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LINEARLY IMPLICIT SPLITTING METHODS FOR HIGHER SPACE-DIMENSIONAL PARABOLIC DIFFERENTIAL EQUATIONS

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Abstract. Splitting methods are recognized as useful tools in the numerical solution of initial boundary value problems of multi(space)-dimensional partial differential equations. Following the method of lines we introduce a new class of linearly implicit splitting methods for the numerical solution of the systems of ordinary differential equations arising from the semidiscretization in space of a parabolic differential equation. In the usual splitting formulas the nonlinear equation systems are solved by Jacobian-based iteration methods. In general, the Jacobian matrices used have a simple structure (often tridiagonal). The linearly implicit splitting formulas directly involve approximations to the Jacobian matrices in the scheme so that only linear equation systems with simple coefficient matrices have to be solved. Furthermore, these formulas are consistent of order two and have good stability properties.

1. Introduction

We consider parabolic differential equations of higher space dimension of the form

$$\frac{\partial u}{\partial t}(t,x) = \sum_{i=1}^{r} G_i\left(t, x_1, \ldots, x_r, u, \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i^2}\right), \tag{1.1}$$

with $t \in [t_0, t_e]$ and $x = (x_1, \ldots, x_r) \in \Omega \subset \mathbb{R}^r$. For simplicity, let Ω be a rectangular, bounded region, whose boundaries are parallel to the coordinate axes. We suppose that the coupling of the space derivatives in the operators G_i is linear. Furthermore, the initial and homogeneous Dirichlet boundary conditions are given by

$$u(t_0, x_1, \ldots, x_r) = u_0(x_1, \ldots, x_r) \qquad \forall x = (x_1, \ldots, x_r) \in \Omega, \tag{1.2}$$

$$\phi(t, x_1, \ldots, x_r) = 0 \qquad \forall t \in [t_0, t_e],\ \forall x = (x_1, \ldots, x_r) \in \partial\Omega. \tag{1.3}$$

For the numerical solution of (1.1)-(1.3), we apply the method of lines (MOL), that is by discretizing the space derivatives via standard second-order finite differences, we get an initial value problem for a system of ordinary differential equations (ODEs)

$$w' = f(t,w) := \sum_{i=1}^{r} f_i(t,w), \quad w(t_0) = w_0 \in \mathbb{R}^m,\ t \in [t_0, t_e], \tag{1.4}$$

where f_i corresponds to the semidiscretized operator G_i $(i = 1(1)r)$ and where m is equal to the number of interior grid points. The function $f(t,w)$ is said to fulfill a *linear splitting relation* and the components $f_i(t,w)$ are called *splitting functions.*

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Since, in general, the system (1.4) is stiff, an implicit method should be used, and since it is large for a small spatial meshsize, there would be high computation costs using fully implicit ODE solvers.

A splitting method consists of two components: a *splitting function* like f in (1.4) and a *splitting formula* to be discussed later. We consider *operator splitting methods* based on the splitting functions f_i as described above (other types of splitting methods can be found in e.g. [7],[8],[15]). Splitting functions arising from the semidiscretization mentioned above have tridiagonal Jacobian matrices $\frac{\partial f_i}{\partial w}$, $i = 1(1)r$. Splitting formulas for solving (1.4) use this special property and decrease therefore the computational costs.

In the following section, we give examples of well-known linear splitting formulas and their stability properties. In the third section, we introduce a new class of linearly implicit splitting methods and investigate its consistency and stability properties. In the last section, we give results of our numerical experiments.

2. Splitting formulas

In [8] autonomous problems (1.1) have been considered and a general class of linear splitting formulas has been given by which many known splitting methods can be generated. For the numerical integration of the nonautonomous ODE (1.4) its analogue is given by the *s-stage linear one-step splitting formula*

$$\begin{aligned} v_{n+1}^{(0)} &= v_n, \\ v_{n+1}^{(j)} &= v_n \ + \ \tau_n \sum_{l=0}^{j} \sum_{i=1}^{r} \lambda_{jli} \ f_i(t_n + c_l \tau_n, v_{n+1}^{(l)}), \ j = 1(1)s, \\ v_{n+1} &= v_{n+1}^{(s)}, \end{aligned} \tag{2.1}$$

where v_n is the numerical solution at the time point $t = t_n$ and $\tau_n = t_{n+1} - t_n$ is the stepsize in time. Special splitting formulas are obtained by specifying the parameters $\lambda_{jli}, c_l \in \mathbb{R}$. Depending on these parameters, we have different consistency and stability results. (Each stage should be implicit with respect to only one of the splitting functions, i.e. if $\lambda_{jjk} \neq 0$ for one $k \in \{1, .., r\}$ then $\lambda_{jji} = 0$ for $i \neq k$.)

2.1. Examples of linear splitting formulas.

In the following, we give three examples of linear splitting formulas. The first example is the well-known *alternating direction implicit method (ADI) of Peaceman and Rachford* (see [8], [11], [14]). This formula can be applied to problems with $r = 2$ and is given by

$$\begin{aligned} v_{n+1}^{(1)} &= v_n \quad + \tfrac{1}{2}\tau_n \left(f_1(t_n + \tfrac{\tau_n}{2}, v_{n+1}^{(1)}) + f_2(t_n, v_n) \right), \\ v_{n+1} &= v_{n+1}^{(1)} + \tfrac{1}{2}\tau_n \left(f_1(t_n + \tfrac{\tau_n}{2}, v_{n+1}^{(1)}) + f_2(t_{n+1}, v_{n+1}) \right). \end{aligned} \tag{2.2}$$

A second example is the *locally one-dimensional method of Yanenko* (see [17])

$$\begin{aligned} v_{n+1}^{(0)} &= v_n, \\ v_{n+1}^{(j)} &= v_{n+1}^{(j-1)} + \tau_n \left[(1-\alpha) f_j(t_n + c_{j-1}\tau_n, v_{n+1}^{(j-1)}) + \alpha f_j(t_n + c_j \tau_n, v_{n+1}^{(j)}) \right], \ j = 1(1)r, \\ v_{n+1} &= v_{n+1}^{(r)}, \end{aligned} \tag{2.3}$$

which can be applied to (1.4) with arbitrary $r \geq 2$, $r \in \mathbb{N}$. Our third example is the $2r$-stage *trapezoidal splitting method*, recently introduced by Hundsdorfer (see [10]):

$$\text{TRAPSP:} \qquad \begin{aligned} v_{n+1}^{(0)} &= v_n, \\ v_{n+1}^{(i)} &= v_{n+1}^{(i-1)} + \tfrac{1}{2}\tau_n\, f_i(t_n, v_{n+1}^{(i-1)}), & i &= 1(1)r, \\ v_{n+1}^{(r+j)} &= v_{n+1}^{(r+j-1)} + \tfrac{1}{2}\tau_n\, f_{r-j+1}(t_{n+1}, v_{n+1}^{(r+j)}), & j &= 1(1)r, \\ v_{n+1} &= v_{n+1}^{(2r)}\ , \end{aligned} \tag{2.4}$$

which can also be applied for arbitrary r.

