

<sup>1</sup>Computing Center, Academia Sinica, Beijing, China. This research was supported in part by ONR Grant N00014-82-K-0184, and Yale University.

<sup>2</sup>Dept. of Computer Science, University of Toronto, Toronto, Ontario, Canada M5S 1A7. This research was supported in part by the Natural Sciences and Engineering Research Council of Canada.

**Nonlinear Implicit One-step Schemes for Solving  
Initial Value Problems for Ordinary Differential  
Equations with Steep Gradients  
Jiachang Sun<sup>1</sup> and Ken Jackson<sup>2</sup>**

Technical Report #215/82

September 1, 1982



**Table of Contents**

1 Introduction . . . . .	2
2 A general theory for nonlinear implicit one-step schemes . . . . .	4
3 Derivation of some geometric schemes . . . . .	12
4 Generalized Mean Scheme (GMS). . . . .	15
5 Some computational considerations for the GMS. . . . .	20
6 Extension to Systems . . . . .	22
7 Numerical Tests . . . . .	23



## ABSTRACT

A general theory for nonlinear implicit one-step schemes for solving initial value problems for ordinary differential equations is presented in this paper. The general expansion of 'symmetric' implicit one-step schemes having second-order is derived and stability and convergence are studied. As examples, some geometric schemes are given.

Based on previous work of the first author on a Generalization of Means, a fourth-order nonlinear implicit one-step scheme (GMS) is presented for solving equations with steep gradients. Also, a hybrid method based on the GMS and a fourth-order linear scheme is discussed. Some numerical results are given.

## 1. Introduction

Many classical methods for solving initial value problems for ordinary differential equations are based on piecewise polynomial interpolation. If the solution of the problem possesses a very steep gradient, these schemes produce poor results. In particular, if a singularity occurs, it is often inappropriate to attempt to represent the solution in the neighborhood of the singularity by a polynomial. In this paper, we consider a class of nonlinear implicit one-step schemes that may be more appropriate for such problems.

A general theory for nonlinear implicit one-step schemes is developed in section 2. Conditions for consistency, stability, and convergence are obtained. Each consistent symmetric scheme is at least second-order, and the condition that it must satisfy to be fourth-order is given. A class of symmetric and homogeneous schemes which are generalizations of the well-known trapezoidal rule is obtained.

The trapezoidal rule is exact for second-degree polynomials. In terms of geometry, a second-degree polynomial is a conic. As examples of nonlinear symmetric implicit schemes, we develop several geometric schemes based upon "circles", "ellipses", "parabolae", and "hyperbolae" in section 3.

On the other hand, in terms of Means, the trapezoidal rule is the Arithmetic Mean of the first derivative of the solution at two neighboring grid points. In section 4, based on the Generalization of Means [9], a fourth-order nonlinear implicit one-step scheme (GMS) is presented for solving problems with steep gradients.

In section 5, we discuss some practical considerations including the use of hybrid methods based upon the GMS and more traditional schemes.

In this paper, the theory of nonlinear implicit one-step schemes is restricted to scalar equations. However, we have used these schemes successfully to solve systems of equations. The application of these schemes to systems is discussed briefly in section 6.

Numerical Results for seven test problems, some of which contain systems of equations, are given in the last section. Two of the examples use an imbedding technique to apply the GMS to the solution of two-point boundary value problems.

## 2. A general theory for nonlinear implicit one-step schemes

Consider the initial value problem (I.V.P.)

$$y' = f(x,y), \quad y(a) = y_a \quad (a < x \leq b) \quad (1)$$

where  $f(x,y)$  is continuous in  $x$  and Lipschitz continuous in  $y$  in the region

$$a \leq x \leq b, \quad -\infty < y < \infty, \quad a \text{ and } b \text{ finite.}$$

We investigate the following general nonlinear implicit one-step scheme

$$Y_{n+1} = Y_n + h S(f_n, f_{n+1}), \quad (2)$$

where

$$h = x_{n+1} - x_n, \quad f_n = f(x_n, Y_n), \quad f_{n+1} = f(x_{n+1}, Y_{n+1}).$$

The local truncation error for scheme (2) is

$$L(f) \equiv y(x_{n+1}) - y(x_n) - hS(f(x_n, y(x_n)), f(x_{n+1}, y(x_{n+1}))), \quad (3)$$

where  $y(x)$  is the solution of (1).

**Definition 1:** [5] The scheme (2) is said to have *order*  $p$  if  $p$  is the largest integer for which  $L(f) = O(h^{p+1})$ .

**Definition 2:** The scheme (2) is said to be consistent with the I.V.P.(1) if  $L(f) = o(h)$ .

We will use the notation  $f(t) \equiv f(t, y(t))$  throughout this paper except where it may be confused.

For  $x_n \leq x \leq x_{n+1}$ , let  $t = (x - x_n)/h$ . Since

$$y(x_{n+1}) - y(x_n) = h \int_0^1 f(t) dt,$$

(3) may be rewritten as

$$L(f) = h \left\{ \int_0^1 f(t) dt - S(f(x_n, y(x_n)), f(x_{n+1}, y(x_{n+1}))) \right\}. \quad (4)$$

By the Integral Mean Value Theorem, there exists a point  $\xi$  between  $x_n$  and  $x_{n+1}$  such that

$$\int_0^1 f(t) dt = f(\xi, y(\xi)).$$

So



$$\frac{L(f)}{h} = f(\xi, y(\xi)) - S(f(x_n, y(x_n)), f(x_{n+1}, y(x_{n+1}))).$$

Furthermore, if  $f'(t) = \frac{df}{dt}$  exists, then

$$\int_0^1 f(t) dt = f(x_n) + \int_0^1 f'(t)(1-t) dt$$

and

$$S(f(x_n), f(x_{n+1})) = S(f(x_n), f(x_n)) + \int_0^1 dS(f(x_n), f(t)).$$

Hence, we have

**Lemma 3:** *Let the function  $S(f, g)$  be continuous in its two variables  $f$  and  $g$ . Then the scheme (2) is consistent with (1) if and only if*

$$S(f, f) = f. \quad (5)$$

Moreover, if both  $f$  and  $S$  have continuous first derivatives, then any scheme (2) satisfying (5) has truncation error

$$L(f) = hf_0^1 \{f'(t)(1-t) - S'(f(x_n, y(x_n)), f(t))\} dt, \quad (6)$$

$$\text{where } f'(t) = \frac{df}{dt}, \quad S'(g, f(t)) = \frac{dS(g, f(t))}{dt}$$

The proof of the following theorem is similar to the one given in [2] for general explicit one-step methods.

**Theorem 4:** *Let*

(i) *the function  $S(f, g)$  be continuous jointly as a function of its two arguments in the region  $fg \geq 0$ , and*

(ii)  *$S(f(x, y), g(x, y))$  satisfy the Lipschitz condition*

$$|S(f(x, y), f(z, w)) - S(f(x, y^*), f(z, w^*))| \leq M (|y - y^*| + |w - w^*|)$$

*for all points in the domain defined by*

$$a \leq x, z \leq b, \quad -\infty < y, y^*, w, w^* < +\infty$$

*under the constraints  $f(x, y)f(z, w) \geq 0$  and  $f(x, y^*)f(z, w^*) \geq 0$ .*

*Then the scheme (2) is convergent if and only if it is consistent.*

In order to get a second-order scheme, note that

$$\int_0^1 f(t) dt = f(x_n) + \frac{h}{2} f'(x_n) + \frac{1}{2} \int_0^1 f''(t)(1-t)^2 dt,$$

$$\int_0^1 dS(f(x_n), f(t)) = h \frac{d}{dx} S(f(x_n), f(x)) \Big|_{x=x_n} + \int_0^1 S''(f(x_n), f(t)) (1-t) dt.$$

Therefore,

**Theorem 5:** *If  $S, f \in C^1$ , then the scheme (2) has a second-order rate of convergence if and only if*

$$S(f, f) = f, \quad \frac{\partial S(g, f)}{\partial f} \Big|_{f=g} = \frac{1}{2}. \quad (7)$$

Moreover, if the second derivatives of  $S$  and  $f$  are continuous, then

$$L(f) = -\frac{h}{2} \int_0^1 \{(1-t)^2 f''(t) - 2(1-t) S''(f(x_n), f(t))\} dt$$

where  $S(f(x_n), f(t)) = S(f(x_n, y(x_n)), f(t, y(t)))$ .

