

# On long time integration of the heat equation

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# ON LONG TIME INTEGRATION OF THE HEAT EQUATION

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ABSTRACT. We construct space-time Petrov–Galerkin discretizations of the heat equation on an unbounded temporal interval, either right-unbounded or left-unbounded. The discrete trial and test spaces are defined using Laguerre polynomials in time and are shown to satisfy the discrete inf-sup condition. Numerical examples are provided.

## 1. INTRODUCTION

1.1. **Model problem.** The subject of this paper is the heat equation on a smoothly bounded domain  $D \subset \mathbb{R}^d$  and an unbounded temporal interval:

$$(1) \quad \partial_t u - \Delta u = f \quad \text{on} \quad (0, \infty) \times D, \quad u|_{\partial D} = 0, \quad u|_{t=0} = g.$$

Given the functions  $f$  and  $g$ , the aim is to find  $u$  for all  $t \in (0, \infty)$ .

We give two space-time variational formulations for (1), and construct stable discrete trial and test spaces employing Laguerre polynomials for the weight  $e^{-\beta t}$  on  $(0, \infty)$  where  $\beta > 0$ .

In [3] the heat equation on a bounded temporal interval was solved by means of a space-time variational formulation and a  $p$  finite element method in time. To accommodate the unbounded temporal interval we devise space-time variational formulations in weighted Bochner spaces. This is similar to the collocation method suggested for long time integration of ordinary differential equations in [5]. Our first space-time variational formulation for (1) and the proof of discrete stability by means of a spectral decomposition in space resembles those of [3]. This is the subject of Section 3. The second space-time variational formulation for (1) is adapted from [6] with the proof of discrete stability from [1]. This is the subject of Section 4. We briefly motivate and discuss a variant of (1) posed on the left-unbounded temporal interval  $(-\infty, 0)$  in Section 5. We comment on numerical examples at the end of each section. Section 6 concludes the paper.

1.2. **Notation.** Let  $V := H_0^1(D)$  denote the Sobolev space equipped with the norm given by the  $H^1$ -seminorm, and  $V'$  its dual, identified via the scalar product of  $H := L^2(D)$ . We thus have the Gelfand triple

$$(2) \quad V \hookrightarrow H \cong H' \hookleftarrow V'$$

with continuous and dense embeddings. We will write  $\langle \cdot, \cdot \rangle$  for the duality pairing on arbitrary Banach spaces, as well as for the scalar product on  $H$ , as should be clear from the context. The scalar product on a Hilbert space  $Y$  is denoted by  $(\cdot, \cdot)_Y$ . Throughout,

$$(3) \quad \beta > 0$$

is constant. If  $J \subset \mathbb{R}$  is an interval then we define the weighted Bochner space  $L_{\pm\beta}^2(J; V)$  as the space of strongly measurable  $V$ -valued functions with finite norm given by

$$(4) \quad \|v\|_{L_{\pm\beta}^2(J; V)}^2 := \int_J \|v\|_V^2 e^{\pm\beta t} dt.$$

We selectively omit the dependence of the integrands on  $t$  for economy of notation. Other weighted Bochner spaces are defined analogously. The space  $H_{\pm\beta}^1(J; V')$  is the subspace of  $L_{\pm\beta}^2(J; V')$  with distributional derivative in the same. The interval of dependence  $J$  may also be omitted when clear from the context.

## 2. LAGUERRE POLYNOMIALS

The Laguerre polynomials on  $(0, \infty)$  for the weight  $e^{-\beta t}$  are

$$(5) \quad L_j(t) := \sqrt{\beta} \sum_{i=0}^j \binom{j}{i} \frac{(-\beta t)^i}{i!}, \quad t \in (0, \infty),$$

where  $j \geq 0$  is the polynomial degree. In particular,

$$(6) \quad L_j(0) = \sqrt{\beta} \quad \forall j \geq 0.$$

The Laguerre polynomials (5) satisfy the orthonormality relations

$$(7) \quad [\mathbf{M}_t]_{ij} := \int_0^\infty L_i(t)L_j(t)e^{-\beta t} dt = \delta_{ij} \quad \forall i, j \geq 0,$$

where  $\delta$  is the Kronecker symbol. Orthogonality (7) implies that

$$(8) \quad [\mathbf{C}_t]_{ij} := \int_0^\infty L_i(t)L'_j(t)e^{-\beta t} dt = \begin{cases} 0, & i \geq j, \\ -\beta, & i < j, \end{cases}$$

because the degree of  $L'_j$  is lower than that of  $L_i$  if  $i \geq j$ , and using integration by parts with (6) if otherwise.

The Gauss–Laguerre quadrature nodes and quadrature weights on  $(0, \infty)$  with weight  $e^{-\beta t}$  are obtained from the usual ones by multiplying both by  $1/\beta$ . The  $k$  Gauss–Laguerre nodes are the zeros of  $L_k$ , and the corresponding quadrature is exact on polynomials of degree at most  $2k - 1$ . The Radau–Laguerre quadrature nodes, that is nodes that include  $t = 0$  and are otherwise optimized to yield a quadrature exact for polynomials of degree  $2k$ , are the  $(k + 1)$  zeros of the polynomial

$$(9) \quad t \mapsto \frac{tL'_{k+1}(t)}{k+1} = -\beta \int_0^t L_k(s)ds = L_{k+1}(t) - L_k(t), \quad t \geq 0.$$

In the following,  $S_k$  denotes the subspace of  $L_{-\beta}^2(0, \infty)$  spanned by the Laguerre polynomials  $L_0, \dots, L_k$ . We recall from [4, p.95] that  $\bigcup_{k \geq 0} S_k$  is dense in  $L_{-\beta}^2(0, \infty)$ .

