8th GRACM International Congress on Computational Mechanics
Volos, 12 July – 15 July 2015

A NEW DIRECT TIME INTEGRATION METHOD FOR THE SEMI-DISCRETE PARABOLIC EQUATION

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Keywords: Semi-Discrete Parabolic Equations, Analog Equation Method, Differential Equations, Numerical Solution.

Abstract. *A direct time integration method is presented for the solution of systems of first order ordinary differential equations, which represent semi-discrete diffusion equations. The proposed method is based on the principle of the analog equation, which converts the N coupled equations into a set of N single term uncoupled first order ordinary differential equations under fictitious source. The solution is obtained from the integral representation of the solution of the substitute single term equations. The stability and convergence of the numerical scheme is proved. The method is simple to implement. It is self starting, unconditionally stable and accurate. It performs well when long time durations are considered as it conserves energy and it can be used as a practical method for integration of the parabolic equations in cases where widely used methods may fail. The method applies to equations of variable coefficients as well as to nonlinear ones. Numerical examples, including linear as well as non linear systems, are treated by the proposed method and its efficiency and accuracy are demonstrated.*

1 INTRODUCTION

The initial value problem for the semidiscrete diffusion equation is stated as

$$\mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{p}(t)\,, \qquad t \in [0,T],\ T > 0 \tag{1}$$

$$\mathbf{u}(0) = \mathbf{u}_0 \tag{2}$$

where $\mathbf{u}(t)$ represents the vector of the unknown functions, $\mathbf{p}(t)$ the external source vector, and $\mathbf{u}_0$ a given vector.

Equation (1) represents the semi-discrete parabolic equations, that is, parabolic equations of which the space variables have been discretized and the time variable is left continuous. The matrices $\mathbf{C}$ and $\mathbf{K}$ may be symmetric or not, depending on the method used for the spatial discretization.

The most well known and commonly used methods for solving Eq. (1) are members of the generalized trapezoidal family or $\alpha-$family of methods, in which the time derivative is approximated by a weighted average of the field function at two consecutive time steps. Some well known members are identified from the value of the parameter α. Thus we have, the forward differences or forward Euler ($\alpha = 0$), The trapezoidal rule or Crank-Nicolson ($\alpha = 1/2$), and backward difference or backward Euler ($\alpha = 1$). The $\alpha-$family of approximations is unconditionally stable for $\alpha \geq 1/2$, while for $\alpha < 1/2$ the methods are stable if a condition $\Delta t < \Delta t_{cr} \equiv 2/(1-2a)\lambda_{\max}$ where $\lambda_{\max}$ is the largest eigenvalue of the matrix $\mathbf{C}^{-1}\mathbf{K}$ is satisfied with $\mathbf{C},\mathbf{K}$ being symmetric and positive definite [1].

In this paper a new direct time integration method is presented for the numerical solution of the initial value problem (1), (2). The proposed method is based on the principle of the analog equation [2], which converts the N coupled equations into a set of N single term uncoupled first order ordinary differential equations under fictitious sources, unknown in the first instance. The fictitious sources are established from the integral representation of the solution of the substitute single term equations. The stability is proved and the convergence is shown through well corroborated numerical results. The method is simple to implement. It is self starting, unconditionally stable and accurate. The stability does not demand symmetric and positive definite coefficient matrices $\mathbf{C},\mathbf{K}$ as the widely used methods, but can solve equations with non symmetric matrices provided that the matrix $\mathbf{C}^{-1}\mathbf{K}$ has positive eigenvalues. This is an important advantage, since the scheme can solve semi-discrete diffusion equations resulting from methods that do not produce symmetric matrices, e.g. the boundary element method. It performs well when long time durations are considered as it conserves energy and, thus, it can be used as a practical method for integration of the parabolic equations in cases where widely used methods do not apply or may fail. It applies also to the case of time dependent coefficient matrices, i.e., $\mathbf{C}(t), \mathbf{K}(t)$, as well as for nonlinear equations. The method is illustrated by solving several equations, including linear as well as non linear systems. The obtained results are in excellent agreement with those obtained from exact solutions.

2 THE LINEAR SYSTEM

2.1 The AEM solution

We illustrate the method with the linear one-degree-of-freedom system

$$c\dot{u} + ku = p(t) \tag{3}$$

$$u(0) = u_0 \tag{4}$$

Let $u = u(t)$ be the sought solution. Then, if the operator d/dt is applied to it, yields

$$\dot{u} = q(t) \tag{5}$$

where $q(t)$ is a fictitious source, unknown in the first instance. Eq. (5) is the analog equation of (3) [3]. It indicates that the solution of Eq. (3) can be obtained by solving Eq. (5) with the initial condition (4), if $q(t)$ is first established. This is implemented as following.

Taking the Laplace transform of Eq. (5) we obtain

$$sU(s) - u(0) = Q(s)$$

or

$$U(s) = \frac{1}{s}u(0) + \frac{1}{s}Q(s)$$

where $U(s), Q(s)$ are the Laplace transforms of $u(t), q(t)$. The inverse Laplace transform of the above expression yields the solution of Eq. (5) in integral form

$$u(t) = u(0) + \int_0^t q(\tau)d\tau \tag{6}$$

Thus the initial value problem of Eqs (3), (4) is transformed into the equivalent Volterra integral equation for $q(t)$.