The ADI method (2.2) and the trapezoidal splitting method (2.4) have classical consistency order two. The LOD method (2.3) is only of order one. All methods have fully implicit stages, which have to be solved by iteration methods.

2.2. **Stability investigations.** In analogy with the stability investigation for ODEs (see [1], [2], [6]), we analyze systems of the form (1.4), where f belongs to certain classes of linear functions defined below. The reason is that the splitting formulas considered are applied to semidiscretized PDEs. The linear ODE systems are assumed to be of the form

$$w'(t) = f(t, w) \ = \ A\, w(t) \ = \ \sum_{i=1}^{r} A_i\, w(t), \qquad w \in \mathbb{R}^m,\ A_i \in \mathbb{R}^{m \times m}\,. \tag{2.5}$$

(Again each A_i corresponds to the discretized derivatives of one space direction.) Applying a linear splitting formula (2.1) to the test problem (2.5), we obtain with $\tau = \tau_n$ the relation

$$v_{n+1} = R(\tau\, A_1, \ldots, \tau\, A_r)\, v_n\ . \tag{2.6}$$

Here, the matrix-valued function R is called the *amplification matrix* and the corresponding rational function the *stability function* of the splitting formula. It is defined by the formal relations

$$\begin{aligned} R^{(0)}(\tau\, A_1, \ldots, \tau\, A_r) &:= I, \qquad I \in \mathbb{R}^{m \times m} \text{ the unit matrix}, \qquad j = 1(1)s \\ R^{(j)}(\tau\, A_1, \ldots, \tau\, A_r) &= (I - \tau\lambda_{jjk}\, A_k)^{-1} \left(I + \sum_{l=0}^{j-1} \sum_{i=1}^{r} \tau\lambda_{jli}\, A_i\, R^{(l)}(\tau\, A_1, \ldots, \tau\, A_r) \right), \\ R(\tau\, A_1, \ldots, \tau\, A_r) &= R^{(s)}(\tau\, A_1, \ldots, \tau\, A_r). \end{aligned}$$

In general, the system (2.5) is large and stiff because of the usually small spatial meshsize. Furthermore, for the matrices A_i we assume $\mu[A_i] \leq 0$ $(i = 1(1)r)$. The logarithmic matrix norm $\mu[.]$ and the vector norm $\|.\|$ are defined corresponding to a given inner product. Therefore, we have for the exact solution of (2.5):

$$\|w(t+\tau)\| \leq \|w(t)\| \qquad \forall\ \tau > 0, \tag{2.7}$$

$$\lim_{\tau\mu[A_i] \to -\infty} w(t+\tau) = 0 \qquad \forall\ i = 1(1)r. \tag{2.8}$$

Ideally, the numerical solution of (2.5) should behave like the exact solution. The analogue of property (2.7) reads $\|v_{n+1}\| \leq \|v_n\|$. Therefore, we shall require

$$\|R(\tau\, A_1, \ldots, \tau\, A_r)\| \leq 1 \qquad \forall\ \tau > 0\ , \tag{2.9}$$

where the matrix norm is subordinate to the vector norm used in (2.7). Secondly, the analogue of (2.8) requires the stability function $R(z_1, \ldots, z_r)$ to satisfy

$$\lim_{\tau\mu[A_i] \to -\infty} \|R(\tau\, A_1, \ldots, \tau\, A_r)\| = 0 \qquad \forall\ i = 1(1)r. \tag{2.10}$$

The relations (2.9) and (2.10) describe stability properties of a splitting formula.

We now introduce two classes of linear functions:

$$\tilde{\mathfrak{A}} \;:= \left\{ f \;:\; f(t,w) = \sum_{i=1}^{r} f_i(t,w) = \sum_{i=1}^{r} A_i\, w,\;\; w \in \mathbb{R}^m,\;\; A_i \in \mathbb{R}^{m\times m} \quad \text{and } \mu[A_i] \le 0 \right\},$$

$$\tilde{\mathfrak{A}}_C := \left\{ f \;:\; f(t,w) = \sum_{i=1}^{r} f_i(t,w) = \sum_{i=1}^{r} A_i\, w,\;\; \mu[A_i] \le 0,\;\; A_i \text{ mutually commuting} \right\} \subset \tilde{\mathfrak{A}}.$$

Definition 2.1. A splitting formula applied to the class $\tilde{\mathfrak{A}}$ and $\tilde{\mathfrak{A}}_C$ is called $\tilde{A}$*-stable* and $\tilde{A}_C$*-stable*, respectively, if its amplification matrix R fulfills (2.9).

Definition 2.2. A splitting formula applied to the class $\tilde{\mathfrak{A}}$ and $\tilde{\mathfrak{A}}_C$ is called $\tilde{L}$*-stable* and $\tilde{L}_C$*-stable* if it is $\tilde{A}$-stable and $\tilde{A}_C$-stable, respectively, and its amplification matrix R fulfills (2.10).

Furthermore, we will use for our investigations a lemma which is based on a result of von Neumann [13] and can also be found in [5].

Lemma 2.1. *Let $\|.\|$ be defined by an inner product and let $A \in \mathbb{R}^{m\times m}$ be a given matrix with $\mu[A] \le \nu$. Let $R(z)$ be a rational function which is analytic in $S(\nu) := \{z \in \mathbb{C} : \mathrm{Re}(z) \le \nu\}$.Then $R(A)$ exists, and in the corresponding matrix norm holds*

$$\|R(A)\| \;\le\; \overline{R}(\nu),$$

where $\overline{R}(\nu) \;:=\; \sup\{\; |R(z)| \;:\; z \in\; S(\nu)\;\}$.