## 3. FIRST VARIATIONAL FORMULATION

**3.1. First variational formulation.** Set  $J := (0, \infty)$ . Define the continuous trial space

$$(10) \quad X := L_{-\beta}^2(J; V)$$

with the norm  $\|\cdot\|_X$  given by (4). The continuous test space is taken as

$$(11) \quad Y := H_{-\beta}^1(J; V') \cap L_{-\beta}^2(J; V),$$

on which

$$(12) \quad \|v\|_Y^2 := \|\partial_t v\|_{L_{-\beta}^2(V')}^2 + \|v\|_{L_{-\beta}^2(V)}^2, \quad v \in Y,$$

is a norm. One can show (see appendix) that

$$(13) \quad \lim_{t \rightarrow \infty} e^{-\beta t} \|v(t)\|_H^2 = 0 \quad \forall v \in Y,$$

and

$$(14) \quad \exists C_Y > 0 : \quad \|v(0)\|_H^2 \leq C_Y \|v\|_Y^2 \quad \forall v \in Y.$$

We introduce a new norm on  $Y$  by

$$(15) \quad \|v\|_Y := \| -\partial_t v + \beta v - \Delta v \|_{L^2_{-\beta}(V')}, \quad v \in Y.$$

From now on,  $Y$  is understood to be equipped with this norm. This norm is indeed equivalent to the foregoing one. We give the proof since the kind of arguments will be used frequently.

*Proof.* Expanding the square of the right hand side of (15) yields

$$(16) \quad \| -\partial_t v + \beta v - \Delta v \|_{L^2_{-\beta}(V')}^2 = \|v\|_Y^2 + T_1 + T_2$$

with

$$(17) \quad T_1 = 2\beta \|v\|_{L^2_{-\beta}(H)}^2 - \int_0^\infty 2\langle \partial_t v, v \rangle e^{-\beta t} dt = \beta \|v\|_{L^2_{-\beta}(H)}^2 + \|v(0)\|_H^2$$

and

$$(18) \quad T_2 = \beta^2 \|v\|_{L^2_{-\beta}(V')}^2 - \beta \int_0^\infty 2\langle \partial_t v, v \rangle_{V'} e^{-\beta t} dt = \beta \|v(0)\|_{V'}^2.$$

By nonnegativity of  $T_1$  and  $T_2$ , the inequality  $\|\cdot\|_Y \geq \|\cdot\|_Y$  is immediate. On the other hand,  $T_1 + T_2 \lesssim \|v\|_Y^2$  follows by continuity of the embedding  $V \hookrightarrow H$  and the trace inequality (14). Hence,  $\|\cdot\|_Y \sim \|\cdot\|_Y$  are equivalent norms on  $Y$ .  $\square$

We identify the dual  $Y'$  of  $Y$  via the scalar product of  $L^2_{-\beta}(J; H)$ , and assume that  $f \in Y'$ . Define the bounded linear operator  $B : X \rightarrow Y'$  by

$$(19) \quad \langle Bw, v \rangle := \int_0^\infty \langle w, -\partial_t v + \beta v - \Delta v \rangle e^{-\beta t} dt, \quad (w, v) \in X \times Y,$$

and the bounded linear functional  $F \in Y'$  by

$$(20) \quad Fv := \langle g, v(0) \rangle + \int_0^\infty \langle f, v \rangle e^{-\beta t} dt, \quad v \in Y.$$

It is clear from the definition of the norm (15) that

$$(21) \quad \|B\| \leq 1.$$

The space-time variational formulation of (1) now reads

$$(22) \quad \text{Find } u \in X : \quad \langle Bu, v \rangle = Fv \quad \forall v \in Y.$$

The definition of  $B$  and  $F$  is motivated by the observation that any smooth and bounded  $u : [0, \infty) \rightarrow V$  that satisfies (1) also satisfies the weak form (22).

**3.2. Stable Galerkin discretization.** Recall that  $S_k$  is spanned by the Laguerre polynomials  $L_0, \dots, L_k$ . Let  $V_\ell \subset V$  be an arbitrary nontrivial finite-dimensional (or merely closed) subspace, and fix a nonnegative integer  $k$ . Given  $k \geq 0$  and  $\ell \geq 0$ , discrete trial and test spaces  $X_L \subset X$  and  $Y_L \subset Y$  are taken as the space-time tensor product spaces

$$(23) \quad X_L := Y_L := S_k \otimes V_\ell.$$

It is interesting to note that in [3], the polynomial degree of the discrete test space was one higher because the condition  $v(T) = 0$  at the final time  $T$  was imposed on the continuous test functions. This is not necessary here thanks to the asymptotic behavior (13).

We now consider the discrete counterpart of (22):

$$(24) \quad \text{Find } u_L \in X_L : \quad \langle Bu_L, v \rangle = Fv \quad \forall v \in Y_L.$$

In order to prove well-posedness of the discrete space-time variational formulation, we introduce  $0 < \kappa_\ell \leq 1$  as the largest number such that

$$(25) \quad \sup_{\chi \in V_\ell \setminus \{0\}} \frac{\langle \chi', \chi \rangle}{\|\chi\|_V} \geq \kappa_\ell \|\chi'\|_{V'} \quad \forall \chi' \in V_\ell.$$

It can be shown that  $\kappa_\ell^{-1}$  is the norm of the  $H$ -orthogonal projector viewed as a mapping  $V \rightarrow V_\ell \subset V$ , see [1, Lemma 6.2]. Therefore,  $\kappa_\ell \gtrsim 1$  for some common finite element spaces  $V_\ell$ . We can now state the following.

