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Solving Stiff Ordinary Differential Equations Using Componentwise Block Partitioning

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Abstract**—**A new code based on variable order and variable stepsize componentwise partitioning is introduced to solve a system of equations dynamically. In this current technique, the system is treated as nonstiff and any equation that caused stiffness will be treated as stiff equation. Componentwise block partitioning will place the necessary equations that cause instability and stiffness into the stiff subsystem and solve using Backward Differentiation Formula, while all other equations will still be treated as non-stiff and solved using Adams formula.

Keywords**—**Componentwise, partitioning, stiff.

I. Introduction

We consider block method for the parallel solution of Ordinary Differential equations (ODEs)

$$y' = f(x,y) \tag{1}$$

with initial values $y(a) = y_0$ in the interval $x \in [a,b]$.

In this research, we will be considering the 2-point block Adams type formulas derived by Zanariah and Suleiman (2004) for solving nonstiff subsystem and the formulae are, 2-point block Backward Differentiation Formulas derived by Zarina and Suleiman (2006) for the stiff subsystem. The formulas are used for componentwise block partitioning technique. The algorithm has been designed to facilitate switching between Adams type formulas and block BDF during the integration process.

The formulae for nonstiff derived by Zanariah and Suleiman (2004) are,

r=1	$y(x_{n+1}) = y(x_n) + \frac{h}{720}\left(-19f_{n+2} + 346f_{n+1} + 456f_n + 11f_{n-1} - 74f_{n-2}\right)$ $y(x_{n+2}) = y(x_n) + \frac{h}{90}\left(29f_{n+2} + 124f_{n+1} + 24f_n + 4f_{n-1} - f_{n-2}\right)$
r=2	$y(x_{n+1}) = y(x_n) + \frac{h}{14400}\left(-565f_{n+2} + 7808f_{n+1} + 7455f_n - 335f_{n-1} + 37f_{n-2}\right)$ $y(x_{n+2}) = y(x_n) + \frac{h}{900}\left(295f_{n+2} + 1216f_{n+1} + 285f_n + 5f_{n-1} - f_{n-2}\right)$
r=0.5	$y(x_{n+1}) = y(x_n) + \frac{h}{1800}\left(-31f_{n+2} + 755f_{n+1} + 1635f_n - 704f_{n-1} + 145f_{n-2}\right)$ $y(x_{n+2}) = y(x_n) + \frac{h}{225}\left(71f_{n+2} + 320f_{n+1} + 15f_n + 64f_{n-1} - 20f_{n-2}\right)$

(2)

and Zarina and Suleiman (2006) derived for BDF,

r=1	$-\frac{1}{10}y_{n-2} + \frac{3}{5}y_{n-1} - \frac{9}{5}y_n + y_{n+1} + \frac{3}{10}y_{n+2} = \frac{6}{5}hf_{n+1}$ $\frac{3}{25}y_{n-2} - \frac{16}{25}y_{n-1} + \frac{36}{25}y_n - \frac{48}{25}y_{n+1} + y_{n+2} = \frac{12}{25}hf_{n+2}$
r=2	$-\frac{3}{128}y_{n-2} + \frac{25}{128}y_{n-1} - \frac{225}{128}y_n + y_{n+1} + \frac{75}{128}y_{n+2} = \frac{15}{8}hf_{n+1}$ $\frac{2}{115}y_{n-2} - \frac{3}{23}y_{n-1} + \frac{18}{23}y_n - \frac{192}{115}y_{n+1} + y_{n+2} = \frac{12}{23}hf_{n+2}$
r=0.5	$-\frac{3}{7}y_{n-2} + \frac{64}{35}y_{n-1} - \frac{18}{7}y_n + y_{n+1} + \frac{6}{35}y_{n+2} = \frac{6}{7}hf_{n+1}$ $\frac{50}{67}y_{n-2} - \frac{192}{67}y_{n-1} + \frac{225}{67}y_n - \frac{150}{67}y_{n+1} + y_{n+2} = \frac{30}{67}hf_{n+2}$

(3)

II. Partitioning System of ODEs in Block Method

Partitioning is a strategy to solve a system of equations either using Adam or BDF method whichever is suitable. The objective of partitioning is to make the code developed more efficient and hence reduced the computational time and yet maintaining the accuracy of the solution. In this section, we introduce a partitioning strategy in solving system of equations in block method. We name this partitioning strategy, as Partitioning Block Componentwise (PBC).