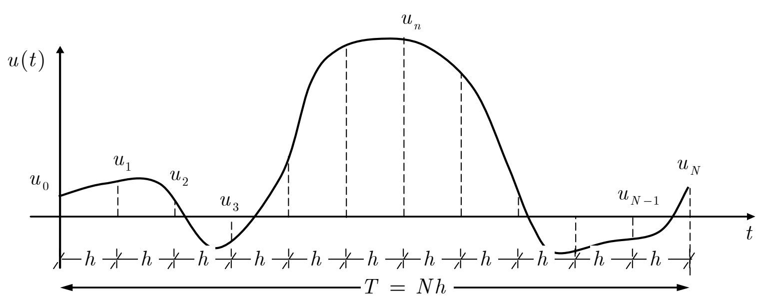

Figure 1. Discretization of the interval $[0, T]$ into N equal intervals $h = T/N$

Eq. (6) is solved numerically within a time interval $[0, T]$. Following a procedure analogous to that presented

in [3], the interval $[0,T]$ is divided into N equal intervals $\Delta t = h$, $h = T / N$, in which $q(t)$ is assumed to vary according to a certain law, e.g. constant, linear etc.
Hence, Eq. (6) at instant $t = nh$ can be written as

$$\begin{aligned} u_n &= u_0 + \int_0^h q(\tau)d\tau + \int_h^{2h} q(\tau)d\tau + \cdots + \int_{(n-1)h}^{nh} q(\tau)d\tau \\ &= u_0 + \sum_{r=1}^{n} \int_{(r-1)h}^{rh} q(\tau)d\tau \\ &= u_0 + \sum_{r=1}^{n-1} \int_{(r-1)h}^{rh} q(\tau)d\tau + \int_{(n-1)h}^{nh} q(\tau)d\tau \\ &= u_{n-1} + \int_{(n-1)h}^{nh} q(\tau)d\tau \end{aligned} \tag{7}$$

2.2 Solution procedure for constant fictitious source $q(t)$

Without excluding higher order variation laws for $q(t)$, we assume that it is constant within the integration interval $[(r-1)h,(r-1)h]$ and equal to the mean value

$$q_r^m = \frac{q_{r-1} + q_r}{2} \tag{8}$$

Substituting Eq. (8) into Eq. (7) gives

$$u_n = u_{n-1} + \frac{h}{2} q_{n-1} + \frac{h}{2} q_n \tag{9}$$

Moreover, Eq. (3) at time $t = nh$ is written as

$$cq_n + ku_n = p_n \tag{10}$$

Eqs (9) and (10) can be combined as

$$\begin{bmatrix} c & k \\ -\dfrac{h}{2} & 1 \end{bmatrix} \begin{Bmatrix} q_n \\ u_n \end{Bmatrix} = \begin{bmatrix} 0 & 0 \\ \dfrac{h}{2} & 1 \end{bmatrix} \begin{Bmatrix} q_{n-1} \\ u_{n-1} \end{Bmatrix} + p_n \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \tag{11}$$

The coefficient matrix in Eq. (11) is not singular for sufficient small h and the system can be solved successively for $n = 1,2,\ldots$ to yield the solution u_n and the derivative, $\dot{u}_n = q_n$ at instant $t = nh \leq T$. For $n = 1$, the value q_0 appears in the right hand side of Eq. (11). This quantity can be readily obtained from Eq. (3) for $t = 0$. This yields

$$q_0 = \left(p_0 - ku_0\right) / c \tag{12}$$

Equation (11) can be also written as

$$\mathbf{U}_n = \mathbf{A}\mathbf{U}_{n-1} + \mathbf{b}p_n, \qquad n = 1,2,\ldots N \tag{13}$$

in which

$$\mathbf{U}_n = \begin{Bmatrix} q_n \\ u_n \end{Bmatrix}, \qquad \mathbf{A} = \begin{bmatrix} c & k \\ -\dfrac{h}{2} & 1 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 0 \\ \dfrac{h}{2} & 1 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} c & k \\ -\dfrac{h}{2} & 1 \end{bmatrix}^{-1} \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \tag{14a,b,c}$$

For the multi-degree of freedom system, the analog equations corresponding to Eq. (5) is the set of the L uncoupled equations

$$\dot{\mathbf{u}} = \mathbf{q}(t) \tag{15}$$

where $\dot{\mathbf{u}}, \mathbf{q}(t)$ are $L \times 1$ vectors. Thus, the numerical scheme for the solution becomes

$$\mathbf{U}_n = \mathbf{A}\mathbf{U}_{n-1} + \mathbf{b}\mathbf{p}_n , \qquad n = 1,2,\ldots,N \tag{16}$$

where

$$\mathbf{U}_n = \begin{Bmatrix} \mathbf{q}_n \\ \mathbf{u}_n \end{Bmatrix}, \quad \mathbf{A} = \begin{bmatrix} \mathbf{C} & \mathbf{K} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix} \tag{17a,b}$$

$$\mathbf{b} = \begin{bmatrix} \mathbf{C} & \mathbf{K} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} \begin{Bmatrix} \mathbf{1} \\ \mathbf{0} \end{Bmatrix}, \qquad \mathbf{1} = \begin{Bmatrix} 1 & 1 & \cdots & 1 \end{Bmatrix}^T \tag{17c,d}$$

$$\mathbf{q}_0 = \mathbf{C}^{-1}\left(\mathbf{p}_0 - \mathbf{K}\mathbf{u}_0\right) \tag{18}$$

The solution algorithm is shown in Table 1. Moreover, Table 2 gives the Matlab program based on this algorithm with data employed for Example 2.