**Corollary 6:** *Keeping  $S(f, f) = f$ , the second condition of (7) is equivalent to one of the following four conditions*

$$\begin{aligned} \frac{\partial S(g, f)}{\partial f} \Big|_{g=f} &= \frac{1}{2}, \quad \frac{\partial S(g, f)}{\partial g} \Big|_{g=f} = \frac{1}{2}, \\ \frac{\partial S(g, f)}{\partial f} \Big|_{g=f} &= \frac{\partial S(g, f)}{\partial g} \Big|_{g=f}, \quad \text{and} \quad \frac{\partial S(g, f)}{\partial g} \Big|_{f=g} = \frac{1}{2}. \end{aligned}$$

Suppose now  $S$  and  $f$  both belong to  $C^2$ . Expanding  $f$  about the point  $x_{n+1/2} = (x_n + x_{n+1})/2$ ,

we have

$$\int_0^1 f(t) dt = f_{n+1/2} + \frac{h^2}{24} f''(x_{n+1/2}) + O(h^4). \quad (8)$$

On the other hand,

$$\begin{aligned} S(f(x_n), f(x_{n+1})) &= S(f(x_{n+1/2}), f(x_{n+1/2})) + \frac{\partial S(f(\xi), f(\eta))}{\partial \xi} \Big|_{\xi, \eta = x_{n+1/2}} (x_n - x_{n+1/2}) + \\ &\frac{\partial S(f(\xi), f(\eta))}{\partial \eta} \Big|_{\xi, \eta = x_{n+1/2}} (x_{n+1} - x_{n+1/2}) + \frac{\partial^2 S(f(\xi), f(\eta))}{\partial \xi^2} \Big|_{\xi, \eta = x_{n+1/2}} \frac{(x_n - x_{n+1/2})^2}{2} + \\ &\frac{\partial^2 S(f(\xi), f(\eta))}{\partial \xi \partial \eta} \Big|_{\xi, \eta = x_{n+1/2}} (x_{n+1} - x_{n+1/2})(x_n - x_{n+1/2}) + \frac{\partial^2 S(f(\xi), f(\eta))}{\partial \eta^2} \Big|_{\xi, \eta = x_{n+1/2}} \frac{(x_{n+1} - x_{n+1/2})^2}{2} + \dots \end{aligned}$$

For symmetric schemes,  $S(f,g)=S(g,f)$  and, consequently,

$$S(f(x_n), f(x_{n+1})) = f(x_{n+1/2}) + \frac{h^2}{8} \left\{ \frac{\partial^2 S(f(\xi), f(\eta))}{\partial \xi^2} + \frac{\partial^2 S(f(\xi), f(\eta))}{\partial \eta^2} - 2 \frac{\partial^2 S(f(\xi), f(\eta))}{\partial \eta \partial \xi} \right\} \Big|_{\xi, \eta = x_{n+1/2}} + O(h^4).$$

But

$$\frac{\partial^2 S(f(\xi), f(\eta))}{\partial \xi^2} = \frac{\partial S(f(\xi), f(\eta))}{\partial f(\xi)} f''(\xi) + \frac{\partial^2 S(f(\xi), f(\eta))}{\partial f^2(\xi)} f'^2(\xi),$$

$$\frac{\partial^2 S(f(\xi), f(\eta))}{\partial \xi \partial \eta} = \frac{\partial^2 S(f(\xi), f(\eta))}{\partial f(\eta) \partial f(\xi)} f'(\eta) f'(\xi).$$

Hence, from Corollary 6

$$S(f(x_n), f(x_{n+1})) = f(x_{n+1/2}) + \frac{h^2}{8} \left\{ f'' + 2f'^2 \left[ \frac{\partial^2 S(f,g)}{\partial f^2} - \frac{\partial^2 S(f,g)}{\partial f \partial g} \right] \Big|_{f,g=f(x_{n+1/2})} \right\} + O(h^4). \quad (9)$$

Substituting (9) and (8) into (4), we obtain the following theorem.

**Theorem 7:** *If  $S$  and  $f \in C^2$ , then each symmetric consistent scheme*

$$S(f,f) = f, \quad S(f,g) = S(g,f) \quad (10)$$

*has a second-order rate of convergence, at least. Moreover, if the fourth derivatives of  $f$  and  $S$  are continuous, then*

$$L(f) = -\frac{h^3}{12} \left\{ f''' + 3f'^2 \left[ \frac{\partial^2 S(f,g)}{\partial f^2} - \frac{\partial^2 S(f,g)}{\partial f \partial g} \right] \Big|_{f,g=f(x_{n+1/2})} \right\} + O(h^5). \quad (11)$$

It should be noted that symmetry is a sufficient but not necessary condition for a scheme to be second-order. For example, the scheme

$$Y_{n+1} = Y_n + h \frac{(f_n + f_{n+1})/2 + f_n^2 f_{n+1}}{1 + f_n(f_n + f_{n+1})/2}$$

is second-order but not symmetric.

**Corollary 8:** *A symmetric scheme is fourth-order if*

$$\left\{ \frac{\partial^2 S(f,g)}{\partial f^2} - \frac{\partial^2 S(f,g)}{\partial f \partial g} \right\} \Big|_{f,g=f(x_{n+1/2})} = - \frac{f''}{3f'^2} \Big|_{x=x_{n+1/2}} \quad (12)$$

Now we consider a general representation of consistent symmetric schemes (2). Let

$$\xi = \frac{f-g}{2}, \quad \eta = \frac{f+g}{2},$$

and assume  $S(f,g)$  can be expanded in terms of its two variables  $f$  and  $g$ :

$$S(f,g) \equiv \bar{S}(\xi,\eta) = \sum_{k,j} \alpha_{k,j} \xi^k \eta^j.$$

Using conditions (10), each consistent symmetric implicit one-step scheme (2) has the expansion

$$S(f,g) = \frac{f+g}{2} + \sum_{k \geq 0, j} \alpha_{2k,j} \left(\frac{f-g}{2}\right)^{2k+2} \left(\frac{f+g}{2}\right)^j, \quad (13)$$

where  $\alpha_{2k,j}$  are real constants to be chosen.

Furthermore, it is often useful to restrict the class of schemes to be homogeneous in the sense that

$$S(cf, cg) = cS(f,g) \quad (14)$$

for any constant  $c$ . For these schemes, we obtain the following conclusion:

**Theorem 9:** *Assume  $S$  can be expanded in terms of its two variables  $f$  and  $g$ . Then each homogeneous consistent symmetric nonlinear implicit one-step scheme (2) has the following expansion*

$$S(f,g) = \frac{f+g}{2} \left\{ 1 - \sum_{k \geq 0} \alpha_k \left(\frac{f-g}{f+g}\right)^{2k+2} \right\}. \quad (15)$$

where  $\alpha_k$  are real constants to be determined.

