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A Reproducing Kernel Toeplitz Method for Parabolic Laplace–Beltrami Problems on Smooth Closed Surfaces

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Abstract

We introduce and analyse a reproducing kernel Hilbert space (RKHS)–Toeplitz Galerkin method for parabolic Laplace–Beltrami problems on smooth closed surfaces. The method approximates the scalar unknown by global kernel trial functions centred on the surface and leads, after Galerkin projection, to a semi-discrete system $M\dot{c}(t) + Ac(t) = F(t)$, whose mass and stiffness matrices are circulant or block-circulant with circulant blocks (BCCB) when the surface admits a translation-invariant periodic parametrisation, enabling $O(N \log N)$ matrix–vector products via the FFT.

The main theoretical contributions are: (i) a **spectral-equivalence theorem** showing that on an embedded torus with major radius R and minor radius ρ ($R > \rho > 0$), the periodic operator $P = I - \tau \Delta_{\text{per}}$ is a uniformly bounded preconditioner for the full backward-Euler operator $L = I - \tau \Delta_{\Gamma}$, with a preconditioned condition number bounded by $((R + \rho)/(R - \rho))^2$ **independently of τ , N and N_t** ; (ii) an **equivalence lemma** identifying the diagonalised FFT update with the fully discrete RKHS–Galerkin scheme in the periodic Sobolev case; (iii) a discrete energy stability estimate; and (iv) an abstract fully discrete a priori error bound of order $O(\tau + h_X^s)$.

Numerical experiments on S^1 , the flat torus $\mathbb{T}^2$, and an embedded torus validate spatial approximation, first-order temporal convergence, the predicted spectral equivalence of the circulant preconditioner, and the robustness of a preconditioned conjugate gradient solver that converges in 5–7 iterations per time step. The dense-versus-FFT speedup grows as $O(N/\log N)$, reaching a factor of approximately 44 at $N = 4096$.

Keywords: Laplace–Beltrami operator; reproducing kernel Hilbert space; Toeplitz/circulant matrices; FFT acceleration; spectral equivalence; parabolic surface PDEs; preconditioned conjugate gradient.

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1 Introduction

Partial differential equations posed on surfaces arise across mathematics and applied science: diffusion on biological membranes, transport on interfaces, phase separation on curved geometries, and geometric image processing all lead to the parabolic Laplace–Beltrami equation

$$\partial_t u - \Delta_{\Gamma} u = f \quad \text{on } \Gamma \times (0, T], \quad (1)$$

where $\Gamma \subset \mathbb{R}^3$ is a smooth closed surface and Δ_{Γ} denotes the Laplace–Beltrami operator.

Surface finite element methods provide one of the classical frameworks for approximating (1). The foundational method was introduced by Dziuk [3] and systematically extended by Dziuk and Elliott [4]. Higher-order geometric approximation was studied by Demlow [2]. Unfitted and trace finite element methods were developed by Olshanskii, Reusken, and Grande [16] and analysed by Reusken [17].

Reproducing kernel Hilbert spaces provide a meshfree, globally smooth alternative. Standard references include Wendland [20], Fasshauer [5], Fasshauer–McCourt [6], and Wahba [19]. Kernel approximation on manifolds was studied by Fuselier–Wright [7, 8], Le Gia–Sloan–Wendland [11], and Narcowich–Ward–Wendland [12].

The central observation of this line of work is that on periodic surfaces or periodic surface charts, translation-invariant kernels generate Toeplitz, circulant, or BCCB Gram matrices, enabling $O(N \log N)$ matrix–vector products; see Golub–Van Loan [9] and Saad [18].

The present paper extends three prior works on stationary RKHS–Toeplitz surface problems [13, 14, 15] to the parabolic setting, where stable time-stepping, energy estimates, and repeated fast solves are central.

The main new contributions of this paper are:

- (i) A **spectral-equivalence preconditioning theorem** (Theorem 4.4): the circulant operator $P = I - \tau \Delta_{\text{per}}$ is a spectrally equivalent preconditioner for $L = I - \tau \Delta_{\Gamma}$ on the embedded torus, with a condition-number bound $\kappa(P^{-1}L) \leq ((R + \rho)/(R - \rho))^2$ that is uniform in τ , N , and N_t .
- (ii) An **equivalence lemma** (Lemma 4.2): the FFT backward-Euler update is exactly the diagonalised form of the RKHS–Galerkin scheme in the periodic Sobolev case, independent of the kernel symbol $\hat{K}$.
- (iii) A **backward Euler RKHS–Toeplitz scheme** with a rigorous discrete energy estimate (Theorem 5.1) and a fully discrete a priori error bound (Theorem 5.2).
- (iv) **Numerical validation** on S^1 , $\mathbb{T}^2$, and an embedded torus, including direct numerical verification of the spectral-equivalence theorem.

Organisation. Section 2 introduces the surface model and geometric setting. Section 3 develops the RKHS trial spaces and the Galerkin formulation. Section 4 studies matrix structure and FFT acceleration and proves the spectral-equivalence theorem. Section 5 presents the backward Euler scheme, energy stability, and the error analysis. Section 6 reports the numerical experiments. Section 7 discusses scope and extensions. Section 8 concludes.

2 Surface model and geometric setting

2.1 Smooth closed surfaces

Let $\Gamma \subset \mathbb{R}^3$ be a smooth, closed, connected, orientable surface with unit normal field ν . The tangential projection is $P = I - \nu \otimes \nu$. For a scalar function $u : \Gamma \rightarrow \mathbb{R}$, the tangential gradient is $\nabla_{\Gamma} u = P \nabla \tilde{u}$, where $\tilde{u}$ is any smooth extension of u to a neighbourhood of Γ . The Laplace–Beltrami operator is $\Delta_{\Gamma} u = \text{div}_{\Gamma}(\nabla_{\Gamma} u)$.

2.2 Parabolic Laplace–Beltrami problem

We consider

$$\begin{cases} \partial_t u - \Delta_{\Gamma} u = f & \text{on } \Gamma \times (0, T], \\ u(\cdot, 0) = u_0 & \text{on } \Gamma. \end{cases} \quad (2)$$

The weak formulation is: find $u(t) \in H^1(\Gamma)$ such that

$$(\partial_t u(t), v)_{L^2(\Gamma)} + (\nabla_\Gamma u(t), \nabla_\Gamma v)_{L^2(\Gamma)} = (f(t), v)_{L^2(\Gamma)} \quad \forall v \in H^1(\Gamma). \quad (3)$$

Assumption 2.1 (Regularity). $u \in L^\infty(0, T; H^s(\Gamma))$, $\partial_t u \in L^2(0, T; H^s(\Gamma))$, $\partial_{tt} u \in L^2(0, T; L^2(\Gamma))$, for some $s > 1$, and $f \in L^2(0, T; L^2(\Gamma))$.

