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INTERIOR A POSTERIORI ERROR ESTIMATES FOR TIME DISCRETE APPROXIMATIONS OF PARABOLIC PROBLEMS

CHRISTIAN LUBICH AND CHARALAMBOS MAKRIDAKIS

ABSTRACT. We derive a posteriori estimates for single-step methods, including Runge–Kutta and Galerkin methods for the time discretization of linear parabolic equations. We focus on the estimation of the error at the nodes and derive a posteriori estimates that show the full classical order (superconvergence order) in the interior of the spatial domain without any compatibility assumptions.

1. INTRODUCTION

This paper is devoted to a posteriori error estimation of one-step time discretization methods for linear parabolic differential equations. The expected order of accuracy at the time nodes is higher than the order expected in other points provided compatibility conditions are satisfied that are, however, unrealistic with all kinds of (Dirichlet or Neumann or Robin) boundary conditions except periodic boundary conditions. In the case of Runge-Kutta methods, the maximal order at the nodal points is the classical order of the method. Thus if the required compatibility conditions are not fully satisfied an *order reduction* with respect to the classical order is observed.

In the present paper our goal is twofold, we first give a new proof of the a posteriori error bounds at the nodes and next we show that the order reduction does not occur in the a posteriori control of the error in the interior of the spatial domain. Here we use the unified treatment of essentially all single-step time-stepping schemes of [3] and of the corresponding reconstructions. A key novel feature of our analysis is an error representation formula based on Duhamel's principle. Through this expression a direct superconvergence analysis for Runge-Kutta and Galerkin time discretization schemes is possible. Our interior results are a posteriori analogs of the a priori estimates of [9].

For previous a posteriori results using various one step time discretization methods we refer, e.g., to [1, 2, 3, 5, 6, 7, 8, 10, 12]. A posteriori time-superconvergence results for fully discrete schemes based on dG piecewise linear time discretization methods were derived in [5].

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1.1. **Discretization methods.** We consider linear parabolic equations in a Hilbert space setting: Find $u : [0,T] \to D(A)$ satisfying

$$\begin{cases} u'(t) + Au(t) = f(t), \quad 0 < t < T, \\ u(0) = u^0, \end{cases} \tag{1.1}$$

with A a positive definite, self-adjoint, linear operator on a Hilbert space $(H, \langle\cdot,\cdot\rangle)$ with domain $D(A)$ dense in H, and a given forcing term $f : [0,T] \to H$.

We will use the notation and formalism of [3] to describe the numerical methods considered. We consider piecewise polynomial functions in arbitrary partitions $0 = t_0 < t_1 < \cdots < t_N = T$ of $[0,T]$, and let $J_n := (t_{n-1}, t_n]$ and $k_n := t_n - t_{n-1}$. We denote by $\mathcal{V}_q^{\mathrm{d}}, q \in \mathbb{N}_0$, the space of functions that are piecewise polynomials of degree at most q in time in each subinterval J_n with coefficients in $V = D(A^{1/2})$, without continuity requirements at the nodes t_n. The elements of $\mathcal{V}_q^{\mathrm{d}}$ are taken continuous to the left at the nodes t_n; $\mathcal{V}_q(J_n)$ consist of the restrictions to J_n of the elements of $\mathcal{V}_q^{\mathrm{d}}$. The spaces $\mathcal{H}_q^{\mathrm{d}}$ and $\mathcal{H}_q(J_n)$ are defined similarly by requiring that the coefficients are in H. Let $\mathcal{V}_q^{\mathrm{c}}$ and $\mathcal{H}_q^{\mathrm{c}}$ be the spaces of the *continuous* elements of $\mathcal{V}_q^{\mathrm{d}}$ and $\mathcal{H}_q^{\mathrm{d}}$. For $v \in \mathcal{V}_q^{\mathrm{d}}$ we let $v^n := v(t_n)$, $v^{n+} := \lim_{t \downarrow t_n} v(t)$.

To define the time stepping methods we introduce the operator $\mathit{\Pi}_{q-1}$ to be a *projection operator* to piecewise polynomials of degree $q-1$, $\mathit{\Pi}_{q-1} : C([0,T]; H) \to \oplus_{n=1}^N \mathcal{H}_{q-1}(J_n)$. Also, $\widetilde{\mathit{\Pi}}_q : \mathcal{H}_q(J_n) \to \mathcal{H}_\ell(J_n)$ is an operator mapping polynomials of degree q to polynomials of degree ℓ, with $\ell = q$ or $\ell = q-1$; $\mathit{\Pi}_{q-1}$ and $\widetilde{\mathit{\Pi}}_q$ are defined in a reference time interval and then transformed into J_n.