Observe that the trapezoidal rule is the principal part of each homogeneous consistent symmetric nonlinear implicit one-step scheme (2). Hence, in this sense, these nonlinear schemes are an extension of the trapezoidal rule.

Setting  $\alpha_k = 0$  for all  $k > 0$ , we get an 'extended trapezoidal rule' with one extra term:

$$S(f,g) = \frac{f+g}{2} - \frac{\alpha(f-g)^2}{2(f+g)}. \quad (16)$$

From (11),

$$L(f; \alpha) = -\frac{h^3}{12} \left\{ f'' - 3\alpha \frac{f'^2}{f} \right\} + O(h^5). \quad (17)$$

In terms of Means, the scheme (16) represents a linear combination between the Arithmetic Mean and the Harmonic Mean of  $f$  and  $g$ :

$$S(f,g) = (1-\alpha) \frac{f+g}{2} + \alpha \frac{2fg}{f+g}.$$

For example, if  $\alpha = 1$ , the above scheme represents the Harmonic Mean between  $f$  and  $g$ .

Finally, we discuss the stability of the nonlinear implicit one-step scheme (2).

Let  $f(x,y) = \lambda y$  and  $Y_{n+1} = \rho Y_n$ , where  $\rho$  is the "growth factor" in the step. Assuming that the scheme (2) is homogeneous in the sense of (14), we get

$$\rho = 1 + h\lambda S(1, \rho). \quad (18)$$

**Definition 10:** A nonlinear implicit one-step scheme (2) is said to be A-stable if all the roots of its characteristic equation (18) satisfy  $|\rho| < 1$  for any  $\text{Re } h\lambda < 0$ .

For nonlinear implicit one-step schemes, (18) may have more than one root for a fixed  $h\lambda$ , and it may be possible to choose which root the scheme follows, unlike the case for multistep methods.

Hence, the following definition may be of some practical value.

**Definition 11:** A nonlinear implicit one-step scheme (2) is said to be conditionally A-stable if at least one root of its characteristic equation (18) satisfies  $|\rho| < 1$  for any  $\text{Re } h\lambda < 0$ .

**Theorem 12:** For each real symmetric homogeneous scheme  $S(f,g)$ , the characteristic equation (18) transforms the unit circle of the  $\rho$  plane to the imaginary axis of the  $\lambda$  plane.

**Proof:** Since  $\bar{S}(f,\bar{f}) = S(\bar{f},f) = S(f,\bar{f})$ ,  $S(f,\bar{f})$  is real for any  $f$ . Hence, for  $\rho = e^{i\beta}$ ,

$$\lambda h = \frac{e^{i\beta} - 1}{S(e^{i\beta}, 1)} = \frac{e^{i\beta/2} - e^{-i\beta/2}}{S(e^{i\beta/2}, e^{-i\beta/2})} \text{ is purely complex.}$$

A necessary requirement for a homogeneous scheme to be A-stable is that it is stable at infinity.

**Theorem 13:** *A necessary condition for a homogeneous nonlinear implicit one-step scheme (2) to be A-stable is that all roots of*

$$S(1, \rho) = 0 \quad (19)$$

*satisfy  $|\rho| \leq 1$ . To be conditionally A-stable, at least one root of the above equation must satisfy  $|\rho| \leq 1$ .*

As an example, consider the stability of scheme (16) with characteristic equation

$$\rho = 1 + h\lambda \left\{ \frac{\rho+1}{2} - \frac{\alpha(\rho-1)^2}{2(\rho+1)} \right\}. \quad (20)$$

If  $|\rho| = 1$ , then  $\rho = e^{i\beta}$ ,  $0 \leq \beta < 2\pi$ , and

$$\frac{\rho-1}{\rho+1} = i \tan \beta/2.$$

Hence, (20) may be rewritten as

$$h\lambda = \frac{2i \tan \beta/2}{1 + \alpha [\tan \beta/2]^2}.$$

It follows that, if  $|\rho| = 1$ , then  $h\lambda$  is purely complex and lies in the interval  $(-i\alpha^{-1/2}, i\alpha^{-1/2})$  for  $\alpha > 0$ . For  $\alpha \leq 0$ ,  $h\lambda$  may assume any value on the imaginary axis. Also note that, for scheme (16), equation (19) becomes

$$\frac{\rho-1}{\rho+1} = \pm \alpha^{-1/2}.$$

That both roots of  $S(1, \rho)$  are on the unit circle for  $\alpha < 0$  and that one is inside and the other is outside the unit circle for  $\alpha > 0$  follows from the well-known result

**Lemma 14:** *The one-to-one mapping in the complex field*

$$W(z) = \frac{z-1}{z+1} \quad (21)$$

*maps the domains  $|z| < 1$ ,  $|z| = 1$ , and  $|z| > 1$  onto  $\text{Re}W < 0$ ,  $\text{Re}W = 0$ , and  $\text{Re}W > 0$ , respectively.*

The characteristic equation (20) can be rewritten as

$$\alpha W^2(\rho) + \frac{2}{h\lambda} W(\rho) - 1 = 0, \quad (22)$$

where  $W$  is defined in (21).

Since  $W=0$  is not a root of equation (22), any root  $W$  satisfies  $h\lambda \{W^{-1} + (-\alpha)W\} = 2$ . If  $\alpha \leq 0$  and  $\text{Re}h\lambda < 0$ , then  $\text{Re}W < 0$ , whence, by Lemma 14, any root of the characteristic equation (20) for the scheme (16) satisfies  $|\rho| < 1$ .

Also note that, if  $\alpha \neq 0$ , then the roots of quadratic equation (22) satisfy  $W_1 W_2 = -\alpha^{-1}$ . Hence, if  $\alpha > 0$ , then  $\text{Arg}(W_1) + \text{Arg}(W_2) = \pi$  and, consequently, either  $\text{Re}W_1 = \text{Re}W_2 = 0$  or  $\text{Re}W_1$  and  $\text{Re}W_2$  are opposite signs. Therefore, by Lemma 14, either both roots of the characteristic equation (20) for the scheme (16) satisfy  $|\rho|=1$  or one is larger than 1 in magnitude and the other is smaller. We may simply choose the value of  $Y_{n+1}$  in scheme (2) with (16) such that  $\|Y_{n+1}\| < \|Y_n\|$ . Thus, we have proven

**Theorem 15:** *Scheme (16) is A-stable for  $\alpha \leq 0$  and conditionally A-stable for  $\alpha > 0$ .*

For the more general scheme (15) with a finite terms number of terms, the corresponding characteristic equation is

$$\sum_{k \geq 0} \alpha_k \{W(\rho)\}^{2k+2} + \frac{2}{h\lambda} W(\rho) - 1 = 0. \quad (23)$$

By the relationship between coefficients and roots,

$$\sum_{k=1}^{2n+2} W_k^{-1} = \frac{2}{h\lambda}, \quad (24)$$

where  $W_k$  ( $k=1, \dots, 2n+2$ ) are roots of (23). Hence, if  $\text{Re}(h\lambda) < 0$ , then  $\text{Re}W_k < 0$  for at least one root  $W_k$  of (23). Therefore,

**Theorem 16:** *Each scheme (15) with a finite number of terms is conditionally A-stable.*

Remark: Theorem 16 is valid even if the coefficients  $\alpha_k$  of the scheme (15) are complex.