**Proposition 3.1.**  *$X_L$  and  $Y_L$  satisfy the discrete inf-sup condition*

$$(26) \quad \gamma_L := \inf_{w \in X_L \setminus \{0\}} \sup_{v \in Y_L \setminus \{0\}} \frac{\langle Bw, v \rangle}{\|w\|_X \|v\|_Y} \geq \kappa_\ell.$$

*Proof.* Since  $\dim X_L = \dim Y_L$  is finite, it is enough to prove that for any nonzero  $v \in Y_L$  there exists a nonzero  $w \in X_L$  such that

$$(27) \quad \langle Bw, v \rangle \geq \kappa_\ell \|w\|_X \|v\|_Y.$$

Let therefore  $v \in Y_L$  be arbitrary nonzero. Let  $\{\varphi_\lambda\}_{\lambda \in \Lambda}$ , denote the  $H$ -orthonormal basis for  $V_\ell$  defined through the eigenvalue problem

$$(28) \quad \langle -\Delta \varphi_\lambda, \chi \rangle = \lambda^2 \langle \varphi_\lambda, \chi \rangle \quad \forall \chi \in V_\ell.$$

Then  $v = \sum_{\lambda \in \Lambda} q_\lambda \otimes \varphi_\lambda$  with  $q_\lambda \in S_k$ . Set  $p_\lambda := \lambda^{-2}(-q'_\lambda + \beta q_\lambda + \lambda^2 q_\lambda)$  and  $w := \sum_{\lambda \in \Lambda} p_\lambda \otimes \varphi_\lambda$ . Using  $\|\varphi_\lambda\|_V = \lambda$  we find

$$(29) \quad \langle Bw, v \rangle = \sum_{\lambda \in \Lambda} \|\lambda p_\lambda\|_{L^2_{-\beta}(0, \infty)}^2 = \|w\|_X^2.$$

However,  $\|\varphi_\lambda\|_{V'}$  does not equal  $\lambda^{-1}$ , but rather

$$(30) \quad \lambda^{-1} = \sup_{\chi \in V_\ell \setminus \{0\}} \frac{\langle \varphi_\lambda, \chi \rangle}{\|\chi\|_V} \geq \kappa_\ell \|\varphi_\lambda\|_{V'},$$

where the equality is seen by expanding  $\chi$  into the eigenbasis, and the inequality is due to (25). This is now used to show

$$(31) \quad \langle Bw, v \rangle = \sum_{\lambda \in \Lambda} \lambda^{-2} \|-q'_\lambda + \beta q_\lambda + \lambda^2 q_\lambda\|_{L^2_{-\beta}(0, \infty)}^2 \geq \kappa_\ell^2 \|v\|_Y^2$$

by first expanding the summand analogously to (16), estimating using (30),  $\|\varphi_\lambda\|_V = \lambda$ , and  $\|\varphi_\lambda\|_H = 1$ , and then collecting the terms again. Combining (29) and (31) we have the claim (27).  $\square$

Using density of  $\bigcup_{k \geq 0} S_k \otimes V$  in  $Y$  one can prove the following theorem.

**Theorem 3.2.**  *$B : X \rightarrow Y'$  defined in (19) is an isometric isomorphism.*

Boundedness (21), the discrete inf-sup condition (26), and [7, Theorem 2] imply the quasi-optimality estimate

$$(32) \quad \|u - u_L\|_X \leq \gamma_L^{-1} \inf_{w_L \in X_L} \|u - w_L\|_X$$

for any exact solution  $u$  of the continuous space-time variational problem (22).

**3.3. Formulation as a collocation method.** In this subsection we suppose for simplicity that  $f \in S_k \otimes V$  in (20). Then we can formulate the discrete space-time variational formulation (24) equivalently as a collocation method as follows. Let  $\mathcal{N}_{k+1} \subset \mathbb{R}$  denote the  $k+1$  zeros of the Laguerre polynomial  $L_{k+1}$ . Let  $I_{k+1} : C^0(\mathbb{R}; V_\ell) \rightarrow X_L$  denote the polynomial interpolation operator on those nodes. Let  $U_L \in S_{k+1} \otimes V_\ell$  be determined by

$$(33) \quad \langle U_L(0), \chi \rangle = \langle g, \chi \rangle \quad \forall \chi \in V_\ell,$$

together with the following  $(k+1)$  collocation conditions:

$$(34) \quad \langle \partial_t U_L(\tau) - \Delta U_L(\tau) - f(\tau), \chi \rangle = 0 \quad \forall \chi \in V_\ell \quad \forall \tau \in \mathcal{N}_{k+1}.$$

This collocation scheme was investigated in [5, Section 2] for ordinary differential equations. We will show that

$$(35) \quad u_L = I_{k+1} U_L.$$

To that end, observe that the interpolation error  $I_{k+1} U_L - U_L$  is in  $\{L_{k+1} \otimes \chi : \chi \in V_\ell\}$ . By orthogonality of  $L_{k+1}$  to  $S_k$  in  $L^2_{-\beta}(J)$  we therefore have  $\langle BI_{k+1} U_L, v \rangle = \langle BU_L, v \rangle$  for all  $v \in Y_L$ . With this, integration by parts and the asymptotics (13), there follows

$$(36) \quad \langle BI_{k+1} U_L, v \rangle = \int_0^\infty \langle \partial_t U_L - \Delta U_L, v \rangle e^{-\beta t} dt + \langle U_L(0), v(0) \rangle.$$

Given exactness of the Gauss quadrature based on  $\mathcal{N}_{k+1}$  for polynomials of degree at most  $2k+1$ , we use the collocation conditions (34) and the initial condition (33) to find that the right hand side of (36) equals  $Fv$  from (20). Hence  $I_{k+1} U_L$  satisfies the discrete space-time variational formulation (24), which implies the claimed equality (35).