The time discrete approximation U to the solution u of (1.1) is defined as follows: We seek $U \in \mathcal{V}_q^{\mathrm{c}}$ satisfying the initial condition $U(0) = u^0$ as well as

$$U'(t) + \mathit{\Pi}_{q-1} F(t, \widetilde{\mathit{\Pi}}_q U(t)) = 0 \quad \forall t \in J_n, \tag{1.2}$$

where $F(t,v) = Av - f(t)$. An equivalent Galerkin formulation is

$$\int_{J_n} \big[\langle U', v\rangle + \langle \mathit{\Pi}_{q-1} F(t, \widetilde{\mathit{\Pi}}_q U(t)), v\rangle \big]\, dt = 0 \quad \forall v \in \mathcal{V}_{q-1}(J_n), \tag{1.3}$$

for $n = 1, \dots, N$, see [3]. The above formalism covers a large class of one-step time discretization schemes. In particular, the *continuous Galerkin (cG) method* is

$$U'(t) + P_{q-1} F(t, U(t)) = 0 \quad \forall t \in J_n, \tag{1.4}$$

with $\mathit{\Pi}_{q-1} := P_{q-1}$, with P_ℓ denoting the L^2 orthogonal projection operator onto $\mathcal{H}_\ell(J_n)$. Furthermore, in [3] was shown that (1.3) describes other important implicit single-step time stepping methods: the *RK collocation methods* (RK-C) with $\mathit{\Pi}_{q-1} := I_{q-1}$ and $\widetilde{\mathit{\Pi}}_q = I$, with I_{q-1} denoting the interpolation operator at the collocation points; all other *interpolatory RK methods* with $\mathit{\Pi}_{q-1} := I_{q-1}$, and appropriate $\widetilde{\mathit{\Pi}}_q$ (with $\ell = q$) ; the *discontinuous Galerkin (dG) method* with $\mathit{\Pi}_{q-1} := P_{q-1}$ and $\widetilde{\mathit{\Pi}}_q = I_{q-1}$, where I_{q-1} is the interpolation operator at the Radau points $0 < c_1 < \cdots < c_q = 1$ (so $\ell = q-1$).

1.2. **Superconvergence – classical order.** A key assumption for the time-discretization methods related to the accuracy at the time nodes is: We assume that the method (1.2) is associated to q *pairwise distinct* points $c_1, \dots, c_q \in [0,1]$ with the property

$$\int_0^1 \prod_{i=1}^{q} (\tau - c_i) v(\tau)\, d\tau = 0 \quad \text{for all polynomials } v \text{ of degree} \le r. \tag{1.5}$$

This condition induces orthogonality conditions at each interval J_n with $t_{n,i} := t_{n-1} + c_i k_n$, $i = 1, \dots, q$. These points will be associated to projections (or interpolants) used to define the method (1.2); see [3] for details. The *superconvergence order* or *classical order* p of the method at the nodes is denoted

$$p = q + 1 + r\,, \tag{1.6}$$

which is equal to the order of the interpolatory quadrature with nodes c_i.

2. Nodal error analysis in H

2.1. **Main error equation.** As in [3] we compare the solution u to the reconstruction $\hat{U}$ of U defined through

$$\widehat{U}(t) := U(t_{n-1}) - \int_{t_{n-1}}^{t} \widehat{\Pi}_q \big[A \widetilde{\Pi}_q U - f\big](s)\, ds \quad \forall t \in J_n. \tag{2.1}$$

where the projection operators $\widehat{\Pi}_q$ onto $\mathcal{H}_q(J_n), n = 1, \dots, N$, are chosen to agree with Π_{q-1} at $t_{n,i}$:

$$(\widehat{\Pi}_q - \Pi_{q-1}) w(t_{n,i}) = 0, \quad i = 1, \dots, q, \quad \forall w \in C([0,T]; H). \tag{2.2}$$

In view of (1.5) for $v(\tau) = 1$ and (2.2), we obtain $\widehat{U}(t_n) = U(t_n)$ and conclude that $\widehat{U}$ is *continuous*. Furthermore, $\widehat{U}$ satisfies

$$\widehat{U}'(t) = -\widehat{\Pi}_q [A \widetilde{\Pi}_q U(t) - f(t)] = -\widehat{\Pi}_q F(t, \widetilde{\Pi}_q U(t)) \quad \forall t \in J_n, \tag{2.3}$$

which has a similar structure to (1.2). The motivation for introducing $\hat{U}$ goes back to [1, 2] and details for its various properties are discussed in [3]. In the sequel we will specify the choices of the projections for different methods. At this point we just mention two key properties of $\hat{U}$: The first one is the orthogonality property which follows by (2.2)

$$\int_{J_n} \langle (\widehat{\Pi}_q - \Pi_{q-1}) w(s), v(s) \rangle\, ds = 0 \quad \forall w \in C([0,T]; H), \ \ v \in \mathcal{H}_r(J_n), \tag{2.4}$$

for $n = 1, \dots, N$. The second one is a further assumption on Π_{q-1}, namely for all $V \in \mathcal{H}_q(J_n)$,

$$\int_{J_n} \langle V - \Pi_{q-1} V, v \rangle dt = 0 \quad \forall v \in \mathcal{H}_{r-1}(J_n), \tag{2.5}$$

which, in view of (2.4), yields

$$\int_{J_n} \langle \widehat{\Pi}_q V - V, v \rangle dt = 0 \quad \forall v \in \mathcal{H}_{r-1}(J_n). \tag{2.6}$$

Condition (2.5) is verified by both cG and dG methods, for which $\mathit{\Pi}_{q-1} = P_{q-1}$, as well as by RK methods, for which $\mathit{\Pi}_{q-1} = I_{q-1}$.

