Shifted Slope-Comparison Multistep Formulas for ODEs

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Abstract

We present new multistep formulas for initial value problems in ODEs, which we call *Shifted Slope-Comparison (SSC) formulas*. SSC formulas are derived from the functional equation $p'(t) = f(t, p(t))$, where p is a polynomial approximation of the solution. This equation, applied at an evaluation point t_e, produces a nonlinear multistep formula $p'(t_e) = f(t_e, p(t_e))$ which can be used to compute the solution at the next integration point. We show that the choice of t_e is critical for the accuracy and stability of SSC formulas. In particular, we show that there exists a point t^+ which leads to an SSC formula with essentially the same accuracy and stability as Adams-Moulton. More interestingly, we show that there exists a point t^* which leads to an SSC formula which is more precise than BDF's, which is precisely A(α)-stable (a concept which aims at capturing the ideal stability region), and whose stability angle α is essentially similar to BDF's. We also show how to apply the corrector idea of Klopfenstein to further improve the stability region.

1 Introduction

This paper presents new formulas for the solutions of initial value problems

$$y'(t) = f(t, y(t)) \tag{1}$$

on a time interval $[t_0, t_f]$, given initial values $y(t_0) = y_0$. The formulas are derived from the functional equation

$$p'(t) = f(t, p(t)) \tag{2}$$

where p is an approximation of the solution y. In the following, we restrict attention to the cases where the approximation p is a polynomial of degree $\leq k$ that interpolates the points

$$(t_n, y_n), \ldots, (t_{n+k}, y_{n+k}).$$

Hence equation (2), when applied to a specific time t_e, produces an *implicit non-linear multistep* formula

$$p'(t_e) = f(t_e, p(t_e)) \tag{3}$$

which can be used to approximate the value $y(t_{n+k})$. We call these equations *Shifted Slope-Comparison (SSC) formulas (or SSC$_k$ formulas for k steps)* since they can be thought of as comparing the slope $p'(t_e)$ of the approximation p at time t_e with the approximation $f(t_e, p(t_e))$ of the slope $f(t_e, y(t_e))$ of the solution at the same time. Obviously, equation (2) at time t_{n+k} gives a backward differentiation formula (BDF).

The fundamental insight of this paper is that it is of great interest to choose a slope-comparison time different from the interpolation time t_{n+k}. More specifically, we show that there exists a time t^+ such that the SSC$_k$ formula

$$p'(t^+) = f(t^+, p(t^+)) \tag{4}$$

produces a method whose accuracy and stability properties are essentially the same as the k-step Adams-Moulton formula (AM$_k$). More interestingly, we show that there exists a time t^* such that the SSC$_k$ formula

$$p'(t^*) = f(t^*, p(t^*)) \tag{5}$$

produces a method with the following properties:

1. It is $A(\alpha)$-stable, its stability angle α is comparable to the one of BDF$_k$, and its stability region does not intersect with $\mathbb{C}^+$.
2. It is of order k and more precise than BDF$_k$.

In particular, for $k = 2$, the method is precisely A-stable and is as accurate as the trapezoidal rule. Assuming a constant step size h, point t is defined in terms of a ratio τ satisfying

$$t = t_n + \tau h.$$

The ratios τ^+ and τ^* defining t^+ and t^* are roots of polynomials that depend only on the number of steps k and can thus be computed once for all for each k. Finally, we also show how to apply the corrector idea from Klopfenstein [Klo71] to SSC formulas. These corrected formulas significantly improve the stability region while only degrading accuracy slightly. As a consequence, the resulting formulas come close to the ideal stability region [Lam91] while only degrading accuracy slightly.

The rest of the paper characterizes the ratios τ^+ and τ^* as well as the additional parameter arising in the corrected SSC formulas. Section 2 defines the SCC formulas precisely and presents the main tools to carry out the analysis. Section 3 characterizes the ratio τ^+, studies the accuracy and stability of the corresponding SSC formula, and compares it to Adams-Moulton. Section 4 characterizes the ratio τ^*, studies the accuracy and stability of the corresponding SSC formula, and compares it to BDF's. Section 5 shows how to apply the corrector idea from [Klo71] to further improve the stability region.

2 The SSC Formulas

When the step size is a constant h, the SSC$_k$ formula, for a step from (t_{n+k-1}, y_{n+k-1}) to (t_{n+k}, y_{n+k}), can be written in terms of backward differences as

$$\boxed{p'(t) - f(t, p(t)) = 0} \tag{6}$$

where

$$\begin{array}{rcl} p(t) & = & \sum_{j=0}^{k} \zeta_j(\tau) \nabla^j y_{n+k}, \\ p'(t) & = & \frac{1}{h} \sum_{j=1}^{k} \zeta_j^{'}(\tau) \nabla^j y_{n+k}, \\ t & = & t_n + \tau h, \\ \zeta_0(\tau) & = & 1, \\ \zeta_j(\tau) & = & \frac{1}{j!} \prod_{m=0}^{j-1} (\tau + m) \;\; (1 \leq j \leq k), \\ \zeta_j^{'}(\tau) & = & \zeta_j(\tau)\delta_j(\tau) \;\; (1 \leq j \leq k), \\ \delta_j(\tau) & = & \sum_{m=0}^{j-1} \frac{1}{\tau + m} \;\; (1 \leq j \leq k). \end{array} \tag{7}$$

When $t = t_{n+k}$, SSC$_k$ reduces to BDFk:

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+k} - hf(t_{n+k}, y_{n+k}) = 0. \tag{8}$$

Observe that the SSC$_k$ formula is parametrized by the ratio τ and hence it defines a class of SSC$_k$ formulas. In the following, we use SSC$_k(\tau)$ to represent the SSC$_k$ formula for a given τ. We will also make frequent use of the function w defined as

$$w(\tau) = \prod_{j=0}^{k} (\tau - j)$$

as it plays an important role in some of our results. The following theorem characterizes the error of the polynomial interpolation [Atk88].