For our investigations we make the following assumption:

Assumption 1. The amplification matrix $R(\tau\, A_1, \ldots, \tau\, A_r)$ can be factorized in terms $R_{(ki)}(\tau\, A_i)$ which only depend on one of the matrix arguments, i.e.

$$R(\tau\, A_1, \ldots, \tau\, A_r) = \prod_{k} \prod_{i \in \{1,..,r\}} R_{(ki)}(\tau\, A_i). \tag{2.11}$$

Remark 2.1. Stability results for mutually commuting operators for more general amplification matrices, which do not have to fulfill Assumption 1, are presented in [12].

Under Assumption 1, we can estimate by using Lemma 2.1 the norm of the amplification matrix (2.11) of a linear splitting formula. Applying a linear splitting formula to the class $\tilde{\mathfrak{A}}_C$, we get with $R_{(i)}(\tau A_i) := \prod_k R_{(ki)}(\tau A_i)$

$$\|R(\tau\, A_1, \ldots, \tau\, A_r)\| \;\le\; \prod_{i=1}^{r} \|R_{(i)}(\tau\, A_i)\| \;\le\; \prod_{i=1}^{r} \sup\{|R_{(i)}(z)| \;:\; \mathrm{Re}(z) \le 0\}.$$

We have easily proved $\tilde{A}_C$-stability if $|R_{(i)}(z)| \le 1 \;\forall z \in \mathbb{C}^-,\; \forall i = 1(1)r$ (see also Remark 2.1). We now consider the class $\tilde{\mathfrak{A}}$. If the matrices A_i do not commute we can estimate

$$\|R(\tau\, A_1, \ldots, \tau\, A_r)\| \;\le\; \prod_{k} \prod_{i \in \{1,..,r\}} \|R_{(ki)}(\tau\, A_i)\| \;\le\; \prod_{k} \prod_{i \in \{1,..,r\}} \sup\{|R_{(ki)}(z)| \;:\; \mathrm{Re}(z) \le 0\}.$$

Hence, we can in general only prove $\tilde{A}$-stability if each of the $|R_{(ki)}(z)|$ is bounded by 1 for all $z \in \mathbb{C}^-$. For example, the amplification matrix of the ADI method (2.2) is given by

$$R(\tau A_1, \tau A_2) \;=\; \underbrace{(I - \tfrac{\tau}{2} A_2)^{-1}}_{=:R_{(12)}(\tau\, A_2)}\; \underbrace{(I + \tfrac{\tau}{2} A_1)}_{=:R_{(11)}(\tau\, A_1)}\; \underbrace{(I - \tfrac{\tau}{2} A_1)^{-1}}_{=:R_{(21)}(\tau\, A_1)}\; \underbrace{(I + \tfrac{\tau}{2} A_2)}_{=:R_{(22)}(\tau\, A_2)}\;.$$

Although $R(.)$ fulfills Assumption 1, the factors $|R_{(11)}(z)|$ and $|R_{(22)}(z)|$ are not bounded. However, if we apply the formula to the class $\tilde{\mathfrak{A}}_C$, then we can commute terms and obtain

$$R(\tau A_1, \tau A_2) \;=\; \underbrace{(I - \tfrac{\tau}{2}A_2)^{-1}(I + \tfrac{\tau}{2}A_2)}_{=:R_{(2)}(\tau A_2)}\underbrace{(I - \tfrac{\tau}{2}A_1)^{-1}(I + \tfrac{\tau}{2}A_1)}_{=:R_{(1)}(\tau A_1)}.$$

Since $|R_{(1)}(z)|, |R_{(2)}(z)| \leq 1 \;\forall z \in \mathbb{C}^-$ and $|R_{(1)}(-\infty)| = |R_{(2)}(-\infty)| = 1$, the formula (2.2) is $\tilde{A}_C$-stable. Analyzing analogously the other examples we obtain for the LOD method (2.3) the amplification matrix

$$R(\tau A_1, \dots, \tau A_r) = \prod_{i=r}^{1}(I - \tau\alpha A_i)^{-1}(I + \tau(1-\alpha)A_i) \ .$$

The norm of this matrix can easily be estimated and we have $\tilde{A}$-stability for $\alpha \in [\frac{1}{2}, \infty)$ and $\tilde{L}$-stability for $\alpha = 1$. Finally, the trapezoidal splitting method (2.4) is $\tilde{A}_C$-stable because its amplification matrix reads

$$R(\tau A_1, \dots, \tau A_r) = \prod_{i=1}^{r}(I - \tfrac{\tau}{2}A_i)^{-1}\prod_{i=r}^{1}(I + \tfrac{\tau}{2}A_i) \ ,$$

which can be written as

$$R(\tau A_1, \dots, \tau A_r) = \prod_{i=1}^{r}(I - \tfrac{\tau}{2}A_i)^{-1}(I + \tfrac{\tau}{2}A_i) \ ,$$

whenever the A_i commute. Summarizing, there exist splitting formulas for solving (1.4) arising from a semidiscretization of a PDE which are either of consistency order one and $\tilde{L}$-stable or of consistency order two but only $\tilde{A}_C$-stable.

3. Linearly implicit splitting formulas

The aim of our paper is to find splitting formulas which are second-order consistent, $\tilde{L}$-stable and where only linear equations have to be solved. Examples of integration methods for ODEs where only *linear* equation systems have to be solved are the so-called linearly implicit Runge-Kutta methods, e.g. Rosenbrock-type methods or adaptive Runge-Kutta methods (see [16]). These methods have good stability properties and are easy to implement. They directly involve an approximation to the Jacobian matrix in the scheme, but they do not exploit the special splitting relation of the right hand side function in the equation (1.4).

We will now introduce a class of linearly implicit splitting formulas, whose structure is similar to the adaptive Runge-Kutta methods.

