

Arithmetic-mean Runge-Kutta Method and Method of Lines for Solving Mildly Stiff Differential Equations

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ABSTRACT

In this paper, method of lines (MOLs) with five-point central finite-difference coupled with a new third-order arithmetic-mean Runge-Kutta method is used to solve a parabolic partial differential equation. Semidiscretization of the parabolic equation using MOLs, results in a mildly stiff system of first order ordinary differential equation. The new arithmetic-mean Runge-Kutta method is then used to solve the system. Numerical comparison with the forward difference method and the MOLs-classical RK4 suggest that the present approach is more accurate.

Keywords: Arithmetic-mean Runge-Kutta, method of lines, finite difference, mildly stiff equations, forward difference

INTRODUCTION

The method of lines (MOLs) is a general technique commonly used in the process of solving partial differential equations by typically using finite difference relationships for the spatial derivatives and ordinary differential equations for the time derivative. This method is a powerful procedure in the process of discretizing the partial differential equations. It is an approximation philosophy rather than a specific method (Madsen (1975)). The modus operandi of this method is to semidiscretize all except one of the independent variables. When there are two independent variables, one is discretized while the other is left continuous. Some numerical analysts describe this method of lines as a process for semidiscretization of the partial differential equations. This process converts the partial differential equations to a system of first-order ordinary differential equations.

Traditionally, this method has been used for parabolic PDEs. The spatial derivatives are usually replaced by three-point finite differences, which include the forward, backward and central differences. Once the PDEs problem had been approximated by simpler ODEs, then any suitable numerical methods, which deal with stiff problems, can be used to achieve an approximate solution. In this study, the (stage) arithmetic-mean Runge-Kutta method is utilized in the attempt to solve a mildly stiff problem explicitly. This new method was incorporated with the five-point MOLs to work out the problem in PDEs. For linear parabolic PDEs, semidiscretization leads to a system of linear first-order ODEs in time.

Consider the PDE

$$U_t = \alpha^2 U_{xx} ; \quad 0 < x < b$$

with

$$\begin{aligned} U(0,t) &= d_0(t) \\ U(b,t) &= d_1(t); \quad 0 \leq t \leq a \\ U(x,0) &= f(x), \quad 0 \leq x \leq b. \end{aligned} \tag{1}$$

For the five-point method of lines, a mesh on $0 < x < 1$ is introduced. For an integer $m > 0$, $h = \frac{1}{m}$ and $x_j = jh$, $j = 0, 1, 2, \dots, m$. is defined.

This is a method, which compute the approximate solution of $U(x,t)$ at the node points x_1, x_2, \dots, x_{m-1} . The domain of the function $U(x,t)$, namely

$$\{(x,t) | 0 < x < 1, t > 0\},$$

shows that the estimates of $U(x,t)$ are computed along the lines $\{(x_j,t) | t > 0\}$, $j = 1, 2, \dots, m-1$.

The Taylor series expansions is used to derive the central-finite difference for the function U_{xx} , producing

$$U(x+h) = U(x) + hU'(x) + \frac{h^2}{2!}U''(x) + \frac{h^3}{3!}U'''(x) + \frac{h^4}{4!}U^{(iv)}(x) + \dots \tag{2}$$

and

$$U(x-h) = U(x) - hU'(x) + \frac{h^2}{2!}U''(x) - \frac{h^3}{3!}U'''(x) + \frac{h^4}{4!}U^{(iv)}(x) + \dots \tag{3}$$

Manipulating the equations (2) and (3), we obtained the numerical differentiation formula,

$$U''(x) = \frac{-U(x+2h) + 16U(x+h) - 30U(x) + 16U(x-h) - U(x-2h)}{12h^2} + O(h^4) \tag{4}$$

Therefore,

$$U_{xx}(x_j,t) = c^2 \frac{-U(x_{j+2},t) + 16U(x_{j+1},t) - 30U(x_j,t) + 16U(x_{j-1},t) - U(x_{j-2},t)}{h^2} + O(h^4) \tag{5}$$

for $j = 1, 2, \dots, m-1$.