### 3. Derivation of some geometric schemes

The trapezoidal rule can be viewed as the Arithmetic Mean of  $f_n$  and  $f_{n+1}$  since

$$S(f_n, f_{n+1}) = \frac{1}{2}(f_n + f_{n+1}).$$

Let  $f_n = \tan \alpha_n$ ,  $f_{n+1} = \tan \alpha_{n+1}$ ,  $(y(x_{n+1}) - y(x_n))/h = \tan \alpha_{n+1/2}$ . The trapezoidal rule satisfies

$$\tan \alpha_{n+1/2} = \frac{1}{2}(\tan \alpha_n + \tan \alpha_{n+1}). \quad (25)$$

It is easy to see that the scheme (25) is poor if the angle  $\alpha_n$  or  $\alpha_{n+1}$  is close to  $90^\circ$ . In this case, it is natural to replace (25) by the Arithmetic Mean of the angles  $\alpha_n$  and  $\alpha_{n+1}$ :

$$\alpha_{n+1/2} = \frac{1}{2}(\alpha_n + \alpha_{n+1}). \quad (26)$$

The corresponding function  $S(f_n, f_{n+1})$  is

$$S(f_n, f_{n+1}) = \frac{\{(1+f_n^2)(1+f_{n+1}^2)\}^{1/2} + f_n f_{n+1} - 1}{f_n + f_{n+1}}. \quad (27)$$

From analytic geometry, the curve which satisfies (26) everywhere is a circle. So we call (27) a Circle Scheme. The Circle Scheme (27) is not linear with respect to the solution  $y(x)$  or  $f$ , but (26) is linear with respect to the angles. Hence, if the angles are not too large, the Circle Scheme is *close to being linear*. In fact, if we rotate the coordinate system by an angle  $\beta = \alpha_{n+1/2}$ , then the Circle Scheme coincides with the trapezoidal rule in the new coordinates.

Introducing a parameter  $a$  into (27) leads to a class of Elliptic Schemes:

$$E(f_n, f_{n+1}; a) = \frac{\{(a^2+f_n^2)(a^2+f_{n+1}^2)\}^{1/2} + f_n f_{n+1} - a^2}{f_n + f_{n+1}} \quad (28)$$

Note

$$\frac{\partial E(f, g)}{\partial f} = \frac{(a^2+g^2)^{1/2} E}{(a^2+f^2)^{1/2}(f+g)}, \quad \frac{\partial E(f, g)}{\partial g} = \frac{(a^2+f^2)^{1/2} E}{(a^2+g^2)^{1/2}(f+g)},$$



$$\frac{\partial^2 E}{\partial f^2} = \frac{\partial E}{\partial f} \frac{E - 2f}{a^2 + f^2}, \quad \frac{\partial^2 E}{\partial f \partial g} = \frac{\partial E}{\partial f} \frac{E}{a^2 + g^2},$$

$$\frac{\partial^2 E}{\partial f^2} \Big|_{f=g} = -\frac{f}{2(a^2 + f^2)}, \quad \frac{\partial^2 E}{\partial f \partial g} \Big|_{f=g} = \frac{f}{2(a^2 + f^2)}.$$

A straightforward computation leads to the following conclusion.

**Theorem 17:**  $E(f_n, f_{n+1}; a)$  in (28) has the following properties:

$$(f_n + f_{n+1})E \geq 0 \text{ with '=' iff } f_n + f_{n+1} = 0.$$

$$\frac{\partial E}{\partial f_n} \geq 0, \quad \frac{\partial E}{\partial f_{n+1}} \geq 0, \quad (f_n + f_{n+1}) \frac{\partial E}{\partial a} \geq 0.$$

$$\text{Min}(f_n, f_{n+1}) \leq E(f_n, f_{n+1}; a) \leq \text{Max}(f_n, f_{n+1}).$$

$$(f_n f_{n+1})^{1/2} < E(f_n, f_{n+1}; a) < \frac{f_n + f_{n+1}}{2} \quad \text{if } a > (f_n f_{n+1})^{1/2}.$$

$$\frac{2f_n f_{n+1}}{f_n + f_{n+1}} \leq E(f_n, f_{n+1}; a) \leq (f_n f_{n+1})^{1/2} \quad \text{if } a < (f_n f_{n+1})^{1/2}.$$

As a function of  $a$ ,  $E$  has only one fixed point  $a = (f_n f_{n+1})^{1/2}$ , for  $f_n f_{n+1} > 0$ .

Hence, the Elliptic Scheme (28) represents a Mean which lies between the Arithmetic Mean and the Harmonic Mean.

Similarly, we can derive two other geometric schemes: the Parabolic Scheme and the Hyperbolic Scheme. An easy way to derive the Parabolic Scheme is to apply the trapezoidal rule in a coordinate system rotated by an angle  $\alpha = \arctan(a)$  from the original coordinate system:

$$P(f_n, f_{n+1}; a) = \frac{f_n + f_{n+1}}{2} \frac{f_n f_{n+1} + a^2}{a^2 + [(f_n + f_{n+1})/2]^2}. \quad (29)$$

Substituting hyperbolic functions into the formulas (25),(26) instead of trigonometric functions, we get the Hyperbolic Scheme

$$H(f_n, f_{n+1}; a) = \frac{a^2 + f_n f_{n+1} - \{(a^2 - f_n^2)(a^2 - f_{n+1}^2)\}^{1/2}}{f_n + f_{n+1}}. \quad (30)$$

Since schemes (28),(29),(30) are all symmetric, by Theorem 7, we have

**Theorem 18:** *The Elliptic, Parabolic, and Hyperbolic Schemes (28),(29),(30) are second-order. The local truncation error for the Elliptic and Parabolic Schemes is*

$$-\frac{h^3}{12} \left\{ f'' - \frac{3ff'^2}{a^2+f^2} \right\} \Big|_{x=x_n+\frac{h}{2}} + O(h^5),$$

and for Hyperbolic Scheme (30)

$$-\frac{h^3}{12} \left\{ f'' - \frac{3ff'^2}{-a^2+f^2} \right\} \Big|_{x=x_n+\frac{h}{2}} + O(h^5).$$

- Remark: 1. In practice, the Parabolic Scheme has an advantage over the Elliptic and Hyperbolic Schemes in that it does not require square roots. Also, it is valid for all  $f_n, f_{n+1}$  including  $f_n + f_{n+1} = 0$ .
2. The parameter  $a$  can be chosen so that one of the schemes (29) or (30) is fourth-order.
  3. These geometric schemes are not homogeneous unless we multiply the parameter  $a$ , as well as  $f_n$  and  $f_{n+1}$ , by the constant  $c$ .

#### 4. Generalized Mean Scheme (GMS)

In addition to the above Geometric Means, another useful Mean for solving O.D.E.s is the Generalized Mean developed by Jiachang Sun [9].

**Definition 19:** For a given positive sequence  $\mathbf{a} = (a_1, \dots, a_n)$  on a real plane  $(r, t)$ , a Generalized Mean of the sequence  $\{a\}$   $S(a_1, \dots, a_n; r, t)$  is defined by

$$S(a_1, \dots, a_n; r, t) = \left\{ \frac{(n-1)! \Gamma(t+1)}{\Gamma(t+n)} [a_1^r, \dots, a_n^r] y^{n-1+t} \right\}^{1/rt}, \quad (31)$$

where  $[y_1, \dots, y_n]f(y)$  is the  $(n-1)$ -th divided difference of the function  $f(y)$  at the points  $y_1, \dots, y_n$ .

