0.644 < 2/3 = \varepsilon$ on $[-\infty, -\xi_0]$. Besides, $\lim_{n\to+\infty} \|A(\xi)^n\|^{1/n} = \rho(\xi)$. Now, if we take a submultiplicative norm:

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

Hence $(\xi \mapsto \|A(\xi)^{2^n}\|^{2^{-n}})_n$ 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 $G_n(\xi) = O(\varepsilon^n)$ uniformly with respect to ξ.

C.2 Proof of Proposition 6 page 14

In this section, we give a proof of Proposition 6. We first refomulate hypotheses (16) and (51). Then we prove an estimate relating the time derivatives for the fully discrete scheme and for the semi-discrete scheme for (2), following the lines of Thomée [30], Chapter 7.

Assume that (16) and 51 are true. Let us show that without loss of generality, we can further assume that ξ_0, ε are such that:

$$\forall \xi \in [-\xi_0, 0], \ |e^\xi - f(\xi)| \leq C|\xi|^{\rho+1}, \tag{51}$$

$$\forall \xi \in [-\xi_0, 0], \ |f(\xi) - 1| \leq C\,|\xi|\,, \tag{52}$$

$$\forall \xi \in [-\xi_0, 0], \ |f(\xi)| \leq e^{\xi/2}, \tag{53}$$

$$\forall \xi \in]-\infty, -\xi_0], \quad e^{\xi} \leq \varepsilon < 1. \tag{54}$$

There is no loss of generality. Indeed, let $\tilde{\xi}_0, \tilde{\varepsilon}$ as in (16); one can choose $\xi_0 > 0$ small enough to have (51), $\xi_0 \leq \min\left\{\frac{1}{20C}, 1, \tilde{\xi}_0\right\}$ and $f \geq 0$ on $[-\xi_0, 0]$.

Then (52) follows from $|e^{\xi} - 1| + |f(\xi) - e^{\xi}| \leq |e^{\xi} - 1| + C|\xi|^{\rho+1} \leq |\xi| + |\xi|$ for $[-\xi_0, 0]$, and (53) from $f(\xi) - e^{\xi} + e^{\xi} - e^{\xi/2} \leq C|\xi|^{\rho+1} - \frac{1}{20}|\xi| \leq 0$ if $\xi \in [\xi_0, 0]$.

Last (54) holds with $\varepsilon = \max\left\{\tilde{\varepsilon}, e^{-\xi_0}, \max\left\{|f(\xi)|\,;\ \xi \in [-\tilde{\xi}_0, -\xi_0]\right\}\right\}$.

Then all the conditions in (16) hold for these new definitions of ξ_0 and ε. The first two points because $\xi_0 \leq \tilde{\xi}_0$ and $\varepsilon \geq \tilde{\varepsilon}$, the third one because $\varepsilon \geq \max\left\{|f(\xi)|\,;\ \xi \in [-\tilde{\xi}_0, -\xi_0]\right\}$.

Lemma 6 *Under the same assumptions as in Proposition 6, the following inequality hold:*

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

where C does not depend on k, h and S_h.

Proof With (19) and (13):

$$V_{h,k}^{n+1} - V_{h,k}^{n} - k\partial_t V_h(t_{n+1/2}) = \sum_{j=1}^{N_h} a_{h,j} \left(\left(G_{n+1} - G_n\right)\left(-k\lambda_{h,j}\right) + k\lambda_{h,j} e^{-(n+\frac{1}{2})k\lambda_{h,j}} \right) w_{h,j}. \tag{55}$$

