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Representation of the Local Error for Higher-order Exponential Splitting Schemes Involving Two or Three Sub-operators

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Abstract. We consider the numerical treatment of abstract evolution equations

$$\partial_t u(t) = Hu(t) = Au(t) + Bu(t)\ [+Cu(t)], \quad u(0) \text{ given},$$

by higher-order exponential splitting schemes. The main focus is on linear problems. A single step of an exponential splitting scheme with stepsize t and s sub-steps comprises a multiplicative composition of sub-flows of the form $\mathscr{S}_j(t) = [\mathrm{e}^{tc_jC}]\,\mathrm{e}^{tb_jB}\,\mathrm{e}^{ta_jA},\ j = 1\ldots s$. We present an algebraic theory of the structure of the local error. The leading term is a linear combination of iterated commutators of the sub-operators A, B [and C] involved. This fact can be exploited for the automatic setup of order conditions, i.e., systems of polynomial equations for the coefficients a_j, b_j [and c_j] which have to be satisfied for a desired order p.

In view of application to partial differential equations, an explicit, exact representation of the local error is of interest. This can be obtained by performing a multiple variation-of-constants integral expansion involving higher-order defect terms. The latter satisfy a multinomial expansion, and the building blocks in this expansion are determined via yet another recursively defined integral representation. We describe the rich combinatorial structure of this local error expansion which is influenced by iterated commutators of the given sub-operators. A defect-based a posteriori local error estimator is also proposed.

Keywords: linear evolution equations, high-order exponential operator splitting methods, local error, a posteriori local error estimation
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EXPONENTIAL SPLITTING SCHEMES: INTRODUCTION AND OVERVIEW

We consider linear evolution equations where the operator on the right-hand side is split into two or three parts,

$$\begin{cases} \partial_t u(t) = Hu(t) = Au(t) + Bu(t)\ [+Cu(t)], \quad t \geq 0, \\ \mathrm{u}(0) \text{ given}, \end{cases} \tag{1}$$

and where the exact flow

$$\mathscr{E}_H(t)u = \mathrm{e}^{tH}u \tag{2}$$

is approximated, over time steps t, by an s-fold exponential splitting method of the form

$$\mathscr{S}(t)u = \mathscr{S}_s(t)\mathscr{S}_{s-1}(t)\cdots\mathscr{S}_1(t)u, \quad \text{with subflows} \quad \mathscr{S}_j(t) = \mathscr{E}_{C_j}(t)\mathscr{E}_{B_j}(t)\mathscr{E}_{A_j}(t) = \mathrm{e}^{tC_j}\,\mathrm{e}^{tB_j}\,\mathrm{e}^{tA_j}. \tag{3}$$

Here, $A_j = a_jA, B_j = b_jB, C_j = c_jC$, with appropriately chosen (real or complex) coefficients $\big(a_j, b_j, c_j\big)_{j=1}^{s}$, such that a particular approximation order is obtained, see Section "Local Error and Order Conditions".

The purpose of this note is to summarize (omitting detailed proofs) the theory from [1, 2] and [3], where the structure of the local error is described in detail. In particular, the theory from [1], devoted to the case of splitting into two operators (e.g., $C = 0$), is extended in [2] to the case of three operators, and the special structure of the leading term of the local error has been described in [3]. We summarize these results; moreover, we indicate how an a posteriori error estimate can be obtained via evaluation of the defect of the splitting solution.

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Notation

For the sake of brevity we often omit the argument t: $\mathscr{S}(t) = \mathscr{S}$, etc., if the context allows. We write

$$\mathscr{S}_j = \mathscr{S}_j^{[0]}, \qquad \mathscr{S} = \mathscr{S}^{[0]}. \tag{4}$$

Let

$$\mathscr{V}_j = \mathscr{V}_j^{[0]} := \mathscr{E}_{A_j}, \quad \mathscr{W}_j = \mathscr{W}_j^{[0]} := \mathscr{E}_{C_j}\mathscr{E}_{B_j}, \tag{5}$$

such that $\mathscr{S}_j^{[0]} = \mathscr{W}_j^{[0]}\mathscr{V}_j^{[0]}$.