Definition 3.1. A *locally one-dimensional, linearly implicit splitting formula (LISM)* for solving (1.4) is given by the following scheme

$$
\begin{aligned}
v_{n+1}^{(0)} &= v_n \\
v_{n+1}^{(s)} &= R_0^{(s)}(a_s\tau T_s)\, v_{n+1}^{(s-1)} + \tau\, R_1^{(s)}(a_s\tau T_s) \sum_{j=0}^{s-1} b_{sj} K_{sj}\,, \qquad s = 1(1)r, \qquad (3.1)\\
v_{n+1}^{(\tilde{s})} &= R_0^{(\tilde{s})}(a_{\tilde{s}}\tau T_{2r-\tilde{s}+1})\, v_{n+1}^{(\tilde{s}-1)} + \tau\, R_1^{(\tilde{s})}(a_{\tilde{s}}\tau T_{2r+1-\tilde{s}}) \sum_{j=0}^{\tilde{s}-1} b_{\tilde{s}j} K_{2r-\tilde{s}+1,j}\,, \qquad \tilde{s} = r+1(1)2r,\\
v_{n+1} &= v_{n+1}^{(2r)}
\end{aligned}
$$

$$\text{with} \qquad K_{ij} = f_i(t_n + c_j\tau, v_{n+1}^{(j)}) - T_i\, v_{n+1}^{(j)}\,, \qquad i = 1(1)r,\ j = 0(1)2r-1.$$

In principle, the matrices T_s $(s = 1(1)r)$ are arbitrary. However, for reasons of stability, they are supposed to be approximations to the Jacobian matrices $\frac{\partial f_s}{\partial w}$. The scalars a_s, c_s and b_{ij} are parameters of the method. The matrix-valued functions $R_0^{(*)}(.)$, $R_1^{(*)}(.)$ are supposed to correspond to rational functions $R_0^{(*)}(z)$, $z \in \mathbb{C}$, where

$$R_1^{(*)}(z) = \frac{R_0^{(*)}(z) - 1}{z}$$

and $R_0^{(*)}(z)$ approximates the exponential function e^z (for $z \to 0$) with at least first order of accuracy. Furthermore, we assume, at least for the last r stages, that

$$R_0^{(\tilde{s})}(z) \text{ is analytic for } \mathrm{Re}(z) \le 0 \text{ and } |R_0^{(\tilde{s})}(-\infty)| < \infty, \qquad \tilde{s} = r+1(1)2r. \tag{3.2}$$

Therefore, the last r stages are linearly implicit.

3.1. **Stability investigations.** Applying the LISM (3.1) to the class $\tilde{\mathfrak{A}}$ and choosing $T_s = A_s$ $(s = 1(1)r)$, we obtain the amplification matrix

$$R(\tau A_1, \ldots, \tau A_r) = \prod_{s=2r}^{r+1} R_0^{(s)}(a_s\tau A_{2r-s+1}) \prod_{s=r}^{1} R_0^{(s)}(a_s\tau A_s). \tag{3.3}$$

This matrix fulfills Assumption 1 and by the choice of the functions $R_0^{(s)}$ we can directly influence the stability of the LISM. Choosing, for example,

$$R_0^{(s)}(z) = \frac{1}{1-z}, \qquad \forall\ s = 1(1)2r,$$

we have $\tilde{L}$-stability, because

$$|R_0^{(s)}(z)| < 1, \quad \forall\ z \in \mathbb{C},\ \mathrm{Re}(z) < 0, \quad \text{and} \quad R_0^{(s)}(-\infty) = 0. \tag{3.4}$$

(Functions which satisfy (3.4) are called *L-acceptable.*) However, the following analysis will show that we cannot achieve consistency order two for this choice. Fortunately, it can be shown that there are possibilities for the choice of the matrix functions such that we do obtain $\tilde{L}$-stability and consistency order two.

3.2. **Consistency order.** In this subsection, we will give order conditions for the classical consistency in time of the LISM (3.1). Following the usual approach (see [3]), we compare the exact solution $w(t_{n+1})$ with the numerical solution $\tilde{v}_{n+1}$ after one single step starting with the exact solution $w(t_n)$, i.e. $v_n = w(t_n)$. Using the Taylor expansions of the numerical solution and of the exact solution at the time point t_n and requiring consistency order two, i.e.

$$\tilde{v}_{n+1} - w(t_{n+1}) \;=\; \mathcal{O}(\tau^3),$$

we obtain order conditions for determining the parameters of the method (3.1).

We assume that the rational functions $R_0^{(s)}(z)$ are approximations to e^z of at least order one, i.e.

$$R_0^{(s)}(z) = 1 + z + d_s\, z^2 + \mathcal{O}(z^3),$$

where d_s is a parameter to be specified later. Furthermore, we distinguish two cases for choosing the matrices T_s, viz. $T_s = \frac{\partial f_s}{\partial w} + \mathcal{O}(\tau)$ and T_s arbitrary.

1. In the case $T_s = \frac{\partial f_s}{\partial w} + \mathcal{O}(\tau)$ we obtain, under the assumption $a_s = \sum_{j=0}^{s-1} b_{sj}$, for $s = 1(1)r$ the following order conditions for order two

$$
\begin{aligned}
1 &= a_s + a_{2r-s+1} && (\text{differential} \quad f_s)\,,\\
\frac{1}{2} &= \sum_{j=0}^{s-1} b_{sj}\, c_j \;+\; \sum_{j=0}^{2r-s} b_{2r-s+1,j}\, c_j && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial t}\right),\\
\frac{1}{2} &= d_s\, a_s^2 + d_{2r-s+1}\, a_{2r-s+1}^2 + a_s\, a_{2r-s+1} && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial w} f_s\right),\\
\frac{1}{2} &= a_i\;, \quad i = 1(1)r, && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial w} f_i,\; i \neq s\right).
\end{aligned}
$$

Simplifying these equations we have

$$\frac{1}{2} = a_s = \sum_{j=0}^{s-1} b_{sj}\;, \quad s = 1(1)2r,$$

$$1 = d_s + d_{2r-s+1}, \quad \frac{1}{2} = \sum_{j=0}^{s-1} (b_{sj} + b_{2r-s+1,j})\, c_j \;+\; \sum_{j=s}^{2r-s} b_{2r-s+1,j}\, c_j\;, \quad s = 1(1)r.$$

