Setup of order conditions for splitting methods

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Introduction

Evolution equations, splitting methods, and order conditions

- Evolution equation ($u = u(t)$):

$$\partial_t u = H(u) = A(u) + B(u) \; [+C(u) + \ldots]$$

Initial condition $u(0) = u_0$ given
Flow (exact solution): $u(t) = \mathcal{E}_H(t, u_0)$

- Subproblems

$$\partial_t u = A(u)$$
$$\partial_t u = B(u)$$

"easily" solvable, respective flows: $u(t) = \mathcal{E}_A(t, u_0)$, $u(t) = \mathcal{E}_B(t, u_0)$

- Prototypical example: Schrödinger equation

$$\partial_t \psi = \frac{1}{2}\mathrm{i}\Delta\psi - \mathrm{i}V\psi$$

- Numerical integration method: compute recursively approximations $u_0 \mapsto u_1 \mapsto u_2 \mapsto \dots$ of the exact solution on grid $t_0, t_1, t_2, \dots$ with stepsize $\Delta t = h$, $t_n = t_0 + nh$.
  Consider only one step starting at some $u = u_n$.
- Idea of splitting methods: Approximate flow $\mathcal{E}_H$ of full problem by recombination of sub-flows $\mathcal{E}_A$ and $\mathcal{E}_B$
- Examples:

$$\mathcal{E}_H(h,u) \approx \mathcal{E}_B(h, \mathcal{E}_A(h,u)) \qquad \text{(Lie-Trotter splitting, first order)}$$
$$\mathcal{E}_H(h,u) \approx \mathcal{E}_A(\tfrac{1}{2}h, \mathcal{E}_B(h, \mathcal{E}_A(\tfrac{1}{2}h,u))) \qquad \text{(Strang splitting, second order)}$$

- Higher order (s stages):

$$\mathcal{E}_H(h,u) \approx \mathcal{S}(h,u) = \mathcal{E}_B(b_s h, \cdot) \circ \mathcal{E}_A(a_s h, \cdot) \circ \cdots \circ \mathcal{E}_B(b_1 h, \cdot) \circ \mathcal{E}_A(a_1 h, \cdot)(u)$$

- Problem: How to determine coefficients $a_1, b_1, \dots, a_s, b_s$ such that local error satisfies

$$\mathcal{L}(h,u) = \mathcal{S}(h,u) - \mathcal{E}_H(h,u) = O(h^{p+1})$$

- Taylor expansion of local error will lead to (multivariate) polynomial equations in the coefficients $a_1, b_1, \dots, a_s, b_s \rightsquigarrow$ order conditions

- Two tasks:

    1. Setup of these polynomial equation
    2. Solve these polynomial equations

  Here: only the first item is considered (second item: very challenging!)

- Implementaion in Maple on multi-core machine described in the paper: more or less obsolete

- We found better approach (unfortunately only after the paper was already accepted)

- Implementation in the Julia programming language

Local error representation via Taylor expansion

Simplest cases and general structure

Local error representation via Taylor expansion

Lie-Trotter AB type splitting, linear case

- Consider $Hu = Au + Bu$ (linear). In general: $AB \neq BA$
- **Lie-Trotter** splitting (order $p = 1$):

$$\mathrm{e}^{hH}u \approx \mathcal{S}(h)u := \mathrm{e}^{hB}\mathrm{e}^{hA}u \quad (\text{'='} \text{ for } AB = BA)$$

Local error via Taylor expansion:

$$\frac{d}{dt}\mathrm{e}^{tH} = (A+B)\mathrm{e}^{t(A+B)} = A + B \text{ at } t = 0$$

$$\frac{d}{dt}\mathcal{S}(t) = \mathrm{e}^{tB}\mathrm{e}^{tA}A + B\,\mathrm{e}^{tB}\mathrm{e}^{tA} = A + B \text{ at } t = 0$$

but

$$\frac{d^2}{dt^2}\mathrm{e}^{tH} = (A+B)^2 = A^2 + AB + BA + B^2 \text{ at } t = 0$$

$$\frac{d^2}{dt^2}\mathcal{S}(t) = \quad \ldots \quad = A^2 + BA + BA + B^2 \text{ at } t = 0$$

$\rightsquigarrow$ local error

$$\mathcal{L}(h)u := \big(\mathcal{S}(h) - \mathrm{e}^{hH}\big)u = -\tfrac{1}{2}h^2[A,B](u) + \mathcal{O}(h^3)$$

with commutator $[A,B](u) = (AB - BA)\cdot u$

Local error representation via Taylor expansion

Lie-Trotter AB type splitting, nonlinear case

- **Lie-Trotter** splitting for $H(u) = A(u) + B(u)$ (nonlinear):

$$\mathcal{E}_H(h,u) \approx \mathcal{S}(h,u) := \mathcal{E}_B(h, \mathcal{E}_A(h,u)),$$

  with first derivatives

$$\frac{d}{dt}\mathcal{E}_H(t,u) = H(\mathcal{E}_H(t,u)) \,,$$

$$\frac{d}{dt}\mathcal{S}(t,u) \; = B(\mathcal{S}(t,u)) + \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t,u)) \cdot A(\mathcal{E}_A(t,u))$$

  (both derivatives are $= A(u) + B(u)$ at $t = 0$)
  and corresponding second derivatives.