Introducing the differential operator

$$\delta(\mathscr{X}) = \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{X} - H\mathscr{X}, \tag{6}$$

the exact evolution operator $\mathscr{E}_H(t)$ satisfies $\delta(\mathscr{E}_H) = 0$. For $j = 1\ldots s$, let

$$\delta_j(\mathscr{X}_j) := \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{X}_j - (A_j + B_j + C_j)\mathscr{X}_j, \tag{7a}$$

$$\rho_j(\mathscr{X}_j) := \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{X}_j - A_j\mathscr{X}_j, \tag{7b}$$

$$\sigma_j(\mathscr{X}_j) := \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{X}_j - \mathscr{X}_j B_j - C_j\mathscr{X}_j. \tag{7c}$$

Furthermore we denote

$$H_j := A_j + B_j + C_j, \tag{8a}$$

$$\underline{H}_j := H_1 + \ldots + H_{j-1}, \tag{8b}$$

and we define a family of iterated commutators according to $A_j^{[0]} := A_j$, $B_j^{[0]} := B_j$, $C_j^{[0]} := C_j$, and recursively for $\ell \geq 1$,

$$A_j^{[\ell]} := [A_j^{[\ell-1]}, \underline{H}_j], \quad B_j^{[\ell]} := [B_j^{[\ell-1]}, \underline{H}_j + A_j], \quad C_j^{[\ell]} := [C_j^{[\ell-1]}, \underline{H}_j + H_j]. \tag{9}$$

Local Error and Order Conditions

Let

$$\mathscr{L}(t) = \mathscr{S}(t) - \mathscr{E}_H(t) \tag{10}$$

denote the local error operator, such that the local error of a single step with stepsize t starting at u is given by $\mathscr{L}(t)u$. Via Taylor expansion of $\mathscr{L}(t)$, asymptotic order p, i.e., $\mathscr{L}(t) = \mathscr{O}(t^{p+1})$, is characterized by the requirement

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{L}(0) = \tfrac{\mathrm{d}^2}{\mathrm{d}t^2}\mathscr{L}(0) = \ldots = \tfrac{\mathrm{d}^p}{\mathrm{d}t^p}\mathscr{L}(0) = 0, \tag{11a}$$

and for a scheme of order p the leading term of the local error is given by

$$\mathscr{L}_0(t) := \tfrac{t^{p+1}}{(p+1)!}\tfrac{\mathrm{d}^{p+1}}{\mathrm{d}t^{p+1}}\mathscr{L}(0), \tag{11b}$$

such that $\mathscr{L}(t) = \mathscr{L}_0(t) + \mathscr{O}(t^{p+2})$. According to [3], for a general splitting method of order p the leading term $\mathscr{L}_0(t)$ has a special structure, namely

$$\mathscr{L}_0(t) = \text{linear combination of } p\text{-th iterated commutators of } A, B, C, \tag{12}$$

with coefficients independent of the given problem. As described in [3], this can be used to set up a recursive algorithm for the generation of order conditions. Furthermore, for a given scheme of order p the coefficients in the linear combination (12) can be determined from the conditions for order $p+1$.

Here we do not discuss order conditions or the construction of higher-order schemes in detail. We assume that a splitting method of order p with s compositions $\mathscr{S}_j$ is given. The goal is to provide an exact representation of $\mathscr{L}(t)$, in contrast to (11b) where only the leading term is indicated.

With the defect

$$\mathscr{D} = \mathscr{S}^{[1]} = \delta(\mathscr{S}^{[0]}) = \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}^{[0]} - H\mathscr{S}^{[0]} \tag{13}$$

of the splitting operator $\mathscr{S}^{[0]}$ with respect to the given evolution equation, we obtain a first, basic integral representation of the local error via the variation-of-constants formula

$$\mathscr{L}(t) = \int_0^t \mathscr{E}_H(t-\tau)\mathscr{D}(\tau)\,\mathrm{d}\tau. \tag{14}$$

LOCAL ERROR THEORY FOR HIGHER-ORDER SCHEMES

Representation of the Local Error via a Multiple Integral

With $\delta(\cdot)$ defined by (6), we recursively define higher-order defect operators $\mathscr{S}^{[q]}$ by

$$\mathscr{S}^{[q]} := \delta(\mathscr{S}^{[q-1]}) = \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}^{[q-1]} - H\mathscr{S}^{[q-1]}, \quad q \geq 1. \tag{15}$$

By successive differentiation of (14) at $t = 0$ it can be seen that the order conditions (11a) are equivalent to

$$\mathscr{S}^{[1]}(0) = \tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}^{[1]}(0) = \ldots = \tfrac{\mathrm{d}^{p-1}}{\mathrm{d}t^{p-1}}\mathscr{S}^{[1]}(0) = 0 \quad \Longleftrightarrow \quad \mathscr{S}^{[1]}(0) = \mathscr{S}^{[2]}(0) = \cdots = \mathscr{S}^{[p]}(0) = 0. \tag{16a}$$

Thus, the local error operator $\mathscr{L} = \mathscr{S}^{[0]} - \mathscr{E}_H$ satisfies the multiple variation-of-constants representation

$$\mathscr{L}(t) = \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_p} \mathscr{E}_H(t - \tau_{p+1})\,\mathscr{S}^{[p+1]}(\tau_{p+1})\,\mathrm{d}\tau_{p+1} \cdots \mathrm{d}\tau_1. \tag{17}$$

In (17) the higher-order defect $\mathscr{S}^{[p+1]}$ appears, and for analyzing the local error this term needs to be represented.

