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Boundary Locus Search for Stiffly Stable Second Derivative Linear Multistep Formulas for Stiff ODEs

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Abstract

High order numerical schemes are mostly desired for the integration of stiff initial value problems. In this paper, stable second derivative linear multistep formulas of high order of accuracy are derived by the inclusion of a nonzero coefficient selected out of k zero coefficients of the third characteristics polynomial of conventional second derivative backward differentiation formulas. One coefficient out of k zero coefficients is assumed nonzero one at a time and this results in the development of k new second derivative linear multistep formulas. Boundary locus technique is thereafter used to analyze the stability of these new k second derivative linear multistep formulas. Stable members of these formulas are shown to be $A-$stable for order $p \le 4$ and $A(\alpha)$-stable for order $p \le 11$. Numerical examples are included to justify the suitability of these schemes as numerical integrators for stiff initial value problem.

***Keywords*: $A-$Stability; Stiffly stable; Initial value problem (ivp); Ordinary differential equation (ode).**

I INTRODUCTION

The development of efficient and suitable numerical methods for the integration of stiff initial value problems (ivps) in ordinary differential equations (ode) has attracted a great deal of research attention. A potentially good numerical integrator for stiff ivps in ode is required to be A-stable (a numerical integrator is said to be A-stable, if its region of absolute stability contains the entire left of the complex plane). However, the requirement of A-stability puts some limitations on the choice of class of linear multistep formulas (LMF) suitable for the integration of stiff ivps in odes; this is due to the fact that explicit LMF cannot be A-stable and A-stable implicit LMF cannot exceed order $p = 2$ [1]. Consequently, researches are geared towards the development of higher order A-stable LMF and this has been achieved through two broad paths, these are: (a) by incorporating higher derivatives of the exact solution into the classical LMF or (b) by incorporating supplementary stages, extra division points or future points [2]. Several authors have derived methods that utilize the path that incorporates higher derivatives, of which examples of second derivative LMF can be found in [3-6]. For some stiff ivps, obtaining higher derivatives may not be possible. In cases where higher derivatives exist, they are cumbersome to obtain. That makes the second derivative methods most successful in this search direction for high order stable methods [6]. It is a well known fact that by adding an extra term to formula of a numerical scheme increases the order of accuracy and also modifies the region of absolute stability [4]. In this paper, a new class of stiffly stable methods for numerical solution of stiff ivps in ode is derived by the inclusion of an extra term into the third characteristics polynomial of the well known second derivative backward differentiation formulas (SDBDF) [7]. This follows the idea utilized in [6,8] to improving the order of accuracy of the backward differentiation formulas (BDF). This paper is arranged as follows: section 2 is on second derivative linear multistep formulas, section 3 is on stability analysis of the proposed method. Numerical examples are presented in section 4, conclusion is in section 5.

II. Second derivative linear multistep formulas

Consider the $k-$step second derivative linear multistep formulas (SDLMF),

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\sum_{j=0}^{k}\beta_j f_{n+j} + h^2\sum_{j=0}^{k}\gamma_j g_{n+j}. \qquad (1)$$

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where $\alpha_j, \beta_j, \gamma_j$ are real constant coefficients to be determined, y_{n+j} is the approximate numerical solution obtained at t_{n+j},

$$f_{n+k} \equiv f(t_{n+k}, y_{n+k}) \text{ and } \qquad g_{n+k} \equiv \left.\frac{df(t,y)}{dt}\right|_{t=t_{n+k}} \qquad (2)$$

for integrating the stiff initial value problem

$$y' = f(t,y), \quad y(t_0) = y_0, \quad y: R \to R^m, \quad f: R \times R^m \to R^m,$$
$$t \in [a,b]. \qquad (3)$$

If β_k and γ_k are both zero then (1) is explicit, and implicit otherwise. Taylor series expansion of the linear difference operator associated with SDLMF (1),

$$L(t, y(t); h) = \sum_{j=0}^{k} (\alpha_j y(t_{n+j}) - h\beta_j y'(t_{n+j})$$
$$-h^2 \gamma_j y''(t_{n+j})) \qquad (4)$$

about t_n shows that the scheme (1) is of order p if and only if

$$\frac{1}{q!}\sum_{j=0}^{k} j^q \alpha_j = \frac{1}{(q-1)!}\sum_{j=0}^{k} j^{q-1}\beta_j + \frac{1}{(q-2)!}\sum_{j=0}^{k} j^{q-2}\gamma_j,$$
$$0 \le q \le p. \qquad (5)$$