- $\rightsquigarrow$ Local error via Taylor expansion:

$$\mathcal{L}(h,u) = \mathcal{S}(h,u) - \mathcal{E}_H(h,u) = \, -\tfrac{1}{2} h^2 [A,B](u) + \mathcal{O}(h^3)$$

  with commutator $[A,B](u) = A'(u) \cdot B(u) - B'(u) \cdot A(u)$

Local error representation via Taylor expansion

Strang AB type splitting

- **Strang** splitting (symmetric, order $p = 2$):

  $$\mathcal{E}_H(h,u) \approx \mathcal{S}(h,u) := \mathcal{E}_B(\tfrac{h}{2}, \mathcal{E}_A(h, \mathcal{E}_B(\tfrac{h}{2}, u)))$$

  Local error via Taylor expansion:

  $$\mathcal{L}(h,u) = \mathcal{S}(h,u) - \mathcal{E}_H(h,u) = \frac{h^3}{6}\frac{d^3}{dt^3}\mathcal{L}(0,u) + \mathcal{O}(h^4)$$

  Leading term $\frac{d^3}{dt^3}\mathcal{L}(0,u)$ = linear combination of second-order commutators

  $$[A,[A,B]](u) \quad \text{and} \quad [[A,B],B](u)$$

  with coefficients independent of h, u

Local error representation via Taylor expansion

Lie-Trotter and Strang ABC type splittings

- **Lie-Trotter:**

$$\mathcal{E}_H(h,u) \approx \mathcal{S}(h,u) := \mathcal{E}_C(h, \mathcal{E}_B(h, \mathcal{E}_A(h,u)))$$

Local error via Taylor expansion:

$$\mathcal{L}(h,u) = \mathcal{S}(h,u) - \mathcal{E}_H(h,u) = \frac{h^2}{2}\frac{d^2}{dt^2}\mathcal{L}(0,u) + \mathcal{O}(h^4)$$

Leading term $\frac{d^2}{dt^2}\mathcal{L}(0,u)$ = linear combination of commutators $K(u)$,

$$K \in \{[A,B],[A,C],[B,C]\}$$

- **Strang:**

$$\mathcal{E}_H(h,u) \approx \mathcal{S}(h,u) := \mathcal{E}_A(\tfrac{h}{2}, \mathcal{E}_B(\tfrac{h}{2}, \mathcal{E}_C(h, \mathcal{E}_B(\tfrac{h}{2}, \mathcal{E}_A(\tfrac{h}{2}, u)))))$$

Local error via Taylor expansion:

$$\mathcal{L}(h,u) = \mathcal{S}(h,u) - \mathcal{E}_H(h,u) = \frac{h^3}{6}\frac{d^3}{dt^3}\mathcal{L}(0,u) + \mathcal{O}(h^4)$$

Leading term $\frac{d^3}{dt^3}\mathcal{L}(0,u)$ = linear combination of commutators $K(u)$,

$$K \in \{[A,[A,B]],[A,[A,C]],[[A,B],B],[[A,B],C],$$
$$[[A,C],B],[[A,C],C],[B,[B,C]],[[B,C],C]\}$$

Local error representation via Taylor expansion

Ansatz for higher-order schemes; representation of the derivatives of the local error

- For the study of order conditions, formally considering the linear case is sufficient.

- Ansatz for higher-order s-stage ABC type splitting ($H = A+B+C$):

$$\mathrm{e}^{hH} \approx S(h) := \mathcal{S}_s(h) \,\cdots\, \mathcal{S}_1(h), \quad S_j(h) = \mathrm{e}^{hC_j}\,\mathrm{e}^{hB_j}\,\mathrm{e}^{hA_j}$$

  with $A_j = a_j A$, $B_j = b_j B$, $C_j = c_j C$, where the coefficients $\{a_j, b_j, c_j,\ j = 1 \ldots s\}$ are to be determined.

- q-th derivatives of local error operator $\mathcal{L}(t) = \mathcal{S}(t) - \mathrm{e}^{tH}$ at $t = 0$:
  With $\boldsymbol{k} = (k_1, \ldots, k_s) \in \mathbb{N}_0^s$, $\boldsymbol{l} = (l_A, l_B, l_C) \in \mathbb{N}_0^3$,

$$\tfrac{d^q}{dt^q}\mathcal{L}(0) = \sum_{|\boldsymbol{k}|=q} \binom{q}{\boldsymbol{k}} \prod_{j=s\ldots 1} \sum_{|\boldsymbol{l}|=k_j} \binom{k_j}{\boldsymbol{l}} C_j^{\,l_C} B_j^{\,l_B} A_j^{\,l_A} - (A+B+C)^q$$

  (Leibniz formula) $\rightarrow$ for use in Taylor ansatz.