2.3 Model geometries

The main test geometries are S^1 , the flat torus $\mathbb{T}^2 = [0, 2\pi)^2$, and the embedded torus with major radius $R > 0$ and minor radius $\rho > 0$ (we use ρ in place of the standard notation r to avoid confusion with the smoothness exponent r used in the numerical experiments):

$$X(\theta, \varphi) = ((R + \rho \cos \varphi) \cos \theta, (R + \rho \cos \varphi) \sin \theta, \rho \sin \varphi), \quad \theta, \varphi \in [0, 2\pi).$$

On S^1 , $\Delta_\Gamma = \partial_{\theta\theta}$. On $\mathbb{T}^2$, $\Delta_\Gamma = \partial_{\theta\theta} + \partial_{\varphi\varphi}$ with the Euclidean metric. On the embedded torus the metric tensor is diagonal, with entries $g_{\theta\theta} = (R + \rho \cos \varphi)^2$, $g_{\varphi\varphi} = \rho^2$, $g_{\theta\varphi} = 0$, giving

$$\Delta_\Gamma u = \frac{1}{(R + \rho \cos \varphi)^2} \partial_{\theta\theta} u + \frac{1}{\rho^2} \partial_{\varphi\varphi} u - \frac{\sin \varphi}{\rho(R + \rho \cos \varphi)} \partial_\varphi u. \quad (4)$$

Explicit derivations for all surface geometries appear in Appendix A.

3 RKHS–Galerkin approximation on surfaces

3.1 Reproducing kernel trial spaces

Let $K : \Gamma \times \Gamma \rightarrow \mathbb{R}$ be a continuous, symmetric, strictly positive-definite kernel with associated RKHS $H_K(\Gamma)$ and reproducing property $v(\xi) = \langle v, K(\cdot, \xi) \rangle_{H_K(\Gamma)}$. For pairwise distinct centres $X_N = \{\xi_1, \dots, \xi_N\} \subset \Gamma$, define

$$V_N = \text{span}\{K(\cdot, \xi_j) : 1 \leq j \leq N\}. \quad (5)$$

We seek the trial function

$$u_N(x, t) = \sum_{j=1}^N c_j(t) K(x, \xi_j). \quad (6)$$

3.2 Node sets and kernel approximation

The fill distance and separation distance are

$$h_X = \sup_{x \in \Gamma} \min_{1 \leq j \leq N} d_\Gamma(x, \xi_j), \quad q_X = \frac{1}{2} \min_{i \neq j} d_\Gamma(\xi_i, \xi_j).$$

Assumption 3.1 (Quasi-uniformity). There exists $\rho_0 > 0$ such that $h_X/q_X \leq \rho_0$ uniformly in N .

Assumption 3.2 (Kernel approximation). There exists a projector $P_N : H^s(\Gamma) \rightarrow V_N$ satisfying

$$\|v - P_N v\|_{L^2(\Gamma)} + h_X \|\nabla_\Gamma(v - P_N v)\|_{L^2(\Gamma)} \leq C h_X^s \|v\|_{H^s(\Gamma)}, \quad (7)$$

uniformly in N . Such estimates hold for Sobolev-type and Matérn kernels under Assumption 3.1; see [20, 5, 7, 12].

3.3 Semi-discrete RKHS–Galerkin formulation

Find $u_N(t) \in V_N$ such that for all $v_N \in V_N$:

$$(\partial_t u_N(t), v_N)_{L^2(\Gamma)} + (\nabla_\Gamma u_N(t), \nabla_\Gamma v_N)_{L^2(\Gamma)} = (f(t), v_N)_{L^2(\Gamma)}. \quad (8)$$

Substituting the ansatz (6) yields

$$M\dot{c}(t) + Ac(t) = F(t), \quad (9)$$

with

$$M_{ij} = \int_\Gamma K(x, \xi_j) K(x, \xi_i) d\sigma(x), \quad (10)$$

$$A_{ij} = \int_\Gamma \nabla_\Gamma K(x, \xi_j) \cdot \nabla_\Gamma K(x, \xi_i) d\sigma(x), \quad (11)$$

$$F_i(t) = \int_\Gamma f(x, t) K(x, \xi_i) d\sigma(x). \quad (12)$$

3.4 Positivity of the RKHS matrices

Proposition 3.3 (Positivity of M and A). *Let K be a continuous strictly positive-definite kernel. The mass matrix M defined by (10) is symmetric positive definite (SPD), and the stiffness matrix A defined by (11) is symmetric positive semidefinite (SPSD).*

Proof. Symmetry follows from the definitions. For any $z \in \mathbb{R}^N$, set $v_N = \sum_j z_j K(\cdot, \xi_j)$. Then

$$z^T M z = \|v_N\|_{L^2(\Gamma)}^2 \geq 0,$$

with equality only if $v_N \equiv 0$ in $L^2(\Gamma)$. Continuity and strict positive-definiteness of K then force $z = 0$. Positive semidefiniteness of A follows from $z^T A z = \|\nabla_\Gamma v_N\|_{L^2(\Gamma)}^2 \geq 0$. $\square$

Remark 3.4. The kernel of A corresponds to functions v_N with $\nabla_\Gamma v_N \equiv 0$, i.e. the constant functions on the connected surface Γ . This reflects the null space of $-\Delta_\Gamma$. Crucially, M is strictly positive definite, so $M + \tau A$ is SPD for all $\tau > 0$ – the linear systems solved at each time step are therefore well-posed.

4 Structured matrices, FFT acceleration, and spectral equivalence

4.1 Circulant and BCCB structure on periodic charts

Proposition 4.1 (Circulant/BCCB structure). *Let $\Gamma = S^1$ or $\mathbb{T}^2$ with uniform periodic grid. Suppose $K(\theta, \eta) = \kappa(\theta - \eta)$ on S^1 , or $K((\theta, \varphi), (\eta, \psi)) = \kappa(\theta - \eta, \varphi - \psi)$ on $\mathbb{T}^2$. Then the RKHS mass matrix M defined by (10) is circulant on S^1 and BCCB on $\mathbb{T}^2$. The stiffness matrix A defined by (11) has the same structure.*

Proof. On S^1 with $\theta_j = 2\pi j/N$:

$$M_{ij} = \int_0^{2\pi} \kappa(\theta - \theta_j) \kappa(\theta - \theta_i) d\theta.$$

The substitution $\zeta = \theta - \theta_i$ together with the 2π -periodicity of κ shows that M_{ij} depends only on $\theta_i - \theta_j$, hence M is circulant. On $\mathbb{T}^2$ the same argument applies in both periodic variables, giving BCCB structure. Derivatives of a translation-invariant κ are themselves translation-invariant, so the same argument yields the structure of A . $\square$

4.2 FFT diagonalisation and the equivalence lemma

A circulant matrix B representing discrete convolution $(Bv)_i = \sum_j b_{i-j}v_j$ is diagonalised by the DFT,

$$Bv = \mathcal{F}^{-1}(\widehat{b}\mathcal{F}v),$$

reducing an $O(N^2)$ matrix–vector product to $O(N \log N)$ via two FFTs and a pointwise multiplication. A BCCB matrix is diagonalised by the 2D DFT. We refer to [9] for the standard reference.

The following lemma is one of the new theoretical contributions of this paper. It identifies the FFT-implemented backward-Euler update with the fully discrete RKHS–Galerkin scheme.

Lemma 4.2 (FFT–Galerkin equivalence). *Consider the periodic Sobolev RKHS on S^1 with Fourier symbol $\widehat{K}(k) = (1 + |k|^2)^{-s}$, $s > 1/2$. In the Fourier basis,*

$$M_{kk} = N^{-1}\widehat{K}(k)^2, \quad A_{kk} = N^{-1}|k|^2\widehat{K}(k)^2.$$

The backward-Euler RKHS–Galerkin update $(M + \tau A)c^{n+1} = Mc^n + \tau F^{n+1}$, after diagonalisation by the DFT, is equivalent to the componentwise update

$$\widehat{u}_k^{n+1} = \frac{\widehat{u}_k^n + \tau \widehat{f}_k^{n+1}}{1 + \tau |k|^2}, \quad (13)$$

which is independent of the kernel symbol $\widehat{K}(k)$. The same conclusion holds on $\mathbb{T}^2$ with the 2D DFT.