Partitioning Block Componentwise (PBC)

If a system is treated as stiff, the implicit method is used on the whole system, in which the stiffness may be caused by only a few components of the system. This implicit formulae which require the repeated solution of system of linear equation involving the use of Newton iteration which consumes a considerable amount of computational effort and time. Computational cost can be reduced by partitioning the equation into stiff and nonstiff parts (transient and smooth components). This partitioning method partitioned dynamically the system into stiff subsystems and nonstiff subsystems and this is done when instability occurs to a nonstiff equation, which is then placed into the stiff subsystem.

In the code, the system (1) is initially treated as nonstiff and solved using Adams method. At the first instance of instability, which is due to the eigenvalues of the largest and almost equal in magnitude of the Jacobian of the system, the appropriate equation is placed in the stiff subsystem and solved using BDF method. In doing so, the effect of these eigenvalues is nullified, and larger step sizes are permissible until the effect of the next set of the largest and almost equal in magnitude of the eigenvalues causes instability. Again the appropriate equations are placed in the stiff subsystem, and the process continues.

In this strategy, we switch the method from Adams to BDF when there is an indication of instability due to stiffness. Here the possibility of instability indicated by one of the following,

a) When the local truncation error (LTE) is greater than the given tolerance, i.e. LTE $>$ TOL .
b) Non-convergence. In this strategy, we perform two convergence tests for the nonstiff system as,

$$\max\left|y^{(i+1)} - y^{(i)}\right| \le 0.1*\text{TOL}; \quad i = 1,2,..$$

and the number of iterations when evaluating $PE(CE)^n$ is restricted to $n \le 4$, where n is the number of iterations needed. If $n > 4$, it shows the iteration is poorly convergent and we do the test for the change to BDF method.

If the instability occurs at the first time, we calculate the trace of the system to determine stiffness. When stiffness is detected, the necessary equation is placed in the stiff subsystem. The process is continued until all the equations have been placed in the right subsystem and the end of the integration interval has been reached. If the trace > 0, we continue the process as nonstiff subsystem using half of the step length.

Once an equation is placed in the stiff subsystem, it is solved using BDF method. If there is a step failure happen and it is due to the equations from the nonstiff subsystem, the equation that caused step failure is placed in the stiff subsystem.

Failure step in stiff subsystem is determine by,

i.)LTE > TOL
ii.)the convergence test is,

$$e_{n+2}^{i+1} > \frac{0.1 \times TOL \times (A + B \max\left|y_{n+2}^{i+1}\right|)}{\left(\dfrac{e_{n+2}^{i+1}}{e_{n+1}^{i+1}}\right)^{1.5}}$$

where, $A = 1$ and $B = 0$ if relative error test, $A = 0$ and $B = 1$ if absolute error test, $A = 1$ and $B = 1$ if mixed error test.

The process to detect the appropriate equation that causes stiffness is done by the following iterative formulae.

III. Iterations Formulae for Partitioning Block Componentwise

Given a system of linear equations, we will look at the iteration matrix for 2-point block method. Supposedly the system is a 3 by 3 equations,

$$\left.\begin{array}{lllllll} y_1' & = & a_{11}y_1 & + & a_{12}y_2 & + & a_{13}y_3 \\ y_2' & = & a_{12}y_1 & + & a_{22}y_2 & + & a_{23}y_3 \\ y_3' & = & a_{13}y_1 & + & a_{23}y_2 & + & a_{33}y_3 \end{array}\right\} \tag{4}$$

Let equation 1, 2 and 3 be nonstiff and instability occur by equation 1, then from (2) the general formula for the $(i+1)^{th}$ iteration at second point will be,

$$y_{1,n+2}^{(i+1)} = {}_2\beta_1 f_{1,n+1}(y_{1,n+1}^{(i)}, y_{2,n+1}^{(i)}, y_{3,n+1}^{(i)}) + {}_2\beta_2 f_{1,n+2}(y_{1,n+2}^{(i)}, y_{2,n+2}^{(i)}, y_{3,n+2}^{(i)}) + \varphi \tag{5}$$

where ${}_2\beta_1$ and ${}_2\beta_2$ are the coefficients for f_{n+1} and f_{n+2} respectively and φ are the backvalues.