We state now the *main error equation*, which is the starting point of our analysis. Let $\widehat{R}$ be the residual of $\widehat{U}$,

$$-\widehat{R}(t) := \widehat{U}'(t) + A\widehat{U}(t) - f(t). \tag{2.7}$$

Subtracting (2.7) from the differential equation in (1.1), we obtain the equation

$$\hat{e}'(t) + A\hat{e}(t) = \widehat{R}(t), \tag{2.8}$$

for the error $\hat{e} := u - \widehat{U}$, which we rewrite in the form

$$\hat{e}'(t) + A\hat{e}(t) = R_{\widehat{U}}(t) + R_{\widetilde{\mathit{\Pi}}_q}(t) + R_{\widehat{\mathit{\Pi}}_q}(t) + R_f(t) \tag{2.9}$$

with

$$R_{\widehat{U}} := A(U - \widehat{U}), \quad R_{\widehat{\mathit{\Pi}}_q} := A(\widehat{\mathit{\Pi}}_q - I)\widetilde{\mathit{\Pi}}_q U, \quad R_f := f - \widehat{\mathit{\Pi}}_q f, \tag{2.10}$$

and

$$R_{\widetilde{\mathit{\Pi}}_q}(t) := A(\widetilde{\mathit{\Pi}}_q U - U). \tag{2.11}$$

Notice that $R_{\widehat{\mathit{\Pi}}_q}$ vanishes when $\widehat{\mathit{\Pi}}_q$ is a projector over $\mathcal{H}_q(J_n)$ whereas $R_{\widetilde{\mathit{\Pi}}_q}$ vanishes when $\widetilde{\mathit{\Pi}}_q = I$.

2.2. **Error representation via Duhamel's principle.** We now apply Duhamel 's principle to (2.8):

$$\hat{e}(t) = \int_0^t E_A(t-s)\widehat{R}(s)\, ds\,, \tag{2.12}$$

where $E_A(t) = e^{-At}$ is the solution operator of the homogeneous equation

$$v'(t) + Av(t) = 0, \quad v(0) = w, \tag{2.13}$$

i.e., $v(t) = E_A(t)w$. The family of operators $E_A(t)$ is athe ope semigroup of contractions on H with generator $-A$. The following properties are well known, cf., e.g., Crouzeix [4], Thomée [12],

$$\frac{d^\ell}{dt^\ell} E_A(t)w = (-A)^\ell E_A(t)w\,, \quad \ell \geq 0\,, \tag{2.14}$$

and

$$|A^\ell E_A(t)w| \leq C_A \frac{1}{t^{\ell-m}} |A^m w| \quad \ell \geq m \geq 0\,. \tag{2.15}$$

Since A and E_A commute, (2.15) implies

$$|\, E_A(t)\, A^\ell w| \leq C_A \frac{1}{t^{\ell-m}} |A^m w|\,, \quad \ell \geq m \geq 0\,, \tag{2.16}$$

whence $|E_A w| \leq C_A t^{-m} |A^{-m} w|$.

Starting from (2.12) we derive now a different error representation formula involving time derivatives of E_A. In the interval $t_{n-1} \le s \le t_n$ we define the scaled jth antiderivative of $\widehat{R}$ as

$$\widehat{R}^{[j]}_n(s) := k_n^{-j} \int_{t_{n-1}}^{s} \int_{t_{n-1}}^{s_{j-1}} \cdots \int_{t_{n-1}}^{s_1} \widehat{R}(\tau)\ ds_1 ds_2 \dots ds_{j-1} d\tau\,, \quad j \ge 1\,. \tag{2.17}$$

Then, one has,

$$k_n^j \widehat{R}^{[j]}_n(s) = \int_{t_{n-1}}^{s} \frac{(s-\tau)^{j-1}}{(j-1)!}\, \widehat{R}(\tau) d\tau\,, \quad j \ge 1\,. \tag{2.18}$$

Using (2.14) ,(2.18) and integrating by parts in (2.12) we obtain,

$$\begin{aligned} \int_{t_{n-1}}^{t} E_A(t-s)\widehat{R}(s)\,ds &= \int_{t_{n-1}}^{t} E_A(t-s) k_n \frac{d}{ds} \widehat{R}^{[1]}_n(s)\,ds \\ &= \int_{t_{n-1}}^{t} E_A(t-s) A\, k_n \widehat{R}^{[1]}_n(s)\,ds + k_n \widehat{R}^{[1]}_n(t)\,. \end{aligned} \tag{2.19}$$

Further,

$$\begin{aligned} \int_{t_{n-1}}^{t} E_A(t-s) A\, k_n \widehat{R}^{[1]}_n(s)\,ds &= \int_{t_{n-1}}^{t} E_A(t-s) A \frac{d}{ds} k_n^2 \widehat{R}^{[2]}_n(s)\,ds \\ &= \int_{t_{n-1}}^{t} E_A(t-s) A^2\, k_n^2 \widehat{R}^{[2]}_n(s)\,ds + A k_n^2 \widehat{R}^{[2]}_n(t)\,. \end{aligned} \tag{2.20}$$

Thus, for any ρ,

$$\begin{aligned} \int_{t_{n-1}}^{t} E_A(t-s)\widehat{R}(s)\,ds = \int_{t_{n-1}}^{t} & E_A(t-s) A^{\rho}\, k_n^{\rho} \widehat{R}^{[\rho]}_n(s)\,ds \\ &+ \sum_{j=1}^{\rho} A^{j-1} k_n^j \widehat{R}^{[j]}_n(t)\,. \end{aligned} \tag{2.21}$$

Notice that, still for $t \ge t_{n-1}$, and for $s \in J_m$, $E_A(t-s) = E_A(t-t_m)E_A(t_m-s)$, thus

$$\int_{J_m} E_A(t-s)\widehat{R}(s)\,ds = E_A(t-t_m) \int_{t_{m-1}}^{t_m} E_A(t_m-s)\widehat{R}(s)\,ds\,. \tag{2.22}$$

Treating the last integral as (2.21) we have proved the following proposition.

