A New Error Bound for Reduced Basis Approximation of Parabolic Partial Differential Equations

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Abstract

We consider a space-time variational formulation for linear parabolic partial differential equations. We introduce an associated Petrov-Galerkin truth finite element discretization with favorable discrete inf-sup constant β_δ: β_δ is unity for the heat equation; β_δ grows only linearly in time for non-coercive (but asymptotically stable) convection operators. The latter in turn permits effective long-time *a posteriori* error bounds for reduced basis approximations, in sharp contrast to classical (pessimistic) exponentially growing energy estimates.

Résumé

Nous considérons une formulation variationnelle espace-temps pour les équations différentielles paraboliques linéaires. Nous y associons une discrétisation par éléments finis de Petrov-Galerkin pour laquelle la constante de stabilité inf-sup β_δ possède des propriétés agréables : β_δ est unité pour l'équation de la chaleur; β_δ a une croissance seulement linéaire en temps pour des opérateurs de convection non-coercifs (mais asymptotiquement stables). Dans le cadre des approximations par bases réduites, cette dernière propriété permet d'obtenir des bornes efficaces pour l'erreur *a posteriori* en temps long, en net contraste avec les estimateurs d'erreur en énergie classiques (pessimistes) qui présentent une croissance exponentielle.

Key words: parabolic equations, space-time formulation, inf-sup stability, reduced basis, a posteriori estimation
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Soit l'équation aux dérivées partielles parabolique (1) et sa formulation variationnelle espace-temps : $u \in \mathcal{X} := L_2(I \equiv (0,T]; V) \cap H^1_{(0)}(I;V')$, $H^1_{(0)}(I;V') := \{v \in H^1(I;V') : v(0) = 0\}$, vérifie (2) pour l'espace des fonctions test $\mathcal{Y} := L_2(I;V)$; ici $b(w,v) := \int_I [\langle \dot{w}(t), v(t)\rangle_{V'\times V} + a(w(t), v(t))]\, dt$ et $f(v) :=$

$\int_I \langle g(t), v(t)\rangle_{V'\times V} dt$. Les normes sur $\mathcal{X}$ et $\mathcal{Y}$ sont définies par $\|w\|^2_{\mathcal{X}} := \|w\|^2_{L_2(I;V)} + \|\dot{w}\|^2_{L_2(I;V')} + \|w(T)\|^2_H$ et $\|v\|_{\mathcal{Y}} := \|v\|_{L_2(I;V)}$. On considère $V = H^1_0(\Omega)$ (opérateurs spatiaux de 2e ordre), où Ω est le domaine spatial. On montre (Proposition 1 basée sur [6]) que pour des problèmes coercifs, la constante inf-sup β de b est positive et bornée inférieurement.

Nous introduisons ensuite une discrétisation par éléments finis de Petrov-Galerkin : soit $u_\delta \in \mathcal{X}_\delta$ vérifiant $b(u_\delta, v_\delta) = f(v_\delta), \forall v_\delta \in \mathcal{Y}_\delta$; avec $\mathcal{X}_\delta := S_{\Delta t} \otimes V_h$ et $\mathcal{Y}_\delta = Q_{\Delta t} \otimes V_h$, $\delta = (\Delta t, h)$, où $S_{\Delta t}, V_h$ et $Q_{\Delta t}$ sont respectivement des éléments finis linéaire par morceaux en temps (de pas Δt) et en espace (de diamètre h), et constants en temps par morceaux. Cette méthode coïncide avec une discrétisation de Crank-Nicolson en temps, ainsi nos résultats s'appliquent directement à ce schéma standard. Nous définissons une norme modifiée sur $\mathcal{X}, ||| \cdot |||_{\mathcal{X},\delta}$, où la partie $\int_I \|w\|^2_V dt$ de $\|\cdot\|_{\mathcal{X}}$ est remplacée par une somme des moyennes de w sur chaque élément temporel. Nous montrons (Proposition 3) que pour l'équation de la chaleur, les constantes inf-sup discrète β_δ et continuité discrète γ_δ sont unités.

Nous considérons maintenant une approximation par bases réduites u_N, comme dans [2]. Nous pouvons construire à la Proposition 5 des bornes sur l'erreur *a posteriori* pour le champ solution u_N et pour la sortie scalaire s_N. L'utilité de ces bornes est très liée à la dépendance de β_δ aux paramètres du problème et au temps final T. La procédure de calcul de ces bornes est similaire à la décomposition hors ligne-en ligne des bases réduites standard.