Now, we use the Generalized Mean (GM) in (31) to construct the Generalized Mean Scheme (GMS), a nonlinear implicit scheme. In this paper we only consider the one-step case. From (31), the GM between  $f_n$  and  $f_{n+1}$  is

$$S(f_n, f_{n+1}; r, t) = \left\{ \frac{1}{1+t} \frac{f_{n+1}^{r(1+t)} - f_n^{r(1+t)}}{f_{n+1}^r - f_n^r} \right\}^{1/rt} \quad (32)$$

where  $r, t$  are real. Substituting (32) into the local truncation error formula (11), we get

**Theorem 20:** Let  $f(x)$  have constant sign for  $x_n \leq x \leq x_{n+1}$ , then each scheme (32) with two real parameters  $(r, t)$  is second-order at least. Moreover,

$$L(f; r) = -\frac{h^3}{12} \left\{ f'' - [3 - r(2+t)] \frac{f'^2}{2f} \right\} \Big|_{x=x_n + \frac{h}{2}} + O(h^5), \quad \text{where } h = x_{n+1} - x_n. \quad (33)$$

To simplify the study of this scheme, we consider the restriction  $rt=1$  on the parameters  $r, t$ .

The scheme (32) reduces to

$$S(f_n, f_{n+1}; r) = \frac{r}{1+r} \frac{f_{n+1}^{1+r} - f_n^{1+r}}{f_{n+1}^r - f_n^r}, \quad (34)$$

where

$$S(f_n, f_{n+1}; 0) = \frac{f_{n+1} - f_n}{\text{Log}(f_{n+1}/f_n)}, \quad S(f_n, f_{n+1}; -1) = \frac{\text{Log}(f_n/f_{n+1})}{f_{n+1}^{-1} - f_n^{-1}}, \quad (35)$$

and the local truncation error (33) becomes

$$L(f; r) = -\frac{h^3}{12} \left\{ f'' - (1-r) \frac{f'^2}{f} \right\} + O(h^5). \quad (36)$$

It is obvious that for  $r = 0$  the scheme (35) is A-stable in the sense of the previous definition, because this scheme is exact for any exponential function. In general, the characteristic equation (18) for (34) is

$$\rho = 1 + \frac{\lambda h r}{1+r} \frac{\rho^{1+r} - 1}{\rho^r - 1}$$

or

$$(\rho-1) \frac{\rho^r - 1}{\rho^{1+r} - 1} = \frac{\lambda h r}{1+r}. \quad (37)$$

Note that

$$(\rho-1) \frac{\rho^r - 1}{\rho^{1+r} - 1} = \frac{|\rho|^{2(1+r)} - \bar{\rho}|\rho|^{2r} - \bar{\rho}^r|\rho|^2 + \bar{\rho}^{1+r} - \rho^{1+r} + \rho^r + \rho - 1}{(\rho^{1+r} - 1)(\bar{\rho}^{1+r} - 1)}.$$

Let  $\rho = Re^{i\beta}$ . Then the real part of the numerator is

$$R^{2(1+r)} - (R^{1+2r}-R)\cos\beta - (R^{2+r}-R^r)\cos r\beta - 1$$

which, for  $r > 0$  and  $R > 1$ , is greater than or equal to

$$R^{2(1+r)} - (R^{1+2r}-R) - (R^{2+r}-R^r) - 1 = (R-1)(R^r-1)(R^{1+r}-1) > 0,$$

whence  $\text{Re}\lambda h > 0$  in (37). Consequently, if  $r > 0$ , then the scheme (34) is A-stable.

For  $r < 0$ ,  $r \neq -1$ , rewrite (37) as

$$\left(1 - \frac{r}{1+r} \lambda h\right) \rho^{1+r} - \rho^r - \rho + \left(1 + \frac{r}{1+r} \lambda h\right) = 0. \quad (38)$$

First, assume  $r$  is a rational number:  $r = -m/n$ , where  $m$  and  $n$  are two positive integers.

Substituting  $Z = \rho^{1/n}$  into (38) and multiplying by  $Z^m$ , we get

$$Z^{n+m} - \left(1 - \frac{r}{1+r} \lambda h\right) Z^n - \left(1 + \frac{r}{1+r} \lambda h\right) Z^m + 1 = 0.$$

Since the product of roots of the above equation equals  $(-1)^{m+n}$ , if any root is greater than 1 in magnitude, then at least one root is less than 1 in magnitude. By continuity, this holds for all real  $r < 0$ , including  $r = -1$ . Therefore, if  $r < 0$ , then the scheme (34), (35) is conditionally A-stable.

In summary, we have proven

**Theorem 21:** *The scheme (34),(35) is A-stable for each parameter  $r \geq 0$  and is conditionally A-stable for  $r < 0$ .*

Given a fixed  $r$ , scheme (34) is exact for equations  $y' = f(x,y(x)) = C_1(x - C_0)^{1/r}$ , where  $C_0$  and  $C_1$  are constants, just as the trapezoidal rule is exact when  $f$  is a linear function of  $x$ . This explains why the GMS may lead to better results near a singularity, provided we can find a good approximation to  $r$ .

Note that we can interpret the GMS as an Intergrand Approximation Method (Jackson, [4]). That is, the discrete numerical solution  $\{Y_n\}$  can be extended to a continuous approximation  $Y(x)$  to the solution  $y(x)$  of (1) satisfying  $Y(x_n) = y(x_n)$  by

$$Y(x) = Y_a + \int_a^x P[f(\cdot, Y(\cdot)); r](s) ds,$$

where, for  $x \in [x_n, x_{n+1}]$ ,

$$P[g;r](s) = \left\{ g(x_n)^r \frac{x_{n+1}-s}{h} + g(x_{n+1})^r \frac{s-x_n}{h} \right\}^{1/r}.$$

$P[g;r]$  is a nonlinear interpolation operator computed by first raising  $g$  to the power  $r$ , then performing linear interpolation, and finally back transforming by raising the interpolant to the power  $1/r$ . Of course, if  $r=1$ ,  $P$  reduces to a linear interpolation operator.

A similar technique can be employed to enrich a piecewise linear space to solve singular two-point boundary value problems, using either the finite element method or the finite difference method. (See, Jiachang Sun [10], [11]).

In order to obtain a more accurate scheme, we set

$$r = 1 - \frac{f f''}{f'^2} \Big|_{x=x_n + \frac{h}{2}}. \quad (39)$$

From (36), the scheme (34) is fourth-order accurate for this value of  $r$ .

It is worth mentioning that the function in (39)

$$F(f, f', f'') = \frac{f f''}{f'^2} \quad (40)$$

often remains bounded even when  $f$  and its derivatives are unbounded. For instance,  $F$  is a constant for any power function  $f = C_1(x - C_0)^2$ . And, what is more interesting,  $F$  is identically equal to 1 for any exponential function,  $f = C_1 \text{Exp}(C_2(x - C_0))$ .

However, the  $F$  is not easy to compute, as an evaluation of  $f''$  is required. Some high-order schemes based on non-polynomial interpolation developed by Lambert [5] and Lambert and Shaw [6] have not been used widely, possibly because they too require the evaluation of higher derivatives of  $f$ . Furthermore, it is not clear that these methods are applicable to systems of equation.

Fortunately, we can avoid computing  $f''$  in (39) by setting

$$r = \frac{1}{h} \left( \frac{f_{n+1}}{f'_{n+1}} - \frac{f_n}{f'_n} \right). \quad (41)$$

With this approximation, the scheme (34) retains its fourth-order rate of convergence. Also, it retains exact for  $f(x, y(x)) = C_1(x - C_0)^{1/r}$ .