Proposition 2.1. *Let $t \in J_n$, then with $\widehat{R}^{[j]}_n$ defined by* (2.17)*, the following error representation formula holds:*

(2.23)

$$\begin{aligned} \hat{e}(t) = \int_{t_{n-1}}^{t} & E_A(t-s) k_n^{\rho-1} A^{\rho-1} \widehat{R}^{[\rho-1]}_n(s)\,ds + \sum_{j=1}^{\rho-1} k_n^j A^{j-1} \widehat{R}^{[j]}_n(t) \\ &+ \sum_{m=1}^{n-1} \Big(\int_{J_m} E_A(t-s) k_m^{\rho} A^{\rho} \widehat{R}^{[\rho]}_m(s)\,ds + E_A(t-t_m) \sum_{j=1}^{\rho} k_m^j A^{j-1} \widehat{R}^{[j]}_m(t_m) \Big). \end{aligned}$$

The error representation formula (2.23) will be the starting point of our analysis. We mainly consider $t = t_n$, which leads to a posteriori error control at the time nodes. We will treat separately Galerkin schemes and Runge-Kutta methods. We use (2.16) in the above error representation formula to obtain

$$|e(t_n)| = |\hat{e}(t_n)| \le C_A \int_{J_n} \Big| k_n^{\rho-1} A^{\rho-1}\, \widehat{R}_n^{[\rho-1]}(s) \Big|\, ds + \Big| \sum_{j=1}^{\rho-1} k_n^j A^{j-1} \widehat{R}_n^{[j]}(t_n) \Big|$$
$$+ C_A \sum_{m=1}^{n-1} \Big(\int_{J_m} \Big| \frac{1}{(t_n - s)}\, k_m^{\rho} A^{\rho-1}\, \widehat{R}_m^{[\rho]}(s) \Big|\, ds + \Big| \sum_{j=1}^{\rho} k_m^j A^{j-1} \widehat{R}_m^{[j]}(t_m) \Big| \Big) .$$

The terms in the above relation are treated in a different manner. The expression (2.18) yields

$$\int_{J_n} \Big| k_n^{\rho-1} A^{\rho-1}\, \widehat{R}_n^{[\rho-1]}(s) \Big|\, ds \le \frac{k_n^{\rho}}{\rho!} \sup_{s\in J_n} \big| A^{\rho-1} \widehat{R}(s) \big| ,$$

and

$$\sum_{m=1}^{n-1} \int_{J_m} \Big| \frac{1}{(t_n - s)}\, k_m^{\rho} A^{\rho-1}\, \widehat{R}_m^{[\rho]}(s) \Big|\, ds \le \max_m \frac{k_m^{\rho}}{\rho!} \sup_{s\in J_m} \big| A^{\rho-1} \widehat{R}(s) \big| \int_0^{t_{n-1}} \frac{1}{t_n - s} ds$$
$$\le \log \frac{t_n}{k_n} \max_{0\le m\le n} \frac{k_m^{\rho}}{\rho!} \sup_{s\in J_m} \big| A^{\rho-1} \widehat{R}(s) \big| .$$

Let

$$L_n := \log \frac{t_n}{k_n} + 1, \tag{2.24}$$

then we have

$$|e(t_n)| \le C_A L_n \max_{1\le m\le n} \frac{k_m^{\rho}}{\rho!} \sup_{s\in J_m} \big| A^{\rho-1} \widehat{R}(s) \big| + \sum_{m=1}^{n} \Big| \sum_{j=1}^{\rho} k_m^j A^{j-1} \widehat{R}_m^{[j]}(t_m) \Big| . \tag{2.25}$$

We are ready now to derive the main estimates of this section.

2.3. **Nodal estimates for Galerkin schemes.** In the case of Galerkin schemes (continuous or discontinuous) the error estimates are direct consequences of (2.25). The main point here is that the terms involving $\widehat{R}_m^{[j]}(t_m)$ all vanish due to the orthogonality. In this case we have the following result.

Theorem 2.1. *Let $q \ge 2$ and $\widehat{R} \in D(A^{\rho-1})$ hold for some $1 \le \rho \le q-1$. Then, the error of the* continuous Galerkin *method of order q and of the* discontinuous Galerkin *method dG$(q-1)$ satisfies*

$$|e(t_n)| \le C_A L_n \max_{1\le m\le n} \frac{k_m^{\rho}}{\rho!} |A^{\rho-1} \widehat{R}|_{L^\infty(J_m)}, \tag{2.26}$$

where C_A is the stability constant in (2.15) *and L_n is given in* (2.24).