2. In the case of arbitrary matrices T_s, we obtain, again with $a_s = \sum_{j=0}^{s-1} b_{sj}$, for $s = 1(1)r$, $i \in \{1,..,r\}$ the conditions

$$
\begin{aligned}
& 1 = a_s + a_{2r-s+1} && (\text{differential} \quad f_s)\,,\\
& \frac{1}{2} = \sum_{j=0}^{s-1} b_{sj}\, c_j \;+\; \sum_{j=0}^{2r-s} b_{2r-s+1,j}\, c_j && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial t}\right),\\
i < s: \quad & \frac{1}{2} = a_i \left(\sum_{j=i}^{s-1} b_{sj} + \sum_{j=i}^{2r-s} b_{2r-s+1,j} \right) && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial w} f_i\right),\\
& \frac{1}{2} = a_s \sum_{j=s}^{2r-s} b_{2r-s+1,j} && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial w} f_s\right),\\
i > s: \quad & \frac{1}{2} = a_i \sum_{j=i}^{2r-s} b_{2r-s+1,j} + (1 - a_s) \sum_{j=2r-i+1}^{2r-s} b_{2r-s+1,j} && \left(\text{differential} \quad \tfrac{\partial f_s}{\partial w} f_i\right),
\end{aligned}
$$

$$s < r: \quad \frac{1}{2} = a_s\,, \qquad 1 \;=\; d_s + d_{2r-s+1}\,, \qquad\qquad (\text{differential} \quad T_s\, f_i,\ i \neq s)\,,$$

$$s = r: \quad \frac{1}{2} = d_r\, a_r^2 + d_{r+1}\, a_{r+1}^2 + a_r\, a_{r+1} \qquad\qquad (\text{differential} \quad T_r\, f_r)\,.$$

Example 3.1. Let T_s be arbitrary and let $r = 3$, $a_3 = a_4 = \frac{1}{2}$. Then the order conditions for arbitrary T_s simplify to: $a_1 = a_2 = a_3 = a_4 = a_5 = a_6 = \frac{1}{2}$,

s	b_{s0}	b_{s1}	b_{s2}	b_{s3}	b_{s4}	b_{s5}
1	$\frac{1}{2}$					
2	$\frac{1}{2} + b_{51}$	$-b_{51}$				
3	$\frac{1}{2} + b_{41} + b_{42}$	$-b_{41}$	$-b_{42}$			
4	$-(\frac{1}{2} + b_{41} + b_{42})$	b_{41}	b_{42}	1		
5	$-\frac{1}{2} - b_{51}$	b_{51}	b_{54}	$1 - 2b_{54}$	b_{54}	
6	$-\frac{1}{2}$	b_{65}	b_{64}	$1 - 2(b_{64} + b_{65})$	b_{64}	b_{65}

$$d_s + d_{7-s} = 1, \qquad s = 1, 2, 3,$$

$$c_3 = \frac{1}{2}, \quad 0 = b_{54}(c_2 + c_5 - 1), \quad 0 = b_{64}(c_2 + c_4 - 1) + b_{65}(c_1 + c_5 - 1).$$

For arbitrary r we get analogous tables.

In both cases, it is possible to solve these systems of order conditions. Furthermore, in the order conditions listed above, some parameters are still free. They can be chosen such that the computational costs are reduced with respect to the number of function evaluations and the number of LU-decompositions. For example, this is achieved if $R_0^{(s)}(a_s\tau T_s) = R_0^{(2r-s+1)}(a_{2r-s+1}\tau T_s)$.

3.3. **Examples of linearly implicit splitting methods.** We will introduce methods which we used for our numerical tests in Section 4. A LISM depends also on the special choice of the matrix functions $R_0^{(s)}(.)$. We now give a list of matrix functions used which are at least first order approximations to e^z.

$$\text{F1:} \qquad R_0(a_sT_s) = (I - \gamma\, a_sT_s)^{-2}\, (I + (1-2\gamma)a_sT_s)\,, \quad \gamma = 1 - \tfrac{\sqrt{2}}{2}, \tag{3.5}$$
$$\Longrightarrow \quad R_1(a_sT_s) = (I - \gamma\, a_sT_s)^{-2}\, \left(I - \gamma^2 a_sT_s\right),$$

$$\text{F2:} \qquad R_0(a_sT_s) = \left(I - \tfrac{a_s}{2}T_s\right)^{-1}\, \left(I + \tfrac{a_s}{2}T_s\right) \tag{3.6}$$
$$\Longrightarrow \quad R_1(a_sT_s) = \left(I - \tfrac{a_s}{2}T_s\right)^{-1},$$

$$\text{F3:} \qquad R_0(a_sT_s) = I + a_sT_s \quad \Longrightarrow \quad R_1(a_sT_s) = I, \tag{3.7}$$

$$\text{F4:} \qquad R_0(a_sT_s) = (I - a_sT_s)^{-1} \quad \Longrightarrow \quad R_1(a_sT_s) = (I - a_sT_s)^{-1}\,. \tag{3.8}$$

Combining these matrix functions with the formulas in the examples below we obtain special methods.

Example 3.2. With *LISM1* we denote the following formula for the case, that T_s is an approximation to the Jacobian $\frac{\partial f_s}{\partial w}$: Let $s = 1(1)r$, $\tilde{s} = 2r - s + 1$.

$$\begin{aligned} \text{LISM1:} \qquad v_{n+1}^{(s)} &= R_0\big(\tfrac{\tau}{2}T_s\big)v_{n+1}^{(s-1)} + \tfrac{\tau}{2}R_1\big(\tfrac{\tau}{2}T_s\big)\Big(f_s(t_n, v_n) - T_s v_n\Big), \\ v_{n+1}^{(\tilde{s})} &= R_0(\tfrac{\tau}{2}T_s)v_{n+1}^{(\tilde{s}-1)} + \tfrac{\tau}{2}R_1(\tfrac{\tau}{2}T_s)\Big(f_s(t_n+\tau, v_{n+1}^{(r)}) - T_s v_{n+1}^{(r)}\Big). \end{aligned} \tag{3.9}$$

Example 3.3. *LISM2* is a special formula of example 3.1, where T_s can be arbitrarily: Let $s = 1(1)r$, $\tilde{s} = 2r - s + 1$.

$$\begin{aligned} \text{LISM2:} \qquad v_{n+1}^{(s)} &= R_0\big(\tfrac{\tau}{2}T_s\big)v_{n+1}^{(s-1)} + \tfrac{\tau}{2}R_1\big(\tfrac{\tau}{2}T_s\big)\,K_{s,s-1}, \\ v_{n+1}^{(\tilde{s})} &= R_0(\tfrac{\tau}{2}T_s)v_{n+1}^{(\tilde{s}-1)} + \tau R_1(\tfrac{\tau}{2}T_s)\left(-\tfrac{1}{2}K_{s,s-1} + K_{s,r}\right), \\ K_{s,s-1} &= f_s(t_n + \tfrac{\tau}{2}, v_{n+1}^{(s-1)}) - T_s v_{n+1}^{(s-1)}, \\ K_{s,r} &= f_s(t_n + \tfrac{\tau}{2}, v_{n+1}^{(r)}) - T_s\, v_{n+1}^{(r)}. \end{aligned} \tag{3.10}$$

We note, that we can reuse the already calculated values $K_{s,s-1}$ in the stage $2r - s + 1$.

