Representation and estimation of the local error of higher-order exponential splitting schemes involving two or three sub-operators

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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; the nonlinear case is briefly commented on. A single step of an exponential splitting scheme with stepsize h and s sub-steps comprises a multiplicative composition of sub-flows of the form

$$\mathcal{S}_j(t) = [\mathrm{e}^{hc_jC}]\,\mathrm{e}^{hb_jB}\mathrm{e}^{ha_jA}, \quad j = 1\ldots s.$$

We present an algebraic theory of the structure of the local error. The leading term is a linear combination of higher-degree 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 Leibniz-type 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 higher-degree commutators of the given sub-operators.

It is also indicated how to realize and analyze a practical, asymptotically correct defect-based a posteriori local error estimator. A numerical example based on spectral discretization of the kinetic part of a Schrödinger equation is also presented.