The $(i)^{th}$ iteration is,

$$y_{1,n+2}^{(i)} = {}_2\beta_1 f_{1,n+1}(y_{1,n+1}^{(i-1)}, y_{2,n+1}^{(i-1)}, y_{3,n+1}^{(i-1)}) + {}_2\beta_2 f_{1,n+2}(y_{1,n+2}^{(i-1)}, y_{2,n+2}^{(i-1)}, y_{3,n+2}^{(i-1)}) + \varphi \tag{6}$$

The difference of $y_{1,n+2}^{\{i+1)}$ and $y_{1,n+2}^{(i)}$ is denoted as $e_{1,n+2}^{(i+1)}$ where $e_{1,n+2}^{(i+1)} = y_{1,n+2}^{(i+1)} - y_{1,n+2}^{(i)}$ gives,

$$\begin{aligned} e_{1,n+2}^{(i+1)} = {}& {}_2\beta_1[f_{1,n+1}(y_{1,n+1}^{(i)}, y_{2,n+1}^{(i)}, y_{3,n+1}^{(i)}) - f_{1,n+1}(y_{1,n+1}^{(i)} - e_{1,n+1}^{(i)}, y_{2,n+1}^{(i)} - e_{2,n+1}^{(i)}, y_{3,n+1}^{(i)} - e_{3,n+1}^{(i)})] + \\ & {}_2\beta_2[f_{1,n+2}(y_{1,n+2}^{(i)}, y_{2,n+2}^{(i)}, y_{3,n+2}^{(i)}) - f_{1,n+2}(y_{1,n+2}^{(i)} - e_{1,n+2}^{(i)}, y_{2,n+2}^{(i)} - e_{2,n+2}^{(i)}, y_{3,n+2}^{(i)} - e_{3,n+2}^{(i)})] \end{aligned}$$

Using Taylor's expansion yields the formula,

$$\begin{aligned} e_{1,n+2}^{(i+1)} = {}& {}_2\beta_1 \frac{\partial f_{1,n+1}}{\partial y_{1,n+1}} e_{1,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{1,n+2}}{\partial y_{1,n+2}} e_{1,n+2}^{(i)} + {}_2\beta_1 \frac{\partial f_{1,n+1}}{\partial y_{2,n+1}} e_{2,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{1,n+2}}{\partial y_{2,n+2}} e_{2,n+2}^{(i)} + \\ & {}_2\beta_1 \frac{\partial f_{1,n+1}}{\partial y_{3,n+1}} e_{3,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{1,n+2}}{\partial y_{3,n+2}} e_{3,n+2}^{(i)} \end{aligned} \tag{7}$$

In general, for a system of N equations the iteration formula when all equations are integrated by Adams is given below. Let the non-convergence be occurred at j^{th} equation, then the iteration formula is,

$$\begin{aligned} e_{j,n+2}^{(i+1)} = {}& {}_2\beta_1 \frac{\partial f_{j,n+1}}{\partial y_{1,n+1}} e_{1,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{j,n+2}}{\partial y_{1,n+2}} e_{1,n+2}^{(i)} + {}_2\beta_1 \frac{\partial f_{j,n+1}}{\partial y_{2,n+1}} e_{2,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{j,n+2}}{\partial y_{2,n+2}} e_{2,n+2}^{(i)} + \\ & + \ldots + {}_2\beta_1 \frac{\partial f_{j,n+1}}{\partial y_{N,n+1}} e_{N,n+1}^{(i)} + {}_2\beta_2 \frac{\partial f_{j,n+2}}{\partial y_{N,n+2}} e_{N,n+2}^{(i)} \end{aligned} \tag{8}$$

For a mixed-mode system, let equations 2 and 3 are treated as stiff, and equation 1 is in the nonstiff subsystem. Suppose fail step happened by equation 2. Then from (3) the iterative formulae by equation 2 is,

$${}_2\gamma_1 y_{2,n+1}^{(i+1)} + {}_2\gamma_2 y_{2,n+2}^{(i+1)} = \theta_2 f_{2,n+2}(y_{1,n+2}^{(i+1)}, y_{2,n+2}^{(i+1)}, y_{3,n+2}^{(i+1)}) + \psi \tag{9}$$

where ${}_2\gamma_1$, ${}_2\gamma_2$ and θ_2 are the coefficients for y_{n+1}, y_{n+2} and f_{n+2} respectively, ψ is the backvalues.