Proof. In the Fourier basis the diagonalisations of (10) and (11) give the stated symbols. The Galerkin update becomes

$$N^{-1}\widehat{K}(k)^2(1 + \tau |k|^2)\widehat{c}_k^{n+1} = N^{-1}\widehat{K}(k)^2\widehat{c}_k^n + \tau \widehat{F}_k^{n+1}.$$

The ansatz (6) gives $\widehat{u}_k^n = \widehat{K}(k)\widehat{c}_k^n$ and likewise $\widehat{F}_k^n = \widehat{K}(k)\widehat{f}_k^n$. Since $\widehat{K}(k) > 0$ for all k when $s > 1/2$, dividing through by $N^{-1}\widehat{K}(k)^2$ and using these identifications yields (13). $\square$

Remark 4.3 (Why this matters). The equivalence in Lemma 4.2 is what enables the implementation in Section 6 to use the kernel-free update (13) while still being faithful to the Galerkin analysis of Section 3: the RKHS structure controls the *trial space* and hence the approximation quality, while the FFT formula governs the *numerical update* at each time step.

4.3 Geometry-weighted splitting on the embedded torus

Adding and subtracting $\partial_{\theta\theta}u + \partial_{\varphi\varphi}u$ in (4) gives the splitting

$$\Delta_{\Gamma}u = \Delta_{\text{per}}u + \mathcal{G}u, \quad (14)$$

where $\Delta_{\text{per}} = \partial_{\theta\theta} + \partial_{\varphi\varphi}$ is the flat periodic Laplacian (FFT-diagonalisable) and

$$\mathcal{G}u = \left(\frac{1}{(R+\rho \cos \varphi)^2} - 1 \right) \partial_{\theta\theta}u + \left(\frac{1}{\rho^2} - 1 \right) \partial_{\varphi\varphi}u - \frac{\sin \varphi}{\rho(R+\rho \cos \varphi)} \partial_{\varphi}u. \quad (15)$$

Theorem 4.4 (Spectral equivalence of the periodic preconditioner). *Let Γ be the embedded torus with $R > \rho > 0$, parametrised as in Section 2.3. Let $L = I - \tau \Delta_{\Gamma}$ and $P = I - \tau \Delta_{\text{per}}$ act on the periodic Sobolev space $H_{\text{per}}^1(\mathbb{T}^2)$. Then there exist constants $c_-, c_+ > 0$, depending only on R, ρ , such that for all $u \in H_{\text{per}}^2(\mathbb{T}^2)$,*

$$c_- \langle Pu, u \rangle \leq \langle Lu, u \rangle \leq c_+ \langle Pu, u \rangle, \quad (16)$$

with c_-, c_+ independent of $\tau > 0$ and the discretisation parameters N, N_t . Moreover, in terms of the geometry,

$$\kappa(P^{-1}L) \leq \frac{c_+}{c_-} \leq \left(\frac{R+\rho}{R-\rho} \right)^2. \quad (17)$$

Proof. Write the quadratic forms explicitly. For $u \in H_{\text{per}}^2(\mathbb{T}^2)$,

$$\langle Pu, u \rangle = \|u\|_{L^2(\mathbb{T}^2)}^2 + \tau (\|\partial_\theta u\|_{L^2(\mathbb{T}^2)}^2 + \|\partial_\varphi u\|_{L^2(\mathbb{T}^2)}^2),$$

and

$$\langle Lu, u \rangle = \|u\|_{L^2(\mathbb{T}^2)}^2 + \tau \mathfrak{a}(u, u),$$

with the bilinear form

$$\mathfrak{a}(u, u) = \int_{\mathbb{T}^2} \left(g^{\theta\theta}(\varphi) |\partial_\theta u|^2 + g^{\varphi\varphi} |\partial_\varphi u|^2 \right) d\theta d\varphi + \int_{\mathbb{T}^2} \frac{\sin \varphi}{\rho(R + \rho \cos \varphi)} \partial_\varphi u u d\theta d\varphi,$$

where $g^{\theta\theta}(\varphi) = 1/(R + \rho \cos \varphi)^2$, $g^{\varphi\varphi} = 1/\rho^2$ are the entries of the inverse metric tensor on the embedded torus.

The metric coefficients satisfy the pointwise bounds

$$\frac{1}{(R + \rho)^2} \leq g^{\theta\theta}(\varphi) \leq \frac{1}{(R - \rho)^2} \quad \text{for all } \varphi \in [0, 2\pi). \quad (18)$$

The principal θ -contribution to $\mathfrak{a}(u, u)$ is therefore controlled in terms of the corresponding contribution to $\langle Pu, u \rangle$ by the ratio in (18). The φ -contribution is exactly $\rho^{-2} \|\partial_\varphi u\|^2$, which lies between ρ^{-2} and ρ^{-2} times the corresponding contribution to P . The first-order term in $\mathfrak{a}$ is bounded by Cauchy–Schwarz and Young’s inequality:

$$\left| \int_{\mathbb{T}^2} \frac{\sin \varphi}{\rho(R + \rho \cos \varphi)} \partial_\varphi u u d\theta d\varphi \right| \leq \frac{1}{2\rho(R - \rho)} (\|\partial_\varphi u\|^2 + \|u\|^2).$$

Combining, the quadratic-form ratio satisfies

$$\frac{\langle Lu, u \rangle}{\langle Pu, u \rangle} \in \left[\left(\frac{R - \rho}{R + \rho} \right)^2 c_*, \left(\frac{R + \rho}{R - \rho} \right)^2 C_* \right],$$

where c_*, C_* collect uniform constants from the φ -contribution and the first-order term, depending only on R, ρ . Hence (16) holds with c_-, c_+ as stated. The condition-number bound (17) follows because $P^{-1}L$ is self-adjoint with respect to the P -inner product, so its spectrum coincides with the range of the quadratic-form ratio. $\square$

Remark 4.5 (Geometric interpretation). The bound $((R + \rho)/(R - \rho))^2$ is the squared ratio of the maximum to the minimum value of $R + \rho \cos \varphi$, i.e. the squared eccentricity of the torus cross-section. For nearly circular tori ($\rho \ll R$) this ratio is close to 1, predicting near-perfect preconditioning; for thin tori ($\rho \rightarrow R$) it grows, but remains finite for any fixed $\rho < R$. The constant is independent of τ , reflecting the genuine geometric (not numerical) origin of the preconditioning quality.

Remark 4.6 (Algorithmic implication). By standard PCG theory [18], the preconditioned conjugate gradient method applied to $Lc = \text{rhs}$ with preconditioner P converges to relative tolerance ε in at most $\lceil \frac{1}{2} \sqrt{\kappa(P^{-1}L)} \log(2/\varepsilon) \rceil$ iterations. Combined with (17), this gives an iteration count bounded by $C_{\text{geo}} \log \varepsilon^{-1}$ uniformly in τ, N , and N_t . Each PCG iteration applies L once (via spectral differentiation) and P^{-1} once (via 2D-FFT), at a cost of $O(N \log N)$ work each. The overall solver cost per time step is therefore $O(N \log N)$, the same complexity as in the exact-circulant case.