The error constant is given as

$$C_{p+1} = \sum_{j=0}^{k} (j^{p+1}\alpha_j - (p+1)j^p \beta_j - (p+1)pj^{p-1}\gamma_j). \qquad (6)$$

SDLMF can be written in compact form as

$$\rho(E)\,\mathrm{y}_n = h\sigma(E)\,\mathrm{f}_n + h^2\phi(E)\,\mathrm{g}_n \qquad (7)$$

where $\rho(E) = \sum_{j=0}^{k}\alpha_j E^j; \sigma(E) = \sum_{j=0}^{k}\beta_j E^j$, and $\phi(E) = \sum_{j=0}^{k}\gamma_j E^j$ are the first, second, and third characteristics polynomial associated with the scheme (1) respectively. E is the shift operator (i.e $E^j y_n = y_{n+j}$). Two prominent members of SDLMF are: second derivative multistep method (SDMM) derived in [5, 9] and the second derivative backward differentiation formulas (SDBDF) [7]. These are of the form:

$$y_{n+k} - y_{n+k-1} = \sum_{j=0}^{k}\beta_j f_{n+j} + h^2\gamma_k g_{n+k} \qquad (8)$$

and

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\beta_k f_{n+k} + h^2\gamma_k g_{n+k} \qquad (9)$$

respectively. The SDMM (8) is of order (k+2) while SDBDF (9) is of order (k+1). In Muka and Obiorah [8], boundary locus search for stiffly stable SDLMF is carried out by the inclusion of an extra term to the second characteristics polynomial of (9). In this paper, a new method of the class of SDLMF (1) is proposed by adding a nonzero coefficient to the third characteristics polynomial of the SDBDF (9). This new method will be of order of accuracy (k+2) which is higher than that of SDBDF (9) by unity.

Proposed second derivative linear multistep formula in this paper, is of the form

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\beta_k f_{n+k} + h^2(\gamma_k g_{n+k} + \gamma_{k-\tau} g_{n+k-\tau}), \qquad (10)$$

where $\tau = 1, 2, \cdots, k.$ The parameters $\beta_k, \gamma_k, \gamma_{k-\tau}$, $\tau = 1(1)k,$ and α_k, $j = 0(1)k-1$ are completely determined using $(k+2)\times(k+2)$ systems of linear equations (5). For each $\tau = 1, 2, \cdots, k,$ a new SDLMF is derived, in other words for a $k-$step SDLMF (10), k formulas will be constructed. The coefficients for `$k-$step SDLMF (10) are presented in Table 1 for each τ, this is achieved through the use of MATHEMATICA 10 software.

Lemma

SDLMF (10) is of order k+2.

Proof

$k-$step SDLMF (10) has a total of (k+3) unknowns to be determined. These are determined using the following system of linear equations

$$k^q + \sum_{j=0}^{k-1} j^q \alpha_j = qk^{q-1}\beta_k + q(q-1)(k^{q-2}\gamma_k +$$
$$(k-\tau)^{q-2}\gamma_{k-\tau}), 0 \le q \le k+2 \qquad (11)$$

Since (11) holds, then (10) is of order (k+2).

III. Stability analysis of SDLMF (10)

This section analyzes the SDLMF (10) in terms of zero and $A-$stability. The SDLMF is said to be zero stable if no root of the first characteristics polynomial has modulus greater than unity and that any root with modulus unity is simple [10]. The first characteristics polynomial $\rho(E)$ of $k-$step SDLMF (10) for each τ and parameters given in Table 1 are easily verified to be zero stable. If SDLMF (10) is applied to the test equation $y' = \lambda y, \quad y(t_0) = y_0$, we get the characteristics equation

$$\sum_{j=1}^{k}\alpha_j \chi^j - z\beta_k \chi^k - z^2(g_{n+k}\chi^k + g_{n+k-\tau}\chi^{k-\tau}) = 0, z = \lambda h. \qquad (12)$$

Set $\chi = \exp(i\theta)$ in (12), for $\theta \in [0, 2\pi]$ yields two roots, using the boundary locus method with the aid of MATLAB R2007b software, the stability domain of SDLMF (10) is described. The stability characteristics of $k-$step SDLMF (10) for τ with the maximum $\alpha-$value and order of consistency are shown in Table 2.