Substituting the above formula into the parabolic differential equations,

$$U_t = c^2 U_{xx}, \quad 0 < x < b, \quad (6)$$

yields

$$U_t(x_j, t) = c^2 \frac{-U(x_{j+2}, t) + 16U(x_{j+1}, t) - 30U(x_j, t) + 16U(x_{j-1}, t) - U(x_{j-2}, t)}{h^2} + O(h^4).$$

Letting $u_j(t)$ be the approximation for $U(x_j, t)$ for $j = 0, 1, \dots, m$, the five-point central finite difference used can be formulated as (Chapra and Canale, 1998)

$$u'_j(t) = c^2 \frac{-u_{j+2}(t) + 16u_{j+1}(t) - 30u_j(t) + 16u_{j-1}(t) - u_{j-2}(t)}{12h^2} \quad (7)$$

with the boundary and initial conditions

$u_0(t) = d_0(t)$, $u_m(t) = d_1(t)$ and $u_j(0) = f(x_j)$, for $j = 1, 2, \dots, m-1$ respectively.

The exact solution for this particular problem can be solved using the separable method subject to the transformation of the boundary and initial values to a standard problem. In order to attain the standard case. Let

$$\begin{aligned} U(x, t) &= \text{Steady state} + \text{transient condition} \\ &= d_0(t) + \frac{x}{b} (d_1(t) - d_0(t)) + \hat{U}(x, t) \end{aligned}$$

$\hat{U}(x, t)$ is substituted in (7) and the standard PDEs below is attained.

$$\hat{U}_t = \alpha^2 \hat{U}_{xx}$$

with

$$\begin{aligned} \hat{U}(0, t) &= 0^0 C, \\ \hat{U}(b, t) &= 0^0 C; \quad 0 < t < a \\ \hat{U}(x, 0) &= f(x) - [d_0(t) + \frac{x}{b} (d_1(t) - d_0(t))] \\ &= f(x) - \frac{x}{b} d_1(t) + d_0(t) (\frac{x}{b} - 1); \quad 0 < x < b \end{aligned}$$

Using the separable method, the exact solution for the above problem is given by (Kreyszig, 1999)

$$\hat{U}(x, t) = \sum_{n=1}^{\infty} a_n e^{-(n\pi\alpha)^2 t} \sin(\frac{n\pi x}{b})$$

with

$$a_n = \frac{2}{b} \int_0^b \left(f(x) - [d_0(t) + \frac{\xi}{b} (d_1(t) - d_0(t))] \right) \sin\left(\frac{n\pi\xi}{b}\right) d\xi$$

Therefore, the exact solution for the existing problem can be written as

$$U(x,t) = d_0(t) + \frac{x}{b} (d_1(t) - d_0(t)) + \frac{2}{b} \sum_{n=1}^{\infty} \left(\int_0^b \left(f(x) - [d_0(t) + \frac{\xi}{b} (d_1(t) - d_0(t))] \right) \sin\left(\frac{n\pi\xi}{b}\right) d\xi \right) e^{-(n\pi\alpha)^2 t} \sin\left(\frac{n\pi x}{b}\right).$$

METHOD OF LINES

This technique is used to convert the partial differential equations to a system of first order ordinary differential equations. When there are two independent variables, one is discretized while the other is left continuous.

In this paper, the five-point central finite difference is used in order to semidiscretize the PDEs. The five-point central finite differences (Chapra and Canale, 1998) used in this method of lines to solve a parabolic PDE can be formulated as

$$u'_j(t) = \frac{-u_{j+2}(t) + 16u_{j+1}(t) - 30u_j(t) + 16u_{j-1}(t) - u_{j-2}(t)}{12h^2} \tag{2}$$