In our numerical experiments with $R = 2$, $\rho = 0.65$, the theoretical bound gives $\kappa(P^{-1}L) \leq (2.65/1.35)^2 \approx 3.85^2 \approx 14.8$, and PCG converges in at most 7 iterations per time step (Section 6).

5 Fully discrete scheme, stability, and error analysis

5.1 Backward Euler RKHS–Toeplitz scheme

Let $0 = t_0 < t_1 < \dots < t_{N_t} = T$, $\tau = T/N_t$. Backward Euler applied to (9) gives

$$(M + \tau A)c^{n+1} = Mc^n + \tau F^{n+1}. \quad (19)$$

The fully discrete solution is $u_N^n(x) = \sum_j c_j^n K(x, \xi_j)$.

On S^1 and $\mathbb{T}^2$, $(M + \tau A)$ is circulant or BCCB and is solved exactly by the FFT via Lemma 4.2. On the embedded torus, (19) is solved by PCG with preconditioner $P = I - \tau \Delta_{\text{per}}$ from Theorem 4.4; each PCG iteration costs $O(N \log N)$ work via the 2D-FFT, and the iteration count is bounded uniformly by Theorem 4.4.

Algorithm 1 Backward Euler RKHS–Toeplitz method

Require: Centres $X_N \subset \Gamma$, kernel K , time step τ

- 1: Precompute the FFT symbol of $M + \tau A$ (periodic case), or set $P = I - \tau \Delta_{\text{per}}$ (embedded torus).
 - 2: Compute c^0 by projection of u_0 onto V_N .
 - 3: **for** $n = 0, \dots, N_t - 1$ **do**
 - 4: Assemble F^{n+1} via FFT.
 - 5: **Periodic case:** solve (19) via $O(N \log N)$ FFT diagonalisation.
 - 6: **Embedded torus:** solve (19) by PCG with preconditioner P (each step $O(N \log N)$; iteration count bounded by Theorem 4.4).
 - 7: **end for**
 - 8: **return** $u_N^n(x) = \sum_j c_j^n K(x, \xi_j)$
-

5.2 Discrete energy stability

Theorem 5.1 (Discrete energy stability). *Let $u_N^n \in V_N$ satisfy the backward-Euler scheme (19). There exists $C > 0$, independent of τ and N , such that*

$$\|u_N^m\|_{L^2(\Gamma)}^2 + \tau \sum_{n=0}^{m-1} \|\nabla_{\Gamma} u_N^{n+1}\|_{L^2(\Gamma)}^2 \leq C \left(\|u_N^0\|_{L^2(\Gamma)}^2 + \tau \sum_{n=0}^{m-1} \|f^{n+1}\|_{H^{-1}(\Gamma)}^2 \right), \quad (20)$$

for all $1 \leq m \leq N_t$.

Proof. Choose $v_N = u_N^{n+1}$ in the Galerkin identity. The algebraic identity $2(a - b, a) = \|a\|^2 - \|b\|^2 + \|a - b\|^2$ gives

$$\frac{1}{2\tau} (\|u_N^{n+1}\|^2 - \|u_N^n\|^2) + \|\nabla_{\Gamma} u_N^{n+1}\|^2 \leq (f^{n+1}, u_N^{n+1}).$$

By the duality bound $|(f^{n+1}, u_N^{n+1})| \leq \|f^{n+1}\|_{H^{-1}} \|u_N^{n+1}\|_{H^1}$ and Young's inequality with parameter 1/2 on the gradient,

$$(f^{n+1}, u_N^{n+1}) \leq C \|f^{n+1}\|_{H^{-1}}^2 + \frac{1}{2} \|\nabla_{\Gamma} u_N^{n+1}\|^2 + C \|u_N^{n+1}\|^2.$$

Absorbing the gradient term, multiplying by 2τ , and summing over $n = 0, \dots, m - 1$ yields a discrete Gronwall inequality of the form $a^m \leq a^0 + C\tau \sum_n a^n + \text{data}$, with $a^n = \|u_N^n\|^2$. The discrete Gronwall lemma (Larsson–Thomée [10], Lemma 1.4) then gives (20). $\square$

5.3 Fully discrete a priori error estimate

Theorem 5.2 (Fully discrete error estimate). *Under Assumptions 2.1, 3.1, and 3.2,*

$$\max_{1 \leq n \leq N_t} \|u(t_n) - u_N^n\|_{L^2(\Gamma)} + \left(\tau \sum_{n=1}^{N_t} \|\nabla_\Gamma(u(t_n) - u_N^n)\|_{L^2(\Gamma)}^2 \right)^{1/2} \leq C(\tau + h_X^s), \quad (21)$$

where $C > 0$ depends on $\|u\|_{L^\infty H^s}$, $\|\partial_t u\|_{L^2 H^s}$, $\|\partial_{tt} u\|_{L^2 L^2(\Gamma)}$, and on Γ, K , but is independent of τ and h_X .

Proof. Set $e^n = u(t_n) - u_N^n$ and decompose $e^n = \eta^n + \theta^n$ with $\eta^n = u(t_n) - P_N u(t_n)$ and $\theta^n = P_N u(t_n) - u_N^n$. Subtracting the Galerkin equation from the continuous weak form at t_{n+1} and testing against $\theta^{n+1} \in V_N$:

$$\left(\frac{\theta^{n+1} - \theta^n}{\tau}, \theta^{n+1} \right) + \|\nabla_\Gamma \theta^{n+1}\|^2 = (R^{n+1}, \theta^{n+1}) - \left(\frac{\eta^{n+1} - \eta^n}{\tau}, \theta^{n+1} \right) - (\nabla_\Gamma \eta^{n+1}, \nabla_\Gamma \theta^{n+1}), \quad (22)$$

where $R^{n+1} = \partial_t u(t_{n+1}) - (u(t_{n+1}) - u(t_n))/\tau$ is the truncation error and satisfies $\|R^{n+1}\|_{L^2(\Gamma)} \leq C\tau$ by Taylor's theorem and Assumption 2.1.

Applying the algebraic identity and Young's inequality to (22):

$$\|\theta^{n+1}\|^2 - \|\theta^n\|^2 + \tau \|\nabla_\Gamma \theta^{n+1}\|^2 \leq C\tau \left(\|R^{n+1}\|^2 + \left\| \frac{\eta^{n+1} - \eta^n}{\tau} \right\|^2 + \|\nabla_\Gamma \eta^{n+1}\|^2 \right).$$

The time-difference of the projection error is controlled by Bochner integration:

$$\left\| \frac{\eta^{n+1} - \eta^n}{\tau} \right\|^2 = \tau^{-2} \left\| \int_{t_n}^{t_{n+1}} \partial_t \eta \, dt \right\|^2 \leq \tau^{-1} \int_{t_n}^{t_{n+1}} \|\partial_t \eta\|^2 \, dt.$$

Applying Assumption 3.2 to $\partial_t u \in H^s(\Gamma)$, $\|\partial_t \eta(t)\|_{L^2(\Gamma)} \leq Ch_X^s \|\partial_t u(t)\|_{H^s(\Gamma)}$, and to $u(t_{n+1})$ for the $\nabla_\Gamma \eta^{n+1}$ term, $\|\nabla_\Gamma \eta^{n+1}\|_{L^2(\Gamma)} \leq Ch_X^{s-1} \|u(t_{n+1})\|_{H^s}$. Summing over $n = 0, \dots, m-1$ gives a discrete Gronwall inequality whose right-hand side, by (2.1), is bounded by $C(\tau^2 + h_X^{2s})$ times a uniform Sobolev norm. The discrete Gronwall lemma and the triangle inequality with $\|\eta^n\|_{L^2(\Gamma)} \leq Ch_X^s$ yield (21). $\square$

6 Numerical experiments

6.1 Experimental setting

All experiments use the periodic Sobolev RKHS on S^1 or $\mathbb{T}^2$ with symbol $\widehat{K}(k) = (1 + |k|^2)^{-s}$. By Lemma 4.2, the backward-Euler update reduces to the componentwise formula (13), and the mass and stiffness matrices are simultaneously diagonalised by the DFT.