The collocation solution  $U_L$  is in turn obtained from the Galerkin solution  $u_L$  by reconstruction, which is one step of the Picard iteration. Indeed, define  $\widehat{u}_L \in S_{k+1} \otimes V_\ell$  by

$$(37) \quad \langle \widehat{u}_L(s), \chi \rangle = \langle g, \chi \rangle + \int_0^s \langle f + \Delta u_L, \chi \rangle dt \quad \forall \chi \in V_\ell, \quad s \geq 0.$$

Now,  $\langle \partial_t \widehat{u}_L(\tau), \chi \rangle = \langle f(\tau) + \Delta u_L(\tau), \chi \rangle = \langle f(\tau) + \Delta U_L(\tau), \chi \rangle$  for all  $\tau \in \mathcal{N}_{k+1}$  due to (35). Comparing with the collocation conditions (34), this shows that  $\partial_t \widehat{u}_L$  and  $\partial_t U_L$  coincide at the collocation nodes  $\mathcal{N}_{k+1}$ , and being both polynomials of degree at most  $k$ , they must be the same. Since the reconstruction  $\widehat{u}_L$  also satisfies the same initial condition (33) as the collocation solution  $U_L$ , we obtain the identity  $\widehat{u}_L = U_L$ .

**3.4. Algebraic equations.** Using the Laguerre polynomials as the basis for  $S_k$  and any basis for  $V_\ell$ , the discrete space-time variational formulation (24) leads to the linear system of algebraic equations

$$(38) \quad \mathbf{B} \mathbf{u} = \mathbf{F}.$$

The system matrix has the Kronecker product form

$$(39) \quad \mathbf{B} = -\mathbf{C}_t^\top \otimes \mathbf{M}_x + \mathbf{M}_t \otimes (\beta \mathbf{M}_x + \mathbf{A}_x)$$

where  $\mathbf{M}_x$  and  $\mathbf{A}_x$  are the usual spatial mass and stiffness matrices, while  $\mathbf{C}_t$  and  $\mathbf{M}_t$  are temporal finite element matrices in  $\mathbb{R}^{(k+1) \times (k+1)}$  with the components given in (7)–(8). Negation and transposition of  $\mathbf{C}_t$  reflect the integration by parts in time that was used to define the operator  $B$  in (19). The triangular form of  $\mathbf{C}_t$  with empty diagonal and diagonality of  $\mathbf{M}_t$  allow (38) to be quickly solved by blockwise forward substitution, where in each solve a positive definite Helmholtz problem has to be solved. In the numerical examples below the load functional will be computed approximately by the

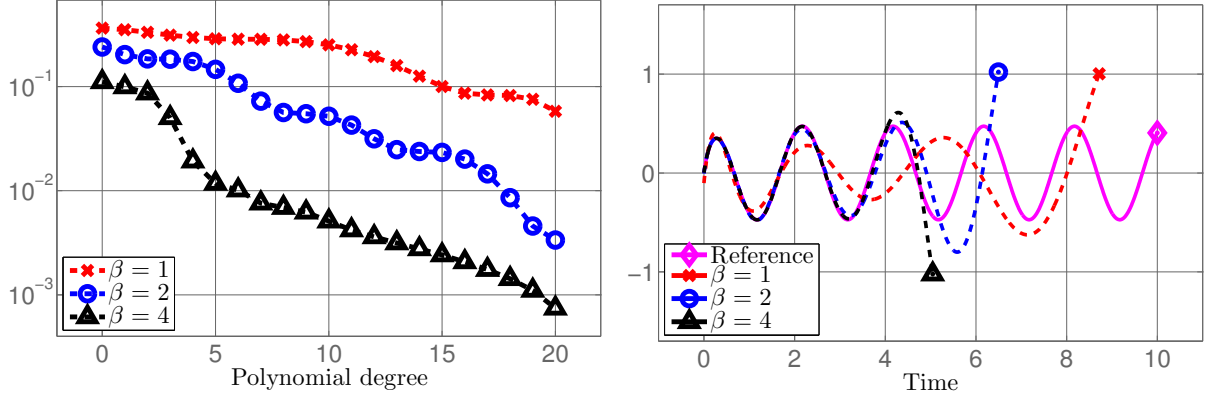


FIGURE 1. Left: Error of the discrete solution in the  $X$  norm as a function of the Laguerre polynomial degree  $k$ , see Section 3.5. Right: Integral of the discrete solution over the spatial domain as a function of time.

Gauss–Laguerre quadrature on 50 nodes. Theoretically, this quadrature is exact for  $\int_0^\infty p(t)e^{-\beta t} dt$  if  $p$  is a polynomial of degree less than 100.

**3.5. Numerical example.** We take  $D = (-1, 1)^2$  in  $\mathbb{R}^2$  and  $f(t, x) = \cos(\pi t)$  for all  $(t, x) \in \mathbb{R} \times D$ . The domain  $D$  is subdivided into  $2 \times 4^5$  congruent triangles, resulting in 961 spatial degrees of freedom for the first order Lagrangian finite elements, defining the subspace  $V_\ell \subset V$ . We use  $\beta = 1, 2, 4$ . Note that the first eigenvalue of the Dirichlet Laplacian on this domain is  $\frac{1}{2}\pi^2 \approx 5$ .