Enfin, nous présentons des résultats numériques pour la constante inf-sup discrète β_δ. Pour des opérateurs *non-coercifs* mais asymptotiquement stables (e.g. convection), on observe que le paramètre inf-sup decroît seulement en $(\mu_1 T)^{-1}$, où μ_1 est la vitesse de déplacement et T le temps final. L'exemple est un domaine spatial unidimensionnel $(0,1)$ avec l'opérateur $\mu_1(x - 1/2)u_x - u_{xx}$ pour $\mu_1 > 2\pi^2$ ($\mu_1 < 2\pi^2$ entraîne un problème coercif). Les estimateurs associés sont beaucoup plus précis que ceux classiques en énergie qui prédisent une croissance exponentielle en $e^{\mu_1 T}$ et qui sont donc inutilisables en pratique.

1. Space-time formulation

We first formulate a general linear parabolic equation. Consider Hilbert spaces $V \hookrightarrow H \hookrightarrow V'$ and an operator $A \in \mathcal{L}(V, V')$, $\langle A\phi, \psi\rangle_{V'\times V} = a(\phi, \psi)$ for $\phi, \psi \in V$. Setting $I := (0, T]$, $T > 0$ and given $g \in L_2(I; V')$, we look for u such that

$$\dot{u}(t) + A\,u(t) = g(t) \text{ in } V',\ t \in I; \qquad u(0) = 0, \tag{1}$$

and an associated output of the form $s := \int_I \ell(u(t))\,dt$ for some $\ell \in V'$. We restrict ourselves to LTI systems even though some of our results can be extended to a more general situation.

For the derivation of the space-time variational form of (1), we introduce the trial space $\mathcal{X} := L_2(I; V) \cap H^1_{(0)}(I; V')$, where $H^1_{(0)}(I; V') := \{v \in H^1(I; V') : v(0) = 0\}$ with norm $\|w\|^2_{\mathcal{X}} := \|w\|^2_{L_2(I;V)} + \|\dot{w}\|^2_{L_2(I;V')} + \|w(T)\|^2_H$ and the test space $\mathcal{Y} := L_2(I; V)$ with norm $\|v\|_{\mathcal{Y}} := \|v\|_{L_2(I;V)}$. Note that $\mathcal{X} = (L_2(I) \otimes V) \cap (H^1_{(0)}(I) \otimes V')$ and $\mathcal{Y} = L_2(I) \otimes V$ which will allow for a tensor product discretization. Then definitions $b(w, v) := \int_I [\langle \dot{w}(t), v(t)\rangle_{V'\times V} + a(w(t), v(t))]\,dt$ and $f(v) := \int_I \langle g(t), v(t)\rangle_{V'\times V} dt$ yield the space-time variational formulation

$$u \in \mathcal{X} : \qquad b(u, v) = f(v), \qquad \forall v \in \mathcal{Y}. \tag{2}$$

The well-posedness of (2) has been shown (under suitable assumptions) in [6, Theorem 5.1].

The approach of [6] can also yield an estimate for the inf-sup constant $\beta := \inf_{w\in\mathcal{X}} \sup_{v\in\mathcal{Y}} \frac{b(w,v)}{\|w\|_{\mathcal{X}}\,\|v\|_{\mathcal{Y}}}$. We define $\varrho := \sup_{0\neq\phi\in V} \frac{\|\phi\|_H}{\|\phi\|_V}$ and $\beta^*_a := \inf_{\phi\in V} \sup_{\psi\in V} \frac{a(\psi,\phi)}{\|\phi\|_V\,\|\psi\|_V}$; we then claim

Proposition 1 *Assume that there exist* $M_a < \infty$, $\alpha > 0$, *and* $\lambda \geq 0$ *such that* $|a(\psi, \phi)| \leq M_a \, \|\psi\|_V \, \|\phi\|_V$ *(continuity) and* $a(\phi, \phi) + \lambda \, \|\phi\|_H^2 \geq \alpha \|\phi\|_V^2$ *(Gårding) for* $v, w \in V$. *Then, we obtain the inf-sup lower bound* $\beta \geq \beta^{LB} := \frac{\min\{1, (\alpha - \lambda\varrho^2) \min\{1, M_a^{-2}\}\}}{\max\{1, (\beta_a^*)^{-1}\}\sqrt{2}}$.