Proof. Recall that both methods are written in the form

$$U'(t) + P_{q-1}F(t, \widetilde{\Pi}_q U(t)) = 0 \quad \forall t \in J_n, \tag{2.27}$$

where $\widetilde{\Pi}_q = I$ for the *cG method*, and for the *dG method* $\widetilde{\Pi}_q = I_{q-1}$, where I_{q-1} is the interpolation operator at the Radau points. Notice that in both cases $\Pi_{q-1} = P_{q-1}$. In view of (2.3),

$$\widehat{U}'(t) + \widehat{\Pi}_q F(t, \widetilde{\Pi}_q U(t)) = 0 \quad \forall t \in J_n, \tag{2.28}$$

with $\widehat{\Pi}_q = P_q$. Therefore in the case of the *cG method* $\widehat{R}(t) = R_{\widehat{U}}(t) + R_{\widetilde{\Pi}_q}(t) + R_{\widehat{\Pi}_q}(t) + R_f(t)$ where

$$R_{\widehat{U}} = A(U - \widehat{U}), \quad R_{\widehat{\Pi}_q} = A(P_q - I)U, \quad R_{\widetilde{\Pi}_q}(t) = 0, \quad R_f = f - P_q f\,. \tag{2.29}$$

Hence by (2.4) we have

$$\int_{J_n} \langle \widehat{R}, v\rangle\, dt = 0 \qquad \forall v \in \mathcal{V}_{q-2}(J_n). \tag{2.30}$$

In view of the definition of $\widehat{R}^{[j]}_m$ of (2.18), we obtain

$$\widehat{R}^{[j]}_m(t_m) = 0, \tag{2.31}$$

so that the terms involving $\widehat{R}^{[j]}_m(t_m)$ in (2.25) vanish and (2.26) follows.

In the case of the dG method, the properties of Gauss-Radau quadrature imply

$$\int_{J_n} \langle A(I_{q-1}U - U), v\rangle\, dt = 0 \quad \forall v \in \mathcal{V}_{q-2}(J_n). \tag{2.32}$$

Thus, given that in the expression for $\widehat{R}$ the difference to the cG case is that $R_{\widetilde{\Pi}_q} + R_{\widehat{\Pi}_q} = A(I_{q-1}U - U)$, (2.30) still holds in this case as well. The proof is thus complete. □

Remark 2.1 (Rate of convergence)**.** One notices that the highest possible order of the residual $\widehat{R}$ for dG is q in (2.26), whereas it is $q+1$ for cG. Hence the highest order in (2.26) is $2q$ in for cG and $2q-1$ for dG, as expected. The difference is due to the fact that in the dG case the residual $\widehat{R}$ contains an additional term of the form $R_{\widetilde{\Pi}_q} = A(U - I_{q-1}U)$. Note, however, that the full order is attained only if $\widehat{R} \in D(A^{q-2})$. For $q > 2$ this is usually not satisfied, since it requires unnatural compatibility conditions at the boundary when A is an elliptic operator with Dirichlet or Neumann boundary conditions.

2.4. **Nodal estimates for collocation methods.** In this section we establish a posteriori estimates for the nodal error for RK collocation methods. We recall that the classical order p of the RK-C method satisfies $q+1 \le p \le 2q$, i.e., $1 \le \rho \le r = p - q - 1$. The main difference to the case of Galerkin schemes is that the terms involving $\widehat{R}^{[j]}_m(t_m)$ give rise to non-zero expressions involving the inhomogeneity f. In this case we choose $\widehat{\Pi}_q = \widehat{I}_q$, [2, 3]. $\widehat{I}_q$ is an extended interpolation operator defined on continuous functions v with the following two key properties

$$\widehat{I}_q v \in \mathcal{H}_q(J_n), \quad (\widehat{I}_q v)(t_{n,i}) = v(t_{n,i}), \quad i = 1, \dots, q\,. \tag{2.33}$$

$\widehat{I}_q$ interpolates v at one more point, either inside J_n either outside given that v is defined at an extended interval. This issue was discussed in detail in [3].

Now, as before we start from $\widehat{R}(t) = R_{\widehat{U}}(t) + R_{\widetilde{\Pi}_q}(t) + R_{\widehat{\Pi}_q}(t) + R_f(t)$ where

$$R_{\widehat{U}} = A(U - \widehat{U}), \quad R_{\widehat{\Pi}_q} = A(\widehat{I}_q - I)U, \quad R_{\widetilde{\Pi}_q}(t) = 0, \quad R_f = f - \widehat{I}_q f\,. \tag{2.34}$$

Therefore by the assumptions on $\widehat{I}_q$ we have

$$\int_{J_n} \langle R_{\widehat{U}} + R_{\widehat{\Pi}_q} + R_{\widetilde{\Pi}_q}(t), v\rangle\, dt = 0 \quad \forall v \in \mathcal{H}_{r-1}(J_n). \tag{2.35}$$

Concerning the remaining term R_f, we introduce the notation

$$E^{[j]}_{f,n} = \int_{J_n} \frac{(t_n - \tau)^{j-1}}{(j-1)!}\, R_f(\tau)\, d\tau\,, \quad 1 \le j \le r\,. \tag{2.36}$$

This is just the quadrature error of the function $(t_n - \tau)^{j-1}/(j-1)! \cdot f(\tau)$ over the interval J_n,

$$E^{[j]}_{f,n} = \int_{J_n} \frac{(t_n - \tau)^{j-1}}{(j-1)!}\, f(\tau)\, d\tau - k_n \sum_{i=1}^{q} b_i\, \frac{((1-c_i)k_n)^{j-1}}{(j-1)!}\, f(t_{n-1} + c_i k_n),$$

which is of optimal order $O(k_n^{p+1})$ if f is p-times continuously differentiable. Then, in view of the definition of $\widehat{R}^{[j]}_n$ of (2.18) and due to (2.35), we have

$$k_n^j \widehat{R}^{[j]}_n(t_n) = E^{[j]}_{f,n}\,.$$

With (2.25) we therefore obtain the following result. A similar result holds for perturbed collocation methods, [11], compare to [3].