In Figure 1, left, we monitor the convergence of the discrete solution in the norm of  $X$  as the dimension  $\dim S_k = k + 1$  of the polynomial space is increased. We observe exponential convergence in  $k$ . The computation time is on the order of 1.5 seconds for the largest problem in Matlab using direct solves for the blockwise forward substitution.

In Figure 1, right, we document the integral of the discrete solution over the the spatial domain  $D$  with Laguerre polynomial degree  $k = 10$  as a function of time, together with a reference value computed by time stepping. One can see that the value starts to oscillate wildly sooner with larger  $\beta$ , but the value is approximately conserved over longer times with smaller  $\beta$ . Similar behavior was observed for test cases where the exact solution converges as  $t \rightarrow \infty$  to a nontrivial steady state.

## 4. SECOND VARIATIONAL FORMULATION

**4.1. Second variational formulation.** Set  $J := (0, \infty)$ . Define the continuous trial space

$$(40) \quad X := L^2_{-\beta}(J; V) \cap H^1_{-\beta}(J; V').$$

On  $X$  we have the norm

$$(41) \quad \|w\|_X^2 := \|\partial_t w\|_{L^2_{-\beta}(V')}^2 + \|w\|_{L^2_{-\beta}(V)}^2 + \beta \|w\|_{L^2_{-\beta}(H)}^2.$$

Dropping the  $\beta$  term we obtain an equivalent norm by continuity of the embedding  $V \hookrightarrow H$ . From (13) and  $\partial_t \|w\|_H^2 = \langle \partial_t w, w \rangle$  we obtain the identity

$$(42) \quad \|w\|_X^2 = \|w(0)\|_H^2 + \|\partial_t w - \Delta w\|_{L^2_{-\beta}(V')}^2 \quad \forall w \in X$$

that motivates the choice (41). The continuous test space is defined as

$$(43) \quad Y := Y_0 \times Y_1 := H \times L^2_{-\beta}(J; V),$$

with the natural Hilbertian norm. The dual of  $Y$  is identified using the scalar product of  $L^2_{-\beta}(J; H)$  as  $Y' = H \times L^2_{-\beta}(J; V')$ . We assume that  $(g, f) \in Y'$  for the data in (1).

Define the bounded linear operator  $B : X \rightarrow Y'$  by

$$(44) \quad \langle Bw, v \rangle := \langle w(0), v_0 \rangle + \int_0^\infty \langle \partial_t u - \Delta u, v_1 \rangle e^{-\beta t} dt, \quad w \in X, \quad (v_0, v_1) \in Y,$$

and the bounded linear functional  $F \in Y'$  by

$$(45) \quad Fv := \langle g, v_0 \rangle + \int_0^\infty \langle f, v_1 \rangle e^{-\beta t} dt, \quad (v_0, v_1) \in Y.$$

Using the identity (42) one finds

$$(46) \quad \|B\| \leq 1.$$

The continuous space-time variational formulation of (1) now reads as in (22).

**4.2. Stable minimal residual discretization.** Recall that  $S_k$  denotes the space spanned by the Laguerre polynomials  $L_0, \dots, L_k$ . Let  $V_\ell \subset V$  be an arbitrary nontrivial finite-dimensional (or closed) subspace, and fix a nonnegative integer  $k$ . Given  $k \geq 0$  and  $\ell \geq 0$  we define the discrete trial and test spaces  $X_L \subset X$  and  $Y_L \subset Y$  as

$$(47) \quad X_L := S_k \otimes V_\ell \quad \text{and} \quad Y_L := V_\ell \times [S_k \otimes V_\ell].$$

Due to  $\dim X_L + 1 = \dim Y_L$  we cannot replace  $X$  by  $X_L$  and  $Y$  by  $Y_L$  in the continuous space-time variational formulation (22). Instead, as suggested in [1], we introduce the residual minimization problem

$$(48) \quad \text{Find } u_L \in X_L : \quad R_L(u_L) \leq R_L(w_L) \quad \forall w_L \in X_L,$$

where  $R_L$  is the discrete functional residual (here,  $S(Y_L)$  denotes the unit sphere of  $Y_L$ )

$$(49) \quad R_L(w_L) := \sup_{v \in S(Y_L)} |\langle Bw_L - F, v \rangle|, \quad w_L \in X_L.$$

Under the discrete inf-sup condition  $\gamma_L > 0$ , established in Proposition 4.1 below, one can show that  $u_L$  is well-defined and the mapping  $F \mapsto u_L$  is continuous with norm at most  $\gamma_L^{-1}$ . Therefore,  $u \mapsto u_L$  is a projection whose norm is at most  $\gamma_L^{-1} \|B\|$ . Boundedness (46) and [7, Theorem 2] imply the quasi-optimality estimate (32) for any solution  $u \in X$  of the continuous space-time variational formulation.