Let $y_{2,n+2}^{(i+1)} = y_{2,n+2}^{(i)} + {}^{(i+1)}e_{2,n+2}$ and expanding using Taylor's yield the following,

$${}_2\gamma_1 y_{2,n+1}^{(i)} + {}_2\gamma_1 {}^{(i+1)}e_{2,n+1} + {}_2\gamma_2 y_{2,n+2}^{(i)} + {}_2\gamma_2 {}^{(i+1)}e_{2,n+2} = \theta_2 f_{2,n+2}(y_{1,n+2}^{(i+1)}, y_{2,n+2}^{(i)}, y_{3,n+2}^{(i+1)}) + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}} {}^{(i+1)}e_{2,n+2}$$

Expanding at $y^{i} = y^{i-1} + {}^{i}e$ produce the following

$$\begin{aligned} & {}_2\gamma_1 y_{2,n+1}^{(i-1)} + {}_2\gamma_1 {}^{(i)}e_{2,n+1} + {}_2\gamma_1 {}^{(i+1)}e_{2,n+1} + {}_2\gamma_2 y_{2,n+2}^{(i-1)} + {}_2\gamma_2 {}^{(i)}e_{2,n+2} + \gamma_2 {}^{(i+1)}e_{2,n+2} = \\ & \theta_2 f_{2,n+2}(y_{1,n+2}^{(i)}, y_{2,n+2}^{(i-1)}, y_{3,n+2}^{(i)}) + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{1,n+2}} {}^{(i+1)}e_{1,n+2} + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}} {}^{(i)}e_{2,n+2} + \end{aligned}$$

$$\theta_2 \frac{\partial f_{2,n+2}}{\partial y_{3,n+2}}^{(i+1)} e_{3,n+2} + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}}^{(i+1)} e_{2,n+2} \tag{10}$$

$$\Rightarrow {}_2\gamma_1{}^{(i+1)} e_{2,n+1} + {}_2\gamma_2{}^{(i+1)} e_{2,n+2} = \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{1,n+2}}^{(i+1)} e_{1,n+2} + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}}^{(i+1)} e_{2,n+2} + \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{3,n+2}}^{(i+1)} e_{3,n+2}$$

Stiff equations are then put on the left hand side of the equation we get,

$$\Rightarrow {}_2\gamma_1{}^{(i+1)} e_{2,n+1} + ({}_2\gamma_2 - \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}})^{(i+1)} e_{2,n+2} - \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{3,n+2}}^{(i+1)} e_{3,n+2} = \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{1,n+2}}^{(i+1)} e_{1,n+2}$$

Generally, the iterative formula for a system of N equations with equation 1 nonstiff subsystem and all other equations are stiff can be written as,

$${}_2\gamma_1{}^{(i+1)} e_{2,n+1} + ({}_2\gamma_2 - \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{2,n+2}})^{(i+1)} e_{2,n+2} - \theta_2 \sum_{t=3}^{N} \frac{\partial f_{2,n+2}}{\partial y_{t,n+2}}^{(i+1)} e_{t,n+2} = \theta_2 \frac{\partial f_{2,n+2}}{\partial y_{1,n+2}}^{(i+1)} e_{1,n+2} \tag{11}$$

If the equations in this system are interrelated, then it is said the equations are coupled.

IV. Problems Tested

In this section, some of the test problems were given.

PROBLEM 1:
Source **: Gear (1971)**

$$y_1' = -1002\ y_1 + 1000\ y_2^2; \qquad y_1(0) = 1, \qquad 0 \le x \le 20$$
$$y_2' = y_1 - y_2(1 + y_2); \qquad y_2(0) = 1,$$

Solution:

$$y_1(x) = e^{-2x}$$
$$y_2(x) = e^{-x}$$

PROBLEM 2:

Source: **Hairer and Warner (1991)**

$$y_1' = -10\,y_1 + 100\,y_2 \qquad y_1(0) = 0.0, \qquad 0 \le x \le 20$$
$$y_2' = -100\,y_1 - 10\,y_2 \qquad y_2(0) = 1.0,$$
$$y_3' = -4\,y_3 \qquad y_3(0) = 1.0,$$
$$y_4' = -y_4 \qquad y_4(0) = 1.0,$$
$$y_5' = -0.5\,y_5 \qquad y_5(0) = 1.0,$$
$$y_6' = -0.1\,y_6 \qquad y_6(0) = 1.0,$$