Theorem 1 (Error in Polynomial Interpolation) *Let $p(t)$ be the polynomial interpolating the function $y(t)$ at the points $t_0, \ldots, t_k$. Then,*

1. $\exists \xi \in \mathcal{H}\{t_0, \ldots, t_k, t\} : y(t) - p(t) = w(\tau) \frac{y^{(k+1)}(\xi)}{(k+1)!} h^{k+1}$;
2. $\exists \xi_1, \xi_2 \in \mathcal{H}\{t_0, \ldots, t_k, t\} : y'(t) - p'(t) = w'(\tau) \frac{y^{(k+1)}(\xi_1)}{(k+1)!} h^k + w(\tau) \frac{y^{(k+2)}(\xi_2)}{(k+2)!} h^{k+1}$;

where $\mathcal{H}A$ is the hull of set A.

SSC formulas are non-linear multistep methods because of the the term $f(t, p(t))$. Consider the linear form of an SSC formula, i.e., the linear multistep method (LMM)

$$\sum_{j=0}^{k} \alpha_j(\tau) y_{n+j} = h \sum_{j=0}^{k} \beta_j(\tau) f_{n+j} \tag{9}$$

where ($j = 0, \ldots, k$)

$$\begin{array}{rcl} \alpha_j(\tau) & = & \varphi'_j(\tau) \\ \beta_j(\tau) & = & \varphi_j(\tau) \\ \varphi_j(\tau) & = & \prod_{\substack{m=0 \\ m \neq j}}^{k} \frac{\tau+k-m}{j-m} \\ f_{n+j} & = & f(t_{n+j}, y_{n+j}). \end{array} \tag{10}$$

We can easily verify that, for all τ, the formula (9) is normalized, i.e., $\sum_{j=0}^{k} \beta_j(\tau) = 1$. We now show that

1. Formulas (6) and (9) have order at least k;
2. when either formula (6) or (9) has order k, the formulas have the same order and the same error constant (i.e., they have the same accuracy);
3. the formulas (6) and (9) have the same linear stability.

2.1 Accuracy

Consider the linear difference operator

$$\mathcal{L}[y(t_n), h] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - h \sum_{j=0}^{k} \beta_j(\tau) y'(t_{n+j}) \tag{11}$$

of the linear multistep method (9) and let us associate a difference operator with SSC_k

$$\Phi[y(t_n), h, \tau] = \sum_{j=0}^{k} \alpha_j(\tau) y(t_{n+j}) - hf(t, \sum_{j=0}^{k} \beta_j(\tau) y(t_{n+j})). \tag{12}$$

¿From Theorem 1, it follows easily that $\mathcal{L}$ and Φ can be expanded as

$$\begin{array}{lcl} \mathcal{L}[y(t_n), h] & = & C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + O(h^{k+2}), \\ \Phi[y(t_n), h, \tau] & = & C_{k+1}(\tau) h^{k+1} y^{(k+1)}(t_n) + O(h^{k+2}). \end{array} \tag{13}$$

Therefore, when $C_{k+1}(\tau) \neq 0$, the SSC_k formula (6) and the LMM_k formula (9) have the same order k and the same error constant $C_{k+1}(\tau)$. When $C_{k+1}(\tau) = 0$, both formulas have order at least $k+1$ but they do not have the same error constant in general.

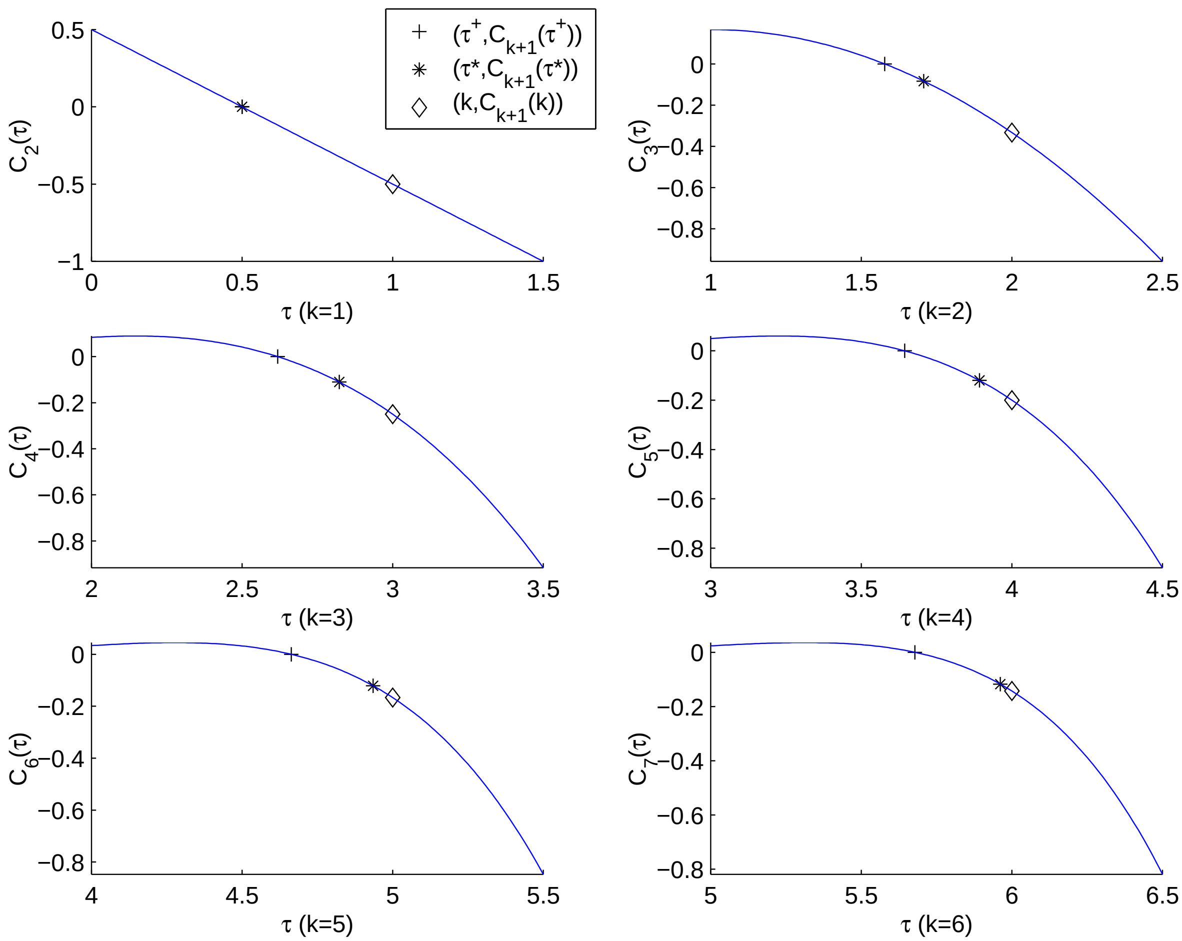

Figure 1: The Error Constant $C_{k+1}(\tau)$ as a Function of τ.