Recurrence Relations for the Higher-order Defect Terms

Lemma 1 *[1, 2] The higher-order defect operators $\mathscr{S}^{[q]}$ defined by* (15) *admit the multinomial expansion*

$$\mathscr{S}^{[q]} = \sum_{\boldsymbol{k} \in \mathbb{N}_0^s,\, |\boldsymbol{k}| = q} \binom{q}{\boldsymbol{k}} \mathscr{S}_s^{[k_s]} \cdots \mathscr{S}_1^{[k_1]}, \quad q \geq 0, \tag{18a}$$

where the $\mathscr{S}_j^{[k]}$ are recursively defined by $\mathscr{S}_j^{[0]} = \mathscr{S}_j$ and, with $\underline{H}_j$ from (8b) *and $\delta_j(\cdot)$ from* (7a)*,*

$$\mathscr{S}_j^{[k+1]} := [\mathscr{S}_j^{[k]}, \underline{H}_j] + \delta_j(\mathscr{S}_j^{[k]}), \quad k \geq 0. \tag{18b}$$

The next step is to represent the $\mathscr{S}_j^{[k]}$. Consider $\mathscr{V}_j^{[0]}$ and $\mathscr{W}_j^{[0]}$ defined by (5), satisfying the initial value problems

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{V}_j^{[0]} = A_j \mathscr{V}_j^{[0]}, \quad \mathscr{V}_j^{[0]}(0) = I, \tag{19a}$$

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{W}_j^{[0]} = \mathscr{W}_j^{[0]} B_j + C_j \mathscr{W}_j^{[0]}, \quad \mathscr{W}_j^{[0]}(0) = I. \tag{19b}$$

With $\rho_j(\cdot)$, $\sigma_j(\cdot)$ from (7b),(7c), the evolution equations (19) can be written as $\rho_j(\mathscr{V}^{[j]}) = 0$ and $\sigma_j(\mathscr{W}^{[j]}) = 0$. For $k \geq 0$, let $\mathscr{V}_j^{[k]}$ and $\mathscr{W}_j^{[k]}$ be recursively defined by

$$\mathscr{V}_j^{[k+1]} := [\mathscr{V}_j^{[k]}, \underline{H}_j] + \rho_j(\mathscr{V}_j^{[k]}), \tag{20a}$$

$$\mathscr{W}_j^{[k+1]} := [\mathscr{W}_j^{[k]}, \underline{H}_j + A_j + B_j] + \sigma_j(\mathscr{W}_j^{[k]}). \tag{20b}$$

The $\mathscr{V}_j^{[k]}$ and $\mathscr{W}_j^{[k]}$ are building blocks for the $\mathscr{S}_j^{[k]}$ from (18):

Lemma 2 *[2] The higher-order defect terms $\mathscr{S}_j^{[k]}$ defined by* (18b) *admit the binomial expansion*[1]

$$\mathscr{S}_j^{[k]} = \sum_{\ell=0}^{k} \binom{k}{\ell} \mathscr{W}_j^{[k-\ell]} \mathscr{V}_j^{[\ell]}, \quad k \geq 0, \quad j = 1 \ldots s. \tag{21}$$

Recursive representations for the $\mathscr{V}_j^{[k]}$ and $\mathscr{W}_j^{[k]}$ are provided by the following Lemma.

---

[1] For the special case $A = 0$ (splitting into two operators) we have $\mathscr{V}_0^{[\ell]} = I$, $\mathscr{V}_j^{[\ell]} = 0$ for $j \geq 1$, and $\mathscr{S}_j^{[k]} = \mathscr{W}_j^{[k]}$ for $j \geq 0$. This corresponds to the special case considered in [1].