A. Data for $\mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{p}(t)$ Read: $\mathbf{C}$, $\mathbf{K}$, $\mathbf{u}_0$, $\mathbf{p}(t)$, T
B. Initial computations Choose : $h := \Delta t$ and compute $n_{\max}$ Compute : $\mathbf{q}_0 := \mathbf{C}^{-1}(\mathbf{p}_0 - \mathbf{K}\mathbf{u}_0)$ Formulate $\mathbf{U}_0 := \begin{Bmatrix} \dot{\mathbf{u}}_0 & \mathbf{u}_0 \end{Bmatrix}^T$ Compute : $\mathbf{A} := \begin{bmatrix} \mathbf{C} & \mathbf{K} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}$, b:= $\begin{bmatrix} \mathbf{C} & \mathbf{K} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{I} \\ \mathbf{0} \end{bmatrix}$
C. Compute solution for $n := 1$ to $n_{\max}$ $\mathbf{U}_n = \mathbf{A}\mathbf{U}_{n-1} + \mathbf{b}\mathbf{p}_n$ end

Table 1 Algorithm for the numerical solution of the semi-discretized linear parabolic equations

2.3 Stability of the numerical scheme

Applying Eq. (17) for $n = 1,2,\ldots$ yields

$$\begin{aligned}
\mathbf{U}_1 &= \mathbf{A}\mathbf{U}_o + \mathbf{b}p_1 \\
\mathbf{U}_2 &= \mathbf{A}\mathbf{U}_1 + \mathbf{b}p_2 \\
&= \mathbf{A}(\mathbf{A}\mathbf{U}_o + \mathbf{b}p_1) + \mathbf{b}p_2 \\
&= \mathbf{A}^2\mathbf{U}_o + \mathbf{A}\mathbf{b}p_1 + \mathbf{b}p_2 \\
\cdots &= \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\mathbf{U}_n &= \mathbf{A}^n\mathbf{U}_o + (\mathbf{A}^{n-1}p_1 + \mathbf{A}^{n-2}p_2 + \ldots \mathbf{A}^0 p_n)\mathbf{b}
\end{aligned} \tag{19}$$

We observe that the last of Eqs (19) gives the solution vector $\mathbf{U}_n$ at instant $t_n = nh$ using only the known vector $\mathbf{U}_0$ at $t = 0$. The matrix $\mathbf{A}$ and the vector $\mathbf{b}$ are computed only once.

```
%======================================================================
% Script file: parabolic_equation_mult_linear
% This Matlab program solves the system of N linear semi-discrete
% diffusion equations C*du/dt+K*u=p(t) using the method developed by
% Katsikadelis
%======================================================================
clear all
%======================================================================
%% Data
%======================================================================
N=2;                  % number of equations
T=10;                 % total time
h=0.1;                % time step
nmax=ceil(T/h);       % number of time instants
t_tot=h*nmax;
t=h:h:t_tot;
u0=[1; 0];            % Initial condition
C=[5 4; 4 5];         % Coefficient matrix  C
K=[25 20; 20 20];     % Coefficient matrix  K
% External source p(t)
p0=[28.5;  24.6];
p=[57/2*exp(-1/10*t).*cos(t)+73/5*exp(-1/10*t).*sin(t)
  123/5*exp(-1/10*t).*cos(t)+31/2*exp(-1/10*t).*sin(t)];
%======================================================================
%% Solution
%======================================================================
q0=inv(C)*(-K*u0+p0);
U0=[q0; u0];
D=[C    K
   -h/2*eye(N) eye(N)];
B=[zeros(N)  zeros(N)
    h/2*eye(N) eye(N)];
A=inv(D)*B;
b=inv(D)*[eye(N); zeros(N)];
U=zeros(2*N,nmax);
U(:,1)=A*U0+b*p(:,1);
for i=2:nmax
    U(:,i)=A*U(:,i-1)+b*p(:,i);
end
du=U(1:N,:);        % Derivative of the solution du/dt
u=U(N+1:2*N,:);   % Solution
%======================================================================
%% Plot solution
%======================================================================
%exact solution
uex=[exp(-0.1*t).*cos(t)
      exp(-0.1*t).*sin(t)];
figure(1);plot (t,u(:,:),'m.',t,u(:,:),'k');grid;
```

Table 2. Matlab program for the solution of the initial value problem (1), (2).

The matrix $\mathbf{A}$ is the amplification matrix. In order that the solution is stable, $\mathbf{A}^n$ must be bounded. This is true if the spectral radius $\rho(\mathbf{A})$ satisfies the condition

$$\rho(\mathbf{A}) = \max\left(\lambda_i\right) \leq 1 \tag{20}$$

where λ_i are the eigenvalues of $\mathbf{A}$. If $\rho(\mathbf{A}) < 1$ the method is strongly stable. Condition (20) is satisfied, if the eigenvalues of the matrix $\hat{\mathbf{K}} = \mathbf{C}^{-1}\mathbf{K}$ are positive.

PROOF.