Figure 1 depicts the error constant $C_{k+1}(\tau)$ as a function of the ratio τ for $k = 1, \ldots 6$. It also depicts the ratios τ^+ and τ^* mentioned in the introduction. Observe that $\tau = k$ gives the accuracy at the next interpolation point t_{n+k}. The figure indicates that the error constant decreases between τ^+ (point t^+) and k (point t_{n+k}). The error constant is zero at time τ^+, indicating that the method is of order $k+1$ with this choice. In addition, the method is always more accurate at ratio τ^* (point t^*) than at ratio k (point t_{n+k}). Observe also that, for $k = 1$, τ^+ and τ^* are the same ratios.

2.2 Stability

When the ODE is a linear system $y' = Ay$, the SSC$_k$ formula (6) and the LMM$_k$ formula (9) become equivalent. Therefore, the SSC$_k$ formula has the linear stability of (9).

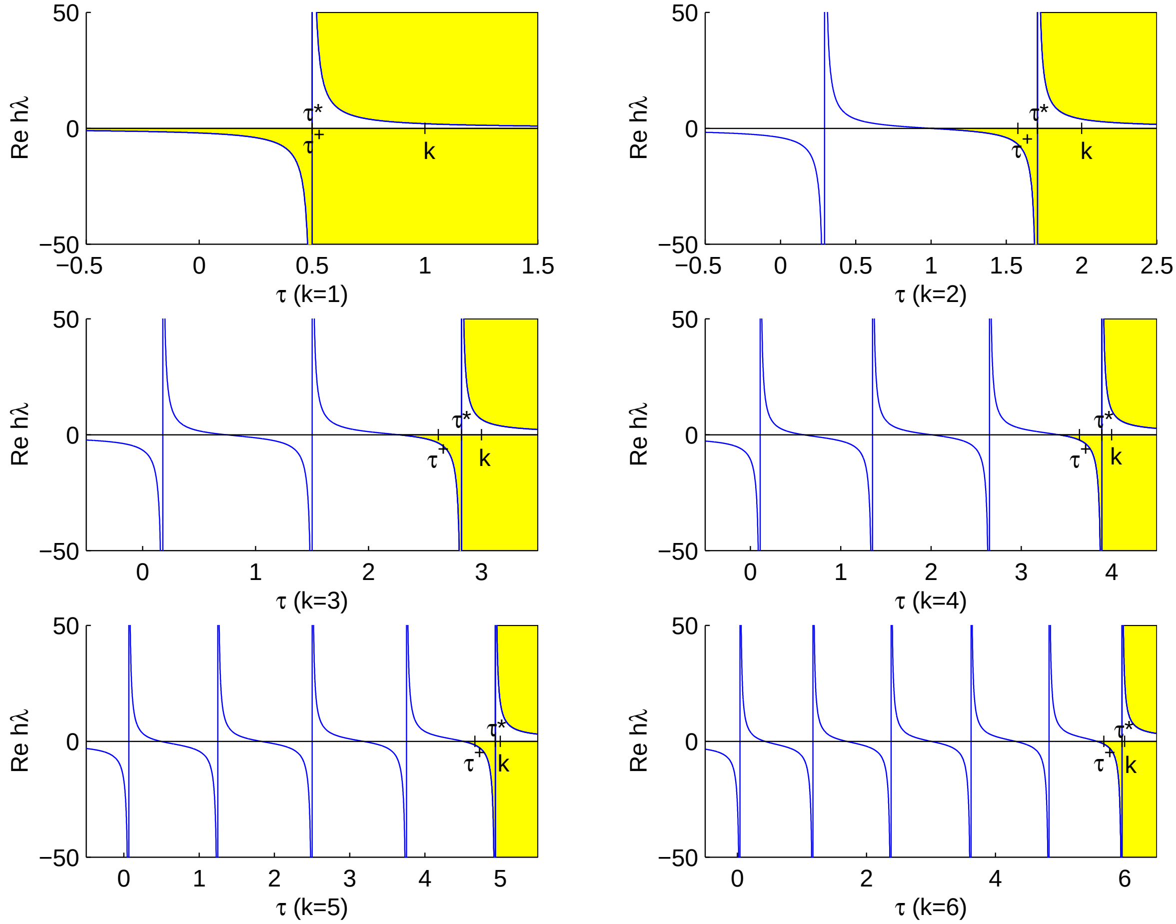

Figure 2: The Function $\hat{h}(\tau, \pi)$ and Stability Interval of SSC as a Function of τ.

Consider the first and second characteristic polynomials associated with SSC$_k(\tau)$:

$$\begin{aligned} \rho(\tau, x) &= \textstyle\sum_{j=0}^{k} \alpha_j(\tau) x^j \\ \sigma(\tau, x) &= \textstyle\sum_{j=0}^{k} \beta_j(\tau) x^j . \end{aligned}$$

We use the definition of [Lam91] for the stability region which is thus an *open set*. The boundary of the stability region $\mathcal{R}_A$ of SSC$_k(\tau)$ is (part of) the locus

$$\hat{h}(\tau,\theta) = \rho(\tau, e^{i\theta})/\sigma(\tau, e^{i\theta}) \tag{14}$$

where $0 \le \theta \le 2\pi$. Figure 2 gives a preview of the stability region of SSC formulas.