Computing experiments show that there is only a slight difference in accuracy between using (39) and (41) in the scheme (34); sometimes one is a little more accurate, and sometimes the other. But (41) saves computing time, and  $f''$  is not required.

An alternative derivation of the GMS is obtained by taking

$$Ff = f^{1/r} \quad (r \neq 0), \quad F^{-1}f = f^r, \quad G(u) = \int_{u_0}^u F\xi \, d\xi. \quad (42)$$

With this notation, (34) may be written as

$$S(f_n, f_{n+1}) = [F^{-1}f_{n+1}, F^{-1}f_n] G(y) \equiv \frac{G(F^{-1}f_{n+1}) - G(F^{-1}f_n)}{F^{-1}f_{n+1} - F^{-1}f_n}. \quad (43)$$

This formulation can be generalized by considering other functions  $F$ . Using Theorem 7 and the

local truncation error formula (11), we have

**Theorem 22:** *For any one-to-one map  $F$ , (43) defines a second-order one-step implicit scheme with local truncation error*

$$L(f; F) = -\frac{h^3}{12} \left\{ f'' + f'^2 \frac{d^2 F^{-1} f}{df^2} \left( \frac{dF^{-1} f}{df} \right)^{-1} \right\} \Big|_{x=x_{n+1/2}} + O(h^5). \quad (44)$$

This formulation unifies most of schemes described in this and the previous section. Some examples follow.

1.  $Ff = f$  leads to the trapezoidal rule.
2.  $Ff = e^{rf}$  leads to the scheme (35). (It is independent of the parameter  $r$ ).
3.  $Ff = \frac{af}{(1-f^2)^{1/2}}$  leads to the Elliptic Scheme (28).
4.  $Ff = \frac{af}{(1+f^2)^{1/2}}$  leads to the Hyperbolic Scheme (30).

Many other schemes can be derived using this formulation.

## 5. Some computational considerations for the GMS

First, we consider how to solve the implicit equation (2). For an initial value system (1) with steep gradients, functional iteration may be employed:

$$Y_{n+1}^{(k)} = Y_n + h S( f_n, f_{n+1}^{(k-1)} ; r^{(k-1)} ), \quad (45)$$

where

$$r^{(k-1)} = \frac{1}{h} \left( \frac{f_{n+1}^{(k-1)}}{f_{n+1}^{(k-1)'}} - \frac{f_n}{f_n'} \right). \quad (46)$$

For stiff problems, a Newton iteration should be used instead.

As a simple stopping criterion for the iteration, we use

$$\| Y_{n+1}^{(k)} - Y_{n+1}^{(k-1)} \| < \epsilon_y,$$

where  $\epsilon_y$  is a parameter to be specified.

The starting value,  $Y_{n+1}^{(0)}$ , is computed by a conventional explicit method. For simplicity, we use the Euler Method for the numerical tests in the last section. Of course, a more accurate predictor may be used.

The rate of convergence of the iteration (45) depends upon the value of the "contraction factor"

$$h \frac{dS}{df} = h \frac{\partial S}{\partial f} \frac{\partial f}{\partial y} + h \frac{\partial S}{\partial r} \frac{\partial r}{\partial y}, \quad (47)$$

where, for the GMS,

$$\frac{\partial S}{\partial r} = \frac{S}{(1+r)^2} + \frac{r}{1+r} \left\{ \frac{f^{1+r} \text{Log} f - f_n^{1+r} \text{Log} f_n}{f^r - f_n^r} - \frac{f^r \text{Log} f - f_n^r \text{Log} f_n}{f^r - f_n^r} S \right\}.$$

If  $f$  is continuous, then,

$$S \rightarrow \frac{1+r}{r} f_n, \quad \text{as } h \rightarrow 0, f \rightarrow f_n,$$

and

$$\frac{\partial S}{\partial r} \rightarrow \frac{f_n}{r(1+r)} + \frac{r}{1+r} \left\{ \frac{1+r}{r} f_n \text{Log} f_n + \frac{1}{r} f_n - \frac{1+r}{r} (f_n \text{Log} f_n + \frac{1}{r} f_n) \right\} = 0.$$

Also, from Theorem 5,  $\partial S / \partial f \rightarrow 1/2$  as  $h \rightarrow 0$ . Therefore, for sufficiently small  $h$ , iteration (45) is



convergent and, moreover, its rate of convergence is close to that of the trapezoidal rule using the same functional iteration procedure.

It is worth mentioning that the GMS is particularly well-suited to solving problems having steep gradients, especially those problems for which  $f(x,y(x))$  behaves like a piecewise power function of  $x$ . In practice, it may be more efficient to use the GMS only on the sections of the problem having steep gradients and a conventional scheme on the sections of the problem where  $f(x,y(x))$  is well-behaved. We consider two fourth-order hybrid schemes of this type. If  $|f_n| \leq f^*$ , then MixI uses the cubic Hermite scheme (modified trapezoidal rule)

$$Y_{n+1} = Y_n + h \frac{f_n + f_{n+1}}{2} + \frac{h^3}{12} (f'_n - f'_{n+1}). \quad (48)$$

And MixII uses the classical fourth-order Runge-Kutta scheme in place of (48). If  $|f_n| > f^*$ , then both MixI and MixII use

$$S(f_n, f_{n+1}) = \frac{f_{n+1} - f_n}{\text{Log}(f_{n+1}/f_n)}, \quad \text{if } |r| \leq er^*,$$

$$S(f_n, f_{n+1}) = \frac{\text{Log}(f_n/f_{n+1})}{f_{n+1}^{-1} - f_n^{-1}}, \quad \text{if } |r+1| \leq er^*,$$

and

$$S(f_n, f_{n+1}) = \frac{r}{1+r} \frac{f_{n+1}(f_{n+1}/f_n)^r - f_n}{(f_{n+1}/f_n)^r - 1}, \quad \text{otherwise,} \quad (49)$$

where  $f^*$  and  $er^*$  are constants. In our numerical tests, we take  $f^* = 2$  and  $er^* = 0.01$ .

## 6. Extension to Systems

So far, our discussion has been restricted to scalar equations. However, we have used nonlinear implicit one-step schemes successfully to solve systems of equations; some numerical results are presented in the last section.

For systems, we apply the scheme (2) to the individual components of the system. The parameter  $r$  is a vector whose components elements are determined componentwise by formula (46), where

$$f' = \frac{d}{dx}f(x,y(x)) = \frac{\partial f}{\partial x} + \sum_j \frac{\partial f}{\partial x_j}$$

is a vector. Hence, the Jacobi matrix of  $f(x)$  is needed to be computed for finding the index vector  $r$  to get a fourth order scheme. The advantage of (41) over (39) is more significant for systems than for scalar equations.

The analysis of nonlinear schemes for systems of equations is an open problem that we will consider in the future.

## 7. Numerical Tests

In this section, we present some numerical results. Throughout,  $y(x)$  denotes the solution of the problem (1) and  $C(x-\xi)^\rho$  is a piecewise approximation to function of  $y'(x)$ , where  $\rho = 1/r$  is the index of the approximation. If  $\rho < 0$ , the approximate position of the singularity is

$$\xi = x_n + h \left\{ \left( \frac{f_n}{f_{n+1}} \right)^r - 1 \right\}^{-1}.$$

Throughout this section, we use the following abbreviations:

GMS -- the scheme (34);

R-K -- the classical fourth-order Runge-Kutta scheme;

C-H -- cubic Hermite scheme (48);

MixI -- the hybrid scheme composed of GMS and C-H (49);

MixII -- the hybrid scheme composed of GMS and R-K;

L-S -- the scheme proposed by Lambert and Shaw [6];

Error --  $Y_n - y(x)$  for the GMS;

Er(f) -- the error in the first derivative  $Y'_n - y'(x)$  for second-order equations.