For convenience of the proof we write Eq. (1) as

$$\dot{\mathbf{u}} + \hat{\mathbf{K}}\mathbf{u} = \mathbf{C}^{-1}\mathbf{p}(t), \qquad \hat{\mathbf{K}} = \mathbf{C}^{-1}\mathbf{K} \tag{21}$$

Using the formula for the inverse of a block matrix [4], we find

$$\begin{bmatrix} \mathbf{I} & \hat{\mathbf{K}} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} = \begin{bmatrix} \left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1} & -\left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1}\hat{\mathbf{K}} \\ \frac{h}{2}\left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1} & \left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1} \end{bmatrix} \tag{22}$$

hence

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} \mathbf{I} & \hat{\mathbf{K}} \\ -\frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \frac{h}{2}\mathbf{I} & \mathbf{I} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{h}{2}\left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1}\hat{\mathbf{K}} & -\left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1}\hat{\mathbf{K}} \\ \frac{h}{2}\left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1} & \left(\mathbf{I} + \frac{h}{2}\hat{\mathbf{K}}\right)^{-1} \end{bmatrix} \end{aligned} \tag{23}$$

Next we find the eigenvalues of $\mathbf{A}$. For this purpose we write the pertinent eigenvalue problem in the form

$$\begin{aligned} \left(\mathbf{A}_{11} - \lambda\mathbf{I}\right)\mathbf{x}_1 + \mathbf{A}_{12}\mathbf{x}_2 &= \mathbf{0} \\ \mathbf{A}_{21}\mathbf{x}_1 + (\mathbf{A}_{22} - \lambda\mathbf{I})\mathbf{x}_2 &= \mathbf{0} \end{aligned} \tag{24}$$

where $\mathbf{A}_{ij}$ are $L \times L$ matrices.

Equations (24) are solved using Gauss elimination. To avoid inversion of the singular matrix $\left(\mathbf{A}_{11} - \lambda\mathbf{I}\right)$, we reorder Eq (24) as

$$\begin{aligned} \mathbf{A}_{12}\mathbf{x}_2 + \left(\mathbf{A}_{11} - \lambda\mathbf{I}\right)\mathbf{x}_1 &= \mathbf{0} \\ (\mathbf{A}_{22} - \lambda\mathbf{I})\mathbf{x}_2 + \mathbf{A}_{21}\mathbf{x}_1 &= \mathbf{0} \end{aligned} \tag{25}$$

which after elimination of $\mathbf{x}_2$ give

$$\begin{bmatrix} \mathbf{A}_{12} & \mathbf{A}_{11} - \lambda\mathbf{I} \\ \mathbf{0} & -(\mathbf{A}_{22} - \lambda\mathbf{I})\mathbf{A}_{12}^{-1}\left(\mathbf{A}_{11} - \lambda\mathbf{I}\right) + \mathbf{A}_{21} \end{bmatrix} \begin{Bmatrix} \mathbf{x}_2 \\ \mathbf{x}_1 \end{Bmatrix} = \begin{Bmatrix} \mathbf{0} \\ \mathbf{0} \end{Bmatrix} \tag{26}$$

The characteristic equation of the matrix in Eq.(26) is

$$\Pi(\lambda) = \det\mathbf{A}_{12}\,\det\left[-(\mathbf{A}_{22} - \lambda\mathbf{I})\mathbf{A}_{12}^{-1}\left(\mathbf{A}_{11} - \lambda\mathbf{I}\right) + \mathbf{A}_{21}\right] = 0 \tag{27}$$

Taking into account that $\det \mathbf{A}_{12} = -\det\left[\left(\mathbf{I}+\frac{h}{2}\hat{\mathbf{K}}\right)^{-1}\hat{\mathbf{K}}\right] \neq 0$, we have

$$\begin{aligned}\Pi(\lambda) &= \det\left[-(\mathbf{A}_{22}-\lambda\mathbf{I})\mathbf{A}_{12}^{-1}\left(\mathbf{A}_{11}-\lambda\mathbf{I}\right)+\mathbf{A}_{21}\right]=0\\ &= \det\left(\mathbf{A}_{21}-\mathbf{A}_{22}\mathbf{A}_{12}^{-1}\mathbf{A}_{11}+\left(-\mathbf{A}_{12}^{-1}\mathbf{A}_{11}+\mathbf{A}_{22}\mathbf{A}_{12}^{-1}\right)\lambda-\mathbf{A}_{12}^{-1}\lambda^{2}\right)=0\end{aligned} \tag{28}$$

We can readily show that

$$\mathbf{A}_{21}-\mathbf{A}_{22}\mathbf{A}_{12}^{-1}\mathbf{A}_{11}=0 \tag{29}$$

Hence, Eq. (29) becomes

$$\left(\mathbf{A}_{12}^{-1}\mathbf{A}_{11}\mathbf{A}_{12}^{1}+\mathbf{A}_{22}-\lambda\mathbf{I}\right)\lambda=0 \tag{30}$$

From Eq. (30) we conclude that the $2L\times 2L$ matrix $\mathbf{A}$ has L zero eigenvalues, while the other L nonzero eigenvalues are the eigenvalues of the matrix

$$\begin{aligned}\bar{\mathbf{A}} &= \mathbf{A}_{12}^{-1}\mathbf{A}_{11}\mathbf{A}_{12}^{1}+\mathbf{A}_{22}\\ &= \left(\mathbf{I}+\frac{h}{2}\hat{\mathbf{K}}\right)^{-1}(\mathbf{I}-\frac{h}{2}\hat{\mathbf{K}})\end{aligned} \tag{31}$$