Theorem 2.2. *Let the classical order p of a $q-$stage Runge-Kutta collocation method satisfy $p \ge q+2$ and let $\widehat{R}, f \in D(A^{\rho-1})$ for $1 \le \rho \le r = p-q-1$. Then the following a posteriori error estimate is valid at the nodes t_n :*

$$|e(t_n)| \le C_A L_n \max_{1\le m\le n} \frac{k_m^\rho}{\rho!} |A^{\rho-1}\widehat{R}|_{L^\infty(J_m)} + \sum_{m=1}^{n}\sum_{j=1}^{\rho} \Big| A^{j-1} E^{[j]}_{f,m}\Big|.$$

The full classical order p is attained when $\widehat{R}, f \in D(A^{r-1})$, which for $r > 1$ again imposes unnatural compatibility conditions.

Remark 2.2. The estimate in [3] for RK collocation methods is similar. The first term on the right hand side is the same but the term involving the quadrature errors $E^{[j]}_{f,m}$ differs to the one of [3] which is

$$C_A L_n \sum_{j=0}^{\rho-1} \max_{1\le m\le n} \Big(k_m^j |A^{j-1}\big(f - \widehat{I}_{q+\rho-j} f\big)|_{L^\infty(J_m)}\Big). \tag{2.37}$$

The auxiliary interpolator operators $\widehat{I}_\ell$ are defined as follows: Let $\hat{t}_{m,j} \in J_m$, with $j = 1, \ldots, \rho$, be pairwise distinct and different from $t_{m,i}$, with $i = 0, \ldots, q$. The operator $\widehat{I}_\ell$

is an interpolation operator of order ℓ with $\ell = q+1, \dots, q+\rho$, defined on continuous functions v on $[0,T]$ and values on $\mathcal{H}_\ell(J_m)$:

$$(\widehat{I}_\ell v)(\sigma) = v(\sigma), \quad \sigma = t_{m,i}, \hat{t}_{m,j}, \quad i = 0, \dots, q, \quad j = 1, \dots, \ell - q.$$

Here, in contrast to [3] we have chosen not to include the non-homogeneous term in the argument involving the strong stability of E_A. For that reason our bound has one higher power of A. In both cases the required regularity of $\widehat{R}$ remains the same. Nevertheless, the second term in Theorem 2.2 can be controlled by the terms appearing in (2.37). To see why, notice that our assumptions imply

$$\int_{J_\ell} \widehat{I}_q v \, dx = \int_{J_\ell} v \, dx \,, \quad v \in \mathcal{H}_{p-1} \,.$$

Then, with $\widehat{I}_\ell$ as above we have,

$$\begin{aligned} E_{f,m}^{[j]} &= \int_{J_\ell} \frac{(t_m - \tau)^{(j-1)}}{(j-1)!} (f - \widehat{I}_q f)(\tau) d\tau \\ &= \int_{J_m} \frac{(t_m - \tau)^{(j-1)}}{(j-1)!} (f - \widehat{I}_{p-j} f)(\tau) d\tau + \int_{J_m} \frac{(t_m - \tau)^{(j-1)}}{(j-1)!} (\widehat{I}_{p-j} f - \widehat{I}_q f)(\tau) d\tau \,. \end{aligned}$$

The last integral is zero and therefore,

$$\big| A^{j-1} E_{f,m}^{[j]} \big| \le \frac{k_m^j}{(j-1)!} \big| A^{j-1} (f - \widehat{I}_{p-j} f) \big|_{L^\infty(J_m)} \,. \tag{2.38}$$

3. Interior a posteriori error bounds

We prove the following main result, which yields full-order a posteriori error bounds in the interior of the domain without requiring any compatibility conditions on the boundary. By $H^k(S)$ we denote the standard Sobolev space of order k defined on a domain S.

Theorem 3.1. *Let A be the negative Laplacian on a bounded domain $\Omega \subset \mathbb{R}^d$, equipped with Dirichlet boundary conditions. Let $\omega \subset \widehat{\omega} \subset \Omega$ be subdomains such that the boundaries of the three domains have pairwise distances of at least $\delta > 0$.*

Let $q \ge 2$ and $\widehat{R}|_{\widehat{\omega}} \in H^{2\rho}(\widehat{\omega})$ for some $1 \le \rho \le r = p - q - 1$, where p is the classical order of the method. Then, the following holds:

1. The error of the continuous Galerkin method of degree q and of the discontinuous Galerkin method dG$(q-1)$ satisfies

$$\|e(t_n)\|_{L_2(\omega)} \le C_1 \sum_{m=1}^{n} k_m^\rho \int_{J_m} \Big(\|\widehat{R}(t)\|_{H^{2\rho}(\widehat{\omega})} + \|\widehat{R}(t)\|_{L_2(\Omega)} \Big) dt, \tag{3.1}$$

where C_1 depends only on Ω and δ.