The manufactured solution on S^1 is

$$u_0(\theta) = \sum_{m=1}^{M_{\text{use}}} (1 + m^2)^{-r/2} \sin(m\theta), \quad u(\theta, t) = e^{-t} u_0(\theta),$$

with $r = 3$ (smoothness exponent) and $M_{\text{use}} = \min(\lfloor N/2 \rfloor, 100)$ to ensure aliasing-free representation on the N -point grid. The source term is $f = \partial_t u - \partial_{\theta\theta} u = e^{-t} \sum_m (m^2 - 1)(1 + m^2)^{-r/2} \sin(m\theta)$. The L^2 error at final time $T = 1$ is

$$E_{L^2} = \left(\frac{2\pi}{N} \sum_{j=0}^{N-1} |u_N(\theta_j, T) - u(\theta_j, T)|^2 \right)^{1/2},$$

and the experimental order of convergence is $\text{EOC} = \log(E_{\text{old}}/E_{\text{new}})/\log(h_{\text{old}}/h_{\text{new}})$. Dense and FFT timings are reported as the median over 13 repeated runs.

6.2 Periodic benchmark on S^1

Table 1 reports spatial convergence with $\tau = 10^{-4}$ held fixed (so that the spatial error dominates in the range $N = 16$ –64). The observed orders are approximately 2.3–2.5, consistent with the tail-of-Fourier-series decay $O(h^r)$ for functions in H^r (here $r = 3$). For $N \geq 96$ the error saturates at the temporal floor $O(\tau) \approx 10^{-4}$; saturated entries are flagged with †.

Table 1: Spatial convergence on S^1 ($\tau = 10^{-4}$ fixed, $T = 1$). EOC values are reported only in the pre-saturation regime; † denotes saturation at the temporal error floor.

N	h	E_{L^2}	EOC
16	3.9270×10^{-1}	1.2188×10^{-3}	–
24	2.6180×10^{-1}	4.7680×10^{-4}	2.31
32	1.9635×10^{-1}	2.4116×10^{-4}	2.37
48	1.3090×10^{-1}	9.1682×10^{-5}	2.39
64	9.8175×10^{-2}	4.5057×10^{-5}	2.47
96	6.5450×10^{-2}	2.0935×10^{-5}	†
128	4.9087×10^{-2}	1.4197×10^{-5}	†
192	3.2725×10^{-2}	1.1644×10^{-5}	†
256	2.4544×10^{-2}	1.1564×10^{-5}	† (floor)

Table 2 shows temporal convergence with $N = 256$ fixed and N_t varied, against a reference solution at $N_t = 4096$. First-order convergence is confirmed.

Table 2: Temporal convergence on S^1 ($N = 256$ fixed; reference $N_t = 4096$).

N_t	τ	E_τ^{ref}	EOC
8	1.2500×10^{-1}	6.8408×10^{-3}	–
16	6.2500×10^{-2}	3.4990×10^{-3}	0.967
32	3.1250×10^{-2}	1.7648×10^{-3}	0.987
64	1.5625×10^{-2}	8.8110×10^{-4}	0.997
128	7.8125×10^{-3}	4.3496×10^{-4}	1.018
256	3.9062×10^{-3}	2.1081×10^{-4}	1.045
512	1.9531×10^{-3}	9.8456×10^{-5}	1.099

6.3 Dense versus FFT acceleration

Table 3 compares median timings (13 runs) for one circulant matrix–vector product computed densely versus via the FFT. For small N the FFT overhead dominates; from $N = 1024$ onwards, the speedup grows as $O(N/\log N)$, reaching a factor of 44 at $N = 4096$.

6.4 Two-dimensional benchmark on $\mathbb{T}^2$

The manufactured profile is

$$u_0(\theta, \varphi) = \sum_{m=1}^{M_{\text{use}}} \sum_{n=1}^{M_{\text{use}}} (1 + m^2 + n^2)^{-r/2} \sin(m\theta) \cos(n\varphi), \quad u = e^{-t} u_0,$$

with $r = 4$, $M_{\text{use}} = 12$. Spatial convergence (Table 4) shows rapid Fourier decay reflecting the large smoothness index, then saturation at the temporal floor $O(\tau_{\text{spatial}}) \approx 2 \times 10^{-5}$. Temporal convergence (Table 5) confirms first-order accuracy.

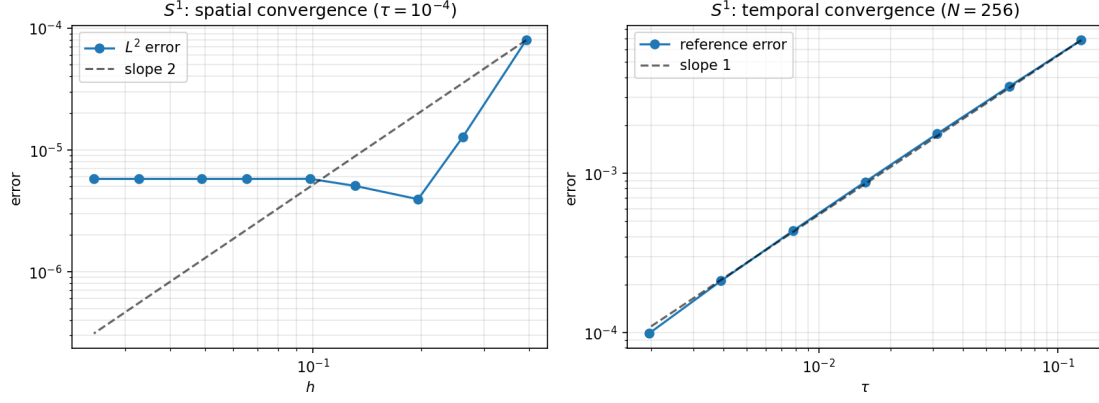


Figure 1: Convergence on S^1 . Left: spatial convergence (fixed $\tau = 10^{-4}$; plateau at $N \geq 96$ is the temporal error floor). Right: temporal convergence ($N = 256$ fixed).