If we combine the methods LISM1 or LISM2 with the rational functions F1 we get the $\tilde{L}$-stable methods *LISM1F1* or *LISM2F1*. Combined with F2 we get the $\tilde{A}$-stable methods *LISM1F2* and *LISM2F2*.

Remark 3.1. The methods LISM1 and LISM2 offer the possibility to perform function and Jacobian evaluations, matrix times vector multiplications and LU-decompositions in parallel.

Example 3.4. *LISM3F3F4* or *LTRAP* denote the following formula: Let $s = 1(1)r$, $\tilde{s} = 2r - s + 1$. We use for $R_0^{(s)}$ the function F3, i.e. the first r stages are explicit. Let $T_s = \frac{\partial f_s}{\partial w}(t_n + \tau, v_{n+1}^{\tilde{s}-1}) + \mathcal{O}(\tau)$ and $R_0^{(\tilde{s})}$ be the function F4. Hence, only the last r stages are implicit.

$$\begin{aligned} \text{LTRAP:} \qquad v_{n+1}^{(s)} &= v_{n+1}^{(s-1)} + \tfrac{\tau}{2}f_s(t_n, v_{n+1}^{(s-1)}), \qquad s = 1(1)r,\ \tilde{s} = 2r - s + 1, \\ v_{n+1}^{(\tilde{s})} &= v_{n+1}^{(\tilde{s}-1)} + \tfrac{\tau}{2}\left(I - \tfrac{\tau}{2}T_s\right)^{-1} f_s(t_n + \tau, v_{n+1}^{(\tilde{s}-1)}). \end{aligned} \tag{3.11}$$

This method is identical with the trapezoidal splitting method (2.4), if the implicit relations in this scheme are solved by one Newton iteration step.

3.4. **B-consistency.** In the numerical integration of stiff problems it often occurs that the order of accuracy of the approximation will be less than expected when the classical order of consistency is taken into account. In the investigations of the foregoing section, where we used the Taylor expansion in the classical way, we do not give attention to the stiffness of the problem (1.4). For stiff problems elementary differentials may become very large even when the solution $w(t)$ is smooth in the sense of

$$\left\| \frac{d^k\, w(t)}{d\, t^k} \right\| \le M_k\ ,\ t \in [0, T],\ k = 1, 2, \dots, \tag{3.12}$$

where the constants M_k are independent of any quantity which influences the stiffness of the problem (1.4) considered. Hence we should try to eliminate these large derivatives from error bounds. For this purpose, Frank, Schneid and Ueberhuber ([4]) introduced the concepts of *B-consistency* and *B-convergence*: Let $\langle .,. \rangle$ be a given inner product on $\mathbb{R}^m$ and let $\nu \in \mathbb{R}$ be a constant. We define the class $\mathfrak{F}_\nu$ of problems (1.4) which satisfy the one-sided Lipschitz condition

$$\langle f(t, w_1) - f(t, w_2), w_1 - w_2 \rangle \le \nu\, \|w_1 - w_2\|^2, \quad t \in [0, T],\ \forall\ w_1, w_2 \in \mathbb{R}^m\ . \tag{3.13}$$

The problems considered in the following are supposed to fulfill

Assumption 2. We assume, that the solution $w(t)$ fulfills (3.12) and that

$$\left\| \frac{d^k}{d\,t^k} f_i(t, w(t)) \right\| \le L_i \;, \qquad t \in [0,T],\; i = 1(1)r,\; k = 1,2,\dots, \tag{3.14}$$

with constants L_i independend of stiffness.

Definition 3.2. A one-step method is called *B-consistent* of order q on the class $\mathfrak{F}_\nu$ if the local error satisfies

$$\|\tilde{v}_{n+1} - w(t_{n+1})\| \le C\,\tau^{q+1}\;, \qquad \forall\; \tau \in (0, \tau^*], \tag{3.15}$$

where the real quantities C and $\tau^* > 0$ are independent of the stiffness of $\mathfrak{F}_\nu$.

For simplicity we consider the class of linear problems (2.5)

$$w'(t) = \sum_{i=1}^{r} A_i\, w(t)\;, \qquad w \in \mathbb{R}^m,\; A_i \in \mathbb{R}^{m\times m},\; \mu[A_i] \le 0. \tag{3.16}$$

The norm of the local error of a LISM (3.1) applied to this class is given by

$$\|\tilde{v}_{n+1} - w(t_{n+1})\| \;\le\; \left\| R(\tau\, A_1, \dots, \tau\, A_r) w(t_n) - \left(I + \tau \sum_{i=1}^{r} A_i \right) w(t_n) \right\| + \frac{\tau^2}{2} M_2.$$

In order to achieve B-consistency order one we have to choose the $R_0^{(i)}(.)$, $i = 1(1)2r$, (see (3.3)) so that

$$\left\| \left[\prod_{s=2r}^{r+1} R_0^{(s)}(a_s \tau A_{2r-s+1}) \prod_{s=r}^{1} R_0^{(s)}(a_s \tau A_s) \;-\; \left(I + \tau \sum_{i=1}^{r} A_i \right) \right] w(t_n) \right\| \le \tau^2\, \bar{C},$$

where $\bar{C}$ is a constant independent of the stiffness of the problem.