Using the spectral decomposition theorem, we can show the eigenvalues of $\bar{\mathbf{A}}$ are

$$\lambda_i=\left(1-\frac{h}{2}\hat{\lambda}_i\right)/\left(1+\frac{h}{2}\hat{\lambda}_i\right) \tag{32}$$

where $\hat{\lambda}_i$ are the eigenvalues of $\hat{\mathbf{K}}$. Therefore the stability condition (20) is satisfied if the eigenvalues of the matrix $\hat{\mathbf{K}}$ are positive. It can be shown that this condition ensures also stability if Eq. (8) is replaced by $q_r^m=\alpha q_{r-1}+\beta q_r$, $\alpha+\beta=1$. The value of α influences only the accuracy. For $a=1/2$ the scheme is second order accurate.

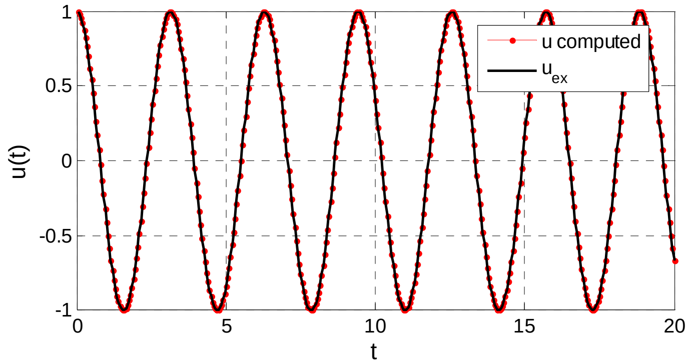

Figure 2. Solution computed and exact in Example 1.

2.5 Numerical examples

Example 1. One-degree of freedom system

Equation (1) has been solved with data: $c=5$, $k=50$, $p(t)=a(-c\omega\sin\omega t+k\cos\omega t)$, $u_0=a$, $a=1$, $\omega=2$. Eq. (1) admits an exact solution $u_{ex}=a\cos\omega t$. The results have been obtained using the Matlab program of Table 2. Fig. 2 shows the solution as compared with the exact solution for $h = 0.05$, while Fig. 3 shows the error $\max|u(t_i) - u_{ex}(t_i)|$ and the mean square error $\mathrm{MSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{i=n}[u(t_i) - u_{ex}(t_i)]^2}$, $0 < t_i \leq 100$ versus the time step h. Finaly, Fig. 4 shows the solution for long duration $(0 \leq t \leq 50000,\ h = 0.01)$. We observe that the scheme remains stable and the error within the same bounds.

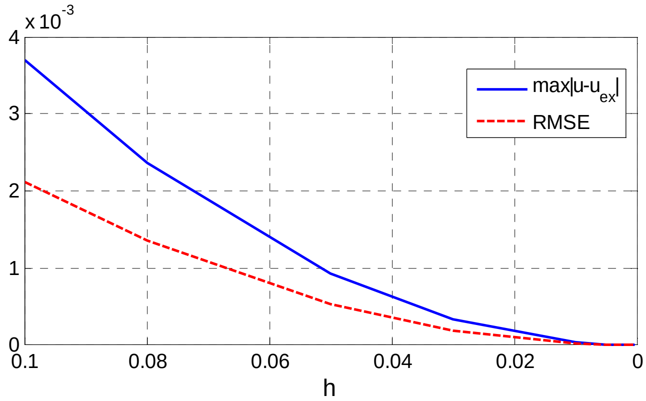

Figure 3. Error $\max|u(t_i) - u_{ex}(t_i)|$ and MSE ($0 < t_i \leq 100$) in Example 1.