2. The error of a q-stage Runge-Kutta collocation method satisfies

$$\begin{aligned}\|e(t_n)\|_{L_2(\omega)} &\leq C_1 \sum_{m=1}^{n} k_m^\rho \int_{J_m} \Big(\|\widehat{R}(t)\|_{H^{2\rho}(\widehat{\omega})} + \|\widehat{R}(t)\|_{L_2(\Omega)} \Big) dt \\ &\quad + C_2 \sum_{m=1}^{n} \sum_{j=1}^{\rho} \Big(\|E_{f,m}^{[j]}\|_{H^{2(j-1)}(\widehat{\omega})} + \|E_{f,m}^{[j]}\|_{L_2(\Omega)} \Big), \end{aligned} \tag{3.2}$$

where $E_{f,m}^{[j]}$ is the quadrature error defined in (2.36) and C_1, C_2 depend only on Ω and δ.

The interior nodal error bounds are of optimal order p when $\widehat{R}$ is sufficiently regular in a neighbourhood of the subdomain ω. The regularity away from ω and the boundary behaviour play no role. We further remark that the dependence of C_1, C_2 on the domain Ω is only through the constants in Poincaré–Friedrichs inequalities. The result could straightforwardly be generalized to any second-order elliptic differential operator with smooth coefficients and appropriate essential boundary conditions.

For the proof we consider a finite chain of domains

$$\omega = \omega_0 \subset \omega_1 \subset \cdots \subset \omega_{\ell-1} = \widehat{\omega} \subset \omega_\ell = \Omega,$$

where $\ell = 2\rho + 2$ and the distance from ω_j to the boundary of ω_{j+1} is for all j bounded from below by a constant times δ. To these regions we associate smooth cutting functions χ_j on Ω such that

$$\chi_j \equiv 1 \quad \text{in } \omega_j\,, \qquad \chi_j \equiv 0 \quad \text{outside } \omega_{j+1}$$

for $j = 0, 1, \ldots, \ell - 1$, and $\chi_\ell \equiv 1$ on Ω. Viewed as multiplication operators, these functions have the following property with respect to the norm $|\cdot|$ of $H = L_2(\Omega)$:

$$|A^{-(j+1)/2}(A\chi_j - \chi_j A)v| \leq \beta\, |A^{-j/2}\chi_{j+1}v|. \tag{3.3}$$

For $A = -\Delta$, this bound is a consequence of the fact that the commutator $A\chi_j - \chi_j A$ is a *first-order* differential operator.

Lemma 3.1. *If operators $\chi_0, \ldots, \chi_\ell$ satisfy (3.3) and $\chi_\ell = \mathrm{id}$, then*

$$|\chi_0 E_A(t)v|^2 \leq |\chi_0 v|^2 + \beta^2 |A^{-1/2}\chi_1 v|^2 + \ldots + \beta^{2\ell} |A^{-\ell/2}\chi_\ell v|^2.$$

Proof. We denote $w(t) = E_A(t)v$ and $B_j = \chi_j A - A\chi_j$. Since $w(t)$ satisfies $w' + Aw = 0$, $w(0) = v$, we have

$$\chi_0 w' + A\chi_0 w = B_0 w, \quad \chi_0 w(0) = \chi_0 v.$$

The standard parabolic energy estimate yields

$$|\chi_0 w(t)|^2 + \int_0^t |A^{1/2}\chi_0 w(s)|^2\, ds \leq |\chi_0 v|^2 + \int_0^t |A^{-1/2}B_0 w(s)|^2\, ds$$

and hence, by (3.3),

$$|\chi_0 w(t)|^2 \leq |\chi_0 v|^2 + \beta^2 \int_0^t |\chi_1 w(s)|^2\, ds.$$

Since $\chi_1 w(t)$ solves $\chi_1 w' + A\chi_1 w = B_1 w,\ \chi_1 w(0) = \chi_1 v$, we obtain by the same argument

$$\int_0^t |\chi_1 w(s)|^2\, ds \le |A^{-1/2}\chi_1 v|^2 + \beta^2 \int_0^t |A^{-1/2}\chi_2 w(s)|^2\, ds.$$

Continuing in this way, we have for $j = 1, \ldots, \ell - 1$

$$\int_0^t |A^{-(j-1)/2}\chi_j w(s)|^2\, ds \le |A^{-j/2}\chi_j v|^2 + \beta^2 \int_0^t |A^{-j/2}\chi_{j+1} w(s)|^2\, ds.$$

Since $\chi_\ell = \mathrm{id}$, for $j = \ell - 1$ the last integral term equals

$$\int_0^t |A^{-(\ell-1)/2} w(s)|^2\, ds \le |A^{-\ell/2} v|^2.$$

Concatenating the above estimates completes the proof. □

Proof. (of Theorem 3.1) We work in the Hilbert space $H = L_2(\Omega)$ with the norm $|\cdot| = \|\cdot\|_{L_2(\Omega)}$. We begin by noting

$$\|e(t_n)\|_{L_2(\omega)} \le |\chi_0 e(t_n)|$$

and $e(t_n) = \widehat{e}(t_n)$. For Galerkin methods we obtain from (2.23) and the Galerkin orthogonality (2.31) that

$$|\chi_0 e(t_n)| \le \sum_{m=1}^{n-1} \int_{J_m} k_m^\rho \left|\chi_0 E_A(t_n - s) A^\rho \widehat{R}_m^{[\rho]}(s)\right| ds.$$