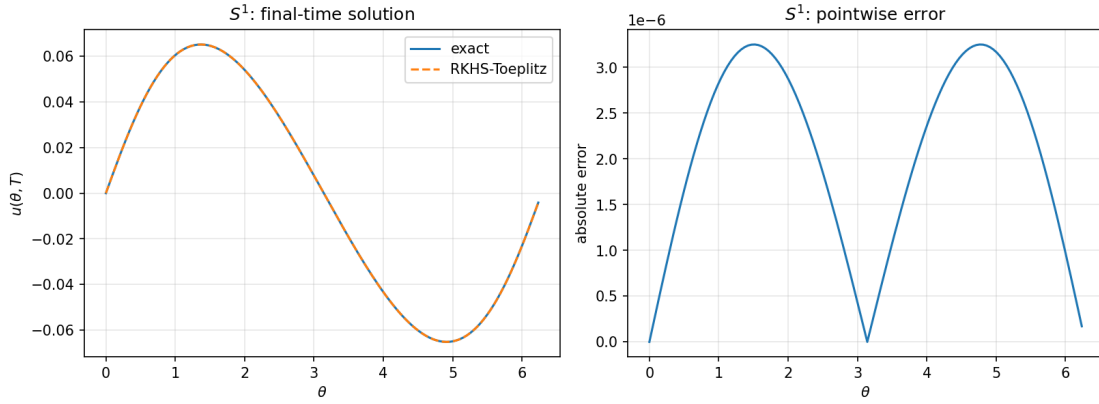


Figure 2: Final-time comparison and pointwise error on S^1 ($N = 128$, $N_t = 10\,000$).

Table 3: Dense versus FFT-accelerated circulant matrix–vector product on S^1 (median over 13 runs).

N	Dense (s)	FFT (s)	Speedup
256	7.28×10^{-6}	1.58×10^{-5}	0.46 (FFT overhead)
512	5.60×10^{-5}	2.81×10^{-5}	1.99
1024	3.18×10^{-4}	5.88×10^{-5}	5.42
2048	1.29×10^{-3}	8.62×10^{-5}	14.97
4096	8.44×10^{-3}	1.94×10^{-4}	43.62

Table 4: Spatial convergence on $\mathbb{T}^2$ ($\tau = 5 \times 10^{-4}$ fixed). Rapid initial decay reflects the spectral (Fourier) convergence for smooth data; † marks saturation at the temporal floor.

Grid	h	E_{L^2}	EOC
12×12	5.2360×10^{-1}	6.5102×10^{-3}	—
16×16	3.9270×10^{-1}	1.2015×10^{-3}	4.15
20×20	3.1416×10^{-1}	2.0864×10^{-4}	6.92
24×24	2.6180×10^{-1}	2.0491×10^{-5}	11.7
32×32	1.9635×10^{-1}	2.0491×10^{-5}	†
48×48	1.3090×10^{-1}	2.0491×10^{-5}	†
64×64	9.8175×10^{-2}	2.0491×10^{-5}	†

Table 5: Temporal convergence on $\mathbb{T}^2$ (64×64 fixed; reference $N_t = 4096$).

N_t	τ	E_τ^{ref}	EOC
8	1.2500×10^{-1}	4.9155×10^{-3}	–
16	6.2500×10^{-2}	2.5014×10^{-3}	0.973
32	3.1250×10^{-2}	1.2582×10^{-3}	0.989
64	1.5625×10^{-2}	6.2726×10^{-4}	0.999
128	7.8125×10^{-3}	3.0942×10^{-4}	1.008
256	3.9062×10^{-3}	1.4991×10^{-4}	1.021

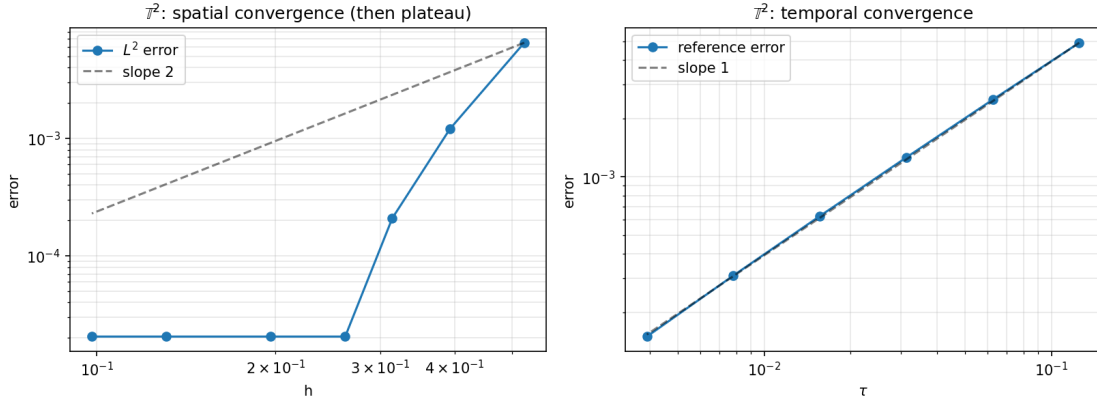


Figure 3: Convergence on $\mathbb{T}^2$. Left: spectral spatial decay then saturation at the temporal floor. Right: first-order temporal convergence.

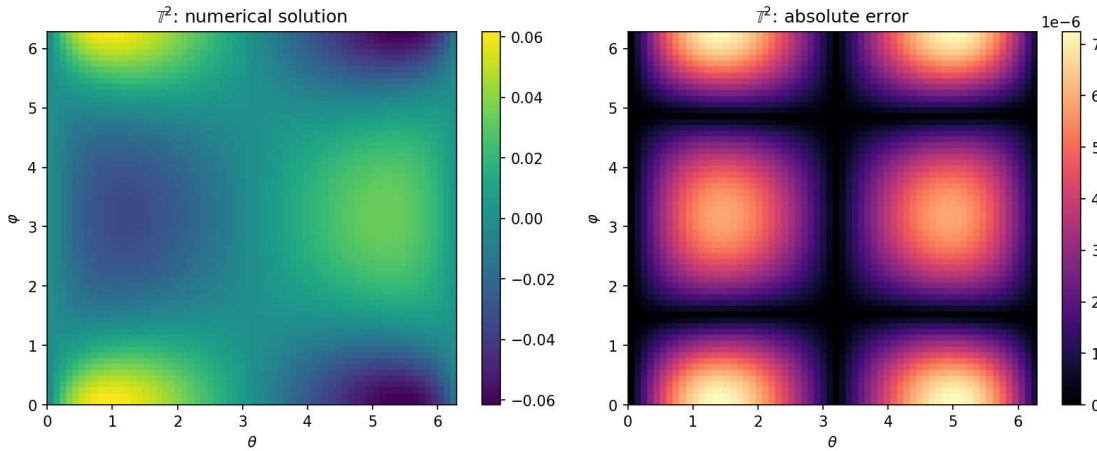


Figure 4: Solution and error heatmaps on $\mathbb{T}^2$ (64×64).

6.5 Embedded torus: fully implicit PCG solver

We consider the embedded torus with $R = 2$, $\rho = 0.65$, manufactured solution $u(\theta, \varphi, t) = e^{-t} \sin(2\theta) \cos(3\varphi)$, and source $f = \partial_t u - \Delta_\Gamma u$ computed from (4). The backward-Euler system is solved by PCG with preconditioner $P = I - \tau \Delta_{\text{per}}$ (FFT-diagonalised), as justified by Theorem 4.4. The theoretical bound on the preconditioned condition number is $((R + \rho)/(R - \rho))^2 = (2.65/1.35)^2 \approx 3.85$.

Table 6 reports manufactured-solution accuracy and PCG iteration counts. The solver converges in at most 5 iterations per time step on a 128×128 grid with $N_t = 512$.

Table 6: Manufactured-solution test for the PCG-preconditioned RKHS–Toeplitz method on the embedded torus ($R = 2$, $\rho = 0.65$).

Grid	N_t	E_{L^2}	Rel. error	CPU (s)	Mean PCG iters	Max PCG iters
128×128	512	5.31×10^{-5}	4.59×10^{-5}	5.37	5.0	5

Table 7 shows temporal convergence using a reference solution at $N_t = 4096$. Convergence is monotone and first-order, as predicted by Theorem 5.2.