Proof. (Sketch) Let $0 \neq w \in \mathcal{X}$. Set $z_w := (A^*)^{-1}\dot{w}$ (where $A^*\colon V \to V'$ denotes the adjoint of V) and set $v_w := z_w + w \in \mathcal{Y}$. Then, $\|v_w\|_{L_2(I;V)}^2 \leq 2 \max\{1, (\beta_a^*)^{-2}\} \|w\|_{\mathcal{X}}^2$. Using the estimates $\|\dot{w}(t)\|_{V'} \leq M_a \|z_w(t)\|_V$, $\langle \dot{w}(t), z_w(t) \rangle_{V' \times V} \geq (\alpha - \lambda\varrho^2) M_a^{-2} \|\dot{w}(t)\|_{V'}^2$ and $a(w(t), z_w(t)) = \frac{1}{2} \frac{d}{dt} \|w(t)\|_H^2$ we arrive at $b(w, v_w) \geq (\alpha - \lambda\varrho^2)(M_a^{-2} \|\dot{w}\|_{L_2(I;V')}^2 + \|w\|_{L_2(I;V)}^2) + \|w(T)\|_H^2 \geq \min\{(\alpha - \lambda\varrho^2) \min\{1, M_a^{-2}\}, 1\} \|w\|_{\mathcal{X}}^2 \geq \beta^{\mathrm{LB}} \|w\|_{\mathcal{X}} \, \|v_w\|_{\mathcal{Y}}$, which proves the claim. □

Remark 2 *Note that* β^{LB} *does not depend on the final time. However, the estimate is only meaningful if* $\alpha \geq \lambda\varrho^2$, *i.e., if the system is coercive. In the non-coercive case,* (1) *is often transformed via* $\hat{u}(t) := \mathrm{e}^{-\lambda t} u(t)$ *to obtain a coercive problem; however, this yields an inf-sup bound that behaves as* $\mathrm{e}^{-\lambda T}$ *— often extremely pessimistic and clearly unsuitable for error estimation in long-time integration.*

2. Petrov-Galerkin Truth Approximation

Let $\mathcal{X}_\delta \subset \mathcal{X}$, $\mathcal{Y}_\delta \subset \mathcal{Y}$ be finite dimensional subspaces and $u_\delta \in \mathcal{X}_\delta$ the discrete approximation of (2), i.e., $b(u_\delta, v_\delta) = f(v_\delta)$, $\forall v_\delta \in \mathcal{Y}_\delta$, $s_\delta = \int_0^T \ell(u_\delta(t)) \, dt$. Henceforth, we concentrate on the case $H = L_2(\Omega)$, $V = H_0^1(\Omega)$. Let $\mathcal{X}_\delta = S_{\Delta t} \otimes V_h$, $\mathcal{Y}_\delta = Q_{\Delta t} \otimes V_h$, $\delta = (\Delta t, h)$, where $S_{\Delta t}$, V_h are piecewise linear and $Q_{\Delta t}$ piecewise constant finite elements with respect to triangulations $\mathcal{T}_h^{\text{space}}$ in space and $\mathcal{T}_{\Delta t}^{\text{time}} \equiv \{t^{i-1} \equiv (i-1)\Delta t < t \leq i \, \Delta t \equiv t^i, 1 \leq i \leq r\}$ in time for $\Delta t := T/r$. This coincides with the Crank–Nicolson (CN) scheme if a trapezoidal approximation of the right-hand side temporal integration is used; hence, we can derive error bounds for the CN scheme via our space-time formulation.

We introduce a different norm on $\mathcal{X}$: For $w \in \mathcal{X}$ and $I^i := (t^{i-1}, t^i)$, set $\bar{w}^i := (\Delta t)^{-1} \int_{I^i} w(t) \, dt \in V$ and $\bar{w} := \sum_{i=1}^r \chi_{I^i} \otimes \bar{w}^i \in L_2(I; V)$, where χ_{I^i} is the characteristic function on I^i; then, set $|||w|||_{\mathcal{X},\delta}^2 := \|\dot{w}\|_{L_2(I;V')}^2 + \|\bar{w}\|_{L_2(I;V)}^2 + \|w(T)\|_H^2$ and the inf-sup parameter $\beta_\delta := \inf_{w_\delta \in \mathcal{X}_\delta} \sup_{v_\delta \in \mathcal{Y}_\delta} \frac{b(w_\delta, v_\delta)}{|||w_\delta|||_{\mathcal{X},\delta} \, \|v_\delta\|_{\mathcal{Y}}}$ as well as the stability parameter $\gamma_\delta := \sup_{w_\delta \in \mathcal{X}_\delta} \sup_{v_\delta \in \mathcal{Y}_\delta} \frac{b(w_\delta, v_\delta)}{|||w_\delta|||_{\mathcal{X},\delta} \, \|v_\delta\|_{\mathcal{Y}}}$.