By Lemma 3.1 with $\ell = 2\rho + 2$ we have, for $w = \widehat{R}_m^{[\rho]}(s)$,

$$\left|\chi_0 E_A(t_n - s) A^\rho w\right|^2 \le \left|\chi_0 A^\rho w\right|^2 + \beta^2 \left|A^{-1/2}\chi_1 A^\rho w\right|^2 + \ldots \beta^{2\ell} \left|A^{-\ell/2}\chi_\ell A^\rho w\right|^2.$$

We now show that we can estimate

$$\left|A^{-j/2}\chi_j A^\rho w\right| \le C\, \|w\|_{H^{2\rho-j}(\omega_{j+2})}.$$

For this we use a duality argument:

$$\left|A^{-j/2}\chi_j A^\rho w\right| = \sup_{\varphi\in C_0^\infty(\Omega),\, \varphi\ne 0} \frac{\langle \chi_j A^\rho w, \varphi\rangle}{|A^{j/2}\varphi|} = \sup_{\varphi\ne 0} \frac{\langle A^{\rho-j/2}\chi_{j+1} w, A^{j/2}\chi_j\varphi\rangle}{|A^{j/2}\varphi|}.$$

Since the norm $|A^{j/2}\cdot|$ is equivalent to the $H^j(\Omega)$ Sobolev norm on $C_0^\infty(\Omega)$, we have

$$\left|A^{j/2}\chi_j\varphi\right| \le C' \left|A^{j/2}\varphi\right| \qquad \forall\, \varphi \in C_0^\infty(\Omega).$$

Hence,

$$\left|A^{-j/2}\chi_j A^\rho w\right| \le C' \left|A^{\rho-j/2}\chi_{j+1} w\right| \le C''\, \|\chi_{j+1} w\|_{H^{2\rho-j}(\Omega)} \le C\, \|w\|_{H^{2\rho-j}(\omega_{j+2})},$$

which is the desired estimate. Combining the above estimates, we obtain

$$\begin{aligned} |\chi_0 e(t_n)| \ \le\ & C \sum_{m=1}^{n-1} k_m^\rho \int_{J_m} \Big(\|\widehat{R}_m^{[\rho]}(s)\|_{H^{2\rho}(\omega_2)} + \beta \|\widehat{R}_m^{[\rho]}(s)\|_{H^{2\rho-1}(\omega_3)} + \ldots \\ & + \beta^{\ell-3} \|\widehat{R}_m^{[\rho]}(s)\|_{H^1(\omega_{\ell-1})} + (\beta^{\ell-2} + \beta^{\ell-1} + \beta^\ell) \|\widehat{R}_m^{[\rho]}(s)\|_{L_2(\Omega)} \Big) ds, \end{aligned}$$

which implies the error bound of Theorem 3.1 for the Galerkin methods. For the Runge–Kutta methods, there appear in addition the quadrature errors $E_{f,m}^{[j]}$ of (2.36), which are treated in the same way. □

REFERENCES

1. G. Akrivis, Ch. Makridakis and R. H. Nochetto, *A posteriori error estimates for the Crank–Nicolson method for parabolic equations*, Math. Comp. **75** (2006) 511–531.
2. G. Akrivis, Ch. Makridakis and R. H. Nochetto, *Optimal order a posteriori error estimates for a class of Runge–Kutta and Galerkin methods*, Numer. Math. **114** (2009) 133–160.
3. G. Akrivis, Ch. Makridakis and R. H. Nochetto, *Galerkin and RungeKutta methods: unified formulation, a posteriori error estimates and nodal superconvergence*, Numer. Math. **118** (2011) 429–456.
4. M. Crouzeix, *Sur l'approximation des équations différentielles opérationelles linéaires par des méthodes de Runge–Kutta*, Thèse, Université de Paris VI, 1975.
5. K. Eriksson and C. Johnson, *Adaptive finite element methods for parabolic problems. I. A linear model problem*, SIAM J. Numer. Anal. **28** (1991) 43–77.
6. K. Eriksson, C. Johnson and S. Larsson, *Adaptive finite element methods for parabolic problems. VI. Analytic semigroups*, SIAM J. Numer. Anal. **35** (1998) 1315–1325.
7. D. Estep and D. French, *Global error control for the Continuous Galerkin finite element method for ordinary differential equations,* RAIRO Modél. Math. Anal. Numér. **28** (1994) 815–852.
8. A. Lozinski, M. Picasso, and V. Prachittham, *An anisotropic error estimator for the Crank-Nicolson method*: *Application to a parabolic problem*, SIAM J. Sci. Comp. **31** (2009) 2757–2783.
9. Ch. Lubich and A. Ostermann, *Interior estimates for time discretizations of parabolic equations*, Appl. Numer. Math. **18** (1995) 241-251.
10. Ch. Makridakis and R. H. Nochetto, *A posteriori error analysis for higher order dissipative methods for evolution problems*. Numer. Math. **104** (2006) 489–514.
11. S. P. Nørsett, and G. Wanner, *Perturbed collocation and Runge-Kutta methods*, Numer. Math. **38** (1981) 193–208.
12. V. Thomée, *Galerkin Finite Element Methods for Parabolic Problems*. 2^{nd} ed., Springer–Verlag, Berlin, 2006.

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