In order to obtain the inf-sup condition (26) for the operator (44) with the discrete trial and test space (47) we follow a different proof than in the previous section. The present proof is an adaptation of [1, Proof of Theorem 4.1] to the unbounded interval with weight  $e^{-\beta t}$ . It has the advantage that space-time dependent coefficients in  $-\nabla \cdot (a(t, x) \nabla u)$  in place of  $-\Delta u$  can be used. To streamline the proof we introduce the quantity

$$(50) \quad K_L := \inf_{z \in \partial_t X_L \setminus \{0\}} \sup_{v \in Y_L \setminus \{0\}} \frac{\int_0^\infty \langle z, v_1 \rangle e^{-\beta t} dt}{\|z\|_{L^2_{-\beta}(V')} \|v\|_Y}.$$

Expanding  $z$  and  $v_1$  into Laguerre polynomials and using their orthonormality (7), it is quickly seen that  $K_L = \kappa_\ell$  with  $\kappa_\ell > 0$  from (25).

**Proposition 4.1.**  $X_L$  and  $Y_L$  satisfy the discrete inf-sup condition (26).



*Proof.* Define the bounded linear operator  $\Gamma : X_L \rightarrow Y_L$  by  $(\Gamma w, v)_Y := \langle Bw, v \rangle$  for all  $(w, v) \in X_L \times Y_L$ . For any  $w \in X_L$  we shall show that  $\|\Gamma w\|_Y \geq \kappa_\ell \|w\|_X$ , which implies the claimed estimate (26) due to

$$(51) \quad \sup_{v \in Y_L \setminus \{0\}} \frac{\langle Bw, v \rangle}{\|v\|_Y} = \sup_{v \in Y_L \setminus \{0\}} \frac{(\Gamma w, v)_Y}{\|v\|_Y} = \|\Gamma w\|_Y \geq \kappa_\ell \|w\|_X.$$

To that end, let  $v_w$  be the pair  $v_w := (w(0), w)$ . Crucially,  $v_w \in Y_L$ . We expand  $\|\Gamma w\|_Y$  as

$$(52) \quad \|\Gamma w\|_Y^2 = \|\Gamma w - v_w\|_Y^2 + 2(\Gamma w, v_w)_Y - \|v_w\|_Y^2,$$

and estimate the individual terms. The unit sphere in  $Y_L$  is abbreviated as  $S(Y_L)$ . For the first term in (52) we find

$$(53) \quad \|\Gamma w - v_w\|_Y = \sup_{v \in S(Y_L)} (\Gamma w - v_w, v)_Y = \sup_{v \in S(Y_L)} \{\langle Bw, v \rangle - (v_w, v)_Y\}$$

$$(54) \quad = \sup_{v \in S(Y_L)} \int_0^\infty \langle \partial_t w, v_1 \rangle e^{-\beta t} dt \geq K_L \|\partial_t w\|_{L^2_{-\beta}(V')} = \kappa_\ell \|\partial_t w\|_{L^2_{-\beta}(V')}.$$

For the second term in (52) we compute

$$(55) \quad (\Gamma w, v_w)_Y = \int_0^\infty \langle \partial_t w - \Delta w, w \rangle e^{-\beta t} dt + \|w(0)\|_H^2$$

$$(56) \quad = \int_0^\infty \langle \partial_t w, w \rangle e^{-\beta t} dt + \|v_w\|_Y^2$$

$$(57) \quad = -\frac{1}{2} \|w(0)\|_H^2 + \frac{\beta}{2} \|w\|_{L^2_{-\beta}(H)}^2 + \|v_w\|_Y^2.$$

Inserting into (52), collecting, and estimating further we obtain  $\|\Gamma w\|_Y \geq \kappa_\ell \|w\|_X$  as anticipated.  $\square$

The counterpart of Theorem 3.2 also holds.

**4.3. Algebraic equations.** Let  $M : X \rightarrow X'$  and  $N : Y \rightarrow Y'$  denote the Riesz mappings. Pick bases for  $S_k$  and  $V_\ell$  as in Section 3.4. Let  $\mathbf{M}$ ,  $\mathbf{N}$ , and  $\mathbf{B}$  denote the matrices corresponding to their continuous counterparts, and let  $\mathbf{F}$  be the load vector. It is shown in [1] that the discrete residual minimization problem is equivalent to the generalized Gauß normal equations

$$(58) \quad \mathbf{B}^\top \mathbf{N}^{-1} \mathbf{B} \mathbf{u} = \mathbf{B}^\top \mathbf{N}^{-1} \mathbf{F}$$

and  $\mathbf{M}$  is spectrally equivalent to the matrix on the left up to a factor of  $(\|B\|/\gamma_L)^2$ . It is therefore natural to apply the conjugate gradient method to the above algebraic system with  $\mathbf{M}$  as preconditioner. The structure and application of  $\mathbf{M}^{-1}$  and  $\mathbf{N}^{-1}$  is similar to the heat equation on a bounded temporal interval, which is discussed in [2]. Since we expect the numerical results to be very close to those of Section 3.5, we do not elaborate here further.

## 5. LEFT-UNBOUNDED TEMPORAL INTERVAL

With the ansatz of the foregoing sections the quality of the discrete solution deteriorates for large  $t$ , see Figure 1. This is not a contradiction to stability in the weighted space-time norms, but motivates the following question. For  $t_1 \gg 1$ , how can the solution  $u$  at  $t = t_1$  to (1) be computed? Due to the diffusive character of the heat equation, the solution at  $t = t_1$  is mostly determined by values of  $f$  on a temporal interval  $(t_0, t_1)$  with  $1 \ll t_0 \ll t_1$ . It is therefore reasonable to truncate the entire temporal domain to this

subinterval and perform the computation there with the initial condition  $u(t_0) = 0$ , say. Instead of truncating explicitly we set up a discretization by Laguerre polynomials in time that are attached to  $t_1$  and face  $-\infty$ . We expect that in this way the solution  $u$  close to  $t_1$  will be resolved best. Translating in time by  $-t_1$  we arrive at the following variant of the original problem:

$$(59) \quad \partial_t u - \Delta u = f \quad \text{on} \quad (-\infty, 0) \times D, \quad u|_{\partial D} = 0,$$

where given  $f$ , the aim is to find  $u$  at time  $t = 0$ . The right hand sides of (1) and (59) will then differ in general. Note that we do not seek to determine  $u$  for negative times  $t$ , which is an ill-posed problem.