Proposition 3 *Let* $a(\cdot, \cdot)$ *be symmetric, bounded and coercive and set* $\|\phi\|_V^2 := a(\phi, \phi)$, $\phi \in V$; *then we have* $\beta_\delta = \gamma_\delta = 1$.

Proof. (Sketch) Since $v_\delta \in \mathcal{Y}_\delta$ is piecewise constant in time, we have $\int_I a(w_\delta, v_\delta) \, dt = \int_I a(\bar{w}_\delta, v_\delta) \, dt$ for all $w_\delta \in \mathcal{X}_\delta$. Hence, $b(w_\delta, v_\delta) = \int_I a(A_h^{-1} \dot{w}_\delta + \bar{w}_\delta, v_\delta) \, dt$, where $z_\delta := A_h^{-1} \dot{w}_\delta$ is defined by $a(z_\delta, \phi_h) = \langle \dot{w}_\delta, \phi_h \rangle_{V' \times V}$, $\forall \phi_h \in V_h$. Note that $\|A_h^{-1} \dot{w}_\delta\|_V = \|\dot{w}_\delta\|_{V'}$. We may prove that for any $v_\delta \in \mathcal{Y}_\delta$ there exists a unique $z_\delta \in \mathcal{X}_\delta$ such that $\int_I a(A_h^{-1} \dot{z}_\delta + \bar{z}_\delta, q_\delta) \, dt = \int_I a(v_\delta, q_\delta) \, dt$ for all $q_\delta \in \mathcal{Y}_\delta$. Note that $v_\delta := A_h^{-1} \dot{z}_\delta + \bar{z}_\delta \in \mathcal{Y}_\delta$ for $z_\delta \in \mathcal{X}_\delta$ and we obtain $b(w_\delta, v_\delta) = \int_I a(A_h^{-1} \dot{w}_\delta + \bar{w}_\delta, A_h^{-1} \dot{z}_\delta + \bar{z}_\delta) \, dt$ so that $\sup_{v_\delta \in \mathcal{Y}_\delta} \frac{b(w_\delta, v_\delta)}{\|v_\delta\|_{\mathcal{Y}}} = \sup_{v_\delta \in \mathcal{Y}_\delta} (\int_I a(A_h^{-1} \dot{w}_\delta + \bar{w}_\delta, A_h^{-1} \dot{z}_\delta + \bar{z}_\delta) \, dt) / \|A_h^{-1} \dot{z}_\delta + \bar{z}_\delta\|_{\mathcal{Y}} = \|A_h^{-1} \dot{w}_\delta + \bar{w}_\delta\|_{\mathcal{Y}}$. The fact that $\|A_h^{-1} \dot{w}_\delta + \bar{w}_\delta\|_{\mathcal{Y}}^2 = \|A_h^{-1} \dot{w}_\delta\|_{L_2(I;V)}^2 + \|\bar{w}_\delta\|_{L_2(I;V)}^2 + 2 \int_I \langle \dot{w}_\delta, \bar{w}_\delta \rangle_{V' \times V} \, dt = \|\dot{w}_\delta\|_{L_2(I;V')}^2 + \|\bar{w}_\delta\|_{L_2(I;V)}^2 + \|w_\delta(T)\|_H^2 = |||w_\delta|||_{\mathcal{X},\delta}^2$ proves the assertion. □

Remark 4 *Proposition 3 also shows the well-posedness of the discrete problem with continuity and inf-sup constant being unity.*

3. The Reduced Basis Method (RBM)

Now, let $\mu = (\mu_1, \mu_2) \in \mathcal{D} := \mathbb{R}^2$ be a parameter vector and $A = A(\mu) := -\Delta u + \mu_1\, \boldsymbol{\beta}(x) \cdot \nabla u + \mu_2\, u$, i.e., a diffusion-convection-reaction operator with convection field $\boldsymbol{\beta}$. We then introduce a standard Reduced Basis (RB) approximation [1,4,5] for the Crank–Nicolson interpretation of our discrete problem, $u_N(\mu) \in \mathcal{X}_{\Delta t,N} = S_{\Delta t} \otimes V_N$; here $V_N \subset V_h$ is an RB space provided for example by the POD-Greedy procedure of [2]. The RB output is then given by $s_N = \int_I \ell(u_N(t))dt (= \int_I \ell(\bar{u}_N(t))dt)$. (It is possible, alternatively, to consider a space–time RB approximation as well [7].) It is then simple [5] to demonstrate