In the figure, the curves are the real function $\hat{h}(\tau,\pi)$ and the shaded regions represent the stability interval, i.e., the intersection of $\mathcal{R}_A$ with the real axis, as a function of τ. These shaded regions can be determined by the stability interval of the SSC(k)'s and by using the fact that the stability region of any convergent linear multistep method cannot contain the positive real axis in the neighborhood of the origin (e.g., [Lam91]). Figure 2 also indicates the ratios τ^+ and τ^*. Of course, once again, the next interpolation point t_{n+k} is given by $\tau = k$ for an SSC$_k$ formula. The figure shows that the stability interval increases when the evaluation point moves from t_{n+k-1} ($\tau = k-1$) to t_{n+k} ($\tau = k$). Observe also that the value t^* specified by ratio τ^* is a very attractive evaluation point, since its stability interval is precisely $\mathbb{R}_0^-$ (more detailed pictures are given later in the paper). The stability interval at time t^+ also does not intersect $\mathbb{R}^+$ but is significantly smaller than the stability interval for t^*. Points before the last two interpolation points need not be considered, since the corresponding SSC formulas are not zero-stable.

2.3 Linear versus Nonlinear Formulas

It is interesting to note that the formula (9) requires one more evaluation of the function f than the formula (6), because the value $f(t_{n+k}, y_{n+k})$ is needed in the next step to compute y_{n+k+1}. When $C_{k+1}(\tau) \neq 0$, since the formulas (6) and (9) have same accuracy and stability, (6) is to be preferred to (9) for computational reasons. However, when $C_{k+1}(\tau) = 0$, the formulas do not have the same accuracy in general. In addition, an error estimate for (6) may be more expensive in this case because its local error does not have a simple structure like (9) does. It is thus not clear which of the two formulas should be preferred in this case.

3 SSC's for Non-Stiff Problems

We now characterize the ratio τ^+ and show that it produces a k-step method with essentially the same properties as the k-step Adams-Moulton formula (AM$_k$). The basic intuition is that τ^+ is chosen to obtain the best possible order for the SSC$_k$ formula.

3.1 Shifting for Optimal Order

The following theorem is a direct consequence of Theorem 1 and it is fundamental in characterizing τ^+.

Theorem 2 *If the formula SSC$_k$(τ) is of order $k+1$, then τ is a root of $w'(\tau)$.*

The k roots of $w'(\tau)$ are located in $]0,1[,]1,2[, \ldots,]k-1,k[$. ¿From Figure 1, it is thus clear that the *rightmost* root of $w'(\tau)$ is the only root of practical interest, since the SSC formula is not zero-stable for the other roots. As a consequence, we define τ^+ as the rightmost root of $w'(\tau)$. Table 1 shows the values of τ^+ for various stepnumbers k ($1 \le k \le 6$).

3.2 Comparison to Adams-Moulton

It is interesting to compare SSC$_k$ and AM$_k$ for $2 \le k \le 6$.[1] Table 2 compares the accuracy of both formulas. It gives the error constants for SSC$_k$ and AM$_k$, as well as the step ratio percentage which indicates the

[1]The linear form of SSC$_1(\tau^+)$ is equivalent to the Trapezoidal Rule.

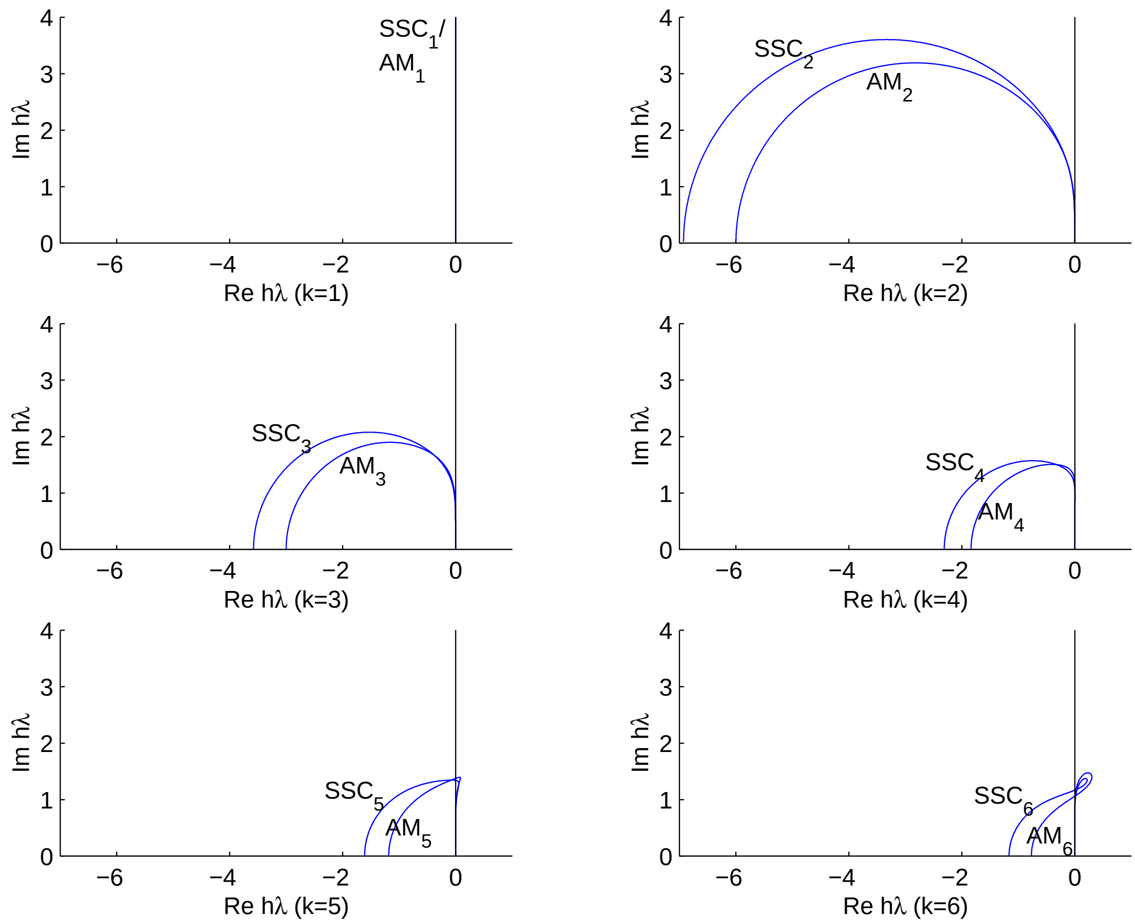

Figure 3: Stability regions of SSC(τ^+) and AM.

k	1	2	3	4	5	6
τ^+	0.5	1.5774	2.6180	3.6444	4.6634	5.6781

Table 1: Values of τ^+ for $1 \leq k \leq 6$.