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

(a) Estimate for $\xi \in [-\xi_0, 0]$. We have:

$$\left(G_{n+1} - G_n\right)(\xi) - \xi e^{(n+\frac{1}{2})\xi} = c(\xi) f(\xi)^n \left(f(\xi) - 1\right) - \xi e^{(n+\frac{1}{2})\xi} + R_n + R_{n+1} \tag{56}$$

where $R_n = G_n(\xi) - c(\xi) f(\xi)^n$. From $(16)_1$: $|R_n| \leq C\varepsilon^n$. As $\left(n^{\rho+1}\varepsilon^n\right)_{n\in\mathbb{N}}$ is bounded, this may also be rewritten as:

$$|R_n| \leq \frac{C}{n^{\rho+1}},\ |R_n + R_{n+1}| \leq \frac{2C}{n^{\rho+1}} \tag{57}$$

For the remaining part in (56), let us decompose it as follows

$$c(\xi) f(\xi)^n \left(f(\xi) - 1\right) - \xi e^{(n+\frac{1}{2})\xi} = \left(c(\xi)\left(f(\xi) - 1\right) - \xi e^{\xi/2}\right) e^{n\xi} + c(\xi)\left(f(\xi) - 1\right)\left(f(\xi)^n - e^{n\xi}\right). \tag{58}$$

For the first term in the right-hand side of (58), with $(16)_{4,5}$ we get:

$$\begin{aligned} c(\xi)\left(f(\xi)-1\right)-\xi e^{\xi/2} &= \left(1+O_{\xi\to 0}(\xi^\rho)\right)\left(e^\xi-1+O_{\xi\to 0}(\xi^{\rho+1})\right)-\xi e^{\xi/2} \\ &= \left(1+O_{\xi\to 0}(\xi^\rho)\right)\left(\xi+\frac{\xi^2}{2}+O_{\xi\to 0}(\xi^{\rho+1})\right)-\xi\left(1+\frac{\xi}{2}+O_{\xi\to 0}(\xi^2)\right) \\ &= O_{\xi\to 0}(\xi^{\rho+1}), \end{aligned}$$

because $\xi^3 = O_{\xi\to 0}(\xi^{\rho+1})$ ($\rho\in\{1,2\}$). Thus

$$\left|\left(c(\xi)\left(f(\xi)-1\right)-\xi e^{\xi/2}\right)e^{n\xi}\right| \le C\left|\xi\right|^{\rho+1} e^{n\xi}. \tag{59}$$

Let us consider now the second term in the right hand side of (58). From $(16)_5$, c is bounded on $[-\xi_0, 0]$. Let us estimate: $f(\xi)^n - e^{n\xi}$. With the identity $a^n-b^n=(a-b)\sum_{j=0}^{n-1} a^j b^{n-j-1}$, we get

$$f(\xi)^n - e^{n\xi} = \left(f(\xi)-e^\xi\right)\sum_{j=0}^{n-1} f(\xi)^j e^{(n-j-1)\xi},$$

so that, with (51), (54)

$$\left|f(\xi)^n - e^{-n\xi}\right| \le C\left|\xi\right|^{\rho+1}\sum_{j=0}^{n-1} e^{(n-j/2-1)\xi} \le C\left|\xi\right|^{\rho+1} n e^{\frac{n}{2}\xi},$$

and therefore, with (52):

$$\left|c(\xi)\left(f(\xi)-1\right)\left(f(\xi)^n-e^{n\xi}\right)\right| \le C\left|\xi\right|^{\rho+2} n e^{\frac{n}{2}\xi}. \tag{60}$$

Equations (59) and (60) yield:

$$\left|c(\xi)f(\xi)^n\left(f(\xi)-1\right)-\xi e^{(n+\frac{1}{2})\xi}\right| \le C\left(\left|\xi\right|^{\rho+1}e^{n\xi}+\left|\xi\right|^{\rho+2} n e^{\frac{n}{2}\xi}\right) = \frac{C}{n^{\rho+1}}\left(\left|n\xi\right|^{\rho+1}e^{n\xi}+\left|n\xi\right|^{\rho+2} e^{\frac{n}{2}\xi}\right),$$

and then, taking into account that the functions $x\mapsto x^{\rho+1}e^x$ and $x\mapsto x^{\rho+2}e^{x/2}$ are bounded on $\mathbb{R}_-$, we get:

$$\left|c(\xi)f(\xi)^n\left(f(\xi)-1\right)-\xi e^{(n+\frac{1}{2})\xi}\right| \le \frac{C}{n^{\rho+1}}. \tag{61}$$