IV. Numerical examples

In this section, SDLMF (10) proposed in this paper is used to generate approximate solutions of three standard problems in examples 1-3 below. The results are compared with those generated by SDMM (8). A constant step size h=0.001 is adopted for the three examples.

Example 1
Consider the IVP

$$y' = -200(y - F(t)) + F'(t), \quad y(0) = 10,$$
$$F(t) = 10 - (10 + t)e^{-t},$$

the exact solution is $y(t) = F(t) + 10e^{-200t}$

Example 2
Consider the system of differential equation

$$\begin{pmatrix} y_1' \\ y_2' \\ y_3' \\ y_4' \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -10 & 0 & 0 \\ 0 & 0 & -100 & 0 \\ 0 & 0 & 0 & -1000 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}$$

with initial conditions

$$y_i(0) = 1, \quad i = 1(1)4,$$

the exact solutions are
$y_1 = e^{-t}$, $y_2 = e^{-10t}$, $y_3 = e^{-100t}$, and $y_4 = e^{-1000t}$.

Example 3

Consider the Van der Pol's ode

$$y_1' = y_2,$$
$$y_2' = \omega^2((1 - y_1^2)y_2 - y_1),$$

with initial value $y(0) = (2,0)^T$ and $\omega = 500.$
MATLAB R2007b software is used and results are presented in Tables 3-5.

Table 1: Coefficients and error constants of SDLMF (10).