We now set  $J := (-\infty, 0)$ , and assume that  $\beta > 0$  is sufficiently small such that

$$(60) \quad 0 < \beta < \inf_{\chi \in V \setminus \{0\}} \frac{\|\chi\|_V^2}{\|\chi\|_H^2}.$$

Thus,  $\beta$  is smaller than the first eigenvalue of the Laplacian with homogeneous Dirichlet boundary conditions. Define the weighted Bochner spaces

$$(61) \quad X := H_\beta^1(J; V') \cap L_\beta^2(J; V) \quad \text{and} \quad Y := L_\beta^2(J; V),$$

endowed with the norm

$$(62) \quad \|w\|_X^2 := \|\partial_t w\|_{L_\beta^2(V')}^2 + \|w\|_{L_\beta^2(V)}^2 - \beta \|w\|_{L_\beta^2(H)}^2 + \|w(0)\|_H^2,$$

and the usual norm on  $Y$ . Note that the weight  $e^{\beta t}$  decays as  $t \rightarrow -\infty$ . Owing to the smallness condition (60), the  $\beta$  term of (62) is controlled by a small multiple of the second term, and can be omitted without changing the generated topology. The motivation for this choice of norm is the observation

$$(63) \quad \|\partial_t w - \Delta w\|_{Y'}^2 = \int_{-\infty}^0 \|\partial_t w - \Delta w\|_{V'}^2 e^{\beta t} dt = \|w\|_X^2.$$

The dual of  $Y$  is identified via the scalar product of  $L_\beta^2(J; H)$  as  $Y' = L_\beta^2(J; V')$  with the obvious norm. We assume that  $f \in Y'$ . We now introduce the bounded linear operator  $B : X \rightarrow Y'$  by

$$(64) \quad \langle Bw, v \rangle := \int_{-\infty}^0 \langle \partial_t w - \Delta w, v \rangle e^{\beta t} dt$$

and the bounded linear functional  $F \in Y'$  by

$$(65) \quad Fv := \int_{-\infty}^0 \langle f, v \rangle e^{\beta t} dt.$$

From (63) we again obtain  $\|B\| \leq 1$ . The continuous space-time variational formulation of (59) reads as in (22). The discrete trial and test spaces  $X_L \subset X$  and  $Y_L \subset Y$  are defined by  $X_L := Y_L := \bar{S}_k \otimes V_\ell$ , where  $\bar{S}_k$  denotes the span of the mirrored Laguerre polynomials  $t \mapsto L_j(-t)$ ,  $j = 0, \dots, k$ , and  $V_\ell \subset V$  is an arbitrary nontrivial finite-dimensional space. The discrete inf-sup condition (26) with  $\gamma_L \geq \kappa_\ell > 0$  can be proven analogously to the proof of Proposition 3.1 in Section 3. Again, the counterpart of Theorem 3.2 holds.

The system matrix in the discrete algebraic system  $\mathbf{B}\mathbf{u} = \mathbf{F}$  now has the form

$$(66) \quad \mathbf{B} = -\mathbf{C}_t \otimes \mathbf{M}_x + \mathbf{M}_t \otimes \mathbf{A}_x$$

where  $\mathbf{C}_t$  is upper triangular with empty diagonal and  $\mathbf{M}_t$  is the identity, see (7)–(8). Therefore, the discrete algebraic solution  $\mathbf{u}$  can be obtained by blockwise back substitution. Negation of the matrix  $\mathbf{C}_t$  reflects the fact that  $L'_j$  in (8) changes sign when  $L_j$  is mirrored onto  $(-\infty, 0)$ .

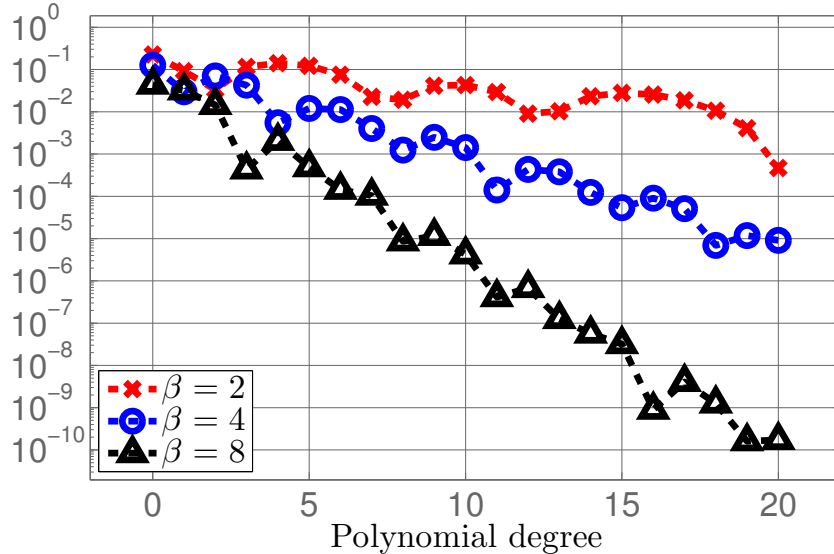


FIGURE 2.  $L^2(D)$  error of the discrete solution at  $t = 0$  as a function of the Laguerre polynomial degree  $k$  for the heat equation on the left-unbounded temporal interval, see Section 5.