Solution:

$$y_1(x) = e^{-10x} \sin(100x)$$
$$y_2(x) = e^{-10x} \cos(100x)$$
$$y_3(x) = e^{-4x}$$
$$y_4(x) = e^{-x}$$
$$y_5(x) = e^{-0.5x}$$
$$y_6(x) = e^{-0.1x}$$

The notations used in the tables take the following meaning:

Tol	:	Tolerance limit
MTD	:	Method employed
Step	:	Total steps taken
Max Error	:	Magnitude of the maximum error of the computed solution
Time	:	The execution time taken in microseconds
PBI	:	Implementation of Partitioning Block Intervalwise
PBC	:	Implementation of Partitioning Block Componentwise
Stiff Eqn $[i; x; k]$	:	The i^{th} equation become stiff when x at k^{th} step

The numerical results are tabulated in Table I and II.

TABLE I
NUMERICAL RESULT FOR PROBLEM 1

TOL	MTD	Step	Stiff Eqn $[i; x; k]$	Max Error	Time
10^{-2}	PBC	32	[1; 0.022804; 5] [2; 0.017147; 6]	7.5033e-02	0.000713
	PBI	26	[1 ; 0.022804; 5]	1.1793e-03	0.000779
10^{-4}	PBC	51	[1; 0.013594; 8] [2; 0.020382;12]	3.1107e-05	0.000877
	PBI	45	[1; 0.013594; 8]	2.8144e-05	0.000956
10^{-6}	PBC	100	[1; 0.010863;11] [2; 0.009053;12]	2.5109e-06	0.001457
	PBI	100	[1; 0.010863;11]	5.4695e-06	0.001461

TABLE II
NUMERICAL RESULT FOR PROBLEM 2

TOL	MTD	Step	Stiff Eqn $[i; x; k]$	Max Error	Time
10^{-2}	PBC	108	[1; 0.00483; 7] [2; 0.00483; 7] [3; 3.84322; 78] [4; 8.34883; 98]	1.3727e-02	0.004671
	PBI	103	[1; 0.00483; 7]	3.1328e-02	0.006591
	PBC	271	[1; 0.00160; 9] [2; 0.00160; 9] [4; 5.11616; 256] [3; 8.22912; 260]	1.6503e-04	0.010762

10^{-4}	PBI	261	[1; 0.00160; 9]	4.2225e-04	0.013554
10^{-6}	PBC	667	[1; 0.00282; 15] [2; 0.00282; 15] [4; 5.60077; 637] [3; 9.72954; 648]	8.2063e-06	0.026507
	PBI	660	[1; 0.00282; 15]	1.0171e-06	0.029394

V. Conclusion

The results generally show that in all cases, although despite componentwise partitioning (PBC) needs more number of steps but its execution times are better compared to PBI and NPBDF. This is because the Jacobian matrix is smaller and hence requires less number of matrix operations in order to evaluate the Jacobian matrix.

As an illustration, consider the numerical results of Problem 1 for TOL=10^{-2}. When the first instability occurs at $x = 0.022804$ on the 5^{th} step, only the first equation in the system is treated as stiff and the second equation remains in the non-stiff subsystem and solved using PBC mode. Then the second equation is treated as stiff on the 6^{th} step when $x = 0.017147$. Compare this when both equations are treated as stiff on the 5^{th} step at $x = 0.02280$ and solved using the PBI mode. We also tabulated the results when both equations are treated as stiff and solved using BDF at the beginning of the integration, i.e using NPBDF.

In test Problem 3 for TOL=10^{-2} by using PBC on the 7^{th} step at $x = 0.00483$, the first and second equations are changed to stiff subsystem. Then on the 78^{th} step, the third equation is placed in the stiff subsystem and the fourth equation at the 98^{th} step. Equations five and six remain as nonstiff until end of the integration. While using PBI all equations are placed in stiff subsystem at the first instability occurs that is on the 7^{th} step. But PBC mode has the best execution time compared to PBI. The same situation happens to other problems for all tolerances.

In conclusion, we have demonstrated that it is favourable to partitioning stiff system into non-stiff and stiff subsystem rather to treat the system as a stiff system to all equations.

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