(b) Estimate for $\xi \leq -\xi_0$. In this case, using (54) and the third assumption in (16), we get:

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

But as we assume that $n \geq 2\dfrac{\ln(1+k\lambda_{h,N_h})}{\ln 1/\varepsilon}$, as $-\xi \leq k\lambda_{h,N_h}$, we have that $(1-\xi)\,\varepsilon^{n/2} \leq 1$. Using the boundedness of $\left(n^{\rho+1}\varepsilon^{n/2}\right)$, we get:

$$\left|G_{n+1}(\xi) - G_n(\xi) - \xi e^{(n+\frac{1}{2})\xi}\right| \leq C\varepsilon^{n/2} \leq \frac{C}{n^{\rho+1}}. \tag{62}$$

(c) Conclusion. From (55), (57), (58), (61), (62), and $n = t_n/k$ we conclude that

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

Proof of Proposition 6 The first assertion is a direct consequence of the definition (10) of K_h, the definition (18) of $K_{h,k}$ and the estimate of Lemma 6.
Let us prove the second one. In view of (13) we have for any $s > 0$:

$$0 \leq -K_h'(s) \leq \frac{K_h(0) - K_h(s)}{s} \leq \frac{K_h(0)}{s} \leq \frac{K(0)}{s}. \tag{63}$$

Indeed, the first inequality holds because K_h' is non positive, the second one holds because K_h is convex, the third one holds because K_h is non negative, the last one follows from 14. Then, using the concavity of K_h', and (63) with $s = t/2$ we get:

$$\forall t > 0,\ 0 \leq K_h''(t) \leq \frac{K_h'(t) - K_h'(t/2)}{t/2} \leq \frac{-K_h'(t/2)}{t/2} \leq 4K(0)t^{-2}. \tag{64}$$

Using the first inequality of the proposition with $\rho = 1$ for the first term, the mean value theorem and (64) for the second one, for $t_n \geq 2k\ln(1+k\lambda_{h,N_h})/\ln(1/\varepsilon)$ and $t \in \,]t_n, t_{n+1}[$, we obtain:

$$\begin{aligned} \left|\left(K_{h,k}' - K_h'\right)(t)\right| = \left|K_{h,k}'(t_{n+1/2}) - K_h'(t)\right| &\leq \left|\left(K_{h,k}' - K_h'\right)(t_{n+1/2})\right| + \left|K_h'(t) - K_h'(t_{n+1/2})\right| \\ &\leq Ckt^{-2} + Ckt^{-2}. \end{aligned} \tag{65}$$

But with (13) we see that $\lim_{t\to+\infty} K_h'(t) = 0$. Also, since from (16) $\lim_{n\to+\infty} G_n(\xi) = 0$ for all $\xi < 0$, we have that $\lim_{n\to\infty} K_{h,k}'(t_{n+1/2}) = \dfrac{1}{k}\sum_{j=1}^{N_h} a_{h,j} \lim_{n\to+\infty} (G_{n+1} - G_n)(-k\lambda_{h;j}) = 0$. Hence, by integration of (65) on $[t, +\infty[$ we get the second estimate of the proposition. The third one is obtained by integrating (65) on $[t, T]$.

D Accuracy for the scheme on the graph: Proof of Theorem 6

In this section, we give the proof of Theorem 6 page 19.