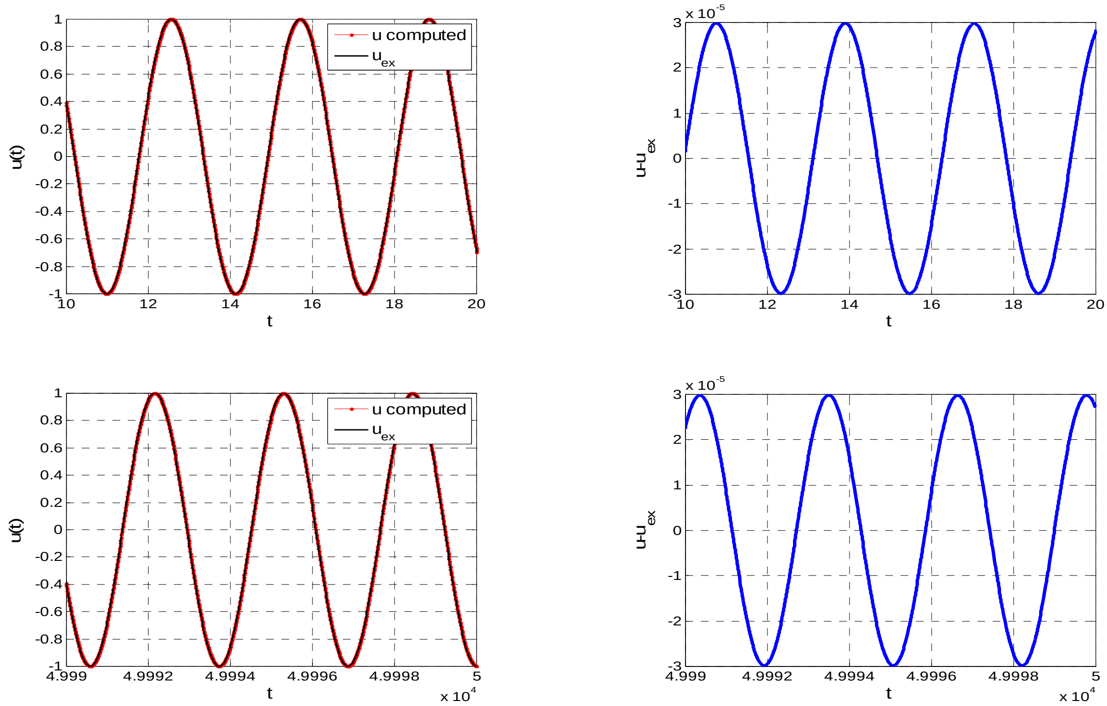

Figure 4. Solution for long duration ($0 \leq t \leq 50000$) Example 1.

Example 2. System of equations

In this example the system of equations

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}\begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \end{Bmatrix} + \begin{bmatrix} 3 & 4 \\ 4 & 4 \end{bmatrix}\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \exp(-0.1t)\begin{Bmatrix} 57\cos t/2 + 73\sin t/5 \\ 123\cos t/5 + 31\sin t/2 \end{Bmatrix} \tag{33}$$

with initial conditions $u_1 = 1,\ u_2 = 0$ is solved. Equation (33) admits an exact solution.

$$\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \exp(-0.1t) \begin{Bmatrix} \cos t \\ \sin t \end{Bmatrix} \tag{34}$$

The computed solution for $T = 10$ and $h = 0.01$ is shown in Fig. 5 as compared with the exact one. Moreover Fig. 6 shows the error $\mathbf{u} - \mathbf{u}_{ex}$.

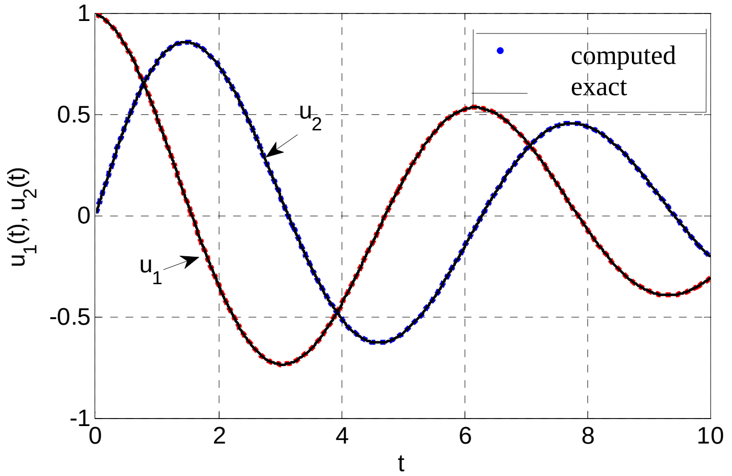

Figure 5. Solution $\mathbf{u} = \{u_1 \quad u_2\}^T$ in Example 2.

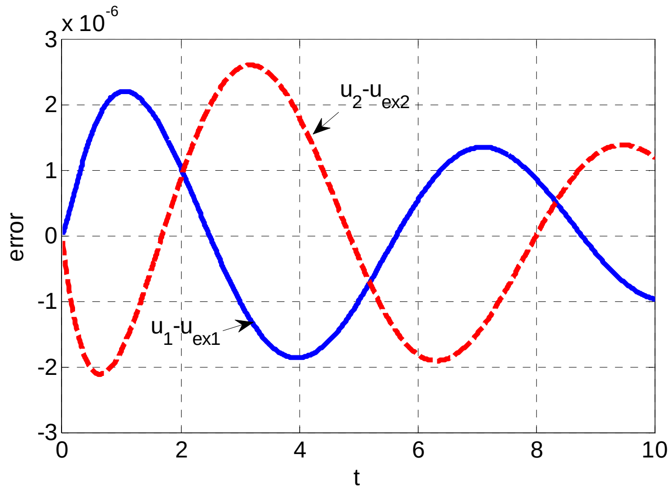

Figure 6. Error $\mathbf{u} - \mathbf{u}_{ex}$ in Example 2.

Example 3. System of equations

In this example the system of equations

$$\begin{bmatrix} 0.1493 & 0.0.8407 \\ 0.2575 & 0.2543 \end{bmatrix} \begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \end{Bmatrix} + \begin{bmatrix} 0.8909 & 0.5472 \\ 0.9593 & 0.1386 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{35}$$

with initial conditions $u_1 = 1, \; u_2 = 0$ is solved. The matrices $\mathbf{C}, \mathbf{K}$ are nonsymmetrical and not positive definite, $eig(\mathbf{C}) = \{-0.2665 \quad 0.6770\}$ $eig(\mathbf{K}) = \{-1.1311 \quad -0.3016\}$. However, the nonsymmetrical matrix $\hat{\mathbf{K}} = \mathbf{C}^{-1}\mathbf{K}$ has positive eigenvalues, $eig(\hat{\mathbf{K}}) = \{3.2245 \quad 0.6973\}$. Therefore, the stability criterion is satisfied. Eq. (35) admits an exact solution

$$u_1 = 1.0095\exp(3.2247t) - 0.0095\exp(0.6974t)$$
$$u_1 = 0.1910\exp(3.2247t) - 0.1910\exp(0.6974t) \quad (36)$$