Theorem

The leading term $\frac{d^{p+1}}{dt^{p+1}}\mathcal{L}(0)$ of the Taylor expansion of the local error of a splitting method of order p is an element of the free Lie algebra generated by $A, B, \ldots$, with Lie-bracket (commutator) $[\cdot,\cdot]$.

More precisely, it is a linear combination of pth order commutators.

- Independent commutators form basis of free Lie algebra
- Example: For $p = 3$, 3 independent 3th order AB-commutators

$$[A,[A,[A,B]]], \quad [A,[[A,B],B]], \quad [[[A,B],B],B],$$

corresponding to the Lyndon-Shirshov basis words

AAAB, AABB, ABBB

of length 4 over the alphabet $(\mathtt{A},\mathtt{B})$

W.Auzinger, W.Herfort:
Local error structures and order conditions in terms of Lie elements for exponential splitting schemes
Opuscula Mathematica 34(2), 243–255, 2014

Algorithmic approach for setup of order conditions

Idea and details of algorithm, Julia implementation

Algorithmic approach for setup of order conditions

Idea of the algorithm, AB type splitting

- s-stage ansatz with unknown (real or complex) coefficients

$$a_j, b_j\,[, c_j], \quad j = 1 \dots s$$

- Desired order p
- For $q = 1, 2, \dots, p$:

  In the expression

$$\tfrac{d^q}{dt^q}\mathcal{L}(0) = \sum_{|\boldsymbol{k}|=q} \binom{q}{\boldsymbol{k}} \prod_{j=s\dots1} \sum_{l=0}^{k_j} \binom{k_j}{l} b_j^l a_j^{k_j-l} B^l A_j^{k_j-l} - (A+B)^q,$$

  where the product $\prod_{j=s\dots1}(\dots)$ and $(A+B)^q$ have been fully expanded (taking into account that A, B are noncommuting),

  search for occurences of Lyndon-Shirshov basis words of length q and extract their coefficients (see algorithmic details below)

- For each basis element we obtain one equation (coefficient $= 0$).

  Rapidly increasing complexity!

Algorithmic approach for setup of order conditions

A basis of the free Lie algebra (Lyndon-Shirshov basis)

Combinatorial words representing Lyndon-Shirshov basis, generated by Duval algorithm (1988).

q	$\#_q$	Lyndon-Shirshov words of length q over alphabet $\{\mathtt{A},\mathtt{B}\}$
1	2	A, B
2	1	AB
3	2	AAB, ABB
4	3	AAAB, AABB, ABBB
5	6	AAAAB, AAABB, AABAB, AABBB, ABABB, ABBBB
6	9	AAAAAB, AAAABB, AAABAB, AAABBB, AABABB, AABBAB, AABBBB, ABABBB, ABBBBB
7	18	...
8	30	...

q	$\#_q$	Lyndon-Shirshov words of length q over alphabet $\{\mathtt{A},\mathtt{B},\mathtt{C}\}$
1	3	A, B, C
2	3	AB, AC, BC
3	8	AAB, AAC, ABB, ABC, ACB, ACC, BBC, BCC
4	18	...
5	48	...
6	115	...

Algorithmic approach for setup of order conditions

Details of the implemented algorithm

Input: q, s

Output: a dictionary eqs of strings, indexed by all Lyndon-Shirshov words W of length q, containing the corresponding equations

for all Lyndon-Shirshov words W of length q **do**
    $eqs[W] = \texttt{"-1"}$ /* each equation contains a term -1 */
end
for all $\mathbf{k} = (k_1, \dots, k_s)$ with $k_j \geq 0$ and $|\mathbf{k}| = k_1 + \cdots + k_s = q$ **do**
    for all $(l_1, \dots, l_s)$ with $0 \leq l_j \leq k_j$ **do**
        $W = \emptyset$ /* empty word */
        for $j = s, s-1, \dots, 1$ **do**
            $W = W\underbrace{\texttt{A}\dots\texttt{A}}_{l_j}\underbrace{\texttt{B}\dots\texttt{B}}_{k_j - l_j}$
        end
        if W is a Lyndon-Shirshov word of length q **then**
            for $j = 1, \dots, s$ **do**
                append to $eqs[W]$ a string representing $+\binom{q}{\boldsymbol{k}}\binom{k_j}{l_j} a_j^{l_j} b_j^{k_j - l_j}$
            end
        end
    end
end

Remarks

Remarks

- The outcome: a system of polynomial equations for the splitting coefficients $a_j, b_j\,[, c_j],\ j = 1 \ldots s$
- For given order p and sufficiently large s: underdetermined system $\leadsto$ search for "optimal" solution, numerically very demanding optimization problem.
- http://www.asc.tuwien.ac.at/~winfried/splitting
- Our Julia implementation available at https://github.com/HaraldHofstaetter/SplittingOrderConditions.jl

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W.Auzinger, H.Hofstätter, D.Ketcheson, O.Koch:
Practical splitting methods for the adaptive integration of nonlinear evolution equations. Part I: Construction of optimized schemes and pairs of schemes
BIT Numer. Math., published online 28 July 2016