Let's first deal with the corrected scheme. We evaluate the contribution to $\theta(k)$ first for $t_n = nk \le \tau$, then for $nk > \tau$, and last for $nk = \tau$. In the first case, using integration by parts with $f = K - K_{h,k,\tau}$:

$$\begin{cases} f_n := \dfrac{1}{k}\displaystyle\int_{t_n}^{t_{n+1}} f(t)\mathrm{d}t = \int_{t_n}^{t_{n+1}} f'(t)\left(1 - \dfrac{t-t_n}{k}\right)\mathrm{d}t + f(t_n), \\ f_{n-1} = -\displaystyle\int_{t_{n-1}}^{t_n} f'(t)\left(1 - \dfrac{t_n - t}{k}\right)\mathrm{d}t + f(t_n), \end{cases} \tag{66}$$

so that

$$\begin{aligned} \sum_{0<nk<\tau} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| &\le \sum_{0<nk<\tau} \int_{t_{n-1}}^{t_{n+1}} \left|K' - K'_{h,k,\tau}\right|(t)\left(1 - \frac{|t-t_n|}{k}\right)\mathrm{d}t \\ &\le \sum_{0<nk<\tau} \int_{t_{n-1}}^{t_{n+1}} \left|K' - K'_{h,k,\tau}\right|(t)\mathrm{d}t \\ &\le 2\int_0^\tau \left|K' - K'_{h,k,\tau}\right|(t)\mathrm{d}t. \end{aligned} \tag{67}$$

Now, let us consider the case where $t_n > \tau$. Then $K_{h,k,\tau} = K_{h,k}$ for all $t \ge \tau$, so that, using (66) with $f = K_{h,k}$ and then the fact that $K'_{h,k}$ is constant on each $]t_n, t_{n+1}[$ we get

$$\begin{aligned} \tilde{K}_n - \tilde{K}_{n-1} &= K'_{h,k}(t_{-1/2})\int_{t_{n-1}}^{t_n}\left(1 - \frac{|t-t_n|}{k}\right)\mathrm{d}t + K'_{h,k}(t_{n+1/2})\int_{t_n}^{t_{n+1}}\left(1 - \frac{|t-t_n|}{k}\right)\mathrm{d}t \\ &= \frac{k}{2}\left(K'_{h,k}(t_{n-1/2}) + K'_{h,k}(t_{n+1/2})\right). \end{aligned}$$

We have

$$|K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| \le \left|\tilde{K}_n - \tilde{K}_{n-1} - kK'(t_n)\right| + |K_n - K_{n-1} - kK'(t_n)|. \tag{68}$$

For the first term on the right hand side, using the above computation, we have:

$$\begin{aligned} \left|\tilde{K}_n - \tilde{K}_{n-1} - kK'(t_n)\right| &= k\left|\frac{1}{2}\left(K'_{h,k}(t_{n-1/2}) + K'_{h,k}(t_{n+1/2})\right) - K'(t_n)\right| \\ &\le \frac{k}{2}\left|K'_{h,k}(t_{n-1/2}) + K'_{h,k}(t_{n+1/2}) - K'(t_{n-1/2}) - K'(t_{n+1/2})\right| \\ &\quad + \frac{k}{2}\left|K'(t_{n-1/2}) + K'(t_{n+1/2}) - 2K'(t_n)\right|. \end{aligned} \tag{69}$$

As,

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

and as from Proposition 10 we have $|K^{(3)}(t)|\leq Ct^{-5/2}$, for the third term in (69), we get:

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

and therefore

$$\left|\tilde{K}_n-\tilde{K}_{n-1}-kK'(t_n)\right|\leq\frac{1}{2}\left|K'_{h,k}(t_{n-1/2})-K'(t_{n-1/2})\right|+\frac{1}{2}\left|K'_{h,k}(t_{n+1/2})-K'(t_{n+1/2})\right|+Ck^3t_n^{-5/2}. \tag{70}$$