A uniform mesh,  $h = x_{n+1} - x_n$ , is used throughout the section. The Fortran program was run in double-precision, on a DEC-System 2060 computer at Yale. The iteration error  $\epsilon_y$  is taken to be  $10^{-10}$ .

Test 1. [6]  $y' = 1 + y^2$ ,  $y(0) = 1$

with solution  $y(x) = \tan(x + \frac{\pi}{4})$  which has a strong singularity at  $x = \frac{\pi}{4}$ .

Table 1.  $x = 0 \quad (0.05) \quad 0.75$

x	y	GMS	$\rho$	$\xi$	L-S	R-K
0.70	11.6814	11.6808	-1.975	0.7828	11.6813	11.6680
0.75	28.2383	28.2305	-1.992	0.7851	28.2378	27.6947

Remark: For the exact solution,  $\rho = -2$ ,  $\xi = \frac{\pi}{4} = 0.7835$ .

Test 2. [6]  $xy' = y + 5x^2e^{y/5x}$ ,  $y(1) = 0$

with solution  $y(x) = -5x\text{Log}(2-x)$  which has a weak singularity at  $x = 2$ .

Table 2.  $x = 0 (0.05) 1.95$

x	y	GMS	$\rho$	$\xi$	L-S	R-K
1.90	21.8745	21.8753	-1.055	2.001	21.8748	21.8746
1.95	29.2084	29.2098	-0.997	2.001	29.2099	29.2077

Remark: For the exact solution,  $\rho = -1$ ,  $\xi = 2$ .

Test 3. [6]  $(1-x)y' = y \text{Log}y$ ,  $y(0) = e^{0.2}$

with solution  $y(x) = e^{0.2/(1-x)}$  which has an essential singularity at  $x = 1$ .

Table 3.  $x = 0 (0.05) 0.95$

x	y	GMS	$\rho$	$\xi$	L-S	R-K
0.90	7.3891	7.3902	-2.521	0.963	7.3954	7.3646
0.95	54.5982	54.8956	-3.126	0.976	57.1189	47.1138

Remark: For the exact solution,  $\rho = -\infty$ ,  $\xi = 1$

These results show that the GMS is more accurate than the classical fourth-order Runge-Kutta scheme in Tests 1 and 3; the accuracy is about the same in Test 2. Also, the GMS is more accurate than the scheme of Lambert and Show in Test 3; the accuracy is about the same in Tests 1 and 2. However, the GMS doesn't need  $f'''$  which the L-S scheme requires.

Test 4. (Artificial) A system of equations consisting of four components:

$$\begin{aligned} y_1' &= -0.1 e^{-y_2}/y_3, & y_1(0) &= .35 \\ y_2' &= 2\{(y_1-0.1)(10y_3)^3\}^{1/2}, & y_2(0) &= 0 \\ y_3' &= e^{2y_2} \text{Log } y_4, & y_3(0) &= 0.1 \\ y_4' &= 2y_3y_4, & y_4(0) &= e^{0.2}. \end{aligned}$$

The solution is

$$\begin{aligned} y_1(x) &= 0.25(1-x)^4 + 0.1, & y_2(x) &= -\text{Log}(1-x), \\ y_3(x) &= 0.1(1-x)^{-2}, & y_4(x) &= e^{0.2/(1-x)}. \end{aligned}$$

Table 4  $h = 0.05$

x	$y_k(x)$	$\rho$	$\xi$	GMS	R-K	C-H
0.900	0.1000	3.01	0.77	0.1000	0.1000	0.1000
(1)						
(2)	2.3026	-1.00	0.91	2.3025	2.1122	2.2580
(3)	10.0000	-3.00	0.97	9.9992	8.8429	9.6617
(4)	7.3890	-0.25	0.96	7.3867	7.0125	7.1183
0.950	0.1000	-11.54	0.27	0.1000	0.0999	*
(1)						
(2)	2.9957	-0.50	0.95	2.4771	3.5606	*
(3)	40.0000	5.53	0.84	36.4946	40.0606	*
(4)	54.5982	-3.27	0.98	50.0038	32.9154	*
	( $h/2 = 0.025$ )			54.4607	46.0766	44.9161

\*: The C-H scheme overflows on the last point using (45).

Remark: On the last point  $x=0.95$  the vector of first derivatives is equal to

(  $-0.16 \times 10^{-3}$ , 2.1,  $1.4 \times 10^3$ ,  $3.8 \times 10^3$  ).

Test 5. A problem with an integrable singularity:

$$y' = \frac{y}{1+x} + (1+x)|x - \frac{1}{2}|^t, \quad y(0) = -\frac{2^{-(1+t)}}{1+t}, \quad -1 < t < 0.$$

The solution is

$$y(x) = \text{Sign}(x - \frac{1}{2}) \frac{1+x}{1+t} |x - \frac{1}{2}|^{1+t}.$$

Table 5. Errors  $x = 0.1 (0.1) 1.0$

x	t=-0.1	t=-0.3	t=-0.5	t=-0.7	* t=-0.7 *
0.1	-0.214-5	-0.115-4	-0.60-5	-0.87-4	0.54-12
0.4	-0.237-4	-0.416-6	0.70-4	-0.19-3	-0.18-10
0.5	0.245-1	0.959-1	0.63+0	-0.74+1	0.29-08
0.6	0.431-1	0.150+0	0.87+0	-0.86+1	0.29-08
0.9	0.507-1	0.178+0	0.10+1	-0.10+2	0.40-08
1.0	0.533-1	0.187+0	0.11+1	-0.11+2	0.42-08

Remark: the right column is the error for another problem

$$y' = (1+t)y(x-0.5)^{-1}, \quad y(0) = \frac{2^{-(1+t)}}{1+t}, \quad -1 < t < 0,$$

the solution of which is:

$$y(x) = (0.5-x)^{1+t}/(1+t), \quad \text{for } x < 1/2$$

$$y(x) = (x-0.5)^{1+t}/(1+t), \quad \text{for } x > 1/2$$

which has a turning point at  $x = \frac{1}{2}$ .

The GMS scheme may be used with invariant imbedding to solve linear two-point boundary value problems with various singularity properties. For these problems,  $y'' = f'$  is available directly and may be used in the computation of the fourth-order GMS scheme using (41) to compute  $r$ .

Consider the two-point boundary value problem

$$y''(x) + p(x)y'(x) + q(x)y(x) = r(x) \tag{50}$$

$$a_0 y(0) + b_0 y'(0) = c_0, \quad a_1 y(1) + b_1 y'(1) = c_1.$$

To solve this problem, we use the sweep method of Gelfand and Formin [1] (p.133). (See, also Miller [7] or Scott [8].)

For  $b_0 \neq 0$ ,

(i) the Initial Value Problem for the Forward Sweep is

$$\begin{aligned} u' &= -q - pu - u^2, & u(0) &= -\frac{a_0}{b_0}, \\ v' &= r - v(u + p), & v(0) &= \frac{c_0}{b_0}. \end{aligned}$$

(ii) and the Initial Value Problem for the Backward Sweep is

$$y' = uy + v, \quad y(1) = \frac{c_1 - b_1 v(1)}{a_1 + b_1 u(1)}.$$

For  $b_0 = 0$ ,

(i) the Initial Value Problem for the Forward Sweep is

$$\begin{aligned} u' &= 1 + u(p + qu), & u(0) &= -\frac{b_0}{a_0}, \\ v' &= u(r + qv), & v(0) &= \frac{c_0}{a_0}. \end{aligned}$$

(ii) and the Initial Value Problem for the Backward Sweep is

$$uy' = y + v, \quad y(1) = \frac{c_1 u(1) - b_1 v(1)}{a_1 u(1) + b_1}.$$

Test 6. An unstable two point boundary value problem

$$y'' - 165y' - 2700y + 4.95e^{15x} = 0,$$

$$y'(0) = 0.015, \quad y(1) = 0.001e^{15}$$

with solution  $y(x) = 0.001 e^{15x}$ .