Applying the formula (2) on a parabolic PDE problem with the details as given:

$$U_t = \alpha^2 U_{xx} ; \quad 0 < x < 1$$

with

$$\begin{aligned} U(0,t) &= 50^0 C, \\ U(1,t) &= 20^0 C; \quad 0 < t < 0.3 \\ U(x,0) &= 70^0 C; \quad 0 \leq x \leq 1 \end{aligned}$$

and $\alpha^2 = 0.1$, $\Delta x = 0.2$. (Rao, 2002), we arrived at a system of ODEs, which could be written as

$$\begin{aligned}\frac{du_1}{dt} &= \frac{5}{24}(-u_{-1} + 16u_0 - 30u_1 + 16u_2 - u_3) \\ \frac{du_2}{dt} &= \frac{5}{24}(-u_0 + 16u_1 - 30u_2 + 16u_3 - u_4) \\ \frac{du_3}{dt} &= \frac{5}{24}(-u_1 + 16u_2 - 30u_3 + 16u_4 - u_5) \\ \frac{du_4}{dt} &= \frac{5}{24}(-u_2 + 16u_3 - 30u_4 + 16u_5 - u_6)\end{aligned}$$

with $u_0 = 50^0$ C and $u_5 = 20^0$ C. In dealing with the five-point central difference approximations to the second derivative, Fisher, as reported by Hicks and Wei (1967), proposed that, at the endpoints, the three-point central difference approximation also be assumed valid. This assumption leads to the requirement that $u_{n+1} = -u_{n-1}$. Therefore, we have $u_{-1} = -u_1$ and $u_6 = -u_4$.

The first order ODEs system above can be represented in the matrix form

$$\begin{pmatrix} \frac{du_1}{dt} \\ \frac{du_2}{dt} \\ \frac{du_3}{dt} \\ \frac{du_4}{dt} \end{pmatrix} = \begin{pmatrix} -29 & 16 & -1 & 0 \\ 16 & -30 & 16 & -1 \\ -1 & 16 & -30 & 16 \\ 0 & -1 & 16 & -29 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$

The eigenvalues for the above matrix are

$$\lambda_1 = \frac{1}{2}(-75 - 17\sqrt{5}), \lambda_2 = \frac{1}{2}(-43 - 15\sqrt{5}), \lambda_3 = \frac{1}{2}(-43 + 15\sqrt{5}), \lambda_4 = \frac{1}{2}(-75 + 17\sqrt{5})$$

The negative eigenvalues above shows that a mildly stiff system of ODEs is formed.

RUNGE-KUTTA METHODS

Arithmetic-Mean Runge-Kutta Method

According to Wazwaz (1994), the standard third-order arithmetic-mean Runge-Kutta formula for solving IVPs of the form $y' = f(x, y)$ may be written in the form

$$y_{n+1} = y_n + \frac{h}{2} \left(\frac{k_1 + k_2}{2} + \frac{k_2 + k_3}{2} \right)$$

where

$$\begin{aligned} k_1 &= f(x_n, y_n) = f \\ k_2 &= f(x_n + a_1 h, y_n + a_1 h k_1) \\ k_3 &= f(x_n + (a_2 + a_3)h, y_n + h a_2 k_1 + h a_3 k_2). \end{aligned}$$

Third-order accuracy was obtained through an adjustment of parameters a_i , $1 \leq i \leq 3$ using a symbolic program and it was found that

$$a_1 = \frac{2}{3}, \quad a_2 = -\frac{1}{3}, \quad a_3 = 1.$$

A new third-order (stage) arithmetic-mean Runge-Kutta formula [4] is represented as

$$y_{n+1} = y_n + h \left[\frac{4+3\sqrt{2}}{4} k_1 + \frac{-3(4+3\sqrt{2})}{4} k_2 + \frac{3(2+\sqrt{2})}{2} k_3 \right]$$

where ,

$$\begin{aligned} k_1 &= f(x_n, y_n) \\ k_2 &= f\left(x_n + \frac{2-\sqrt{2}}{3} h, y_n + \frac{2-\sqrt{2}}{3} h k_1\right) \\ k_3 &= f\left(x_n + \frac{1}{3} h, y_n + \frac{1}{3} \left(\frac{k_1 + k_2}{2}\right) h\right). \end{aligned}$$