k	τ	$\gamma_{k-\mu}$	γ_k	β_k	α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	C_{p+3}
1	1	$-\frac{1}{6}$	$-\frac{1}{3}$	1	-1	1							$\frac{1}{24}$
2	1	$-\frac{4}{87}$	$-\frac{26}{87}$	$\frac{26}{29}$	$\frac{3}{29}$	$-\frac{32}{29}$	1						$\frac{86}{1305}$
	2	$\frac{2}{39}$	$-\frac{8}{39}$	$\frac{10}{13}$	$\frac{3}{13}$	$-\frac{16}{13}$	1						$\frac{2}{117}$
3	1	$\frac{108}{89}$	$\frac{18}{89}$	$-\frac{30}{89}$	$-\frac{8}{89}$	$\frac{135}{89}$	$-\frac{216}{89}$	1					$-\frac{9}{890}$
	2	$\frac{54}{203}$	$-\frac{36}{203}$	$\frac{150}{203}$	$\frac{40}{203}$	$-\frac{27}{203}$	$-\frac{216}{203}$	1					$\frac{9}{1015}$
	3	$-\frac{12}{461}$	$-\frac{78}{461}$	$\frac{330}{461}$	$-\frac{56}{461}$	$\frac{243}{461}$	$-\frac{648}{461}$	1					$\frac{9}{922}$
4	1	$\frac{1728}{2669}$	$\frac{72}{2669}$	$\frac{420}{2669}$	$\frac{27}{2669}$	$-\frac{320}{2669}$	$\frac{2808}{2669}$	$-\frac{5184}{2669}$	1				$-\frac{24}{13345}$
	2	$\frac{432}{379}$	$-\frac{72}{379}$	$\frac{300}{379}$	$-\frac{27}{379}$	$\frac{512}{379}$	$-\frac{864}{379}$	0	1				$\frac{96}{13265}$
	3	$-\frac{192}{1511}$	$-\frac{168}{1511}$	$\frac{780}{1511}$	$-\frac{135}{1511}$	$\frac{64}{1511}$	$\frac{648}{1511}$	$-\frac{1728}{1511}$	1				$\frac{216}{40285}$
	4	$\frac{216}{13693}$	$-\frac{2016}{13693}$	$\frac{9300}{13693}$	$\frac{1107}{13693}$	$-\frac{4864}{13693}$	$\frac{10800}{13693}$	$-\frac{20736}{13693}$	1				$\frac{2976}{479255}$
5	1	$\frac{108000}{208879}$	$-\frac{1800}{208879}$	$\frac{55020}{208879}$	$-\frac{504}{208879}$	$\frac{5625}{208879}$	$-\frac{2000}{208879}$	$\frac{207000}{208879}$	$-\frac{387000}{208879}$	1			$-\frac{75}{132923}$
	2	$-\frac{54000}{701}$	$\frac{1800}{701}$	$-\frac{4620}{701}$	$-\frac{576}{701}$	$\frac{7875}{701}$	$\frac{80000}{701}$	$\frac{144000}{701}$	$-\frac{72000}{701}$	1			$-\frac{600}{4907}$
	3	$-\frac{3000}{4463}$	$-\frac{600}{4463}$	$\frac{2940}{4463}$	$\frac{162}{4463}$	$-\frac{3375}{4463}$	$\frac{5500}{4463}$	0	$\frac{6750}{4463}$	1			$\frac{225}{62482}$
	4	$\frac{27000}{221269}$	$-\frac{28800}{221269}$	$\frac{143220}{221269}$	$\frac{17856}{221269}$	$-\frac{1125}{221269}$	$-\frac{112000}{221269}$	$\frac{234000}{221269}$	$-\frac{360000}{221269}$	1			$\frac{5700}{1548883}$
	5	$-\frac{21600}{2034059}$	$-\frac{268200}{2034059}$	$\frac{1323420}{2034059}$	$-\frac{122184}{2034029}$	$\frac{568125}{2034029}$	$-\frac{1310000}{2034029}$	$\frac{2115000}{2034029}$	$-\frac{3285000}{2034029}$	1			$\frac{8625}{2034059}$
6	1	$\frac{648000}{1401653}$	$-\frac{30600}{1401653}$	$\frac{427140}{1401653}$	$\frac{100}{127423}$	$-\frac{12528}{1401653}$	$\frac{70875}{1401653}$	$-\frac{292000}{1401653}$	$\frac{1390500}{1401653}$	$-\frac{2599600}{1401653}$	1		$-\frac{2150}{9811571}$
	2	$-\frac{162000}{56059}$	$-\frac{1800}{56059}$	$\frac{21420}{56059}$	$\frac{400}{56059}$	$-\frac{5184}{56059}$	$\frac{37124}{56059}$	$-\frac{272000}{56059}$	$\frac{486000}{56059}$	$-\frac{302400}{56059}$	1		$-\frac{500}{392413}$