Corollary 3.1. *Under the Assumption 2, a LISM (3.1) for $r = 2$ is B-consistent of order one on the class of linear problems (1.4) with $f \in \tilde{\mathfrak{A}}_C$, if its amplification matrix has the form*

$$R(\tau\, A_1, \tau\, A_2) = \left(I - \frac{\tau}{2} A_2\right)^{-1} \left(I + \frac{\tau}{2} A_2\right) \left(I - \frac{\tau}{2} A_1\right)^{-1} \left(I + \frac{\tau}{2} A_1\right) \tag{3.17}$$

or

$$R(\tau\, A_1, \tau\, A_2) = \left(I - \frac{\tau}{4} A_2\right)^{-2} \left(I + \frac{\tau}{4} A_2\right)^{2} \left(I - \frac{\tau}{4} A_1\right)^{-2} \left(I + \frac{\tau}{4} A_1\right)^{2}\;. \tag{3.18}$$

Remark 3.2.
1. Splitting methods, which have amplification matrices of the form (3.17) or (3.18), are $\tilde{A}_C$-stable.
2. The statements of Corollary 3.1 can be extended to systems of the form
$$w'(t) = A_1\, w(t) + g_1(t) + A_2\, w(t) + g_2(t), \tag{3.19}$$
where $w, g_i \in \mathbb{R}^m,\; A_i \in \mathbb{R}^{m\times m}, \mu[A_i] \le 0,\; i = 1,2$. Here, the functions $g_i(t)$ can for example contain the boundary values of the underlying PDE with inhomogeneous boundary conditions (see [9],[10],[11]).
3. We could only find Splitting methods, which are $\tilde{L}$-stable and B-consistent of order greater than zero, under the strong assumption, that $A_2\, A_1\, w(t)$ is uniformly bounded. In [10], it is mentioned that this holds, for example, for periodic boundary conditions.
4. For $r = 3$ we obtain B-consistency order one only under very strong assumptions.

Example 3.5. For $r = 2$ the methods LISM1F2, LISM2F2, LTRAP and the trapezoidal splitting method (2.4) are B-consistent of order one on the class of linear problems (3.16).

4. Numerical tests

In this section some numerical results are presented for the methods of section 3.3 and the trapezoidal splitting method (2.4). The implicit relations in TRAPSP are solved by a simplified Newton iteration process. We have implemented the methods with a stepsize control for the time integration using Richardson extrapolation. At the end of the numerical integration process we compare the numerical solution with the exact solution $u_h(t)$ of the PDE in each grid point. In the figures of the examples below we plotted the computing time compared with the logarithm of the relative error

$$ERR = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(\frac{v_i - u_h(t_e)_i}{1+|u_h(t_e)_i|}\right)^2}$$

at the endpoint t_e, where v is the numerical solution at t_e. In these examples we distribute the source terms equally to the splitting functions.

Example 4.1. We consider the 2-dimensional problem

$$u_t \quad = \quad \tfrac{1}{2}x(1-x)u_{xx} + \tfrac{1}{2}(1+\alpha\, x)\, y(1-y)u_{yy} - (1-x)\alpha u$$

on $\Omega = [0,1]^2$ and $t \in [0,1]$. The initial condition and Dirichlet boundary conditions are chosen such that we have the exact solution

$$u(t,x,y) \quad = \quad e^{-(2+\alpha)t}x(1-x)y(1-y).$$

Because the exact solution of the PDE is a polynomial in the space variables of degree less than 4 there is no spatial error in the ODE (1.4) after semidiscretization. The semidiscrete ODE is a linear system of the form (2.5). We consider two cases, $\alpha = 0$ and $\alpha = 100$. For $\alpha = 0$ the matrices A_1 and

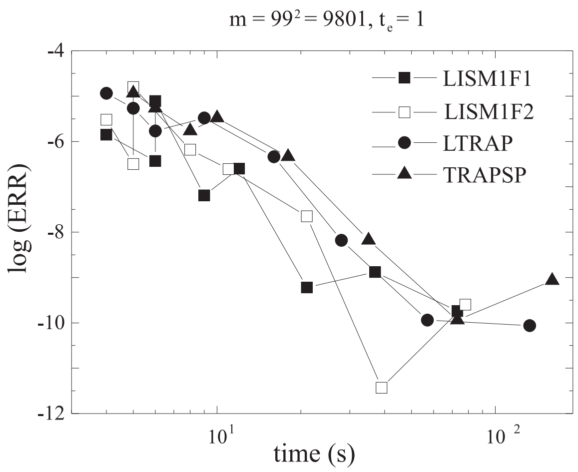

FIGURE 4.1. Example 4.1, $\alpha = 0$, $m = 99^2 = 9801$, $t_e = 1$

A_2 commute, because we use an equidistant grid in space. In Figure 4.1 we see, that all the methods plotted there have similar properties. The $\tilde{L}$- and $\tilde{A}$-stable methods LISM1F1 and LISM1F2 are faster than the $\tilde{A}_C$-stable method TRAPSP and LTRAP for this linear example. For $\alpha = 100$ (see Figure 4.2) the matrices A_1 and A_2 do not commute. The assumptions for the stability of LTRAP and TRAPSP are not satisfied. The methods LISM1F1 and LISM1F2 do not need the assumption of commuting matrices. This seems to be the reason for the better performance of the $\tilde{A}$-stable method LISM1F2. Furthermore, for this example the $\tilde{L}$-stability of the method LISM1F1 pays off.

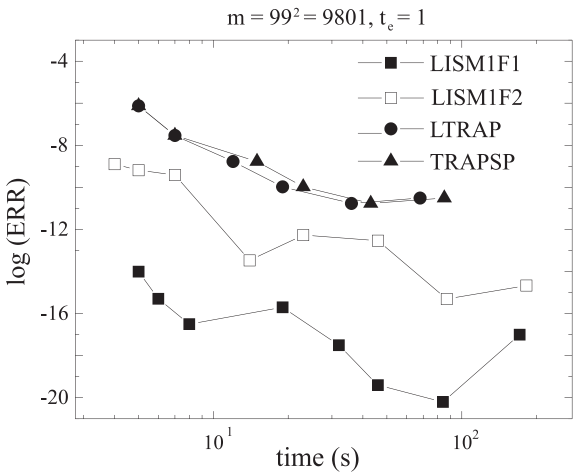

FIGURE 4.2. Example 4.1, $\alpha = 100$, $m = 99^2 = 9801$, $t_e = 1$

Example 4.2. We consider the 2-dimensional, nonlinear diffusion equation

$$u_t \quad = \quad e^u(u_{xx} + u_{yy}) + u\,\left(2\pi^2\,e^u - 1\right), \tag{4.1}$$