Order	Error constant		
k+1	AM	SSC(τ^+)	Step ratio percent
3	-0.042	-0.048	-5%
4	-0.026	-0.033	-6%
5	-0.019	-0.025	-6%
6	-0.014	-0.020	-6%
7	-0.011	-0.017	-5%

Table 2: Accuracy of SSC(τ^+) relative to AM.

necessary step size reduction to achieve the same accuracy in both methods for sufficiently small step sizes. The table shows that SCC$_k$ is slightly less accurate than AM$_k$ and has a step ratio of about -6%. Figure 3 depicts the stability region of SSC$_k$ and AM$_k$. Here the situation is reversed and the stability region of SSC$_k$ is slightly larger than the one of AM$_k$. As a consequence, the two formulas have very similar properties. Observe also that AM$_k$ is slightly cheaper than SSC$_k$.

4 SSC's for Stiff Problems

This section is the core of the paper and it studies SSC$_k$ formulas of order k. The error constant $C_{k+1}(\tau)$ of these formulas is not zero. Hence, in our analysis, we do not distinguish between the SSC formula (6) and its linear form (9), since they have the same accuracy and stability. We will show that it is possible to find a ratio τ^* such that the stability region and the accuracy of SSC$_k$(τ^*) improve upon those of BDF$_k$.

4.1 Precise A(α)-Stability

We first define the concept of precise A(α)-stability formally. It is motivated by Lambert who argues that "on the whole, there seems to be something to be said in favour of what we might call *precisely A-stable* methods, that is, methods whose regions of absolute stability are precisely the left half-plane; the numerical solutions of the test system $y' = Ay$ then tend to zero as n tends to infinity *if and only if* the exact solutions tend to zero as x tends to infinity" ([Lam91], page 232). In other words, the ideal stability region for a method is $\mathbb{C}_0^-$. We will show that SSC$_k$ formulas come close to that ideal.

Definition 1 (Precise A(α)-Stability) *A method with stability region $\mathcal{R}_A$ is said to be* precisely A(α)-stable, $0 < \alpha < \pi/2$, *if it is A(α)-stable and $\mathcal{R}_A \cap \mathbb{C}^+ = \emptyset$; it is said to be* precisely A(0)-stable *if it is A(α)-stable for some $\alpha \in]0, \pi/2[$; it is said to be* precisely A-stable *if $\mathcal{R}_A = \mathbb{C}_0^-$.*

4.2 Shifting for Precise A(α)-Stability

We now show how to choose a ratio τ^* to achieve precise A(α)-Stability. We first give a necessary condition for precise A(0)-stability.

k	1	2	3	4	5	6
τ^*	0.5	1.7071	2.8229	3.8924	4.9350	5.9613

Table 3: Values of τ^* for $1 \leq k \leq 6$.

Lemma 1 *If (τ, θ) is a zero of $\sigma(\tau, e^{i\theta})$, then $\theta = \pi$.*

Theorem 3 (Necessary Condition for Precise A(α)-Stability in SSC) *If the method SSC(τ) is precisely A(0)-stable, then τ is a root of $\sigma(\tau, -1)$.*

Proof Precise A(0)-stability requires that the stability region be an unbounded set. This implies that τ be a pole of $\hat{h}(\tau, \theta)$, i.e., a zero of $\sigma(\tau, e^{i\theta})$ for some θ. By Lemma 1, τ must be a root of $\sigma(\tau, e^{i\pi}) = \sigma(\tau, -1)$. □

Since the roots of $\sigma(\tau, -1)$ are poles of $\hat{h}(\tau, \pi)$, it follows from Figure 1 that only the rightmost root is of practical interest since the SSC formulas are not zero-stable for the other roots. As a consequence, we define τ^* as the rightmost root of $\sigma(\tau, -1)$. Table 3 shows the values of τ^* for various stepnumbers k ($1 \leq k \leq 6$). We now study the properties of SSC$_k$(τ^*). The following proposition is easily verified.

Proposition 1 *τ is a root of $\sigma(\tau, -1)$ iff $\lim_{\substack{\theta \to \pi \\ \theta < \pi}} \mathrm{Im}\, \hat{h}(\tau, \theta) = +\infty$ and $\lim_{\substack{\theta \to \pi \\ \theta > \pi}} \mathrm{Im}\, \hat{h}(\tau, \theta) = -\infty$.*

Recall that a method is convergent iff it is zero-stable and consistent.

Property 1 (Stability Properties of SSC) *Let τ^* be the rightmost root of $\sigma(\tau, -1)$. Then,*

1. *For $1 \leq k \leq 6$, SSC$_k$(τ^*) is convergent and A(0)-stable:*
   - *(a) SSC$_1$(τ^*) and SSC$_2$(τ^*) are precisely A-stable;*
   - *(b) SSC$_3$(τ^*) and SSC$_4$(τ^*) are precisely A(0)-stable;*
   - *(c) SSC$_5$(τ^*) and SSC$_6$(τ^*) are almost precisely A(0)-stable, i.e., the boundary of the stability region marginally invades $\mathbb{C}_0^+$;*
2. *For $k \geq 7$, SSC$_k$(τ^*) is not convergent (i.e., it is consistent but not zero-stable).*

It is important to emphasize that neither the AM formulas nor the BDF's are precisely A(0)-stable: the AM formulas are not A(0)-stable while the stability regions of the BDF's contain part of the positive half-plane $\mathbb{C}^+$. As a consequence, the SSC$_k$ formulas have some appealling stability properties. Note also that, for $k = 1$, we have $\tau^* = \tau^+$. Finally, the formula SSC$_2$(τ^*) shares three common properties with the Trapezoidal Rule:

1. it is precisely A-stable;
2. it is of order 2;
3. its error constant is -1/12.[2]

It can also be verified that the linear SSC$_2$(τ^*) formula becomes equivalent to the Trapezoidal Rule when the latter is used as a starting method to compute the value y_1.

Order	Error constant			Stability angle		
k	BDF	SSC(τ^*)	Step ratio percent	BDF	SSC(τ^*)	Percent change
2	$-1/3$	$-1/12$	59%	$90°$	$90°$	0%
3	-0.25	-0.11	23%	$86°$	$84°$	-2%
4	-0.2	-0.12	11%	$73°$	$73°$	-1%
5	-0.17	-0.12	5%	$52°$	$55°$	6%
6	-0.14	-0.12	3%	$18°$	$25°$	40%

Table 4: Accuracy and stability angle of SSC(τ^*) relative to BDF.