The computed $\mathbf{u} - \mathbf{u}_{ex}$ for $h = 0.01$ is shown in Fig. 7

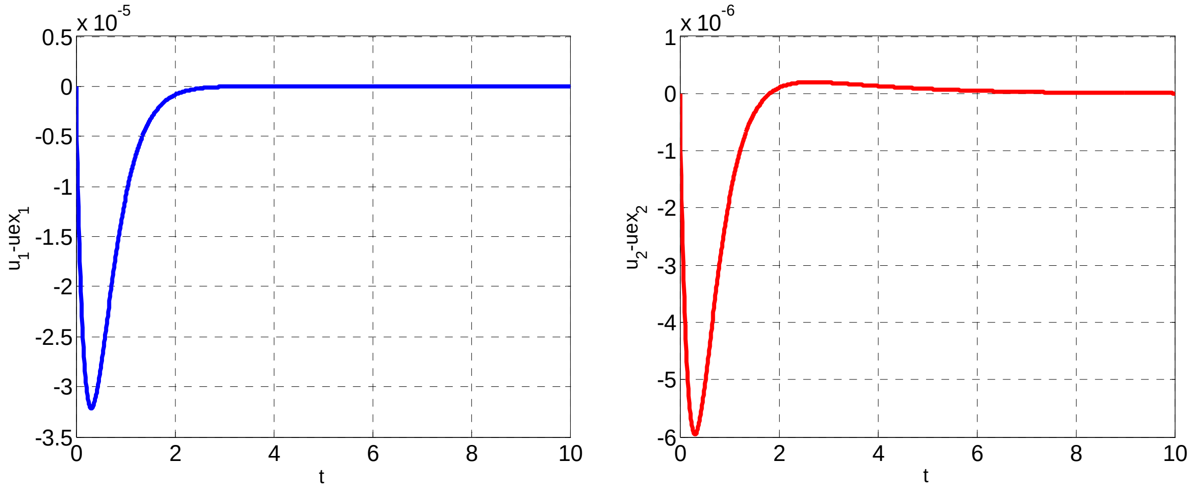

Figure 7. Error $\mathbf{u} - \mathbf{u}_{ex}$ in Example 3.

3 VARIABLE COEFFICIENTS

So far we have developed the method for the solution of Eq. (1) with constant coefficients. Obviously, if the coefficients c and k are functions of the independent variable t, i.e., $c(t), k(t)$, the previously described solution procedure remains the same except that the elements c, k in the first row of the coefficient matrix in the left hand side of Eq. (11) depend on time. Therefore, this coefficient matrix in the respective solution algorithm must be reevaluated in each step. In the following, the efficiency of the method is demonstrated by solving an equation with variable coefficients.

Example 4.Variable coefficients

We consider the initial value problem

$$(5+t)\dot{u} + (1+t^2)u = \left[(0.5 - 0.1t + t^2)\cos(t) - (5+t)\sin(t)\right]\exp(-0.1t), \qquad u_0 = 1 \quad (37)$$

Equation (37) admits an exact solution $u_{ex}(t) = e^{-0.1t}\cos t$. The computed solution for $T = 30$ and $h = 0.01$ is shown in Fig. 8 as compared with the exact one.

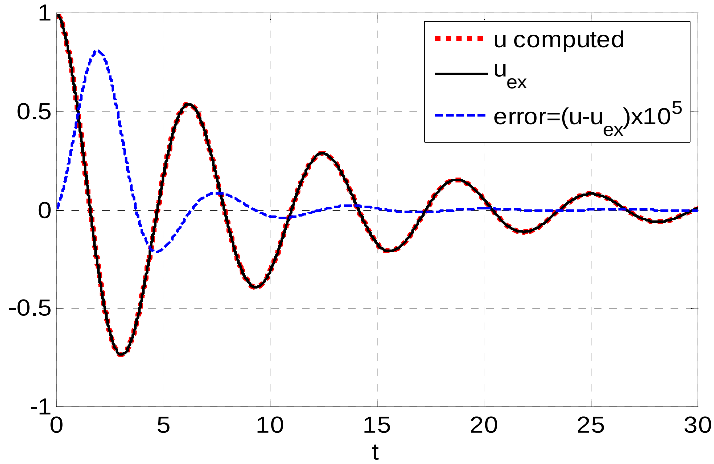

Figure 8. Solution u and error $(u - u_{ex}) \times 10^5$ in Example 4.

5 NONLINEAR EQUATIONS

The solution procedure developed previously for the linear equations can be straightforward extended to nonlinear equations.

The nonlinear initial value problem for multi-degree of freedom systems is described as

$$\mathbf{C}\dot{\mathbf{u}} + \mathbf{F}(\mathbf{u}) = \mathbf{p}(t) \tag{38}$$

$$\mathbf{u}(0) = \mathbf{u}_0 \tag{39}$$

where $\mathbf{C}$ is $L \times L$ known coefficient matrix with $\det(\mathbf{C}) \neq 0$; $\mathbf{F}(\mathbf{u})$ is an $L \times 1$ vector, whose elements are nonlinear functions of the components of $\mathbf{u}$; $\mathbf{p}(t)$ is the external source vector and $\mathbf{u}_0$ a given constant vector.