Similarly:

$$|K_n-K_{n-1}-kK'(t_n)|\leq Ck^3{t_n}^{-5/2}. \tag{71}$$

With (68), (70), (71), noting that

$$\sum_{\tau<nk<T}k^3{t_n}^{-5/2}\leq k^3\sum_{n=\tau/k}^{+\infty}(nk)^{-5/2}=k^{1/2}\sum_{n=\tau/k}^{+\infty}n^{-5/2}\sim\frac{2}{3}k^{1/2}\left(\frac{k}{\tau}\right)^{3/2}$$

we get.

$$\begin{aligned}\sum\nolimits_{\tau<nk<T}&|K_n-K_{n-1}-\tilde{K}_n+\tilde{K}_{n-1}|\\&\leq\sum\nolimits_{\tau<nk<T}\left|\tilde{K}_n-\tilde{K}_{n-1}-kK'(t_n)\right|+\sum\nolimits_{\tau<nk<T}|K_n-K_{n-1}-kK'(t_n)|\\&\leq\frac{k}{2}\sum\nolimits_{\tau<nk<T}\left(\left|K'_{h,k,\tau}-K'\right|(t_{n-1/2})+\left|K'_{h,k,\tau}-K'\right|(t_{n+1/2})\right)+Ck^2\tau^{-3/2}\end{aligned} \tag{72}$$

Last, let us consider the case $t_n=\tau$. We have:

$$\begin{aligned}\int_\tau^{\tau+k}\left|\left(K'_{h,k,\tau}-K'\right)(t)\right|\mathrm{d}t&=\int_\tau^{\tau+k}\left|K'_{h,k,\tau}(t_{n+1/2})-K'(t)\right|\mathrm{d}t\\&\leq\int_\tau^{\tau+k}\left|\left(K'_{h,k,\tau}-K'\right)(t_{n+1/2})\right|\mathrm{d}t+\int_\tau^{\tau+k}\left|K'(t_{n+1/2})-K'(t)\right|\mathrm{d}t.\end{aligned}$$

Indeed, the first equality holds because $K'_{h,k,\tau}=K'_{h,k}$ is constant on $[t_n,t_{n+1}]$.
But $\left|K'(t_{n+1/2})-K'(t)\right|\leq\left|t-t_{n+1/2}\right|\sup_{[(\tau,\tau+k]}|K^{''}|\leqslant\left|t-t_{n+1/2}\right|Ct_n^{-3/2}$. Hence, we get

$$\int_\tau^{\tau+k}\left|\left(K'_{h,k,\tau}-K'\right)(t)\right|\mathrm{d}t\leq\int_\tau^{\tau+k}\left|\left(K'_{h,k,\tau}-K'\right)(t_{n+1/2})\right|\mathrm{d}t+Ck^2\tau^{-3/2}. \tag{73}$$

Now with (67), (72), (73), we get that

$$\sum_{0<nk<T} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| \le 2\int_0^{\tau+k} |K'_{h,k,\tau} - K'|(t)\mathrm{d}t + 2\sum_{\tau\le nk<T} \left|K'_{h,k,\tau} - K'\right|(t_{n+1/2}) + Ck^2\tau^{-3/2}.$$

With Theorem 3, therefore

$$\sum_{0<nk<T} |K_n - K_{n-1} - \tilde{K}_n + \tilde{K}_{n-1}| \le Ck^{m\mu}.$$

For an uncorrected scheme. We have, in the same way:

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

Now, we need to bound $|K_0 - \tilde{K}_0|$. We have

$$|K_0 - \tilde{K}_0| \le |K_{N_k-1} - \tilde{K}_{N_k-1}| + \sum_{0<nk<T} |K_n - K_{n-1} - \tilde{K}_n - \tilde{K}_{n-1}|, \text{ where } N_k = T/k$$

so that is sufficient to estimate $\left|K_{N_k-1} - \tilde{K}_{N_k-1}\right|$. But from the error estimate of the trapezoid formula error:

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

Hence, (9) and (18) yields:

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

All these terms are bounded by $Ck^{m\mu}$. This completes the proof of the theorem. □

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