4.3 Comparison to BDF

We now compare the SSC(τ^*)'s and BDF's. Table 4 compares the error constant and the stability angle of both formulas for various stepnumbers. It can be seen that SSC(τ^*) formulas are more precise for $2 \leq k \leq 6$ and that the gain is significant for small stepnumbers. SSC(τ^*) formulas also have a better stability angle in general (except for $k = 3, 4$). Figure 4 is also very interesting. It compares the stability regions of SSC(τ^*)'s and BDF's for various stepnumbers. Here we clearly see that SSC(τ^*)'s are much closer to the ideal stability region than BDF's. SSC(τ^*)'s have almost no intersection with $\mathbb{C}^+$ contrary to BDF's which have significant intersections.

5 Improving the Stability of SSC

In this section, we show how to use the correction idea from Klopfenstein [Klo71] to improve the stability region of SSC formulas. We start by reviewing the basic idea and then we apply it to the SSC's.

5.1 The Numerical Differentiation Formulas

Klopfenstein [Klo71] introduced a variant of the BDF's, called the numerical differentiation formulas (NDF's), by adding a term to the formula (8):

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j y_{n+k} - hf(t_{n+k}, y_{n+k}) - \kappa\gamma_k \left(y_{n+k} - y_{n+k}^{(0)} \right) = 0 \tag{15}$$

where

$$y_{n+k}^{(0)} = \sum_{j=0}^{k} \nabla^j y_{n+k-1} \tag{16}$$

is a predictor. In this formula, κ is a parameter and $\gamma_k = \sum_{j=1}^{k} \frac{1}{j}$. By noting that

$$y_{n+k} - y_{n+k}^{(0)} = \nabla^{k+1} y_{n+k} \approx h^{k+1} y^{(k+1)} \tag{17}$$

we see that the term added to the formula (8) can be interpreted as a correction term which does not decrease the order of the formula. The corresponding error constant is given by

$$-\frac{1}{k+1} - \kappa\gamma_k. \tag{18}$$

[2] By the second Dahlquist barrier (e.g. [Lam91]), this is the smallest possible error constant (in magnitude) for a second-order A-stable linear multistep method.

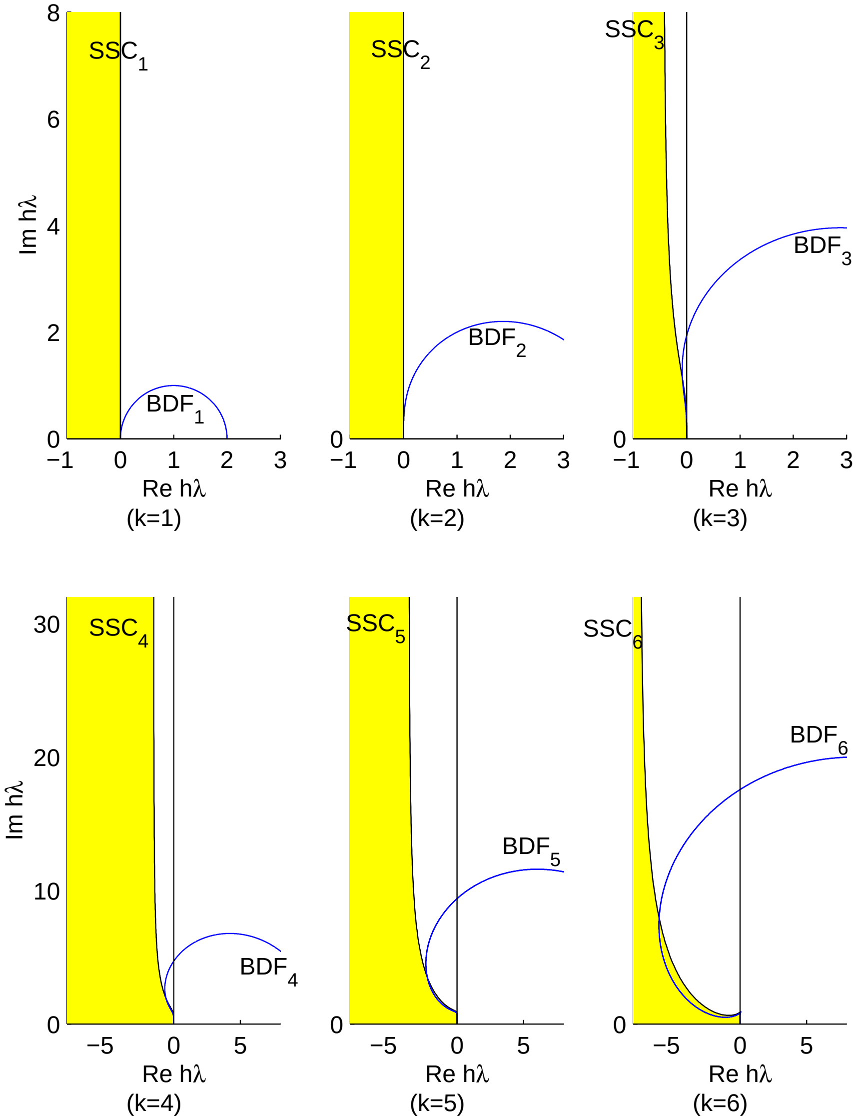

Figure 4: Stability regions of SSC(τ^*) and BDF.

Order	Error constant			Stability angle		
k	BDF	NDF	Step ratio percent	BDF	NDF	Percent change
1	-0.5	-0.31	26%	$90°$	$90°$	0%
2	$-1/3$	$-1/6$	26%	$90°$	$90°$	0%
3	-0.25	-0.1	26%	$86°$	$80°$	-7%
4	-0.2	-0.11	12%	$73°$	$66°$	-10%

Table 5: Accuracy and stability angle of NDF relative to BDF.

Shampine and Reichelt [SR97] proposed values for κ that make the NDF's more accurate than the BDF's while only degrading slightly the stability. Table 5 compares the accuracy and the stability angles of the NDF's proposed by Shampine and Reichelt and the traditional BDF's. As can be seen, the correction improves the accuracy (by about 26% in step ratio percentage on orders 1 to 3) while only decreasing the stability angle slightly.