Lemma 3 *[1, 2]*

(i) The $\mathscr{V}_j^{[k]}$ *defined by* (20a) *satisfy* $\rho_j(\mathscr{V}_j^{[k]}) = \sum_{\ell=1}^{k} \binom{k}{\ell} A_j^{[\ell]} \mathscr{V}_j^{[k-\ell]},\ k \geq 0,\ j = 1 \ldots s$. *That is, the* $\mathscr{V}_j^{[k]}$ *satisfy the recursively defined evolution equations*

$$\tfrac{\mathrm{d}}{\mathrm{d}t} \mathscr{V}_j^{[k]} = A_j \mathscr{V}_j^{[k]} + \sum_{\ell=1}^{k} \binom{k}{\ell} A_j^{[\ell]} \mathscr{V}_j^{[k-\ell]}. \tag{22a}$$

This implies

$$\mathscr{V}_j^{[k]}(t) = \mathscr{E}_{A_j}(t) \mathscr{V}_j^{[k]}(0) + \int_0^t \mathscr{E}_{A_j}(t-\tau) \rho_j(\mathscr{V}_j^{[k]})(\tau)\, \mathrm{d}\tau, \tag{22b}$$

with initial value $\mathscr{V}_j^{[k]}(0) = [\mathscr{V}_j^{[k-1]}(0), \underline{H}_j] + \rho_j(\mathscr{V}_j^{[k-1]})(0)$.

(ii) The $\mathscr{W}_j^{[k]}$ *defined by* (20b) *satisfy* $\sigma_j(\mathscr{W}_j^{[k]}) = \sum_{\ell=1}^{k} \binom{k}{\ell} \big(\mathscr{W}_j^{[k-\ell]} B_j^{[\ell]} + C_j^{[\ell]} \mathscr{W}_j^{[k-\ell]} \big),\ k \geq 0,\ j = 1 \ldots s$. *That is, the* $\mathscr{W}_j^{[k]}$ *satisfy the recursively defined evolution equations*

$$\tfrac{\mathrm{d}}{\mathrm{d}t} \mathscr{W}_j^{[k]} = \mathscr{W}_j^{[k]} B_j + C_j \mathscr{W}_j^{[k]} + \sum_{\ell=1}^{k} \binom{k}{\ell} \big(\mathscr{W}_j^{[k-\ell]} B_j^{[\ell]} + C_j^{[\ell]} \mathscr{W}_j^{[k-\ell]} \big). \tag{23a}$$

This implies

$$\mathscr{W}_j^{[k]}(t) = \mathscr{E}_{C_j}(t) \mathscr{W}_j^{[k]}(0) \mathscr{E}_{B_j}(t) + \int_0^t \mathscr{E}_{C_j}(t-\tau) \sigma_j(\mathscr{W}_j^{[k]})(\tau) \mathscr{E}_{B_j}(t-\tau)\, \mathrm{d}\tau, \tag{23b}$$

with initial value $\mathscr{W}_j^{[k]}(0) = [\mathscr{W}_j^{[k-1]}(0), \underline{H}_j + A_j + B_j] + \sigma_j(\mathscr{W}_j^{[k-1]})(0)$.

A Priori and a Posteriori Local Error Estimates

On the basis of the results from Sections "Representation of the Local Error via a Multiple Integral" and "Recurrence Relations for the Higher-order Defect Terms" it can be shown:

Proposition 1 *[1, 2] For a scheme of order p, i.e., under assumption* (11a)*, the local error satisfies*

$$\mathscr{L}(t)u = \mathscr{O}(t^{p+1}). \tag{24}$$

Here $\mathscr{O}(t^{p+1})$ *means* $\mathscr{C}(t) \cdot t^{p+1}$*, where* $\mathscr{C}(t)$ *is well-defined and bounded provided that all expressions occurring in the recursive representation of* $\mathscr{L}(t)$ *are well-defined and bounded when* $\mathscr{L}(t)$ *is applied to u.*

In applications this means that u needs to satisfy certain regularity requirements, in particular due to the iterated commutators (9) appearing in the representation for $\mathscr{L}(t)$; see in particular Lemma 3.

For practical purposes, according to [1], we aim for estimation of the local error $\mathscr{L}(t)u$ by a computable local error estimator $\widetilde{\mathscr{L}}(t)u$. According to [1, 2] this can be accomplished via an Hermite quadrature approximation to the local error integral (14), exploiting (16a). This approximation is given by

$$\widetilde{\mathscr{L}}(t)u = \tfrac{t}{p+1} \mathscr{D}(t)u, \tag{25}$$

with the defect $\mathscr{D} = \mathscr{S}^{[1]}$ defined by (13). An analysis similar to that for the local error $\mathscr{L}(t)$ shows:

Proposition 2 *[1, 2] The local error estimate* $\widetilde{\mathscr{L}}(t)u$ *defined by* (25) *satisfies*

$$\widetilde{\mathscr{L}}(t)u - \mathscr{L}(t)u = \mathscr{O}(t^{p+2}), \tag{26}$$

that is, under appropriate regularity requirements on u the estimator is asymptotically correct.

In [1, 2] it is also demonstrated how $\mathscr{D}(t)u$ can be evaluated in practice, and numerical examples are presented. A theory of lower-order schemes for fully nonlinear problems and splitting into two operators is presented in [4].

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