For the numerical example, the setup of  $D$ ,  $f$  and  $V_\ell$  is the same as in Section 3.5. We vary the Laguerre polynomial degree  $k = 0, \dots, 20$ , and compute the  $L^2(D)$  error of the discrete solution at  $t = 0$  for  $\beta = 2, 4, 8$ . We used the solution with  $k = 21$  as a reference, which was verified to be consistent with the result obtained by a time-stepping scheme performed on a large temporal interval  $(-T, 0)$  with zero datum at  $-T$ . The computation time for the largest problem is on the order of 1.5 seconds in Matlab using direct solves for the blockwise forward substitution. Figure 2 documents the exponential decay of the  $L^2(D)$  error at  $t = 0$  with respect to the polynomial degree  $k$ . The decay is most prominent for  $\beta = 8$ , although this exponent is not covered by the theory. The error in  $H^1(D)$  behaves similarly.

## 6. CONCLUSIONS

We have devised two space-time variational formulations for the heat equation on the unbounded temporal interval  $(0, \infty)$  using weighted Bochner spaces. Discrete trial and test spaces with Laguerre polynomials in time were shown to be stable for suitable weighted space-time norms. As shown in the numerical example, the discrete solutions converge exponentially with respect to the polynomial degree for sufficiently smooth data in the weighted space-time norm but pointwise accuracy is not given for large times.

This motivated the heat equation posed on the left-unbounded interval  $(-\infty, t_1)$ , aimed at computing the solution at time  $t_1$  for large  $t_1$ , where after a shift in time we assumed  $t_1 = 0$ . A space-time variational formulation and stable discrete trial and test space based on mirrored Laguerre polynomials were given. The numerical example showed exponential convergence with respect to the polynomial degree.

The author thanks Ch. Schwab for motivating the topic.

## APPENDIX

The statement

$$(13) \quad \lim_{t \rightarrow \infty} e^{-\beta t} \|v(t)\|_H^2 = 0 \quad \forall v \in Y$$

can be obtained by contradiction. However, will use another method that will be also instrumental in finding the sharp constant  $C_Y > 0$  in

$$(14') \quad \|v(0)\|_H^2 \leq C_Y \|v\|_Y^2 = C_Y \{ \|\partial_t v\|_{L^2_{-\beta}(V')}^2 + \|v\|_{L^2_{-\beta}(V)}^2 \} \quad \forall v \in Y.$$

Fix  $\lambda > 0$ ,  $\beta > 0$  and  $T > 0$ . We consider the problem of finding the optimal constants  $C_Y > 0$  and  $C_T > 0$  in the estimates

$$(67) \quad \max\{C_Y^{-1}|f(0)|^2, C_T^{-1}e^{-\beta T}|f(T)|^2\} \leq I[f] := \int_0^T \{|\lambda^{-1}f(t)|^2 + |\lambda f(t)|^2\}e^{-\beta t} dt.$$

To find  $C_T$  we may assume that  $f(T) = 1$  and minimize  $I[f]$  in (67), which leads to the boundary value problem

$$(68) \quad -\lambda^{-2}f''(t) + \beta\lambda^{-2}f'(t) + \lambda^2f(t) = 0, \quad t \in (0, T),$$

with boundary conditions  $f'(0) = \epsilon$  and  $f(T) = 1$ , for an initially unknown  $\epsilon \in \mathbb{R}$ . Solving for  $f$  explicitly, we then minimize  $I[f]$  with respect to  $\epsilon$  to find  $\epsilon = 0$  and an explicit value for  $I[f]$ . Similarly, we find the minimal value of  $I[f]$  for the optimal constant  $C_Y$ . We then obtain

$$(69) \quad C_{Y,T} = \lambda^{-2}(\omega \coth(\omega T) \pm \beta/2), \quad \omega := \sqrt{(\beta/2)^2 + \lambda^4}.$$

Letting  $T \rightarrow \infty$  we have  $C_T \leq 1$  independently of  $\lambda > 0$  and  $\beta > 0$ , while  $C_Y$  converges to a function (of  $\beta$  and  $\lambda$ ) that is monotonically increasing in  $\beta/\lambda^2$ . The statement (14) follows from (67) by expanding  $v$  with respect to the  $H$ -orthonormal eigenfunctions  $\varphi_\lambda$ ,  $\lambda \in \Lambda \subset (0, \infty)$ , of the Dirichlet Laplacian which satisfy  $-\Delta\varphi_\lambda = \lambda^2\varphi_\lambda$ . Since  $\Lambda$  is bounded away from zero, the ratio  $\beta/\lambda^2$  is bounded above for any fixed  $\beta$ , hence  $C_Y$  in (14) is finite but depends on  $\beta$ . To obtain (13) we observe that  $\sup_{T>0} C_T \leq 1$  implies that  $E : v \mapsto \limsup_{t \rightarrow \infty} e^{-\beta t} \|v(t)\|_H^2$  is Lipschitz continuous on  $Y$ . Hence  $Y_0 := E^{-1}(\{0\})$  is a closed subset of  $Y$ . But  $S_k \otimes V \subset Y_0$  for any  $k \geq 0$ , and the union of those subspaces over  $k \geq 0$  is dense in  $Y$ . Therefore,  $Y_0 = Y$ , which shows (13).

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