5.2 Corrected SSC Formulas for Stiff Problems

We apply the same corrector idea to the SSC formula (6) to obtain:

$$\boxed{p'(t) - f(t, p(t)) - \kappa\gamma_k \left(y_{n+k} - y_{n+k}^{(0)}\right) = 0.} \tag{19}$$

The formula (19) is denoted SSC$^\kappa$ or, more explicitly, SSC$_k^\kappa$. For any value of κ, the formula SSC$_k^\kappa$ is of order at least k and its error constant is given by

$$C_{k+1}(\tau) - \kappa\gamma_k. \tag{20}$$

The boundary of the stability region of SSC$^\kappa(\tau)$ is (part of) the locus

$$\begin{aligned} \hat{h}_\kappa(\tau,\theta) &= \rho_\kappa(\tau, e^{i\theta})/\sigma_\kappa(\tau, e^{i\theta}) \\ &= \left(e^{i\theta}\rho(\tau, e^{i\theta}) + \kappa\gamma_k \varrho(e^{i\theta})\right)/(e^{i\theta}\sigma(\tau, e^{i\theta})) \\ &= \hat{h}(\tau,\theta) + \kappa\gamma_k \varrho(e^{i\theta})/(e^{i\theta}\sigma(\tau, e^{i\theta})) \end{aligned} \tag{21}$$

where

$$\varrho(x) = \sum_{j=0}^{k} \varphi_j(k+1)x^j - x^{k+1}. \tag{22}$$

The correction preserves the main results about the method.

Theorem 4 (Necessary Condition for Precise A(α)-Stability in SSC$^\kappa$) *For all $\kappa \in \mathbb{R}$, if the method SSC$^\kappa$(τ) is precisely A(0)-stable, then τ is a root of $\sigma(\tau, -1)$.*

Proof By (21), precise A(0)-stability implies that τ be a pole of $\hat{h}_\kappa(\tau,\theta)$, i.e., a zero of $\sigma(\tau, e^{i\theta})$ for some θ. By Lemma 1, τ must be a root of $\sigma(\tau, e^{i\pi}) = \sigma(\tau, -1)$. □

Proposition 2 *For all $\kappa \in \mathbb{R}$, τ is a root of $\sigma(\tau,-1)$ iff $\lim_{\substack{\theta\to\pi \\ \theta<\pi}} \mathrm{Im}\ \hat{h}_\kappa(\tau,\theta) = +\infty$ and $\lim_{\substack{\theta\to\pi \\ \theta>\pi}} \mathrm{Im}\ \hat{h}_\kappa(\tau,\theta) = -\infty$.*

k	1	2	3	4	5	6
κ^*	0	0	0.0129	0.0213	0.0257	0.0274

Table 6: Values of κ^* for $1 \leq k \leq 6$.

5.3 Determination of the Parameters in SSC$^\kappa$

It remains to determine the value of the parameter κ. Contrary to [SR97], our objective is to optimize the stability region of the SSC's. We know from Theorem 4 and Proposition 2 that precise A(0)-stability implies

$$\lim_{\substack{\theta\to\pi\\ \theta<\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = +\infty, \quad \lim_{\substack{\theta\to\pi\\ \theta>\pi}} \text{Im } \hat{h}_\kappa(\tau,\theta) = -\infty. \tag{23}$$

To optimize the stability region, we also impose

$$L = \lim_{\theta\to\pi} \text{Re } \hat{h}_\kappa(\tau,\theta) = 0. \tag{24}$$

This limit L can be computed and is given by

$$L = \left(\sum_{j=0}^{k} A_j \varphi_j(k+1) - A_{k+1}\right) \kappa\gamma_k + \sum_{j=0}^{k} A_{j+1}\alpha_j(\tau) \tag{25}$$

where

$$A_j = B_1 j(-1)^{j+1} + B_2(-1)^j, \quad 0 \leq j \leq k+1, \tag{26}$$

$$B_1 = \left(\sum_{j=0}^{k} \beta_j(\tau)(j+1)(-1)^j\right)^{-1}, \tag{27}$$

$$B_2 = -\frac{B_1^2}{2}\sum_{j=0}^{k} \beta_j(\tau)(j+1)^2(-1)^{j+1}. \tag{28}$$

As a consequence, there exists a unique value κ^* satisfying condition (24) and given by

$$\kappa^* = \frac{\sum_{j=0}^{k} A_{j+1}\alpha_j(\tau)}{\gamma_k\left(A_{k+1} - \sum_{j=0}^{k} A_j\varphi_j(k+1)\right)}. \tag{29}$$

Table 6 shows the values of κ^* for $1 \leq k \leq 6$. As for the SSC's, we can verify that only the rightmost root of $\sigma(\tau,-1)$ is of practical interest for SSC$^{\kappa^*}(\tau)$ since the formula is not zero-stable for the other roots. We now describe the stability properties of the SSC$^{\kappa^*}(\tau^*)$ formulas.

Property 2 (Stability Properties of SSC$^{\kappa^*}$) *Let τ^* be the rightmost root of $\sigma(\tau,-1)$ and κ^* be defined by (29). Then,*

1. *For $1 \leq k \leq 6$, SSC$_k^{\kappa^*}(\tau^*)$ is convergent and A(0)-stable:*
   - *(a) SSC$_1^{\kappa^*}(\tau^*)$ and SSC$_2^{\kappa^*}(\tau^*)$ are precisely A-stable;*
   - *(b) SSC$_3^{\kappa^*}(\tau^*)$ and SSC$_4^{\kappa^*}(\tau^*)$ are precisely A(0)-stable;*

Order	Error constant			Stability angle		
k	BDF	$\mathrm{SSC}^{\kappa^*}(\tau^*)$	Step ratio percent	BDF	$\mathrm{SSC}^{\kappa^*}(\tau^*)$	Percent change
3	-0.25	-0.13	17%	$86°$	$86°$	0%
4	-0.2	-0.16	4%	$73°$	$77°$	5%
5	-0.17	-0.18	-1%	$52°$	$62°$	19%
6	-0.14	-0.18	-4%	$18°$	$36°$	101%

Table 7: Accuracy and stability angle of $\mathrm{SSC}^{\kappa^*}(\tau^*)$ relative to BDF.