Classical Fourth-Order Runge-Kutta Method

The explicit fourth-order classical Runge-Kutta formula for solving initial value problems (IVPs) of the form $y' = f(x, y)$ may be written in the form

$$y_{n+1} = y_n + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4)$$

where

$$\begin{aligned} k_1 &= f(x_n, y_n) \\ k_2 &= f\left(x_n + \frac{1}{2} h, y_n + \frac{1}{2} h k_1\right) \\ k_3 &= f\left(x_n + \frac{1}{2} h, y_n + \frac{1}{2} h k_2\right) \\ k_4 &= f(x_n + h, y_n + h k_3). \end{aligned}$$

The RK4 method is integrated within the MOLs to solve the same problem and the results obtained are compared with numerical results attained using the MOLs- arithmetic-mean Runge-Kutta method.

NUMERICAL RESULTS

Using the third-order (stage) arithmetic-mean Runge-Kutta method, which we derived to solve the system above, we attained the results below:

Table 1. The solution for the five-point MOLs & stage-arithmetic mean Runge-Kutta method on the parabolic PDEs compared to the forward difference and five-point MOLs & classical Runge-Kutta (RK4) methods.

	Exact value	Relative errors		
		Forward Difference	Five-point MOLs- RungeKutta4	Five-point MOLs + Arithmetic-mean RKutta
X = 0.2				
t = 0.06	68.6422168761	2.39242984E-02	1.30653818E-02	7.603114E-03
t = 0.12	66.0658758630	1.76471718E-02	4.62244523E-04	1.113871E-02
t = 0.18	64.1619477795	1.24598427E-02	8.19717789E-03	2.600995E-02
t = 0.24	62.7607571081	9.46960546E-03	1.30761833E-02	3.670719E-02
t = 0.30	61.6611828442	7.90461392E-03	1.58032532E-02	4.462937E-02
X = 0.4				
t = 0.06	69.9947833016	7.45298171E-05	2.05179732E-03	1.129110E-03
t = 0.12	69.7981589510	3.55537961E-03	6.52298036E-03	3.858036E-04
t = 0.18	69.2214302667	6.79240901E-03	9.26422380E-03	1.104470E-03
t = 0.24	68.3337219450	9.05258674E-03	1.00828410E-02	3.372797E-03
t = 0.30	67.2352979293	1.04377994E-02	9.46693608E-03	6.791055E-03
X = 0.6				
t = 0.06	69.9869625901	1.86283408E-04	9.37322322E-03	8.680889E-04
t = 0.12	69.5066860511	9.08813363E-03	2.01658899E-02	8.819577E-03
t = 0.18	68.2179429039	1.44455089E-02	2.40058489E-02	1.167386E-02
t = 0.24	66.4821442738	1.64821590E-02	2.35286335E-02	1.053576E-02
t = 0.30	64.5903609103	1.69102966E-02	2.12656275E-02	7.366128E-03
X = 0.8				
t = 0.06	66.6055422721	6.16396494E-02	4.84800276E-02	5.325217E-02
t = 0.12	60.1647150419	4.84455887E-02	3.02765156E-02	3.372380E-02
t = 0.18	55.4074762158	3.61183427E-02	1.74510979E-02	1.630033E-02
t = 0.24	51.9292648451	2.81154538E-02	1.11194810E-02	3.958998E-03
t = 0.30	49.2673936515	2.29555963E-02	8.33446503E-03	5.140912E-03