	3	$-\frac{12000}{4363}$	$-\frac{600}{4363}$	$\frac{2940}{4363}$	$-\frac{100}{4363}$	$\frac{1512}{4363}$	$-\frac{16875}{4363}$	$\frac{30000}{4363}$	$-\frac{13500}{4363}$	$-\frac{5400}{4363}$	1		$\frac{100}{30541}$
	4	$\frac{3240}{6049}$	$-\frac{720}{6049}$	$\frac{3780}{6049}$	$-\frac{152}{6049}$	$\frac{3456}{6049}$	$-\frac{5265}{6049}$	$-\frac{1280}{6049}$	$\frac{7560}{6049}$	$-\frac{10368}{6049}$	1		$\frac{104}{42343}$
	5	$-\frac{129600}{1345709}$	$-\frac{160200}{1345709}$	$\frac{840420}{1345709}$	$-\frac{80500}{1345709}$	$-\frac{37584}{1345709}$	$\frac{691875}{1345709}$	$-\frac{1420000}{1345709}$	$\frac{1822500}{1345709}$	$-\frac{2322000}{1345709}$	1		$-\frac{25250}{9419963}$
	6	$\frac{6000}{782521}$	$-\frac{94200}{782521}$	$\frac{490980}{782521}$	$\frac{37200}{782521}$	$-\frac{184896}{782521}$	$\frac{462375}{782521}$	$-\frac{784000}{782521}$	$\frac{1026000}{782521}$	$-\frac{1339200}{782521}$	1		$\frac{16700}{5477647}$
7	1	$\frac{137200}{3160481}$	$-\frac{88200}{3160481}$	$\frac{1025780}{3160481}$	$-\frac{8600}{28444329}$	$\frac{34300}{9481443}$	$-\frac{65856}{3160481}$	$\frac{2272375}{28444329}$	$-\frac{2401000}{9481443}$	$\frac{102900}{101951}$	$-\frac{51724450}{28444329}$	1	$\frac{2695}{28444329}$
	2	$-\frac{55566000}{26491247}$	$-\frac{1499400}{26491247}$	$\frac{11920860}{26491247}$	$-\frac{36000}{26491247}$	$\frac{480200}{26491247}$	$-\frac{3259872}{26491247}$	$\frac{16592625}{26491247}$	$-\frac{100156000}{26491247}$	$\frac{175959000}{26491247}$	$-\frac{116071200}{26491247}$	1	$-\frac{6370}{264491247}$
	3	$-\frac{4116000}{43907}$	$-\frac{29400}{43907}$	$\frac{93660}{43907}$	$\frac{7200}{43907}$	$-\frac{102900}{43907}$	$\frac{814968}{43907}$	$-\frac{6559875}{43907}$	$\frac{11662000}{43907}$	$-\frac{6482700}{43907}$	$\frac{617400}{43907}$	1	$\frac{1225}{43907}$
	4	$\frac{3087000}{1566947}$	$-\frac{176400}{1566947}$	$\frac{958860}{1566947}$	$\frac{20800}{1566947}$	$-\frac{343000}{1566947}$	$\frac{4148928}{1566947}$	$-\frac{7245875}{1566947}$	$\frac{2744000}{1566947}$	$\frac{1852200}{1566947}$	$-\frac{2744000}{1566947}$	1	$\frac{2940}{1566947}$
	5	$-\frac{22226400}{47398091}$	$-\frac{5203800}{47398091}$	$\frac{28643580}{47398091}$	$\frac{909000}{47398091}$	$-\frac{22466500}{47398091}$	$\frac{30968784}{47398091}$	$\frac{21223125}{47398091}$	$-\frac{1715000}{47398091}$	$\frac{4630500}{2788123}$	$-\frac{86436000}{47398091}$	1	$\frac{86975}{47398091}$
	6	$\frac{686000}{8606723}$	$-\frac{950600}{8606723}$	$\frac{5213740}{8606723}$	$\frac{400800}{8606723}$	$\frac{1303400}{25820169}$	$-\frac{4642848}{8606723}$	$\frac{9904125}{8606723}$	$-\frac{39788000}{25820169}$	$\frac{14200200}{8606723}$	$-\frac{15640800}{8606723}$	1	$\frac{52430}{25820169}$
	7	$-\frac{1764000}{303126503}$	$-\frac{33780600}{303126503}$	$\frac{184324140}{303126503}$	$-\frac{11878000}{303126503}$	$\frac{63146300}{303126503}$	$-\frac{172699128}{303126503}$	$\frac{320833625}{303126503}$	$-\frac{441784000}{303126503}$	$\frac{486202500}{303126503}$	$-\frac{564947800}{303126503}$	1	$\frac{691145}{302126503}$

Table 2: Stability characteristics of SDLMF (10).

K	1	2	3	4	5	6	7	8	9
τ	1	1	3	4	4	5	6	8	9
α	90°	90°	88°	83.2°	74.8°	62.1°	35.2°	28.3°	7.76°
p	3	4	5	6	7	8	9	10	11

Table 3: Absolute Error using SDMM and SDLMF (10) to integrate Problem in Example 1

t	SDMM	SDLMF	Error SDMM	Error SDLMF
3.0	9.353586300575	9.353564537742	0.000818189358	0.000796426525
4.0	9.743908612962	9.743900992905	0.000327557404	0.000319937347
5.0	9.899061075736	9.899058414668	0.000130280722	0.000127619654
6.0	9.960391491388	9.960390564773	0.000051526215	0.000050599599
7.0	9.984518286045	9.984517964421	0.000020279460	0.000019957835