Table 6.  $x = 0 (0.005) 1$ 

x	NI	Yn	Error	E(C-H)	fn	Er(f)	Ef(C-H)
0.000	2	9.752-4	-2.48-5	2.73-7	1.5-2	-	-
0.005	19	2.106-3	-1.08-5	1.29-7	3.2-2	1.6-4	-1.9-6
0.500	27	1.808	-1.25-8	-3.23-8	27.1	1.9-7	3.3-7
0.900	34	7.294+2	-3.48-11	-1.31-5	1.1+4	-1.8-8	2.8-4
0.950	35	1.544+3	-1.09-11	-2.77-5	2.3+4	1.8-8	6.0-3

Remark: NI -- number of iterations with  $\epsilon_y = 10^{-10}$  for the GMS.

Test 7. A linear singular perturbation problem with constant coefficients

$$Ly = -\epsilon y'' + y' + (1+\epsilon)y = f(x), \quad \text{in } (0,1)$$

$$y(0) = y(1) = 0$$

where  $f(x) = (1+\epsilon)(a-b)x - \epsilon a - b$ ,

$$a = 1 + e^{-(1+\epsilon)/\epsilon}, \quad b = 1 + e^{-1},$$

with true solution

$$y(x) = e^{-(1+\epsilon)(1-x)/\epsilon} + e^{-x} - a + (a-b)x.$$



Table 7.1 Maximum error in Y at the nodes

$\epsilon$	1/h	R-K	GMS	MixI	C-H	MixII
0.1	10	0.31+0	-0.18-1	-0.24-3	0.79-3	0.37-1
	20	0.11-1	0.75-4	-0.12-4	0.47-4	0.99-3
	40	0.45-3	0.10-4	-0.74-6	0.29-5	0.16-3
	80	0.91-5	0.23-5	-0.46-7	0.18-6	0.33-4
0.01	100	0.21+0	-0.24-2	-0.19-4	0.56-3	-0.24-2
	200	0.75-2	0.65-5	-0.12-5	0.34-4	0.10-4
	400	0.30-3	0.81-6	-0.76-7	0.21-5	0.17-5
	800	0.15-4	0.19-6	-0.47-8	0.13-6	0.34-6
0.001	1000	0.20+0	-0.12-3	-0.19-5	0.54-3	-0.12-3

Table 7.2 Maximum error in Y' at the nodes

$\epsilon$	1/h	R-K	GMS	MixI	C-H	MixII
0.1	10	0.34+1	-0.19+0	0.38-3	0.88-2	0.46+0
	20	0.12+0	0.83-3	-0.12-3	0.52-3	0.25-1
	40	0.49-2	0.11-3	-0.80-5	0.32-4	0.73-2
	80	0.41-3	0.25-4	-0.50-6	0.20-5	0.28-2
0.01	100	0.21+2	-0.24+0	-0.19-2	0.57-1	-0.24+0
	200	0.75+0	0.66-3	-0.12-3	0.34-2	0.27-2
	400	0.31-1	0.82-4	-0.76-5	0.21-3	0.76-3
	800	0.16-2	0.19-4	-0.48-6	0.13-4	0.29-3
0.001	1000	0.19+3	-0.12+0	-0.19-2	0.54+0	-0.12+0

Table 7.3 CPU TIME in seconds on a DEC 20.

$\epsilon$	1/h	R-K	GMS	MixI	C-H	MixII
0.1	10	0.08	0.57	0.48	0.38	0.23
	20	0.15	0.52	0.41	0.38	0.21
	40	0.28	0.64	0.54	0.62	0.37
	80	0.55	1.15	0.93	1.12	0.66
0.01	100	1.83	6.66	5.63	6.20	2.62
	200	3.68	7.49	6.78	7.83	4.69
	400	7.30	12.98	11.48	13.96	7.92
	800	14.63	23.36	21.76	24.77	15.62
0.001	1000	21.82	58.30	47.74	50.17	23.40

Table 7.4  $\frac{\epsilon}{h} = 1$ 

	$\epsilon$	R-K	GMS	MixI	C-H	MixII
Error	0.1	0.31+0	-0.18-1	-0.24-3	0.79-3	0.37-1
	0.01	0.21+0	-0.24-2	-0.19-4	0.56-3	-0.24-2
	0.001	0.20+0	-0.12-3	-0.19-5	0.54-3	-0.12-3
Er(f)	0.1	0.34+1	-0.19+0	0.38-3	0.88-2	0.46+0
	0.01	0.21+2	-0.24+0	-0.19-2	0.57-1	-0.24+0
	0.001	0.19+3	-0.12+0	-0.19-2	0.54+0	-0.12+0

*Acknowledgement.* The authors wish to thank Professors M.Schultz and S.Eisenstat for a number of useful discussions and suggestions and for making their visits to Yale University very enjoyable.

## REFERENCES

1. I.Gelfand and S.Fomin, "*Calculus of Variations*", Prentice-Hall, New Jersey, 1963.
2. P.Henrici, "*Discrete Variable Methods in Ordinary Differential Equations*", John Wiley and Sons, 1962.
3. T.E.Hull, "*Numerical Solutions of Initial Value Problems for Ordinary Differential Equations*", "Numerical Solution of Boundary-Value Problems for Ordinary Differential Equations", Edited by A.K.Aziz, Academic Press, N.Y., 1975, pp.3-26.
4. K.R.Jackson, "*Variable Stepsize, Variable Order Integrand Approximation Methods for the Numerical Solution of Ordinary Differential Equations*", Ph. D. Thesis, Department of Computer Science, University of Toronto, Technical Report, #129, 1978.
5. J.D.Lambert, "*Computational Methods in Ordinary Differential Equations*", John Wiley and Sons, London, 1973.
6. J.D.Lambert and B.Shaw, "*A Method for the Numerical Solution  $y'=f(x,y)$  Based on a Self-Adjusting Non-Polynomial Interpolant*", Math. Comp., 20, 1966, pp.11-20.
7. R.E.Miller, "*Use of the Field Method for Numerical Integration of Two-Point Boundary-Value Problems*", AIAA 5, 1967, pp.811-813.
8. M.R.Scott, "*On the Conversion of Boundary-Value Problems into Stable Initial-Value Problems Via Several Invariant Imbedding Algorithms*", "Numerical Solution of Boundary-Value Problems for Ordinary Differential Equations", Edited by A.K.Aziz, Academic Press, N.Y., 1975, pp.89-148.
9. Jiachang Sun, "*Generalizations of the Means and Their Inequalities*", Department of Mathematics, University of California, Santa Barbara, May, 1981. Also submitted to a Chinese Journal ("Mathematical Annals").
10. Jiachang Sun, "*A Galerkin Method on Nonlinear Subsets and Its Application to a Singular Perturbation Problem*", Department of Computer Science, Yale University, Technical Report #217, 1982.
11. Jiachang Sun, "*Semi-linear Difference Schemes for Singular Perturbation Problems in one dimension*", Department of Computer Science, Yale University, Technical Report #216, 1982.