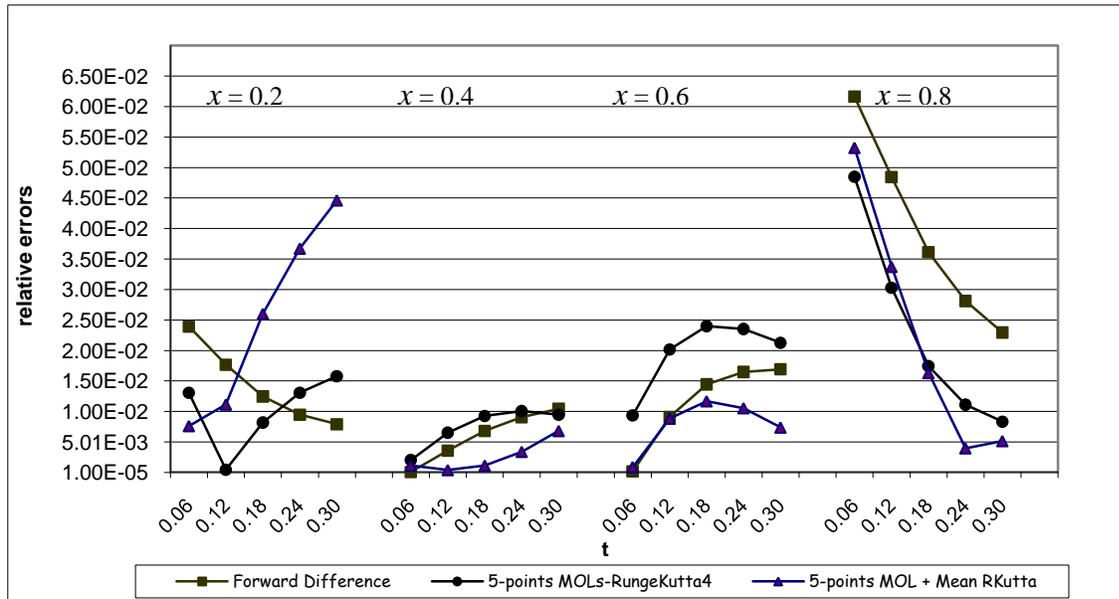


Figure 1: The graphs of relative errors for the five-point MOLs + stage-arithmetic mean Runge-Kutta, forward difference and five-point MOLs + RK4 methods at each point of x .

DISCUSSION & CONCLUSION

The result obtained using the combination of the five-point MOLs and (stage) arithmetic-mean Runge-Kutta method is presented in the table above. In order to compare the relative errors, the results for the forward difference and the coupling of MOLs with the classical Runge-Kutta methods are exhibited. We also plotted the graphs of the relative errors for the three methods at each point, x . We find that the combination of the five-point MOLs and (stage) arithmetic-mean Runge-Kutta method lose a few points at the point $x = 0.2$ but gain back the accuracy at the other points. We had a strong feeling that the assumption for the endpoints of the five-point MOLs given by Fisher as reported by Hicks, which we had benefited in this method, can still be improved in order to gain better accuracy.

We conclude that as a whole, this new creation of blending the five-point MOLs and the (stage) arithmetic-mean Runge-Kutta method works well compared with the other two methods.

REFERENCES

- Ahmad, R. R. & Yaacob, N. (2005), Third-order composite Runge-Kutta method for stiff problems. *Intern. J. Computer Math.* **82(10)**: 1221 – 1226.
- Chapra, S.C & Canale R, P. (1998), *Numerical Methods for Engineers*. McGraw Hill.
- Hicks, J.S and Wei, J. (1967), Numerical Solution of Parabolic Partial Differential Equations With Two-Points Boundary Conditions by Use of Method of Lines. *Journal of the Association for Computing Machinery.* **14(3)**:549 – 562.
- Kreyszig, E. (1999), *Advanced Engineering Mathematics*. John Wiley & Sons. 8th Ed
- Madsen, N.K. (1975), The Methods of Lines for the Numerical Solution of Partial Differential Equations. In Proceeding of the SIGNUM meeting on Software of PDE, 5 - 7. Moffitt Field, California, USA
- Rao, S.S. (2002), *Applied Numerical Methods for Engineers & Scientists*. Prentice Hall.
- Wazwaz, A. (1994), A comparison of Modified Runge-Kutta Formulas Based On A Variety of Means. *Intern. J. Computer Math.* **50**: 105 – 112.