Proposition 5 *The RB error satisfies* $|||u_\delta - u_N|||_{\mathcal{X},\delta} \leq \|r_N\|_{\mathcal{Y}'}/\beta_\delta^{\mathrm{LB}}$*, where* $r_N(v) := f(v) - b(u_N, v)$*,* $\forall v \in \mathcal{Y}$*, and* β_δ^{LB} *is a lower bound for the* β_δ *defined in Proposition 3. Furthermore,* $|s_\delta - s_N| \leq \|\ell\|_{V'}\sqrt{T}\|r_N\|_{\mathcal{Y}'}/\beta_\delta^{LB}$*.*

The utility of these *a posteriori* error bounds is critically dependent on the dependence of β_δ as a function of the parameter μ and final time T, $\beta_\delta(\mu; T)$.

We briefly comment on the computational implications of this space-time error bound. As always, our model problem (as is the case here) must honor the "affine-in-functions-of-parameter" condition [5] to permit effective offline–online computation of the reduced basis approximation and *a posteriori* error bounds. The current formulation introduces the further complication of the space–time norms. In fact, calculation of the dual norm $\|\cdot\|_{\mathcal{Y}'}$ (through the corresponding Riesz representation [5]) does not couple different time steps/elements, and hence the additional online difficulty is relatively minor. (The offline stage for computation of the inf-sup lower bound by the Successive Constraint Method [5,8] does require special treatment, in particular due to the norm $|||\cdot|||_{\mathcal{X},\delta}$.)

4. Numerical Results

We report numerical results for the Crank–Nicolson scheme for various choices of the parameters μ_1, μ_2 as well as for different time steps Δt and uniform mesh sizes h. For simplicity, we consider the univariate case (in space) $\Omega = (0, 1)$ and choose $\boldsymbol{\beta}(x) = x - \frac{1}{2}$. Let us denote by $\beta_\delta(\mu; T)$, $\gamma_\delta(\mu; T)$ the numerical values for the truth inf-sup and continuity constants, respectively, corresponding to parameter μ and final time T. We start by confirming Proposition 3. Thus, we choose $\mu_1 = \mu_2 = 0$; for several values of T, h, and Δt we invariantly obtain 1.000 for both $\beta_\delta(\mu; T)$ and $\gamma_\delta(\mu; T)$, as must be the case.

Next, we investigate the case of convection, $\mu_2 = 0$, in which case a is coercive only for $\mu_1 < 2\pi^2$. We obtain $\beta_\delta((50, 0); 1.0) = 0.050$, $\beta_\delta((50, 0); 2.0) = 0.027$ ($\gamma_\delta = 2.60$) and $\beta_\delta((100, 0); 1.0) = 0.019$, $\beta_\delta((100, 0); 2.0) = 0.010$ ($\gamma_\delta = 5.6$). These numbers are relatively invariant for sufficiently small h and Δt. We observe numerically an overall behavior of $\beta_\delta((\mu_1, 0); T) \sim (\mu_1 T)^{-1}$ and $\gamma_\delta((\mu_1, 0); T) \sim \mu_1$ (the latter is readily proven, but not the former). Note $T = \mathcal{O}(1)$ is effectively a "long time" in convective units, $1/\mu_1$. We emphasize that although the problem is non-coercive, the problem is asymptotically stable in the sense that all eigenvalues σ of $-a(\psi, \phi) = \sigma\langle\psi, \phi\rangle_{V' \times V}$ lie in the left-hand plane; this stability is reflected in the inf-sup behavior. In contrast, a standard energy approach [3] gives effective inf-sup constants on the order of $e^{-\mu_1 T}$ (here about 10^{-8}). Hence, the traditional method fails to provide useful results, whereas our new approach, which reflects the true time-coupled properties of the system, yields relatively sharp error bounds.

Finally, we consider the case $\mu_1 = 0$ which gives rise to an asymptotically unstable (and non-coercive) system for $\mu_2 < -\pi^2$. This means that any error estimate *must* grow exponentially with the final time T. We observe this for our estimator as well, e.g. $\beta_\delta((0, -20); 1.0) = 3.93 \cdot 10^{-5}$ (order of $e^{\mu_2 T}$).

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