where $\Omega = [0,1]^2$ and $t \in [0,10]$. The initial and Dirichlet boundary conditions are chosen so that we have the exact solution

$$u(t,x,y) \quad = \quad e^{-t}\,\sin(\pi\,x)\sin(\pi,y)\ . \tag{4.2}$$

In contrast to the semidiscretization described in Section 1, we calculate for our tests the analytical expression of the spatial error introduced by the semidiscretization and add it to the right hand side of the ODE (1.4). Then the exact solution of this ODE is equal to the exact solution of the PDE (1.1) restricted to the grid and ERR does not depend on an error in space. Otherwise, the spatial error would dominate the overall error if we require small tolerances in the step size control process. Figure 4.3 shows, that the linearly implicit, $\tilde{L}$-stable method LISM1F1 is more accurate and stable

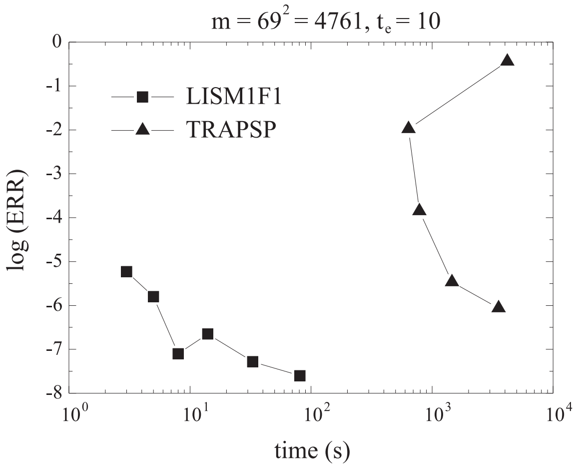

FIGURE 4.3. Example 4.2, $m = 69^2 = 4761$, $t_e = 10$

as the fully implicit, $\tilde{A}_C$-stable method TRAPSP.

Example 4.3. As third example of this section we choose the 3-dimensional PDE

$$\begin{aligned} u_t = u_{xx} + u_{yy} + u_{zz} + e^t\big(&x(1-x)y(1-y)z(1-z) \\ &+ 2y(1-y)z(1-z) + 2x(1-x)z(1-z) + 2x(1-x)y(1-y)\big) \end{aligned}$$

with $\Omega = [0,1]^3$ and $t \in [0,10]$ and homogeneous Dirichlet boundary conditions. The initial condition is chosen so that we get as exact solution

$$u(t,x,y,z) = e^t\, x\,(1-x)\, y\,(1-y)\, z\,(1-z).$$

Using central differences of second order again no spatial error occurs. Figure 4.3 demonstrates that

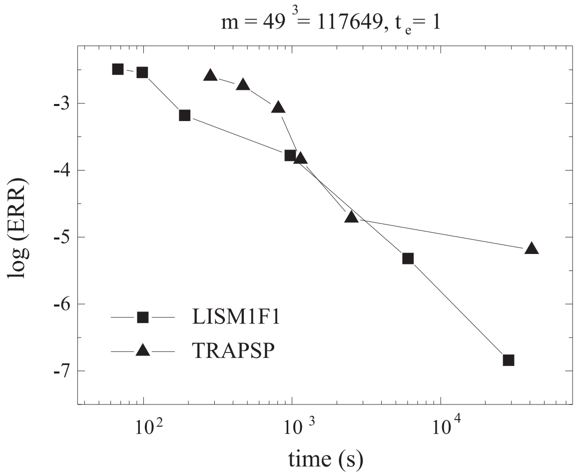

FIGURE 4.4. Example 4.3, $m = 49^3 = 117649$, $t_e = 10$

both methods, LISM1F1 and TRAPSP, work similar and appropriate for very large problems.

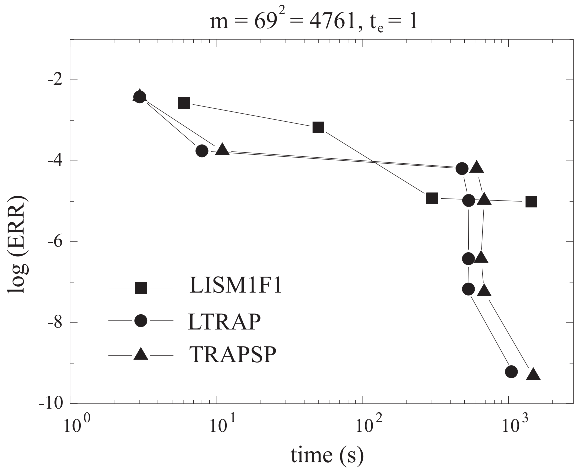

FIGURE 4.5. Example 4.4, $m = 69^2 = 4761$, $t_e = 1$

Example 4.4. Let the 2-dimensional problem

$$u_t = u_{xx} + u_{yy} + e^t\,(x\,(1-x)\,y\,(1-y)\,(16+y) + 2\,y\,(1-y)\,(16+y) + 6\,x\,(1-x)\,(5+y))$$

for $\Omega = [0,1]^2$, $t \in [0,1]$ be given. The function

$$u(t,x,y) = e^t\, x\,(1-x)\, y\,(1-y)\,(16+y)$$

is the solution of the example, if we require $u(0,x,y) = x(1-x)y(1-y)(16+y)$ and homogeneous Dirichlet boundary conditions. Figure 4.5 shows that LISM1F1 is less accurate than LTRAP or TRAPSP. We suppose, that the reason is the better B-consistency order of the trapezoidal method on the class of problems (3.19) (see Remark 3.2).

5. Conclusion

We have derived a class of linearly implicit splitting methods of classical consistency order two, which are $\tilde{A}$- and $\tilde{L}$-stable (independent of the commutativity of the A_i). These methods are attractive for the numerical solution of parabolic differential equations, because they only require the solution of linear equations with tridiagonal matrices. Unfortunately, in contrast to the trapezoidal splitting method TRAPSP (which is only $\tilde{A}_C$-stable), they are in general only of B-consistency order zero. However, our numerical tests indicate that for certain problems $\tilde{L}$-stability (and classical order two) can be more important than B-consistency.

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