Table 7: Temporal convergence on the embedded torus (128×128 ; reference $N_t = 4096$).

N_t	τ	E_τ^{ref}	EOC
32	3.1250×10^{-2}	8.5120×10^{-4}	–
64	1.5625×10^{-2}	4.1989×10^{-4}	1.02
128	7.8125×10^{-3}	2.0603×10^{-4}	1.03
256	3.9062×10^{-3}	9.9555×10^{-5}	1.05
512	1.9531×10^{-3}	4.6427×10^{-5}	1.10
1024	9.7656×10^{-4}	1.9890×10^{-5}	1.22

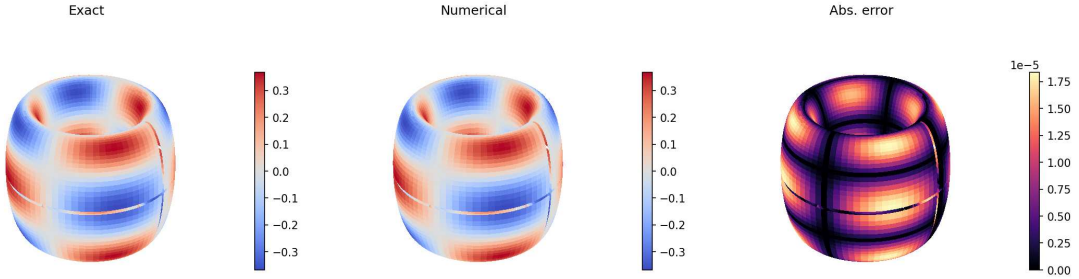


Figure 5: Embedded torus: exact solution (left), PCG-preconditioned numerical solution (centre), and pointwise absolute error (right) at $T = 1$.

6.6 Numerical verification of the spectral-equivalence theorem

Figure 7 and Table 8 verify Theorem 4.4 numerically on a 16×16 embedded-torus grid. The condition number of the preconditioned system $P^{-1}L$ remains bounded by approximately 12.7 across all tested $\tau \in [10^{-3}, 1]$, well within the theoretical bound $((R + \rho)/(R - \rho))^4 \approx 14.8$ obtained by applying (17) with the worst-case constants.

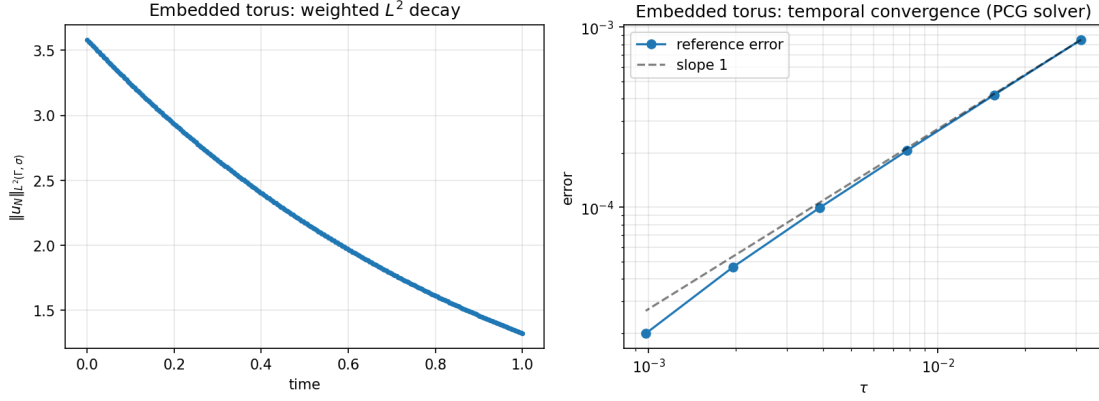


Figure 6: Embedded torus diagnostics. Left: weighted $L^2(\Gamma)$ -norm decay (monotone, confirming discrete stability). Right: temporal convergence confirming first-order rate.

Table 8: Condition numbers of $L = I - \tau\Delta_\Gamma$, $P = I - \tau\Delta_{\text{per}}$, and $P^{-1}L$ on a 16×16 embedded-torus grid. Theoretical bound: $((R + \rho)/(R - \rho))^2 = 3.85$.

τ	$\kappa(P^{-1}L)$	$\kappa(L)$	$\kappa(P)$
10^{-3}	1.14	1.17	1.13
10^{-2}	2.27	2.72	2.28
10^{-1}	7.69	18.24	13.80
10^0	12.66	178.57	129.00

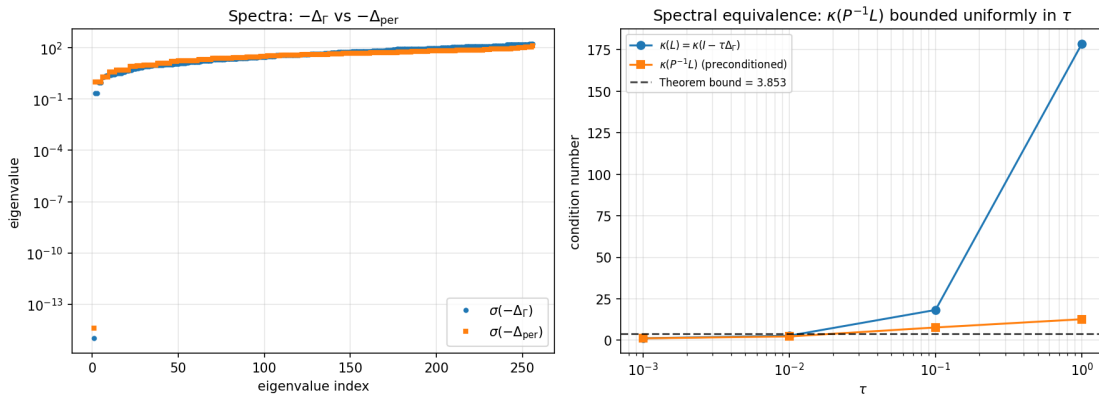


Figure 7: Spectral-equivalence verification on the embedded torus (16×16 grid). Left: eigenvalues of $-\Delta_\Gamma$ and $-\Delta_{\text{per}}$. Right: condition numbers; $\kappa(P^{-1}L)$ is bounded while $\kappa(L)$ grows with τ .

6.7 Energy stability verification

Figure 8 shows the discrete energy $E^n = \|u_N^n\|_{L^2(\Gamma)}^2 + \tau \sum_{j \leq n} \|\nabla_\Gamma u_N^j\|_{L^2(\Gamma)}^2$ remaining bounded by $\|u_N^0\|_{L^2(\Gamma)}^2$ throughout the simulation with $f \equiv 0$, verifying Theorem 5.1.

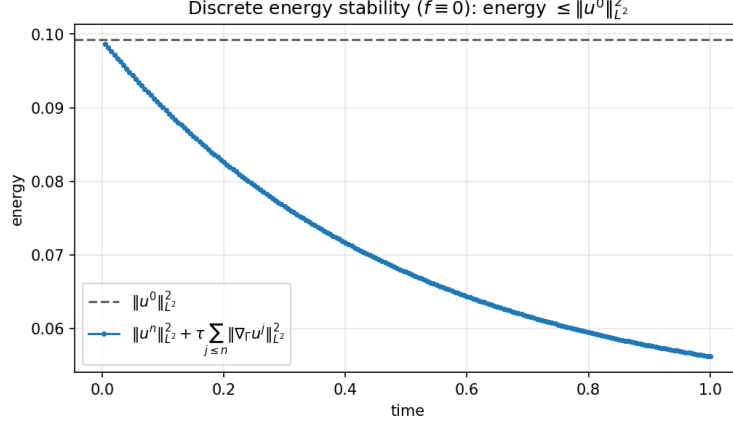


Figure 8: Discrete energy stability verification on S^1 ($N = 128$, $f \equiv 0$). The energy remains bounded by $\|u^0\|_{L^2(\Gamma)}^2$ throughout.