Table 4: Absolute Error using SDMM and SDLMF (10) to integrate Problem in Example 2

T	Methods	$\|y_1(t_n)-y_{1n}\|$	$\|y_2(t_n)-y_{2n}\|$	$\|y_3(t_n)-y_{3n}\|$	$\|y_4(t_n)-y_{4n}\|$
0.1	**SDMM** **SDLMF**	1.76229×10^{-3} 1.76225×10^{-3}	5.47101×10^{-3} 5.46912×10^{-3}	1.43009×10^{-5} 1.43376×10^{-5}	1.285125×10^{-5} 1.867358×10^{-5}
0.2	**SDMM** **SDLMF**	1.553758×10^{-3} 1.553715×10^{-3}	1.348821×10^{-3} 1.348124×10^{-3}	2.7437×10^{-8} 3.6157×10^{-8}	4.815047×10^{-6} 7.039827×10^{-6}
0.3	**SDMM** **SDLMF**	1.368951×10^{-3} 1.36891×10^{-3}	2.507709×10^{-4} 2.505131×10^{-4}	2.2775×10^{-8} 3.0665×10^{-8}	1.789153×10^{-6} 2.622090×10^{-6}
0.4	**SDMM** **SDLMF**	1.20525×10^{-3} 1.20521×10^{-3}	1.514322×10^{-6} 1.418994×10^{-6}	2.0609×10^{-8} 2.7750×10^{-8}	6.62710×10^{-7} 9.72107×10^{-7}
0.5	**SDMM** **SDLMF**	1.060298×10^{-3} 1.060267×10^{-3}	3.299020×10^{-5} 3.302544×10^{-5}	1.8650×10^{-8} 2.5112×10^{-8}	2.45182×10^{-7} 3.59769×10^{-7}

Table 5: Absolute Error using SDMM and SDLMF (10) to integrate Problem in Example 3

t	Methods	$\lvert y_1(t_n) - y_{1n} \rvert$	$\lvert y_2(t_n) - y_{2n} \rvert$
0.1	**SDMM** **SDLMF**	3.1038652×10^{-3} 3.1036961×10^{-3}	1.758217×10^{-3} 1.758170×10^{-3}
0.2	**SDMM** **SDLMF**	2.407847×10^{-3} 2.407710×10^{-3}	1.5408544×10^{-3} 1.54081212×10^{-3}
0.3	**SDMM** **SDLMF**	1.862156×10^{-3} 1.862043×10^{-3}	1.345562×10^{-3} 1.345524×10^{-3}
0.4	**SDMM** **SDLMF**	1.435166×10^{-3} 1.435073×10^{-3}	1.171434×10^{-3} 1.171400×10^{-3}
0.5	**SDMM** **SDLMF**	1.101776×10^{-3} 1.101700×10^{-3}	1.017040×10^{-3} 1.017008×10^{-3}
0.6	**SDMM** **SDLMF**	8.420851×10^{-4} 8.420228×10^{-4}	8.807224×10^{-4} 8.806940×10^{-4}
0.7	**SDMM** **SDLMF**	6.403308×10^{-4} 6.402798×10^{-4}	7.607715×10^{-4} 7.607458×10^{-4}

V Conclusion

A new class of second derivative linear multistep formula (SDLMF) is developed via the inclusion of a non-zero term in the third characteristics polynomial of SDBDF (9). In the derivation of k-step SDBDF (9), (k-1) coefficients of the third characteristics polynomial of SDLMF (7) are set to zero. In the SDLMF (10), the (k-1) zero terms in SDBDF (9) are made non-zero one at a time. This results in the derivation of k numbers of k-step SDLMF (10). The boundary locus technique is thereafter used to select methods that are stable of which Table 2, contains stability characteristics of methods with largest $\alpha -$values of SDLMF (10). The order of accuracy of our proposed method is higher by one when compared with the SDBDF and of the same order of accuracy as Enright's SDMM (8). The SDMM (8) is unstable for order $p > 9.$ Method proposed herein is $A(\alpha) -$stable for order $p \leq 11.$ Numerical results shown in Tables 3-5 reveal that our proposed methods are suitable for integrating linear and nonlinear stiff IVPs.

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