(c) *$SSC_5^{\kappa^*}(\tau^*)$ and $SSC_6^{\kappa^*}(\tau^*)$ are almost precisely A(0)-stable, i.e., the boundary of the stability region marginally invades $\mathbb{C}_0^+$;*

2. *$SSC_7^{\kappa^*}(\tau^*)$ is convergent but not A(0)-stable;*

3. *For $k \geq 8$, $SSC_k^{\kappa^*}(\tau^*)$ is not convergent (i.e., it is consistent but not zero-stable).*

5.4 Comparison to BDF/NDF

It is interesting to compare the corrected SSC formulas with BDF's and NDF's. Table 7 compares the accuracy and the stability angles of $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ for $k = 3..6$. (For $k = 1..2$, $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ = $\mathrm{SSC}_k(\tau^*)$ since $\kappa^* = 0$.) Observe that $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ still compares very well to BDF's as far as the error constant is concerned. In addition, $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ now exhibits significant improvements over BDF's as far as the stability angles are concerned. Figure 5 is also particularly interesting. It clearly indicates the benefits of the correction on the stability region. For $k = 1..4$, the stability region of $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ is essentially the ideal stability region. For $k = 5..6$, $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ also produces a significant improvement over $\mathrm{SSC}_k(\tau^*)$. Clearly, the stability region of $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ significantly improves over those of BDF's and NDF's. Given that the accuracy of $\mathrm{SSC}_k^{\kappa^*}(\tau^*)$ is very competitive with BDF's and NDF's and that its performance is essentially similar, these stability results make it an interesting alternative to these traditional methods.

6 Conclusion

In this paper, we proposed a new class of formulas, called *Shifted Slope-Comparison (SSC) formulas*, for the solution of initial value problems in ODEs. The SSC formulas are derived from the functional equation $p'(t) = f(t, p(t))$, where p is a polynomial approximation of the solution, by carefully choosing an evaluation point t_e. In particular, we showed that there exists a point t^+ which leads to an SSC formula with essentially the same accuracy and stability as Adams-Moulton. More interestingly, we showed that there exists a point t^* which leads to an SSC formula which is more precise than BDF's, which is precisely A(α)-stable, and whose stability angle α is essentially similar to BDF's. Finally, by applying the corrector idea of Klopfenstein, we showed how to improve the stability region of SSC formulas significantly, while only degrading the accuracy slightly. The so-obtained SSC formulas seem to be appealling alternatives to BDF's since they have essentially the ideal stability region, while preserving the same accuracy as BDF's.

Finally, it is worth mentioning that the idea of using an evaluation point t that is different from the current integration point t_{n+k} originated from our research on interval methods for parametric differential equations [JVHD01]. Although the problem and the issues are quite different as discussed in [Jan01], it is interesting to observe that these non-standard evaluation points have interesting theoretical and experimental properties in these two contexts.

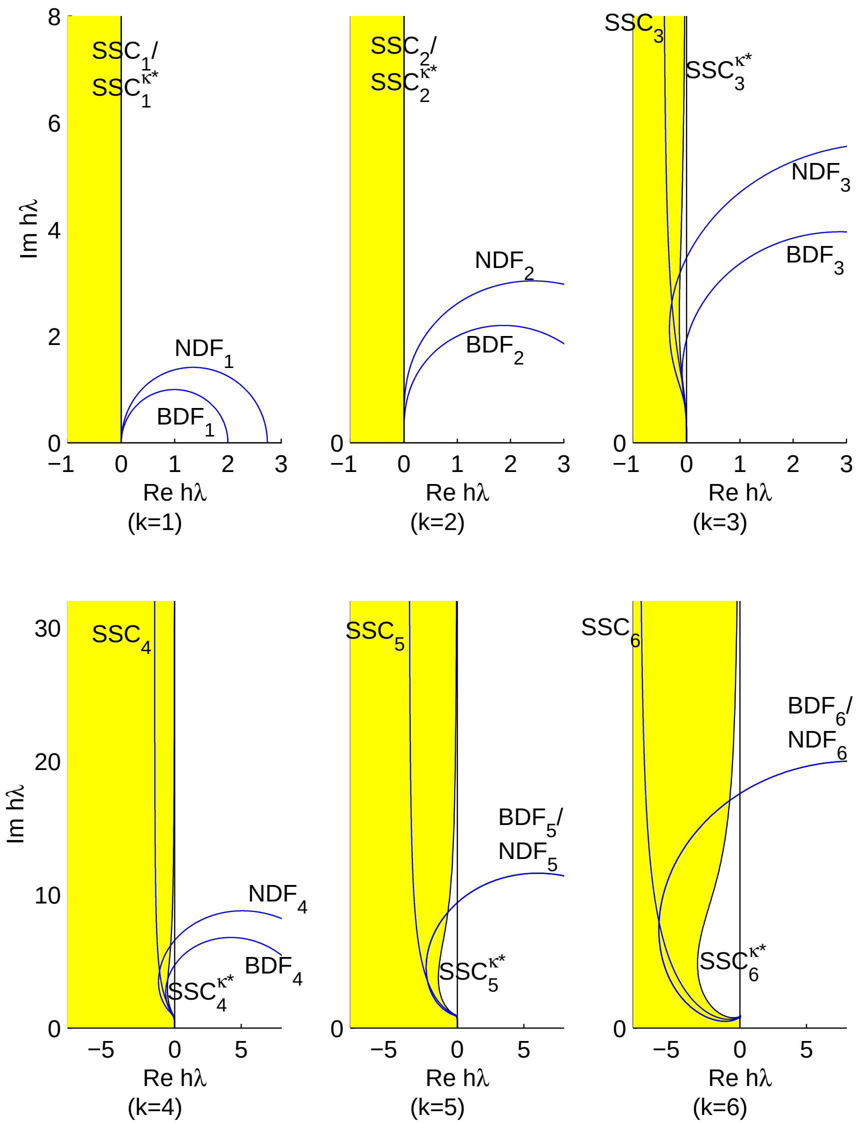

Figure 5: Stability regions of $\mathrm{SSC}^{\kappa^*}(\tau^*)$, BDF, and NDF.

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