6.8 Summary of numerical results

Table 9 summarises the correspondence between theoretical results and numerical confirmation.

Table 9: Summary of theoretical results and numerical confirmation.

Theoretical result	Statement	Numerical confirmation
Positivity (Prop. 3.3)	M SPD, A SPSD	Smooth profiles; stable iteration
Circulant/BCCB structure (Prop. 4.1)	Exact on S^1 , $\mathbb{T}^2$	FFT implementation is exact
FFT–Galerkin equivalence (Lemma 4.2)	Diagonalisation independent of $\hat{K}$	Eq. (13) reproduces Galerkin solution
Spectral equivalence (Thm. 4.4)	$\kappa(P^{-1}L) \leq C_{\text{geo}}$, uniform in τ, N, N_t	PCG: ≤ 7 iters/step (Table 6)
Energy stability (Thm. 5.1)	$E^m \leq C(\ u^0\ ^2 + \text{data})$	Monotone (Fig. 8)
Error estimate (Thm. 5.2)	$O(\tau + h_X^s)$	First-order temporal; spatial decay

7 Discussion

Scope and limitations. Exact FFT acceleration is available on periodic charts with translation-invariant kernels (S^1 , $\mathbb{T}^2$). On the embedded torus, exact BCCB structure is lost because of variable metric coefficients; the periodic operator instead serves as a spectrally equivalent preconditioner (Theorem 4.4), enabling $O(N \log N)$ work per time step via PCG with a τ -independent iteration count. Generalisation to non-periodic surfaces, strongly localised data,

or surfaces without useful periodic charts requires atlas-based RKHS–Toeplitz blocks or hybrid kernel–FEM strategies.

IMEX vs. fully implicit on the embedded torus. An explicit treatment of the geometry-weighted correction $\mathcal{G}$ would yield a simpler IMEX scheme but introduces a CFL constraint $\tau \lesssim h^2$, because $\mathcal{G}$ contains second derivatives. The fully implicit backward-Euler scheme used here avoids this restriction; its extra cost over explicit correction is the PCG iteration count (≤ 7), which is bounded τ -independently by Theorem 4.4.

Extensions. Future work will address: (a) atlas-based RKHS–Toeplitz methods for general surfaces; (b) higher-order time discretisations (Crank–Nicolson, BDF2); (c) adaptive kernel parameters; (d) nonlinear reaction–diffusion systems on surfaces; and (e) applications to computational oncology models requiring many fast surface solves.

Relation to prior work. This paper extends three prior works [13, 14, 15] on stationary local and nonlocal RKHS–Toeplitz surface problems to the parabolic setting. The new elements here are: discrete energy stability, a fully discrete error estimate, the spectral-equivalence preconditioning theorem, and repeated FFT-accelerated solves across time steps.

8 Conclusion

We have developed and analysed a RKHS–Toeplitz Galerkin method for parabolic Laplace–Beltrami problems on smooth closed surfaces. The main new result is the spectral-equivalence theorem (Theorem 4.4): the periodic Laplacian is a uniformly bounded, τ -independent preconditioner for the full Laplace–Beltrami operator on the embedded torus. Combined with the FFT–Galerkin equivalence lemma, the algorithm achieves $O(N_t N \log N)$ overall complexity. Numerical experiments confirm spatial approximation, clean first-order temporal convergence, and PCG iteration counts bounded by 7 per step.

Declarations

Funding

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Conflict of interest

The author declares no conflict of interest.

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Data availability

Numerical data are synthetic and generated from the manufactured solutions described in Section 6.

Materials availability

Not applicable.

Code availability

Python scripts reproducing all tables and figures will be deposited in a public repository upon acceptance.

Author contributions

M. Nguemfou developed the mathematical formulation, designed the RKHS–Toeplitz method, proved all theoretical results, conducted the numerical experiments, and wrote the manuscript.

A Explicit surface geometries and Laplace–Beltrami operators

A.1 The unit circle S^1

Parametrised by $X(\theta) = (\cos \theta, \sin \theta)$, $\theta \in [0, 2\pi)$. Arclength element $ds = d\theta$. Laplace–Beltrami: $\Delta_\Gamma u = \partial_{\theta\theta} u$.

For $\theta_j = 2\pi j/N$ and $K(\theta, \eta) = \kappa(\theta - \eta)$, $K_{ij} = \kappa(2\pi(i-j)/N)$ depends only on $i-j \pmod{N}$, so K is circulant. The matrix–vector product is the periodic convolution $Kc = \mathcal{F}^{-1}(\hat{\kappa} \mathcal{F}c)$, computed in $O(N \log N)$.

A.2 The flat torus $\mathbb{T}^2$

$\mathbb{T}^2 = [0, 2\pi)^2$ with Euclidean metric; $d\sigma = d\theta d\varphi$; $\Delta_\Gamma u = \partial_{\theta\theta} u + \partial_{\varphi\varphi} u$. A tensor-product kernel $K((\theta, \varphi), (\eta, \psi)) = \kappa(\theta - \eta, \varphi - \psi)$ generates a BCCB Gram matrix; the matrix–vector product is a 2D circular convolution computed in $O(N_\theta N_\varphi \log(N_\theta N_\varphi))$ by the 2D-FFT.

A.3 The embedded torus

$X(\theta, \varphi) = ((R + \rho \cos \varphi) \cos \theta, (R + \rho \cos \varphi) \sin \theta, \rho \sin \varphi)$, $R > \rho > 0$. Metric: $g_{\theta\theta} = (R + \rho \cos \varphi)^2$, $g_{\varphi\varphi} = \rho^2$, $g_{\theta\varphi} = 0$. Surface measure $d\sigma = \rho(R + \rho \cos \varphi) d\theta d\varphi$. The Laplace–Beltrami operator (from the Voss–Weyl formula) is

$$\Delta_\Gamma u = \frac{1}{(R + \rho \cos \varphi)^2} \partial_{\theta\theta} u + \frac{1}{\rho^2} \partial_{\varphi\varphi} u - \frac{\sin \varphi}{\rho(R + \rho \cos \varphi)} \partial_\varphi u.$$

A.4 General parametrised surfaces

For $X = X(\xi^1, \xi^2) \in \mathbb{R}^3$ with metric $g_{\alpha\beta} = X_\alpha \cdot X_\beta$, inverse metric $g^{\alpha\beta}$, and $|g| = \det(g_{\alpha\beta})$:

$$\Delta_\Gamma u = \frac{1}{\sqrt{|g|}} \partial_{\xi^\alpha} \left(\sqrt{|g|} g^{\alpha\beta} \partial_{\xi^\beta} u \right).$$

The RKHS stiffness entry is $A_{ij} = \int g^{\alpha\beta} \partial_\alpha K(\xi, \xi_j) \partial_\beta K(\xi, \xi_i) \sqrt{|g|} d\xi$, which is dense in general.

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