The solution procedure is similar to that for the linear systems. Thus, Eq. (38) for $t = 0$ gives the vector

$$\mathbf{q}_0 = \mathbf{C}^{-1}[\mathbf{p}_0 - \mathbf{F}(\mathbf{u}_0)], \qquad \mathbf{q}_0 = \dot{\mathbf{u}} \tag{40}$$

Subsequently, we apply Eq. (38) for $t = t_n$

$$\mathbf{C}\mathbf{q}_n + \mathbf{F}(\mathbf{u}_n) = \mathbf{p}_n \tag{41}$$

Apparently, Eq (9) is valid in this case, too. Thus we may write

$$\mathbf{u}_n = \mathbf{u}_{n-1} + \frac{h}{2}\mathbf{q}_n + \frac{h}{2}\mathbf{q}_{n-1} \tag{42}$$

Eqs (41) and (42) are combined and solved for $\mathbf{q}_n, \mathbf{u}_n$ with $n = 1, 2, \ldots$ ..The solution can be obtained using an iterative procedure in each step. A simple procedure is to substitute Eq. (42) into Eq (41). This yields a non linear equation for $\mathbf{q}_n$, which is solved by employing any ready-to-use subroutine for nonlinear algebraic equations. In our examples the function *fsolve* of Matlab has been employed to obtain the numerical results.

Example 5.

The numerical scheme is employed to solve the initial value problem

$$0.2\dot{u} + u + u^3 = p(t)\,, \quad u(0) = 0 \tag{43a,b}$$

For $p(t) = e^{-0.1t}[(0.01\sin t - 0.2\cos t - \sin t) - 0.2(0.1\sin t - \cos t) + \sin t + e^{-0.2t}(\sin t)^3]$, Eq (43) admits an exact solution $u_{exact}(t) = e^{-0.1t}\sin t$. Fig. 9 shows the solution with $\Delta t = 0.01$ as compared with the exact one and Fig. 10 presents the error $u - u_{ex}$.

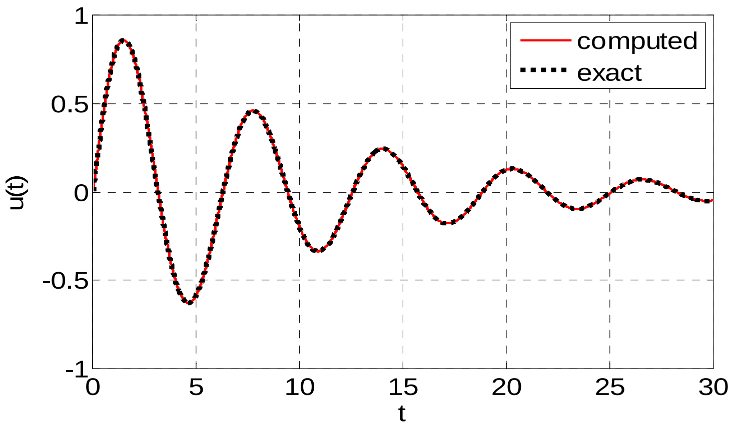

Figure 9. Solution u in Example 5.

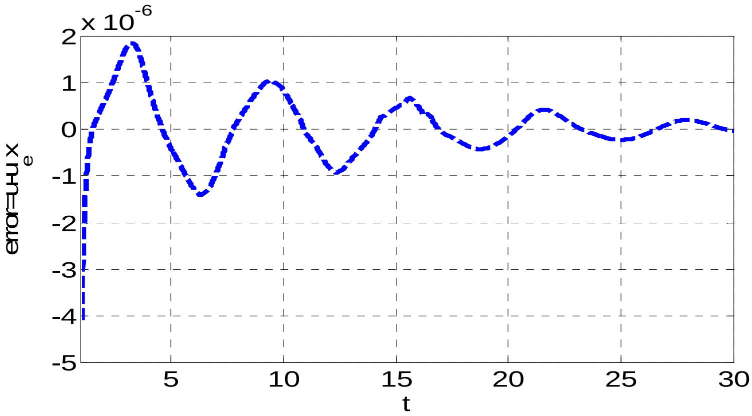

Figure 10. Error $u - u_{ex}$ with $\Delta t = 0.01$ in Example 5.

Example 6

In this example the problem describing the kinetics of an autocatalytic reaction given by Robertson [5] is solved. It is governed by the nonlinear system of equations

$$\begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \end{Bmatrix} = \begin{Bmatrix} -k_1 u_1 + k_3 u_2 u_3 \\ k_1 u_1 - k_2 u_2^2 - k_3 u_2 u_3 \\ k_2 u_2^2 \end{Bmatrix}, \quad \text{with} \quad \begin{Bmatrix} u_1(0) \\ u_2(0) \\ u_3(0) \end{Bmatrix} = \begin{Bmatrix} u_{10} \\ u_{20} \\ u_{30} \end{Bmatrix} \tag{44a,b}$$

where u_1, u_2, u_3 denote the concentrations of the three involved chemical species and k_1, k_2, k_3 are the rate constants.

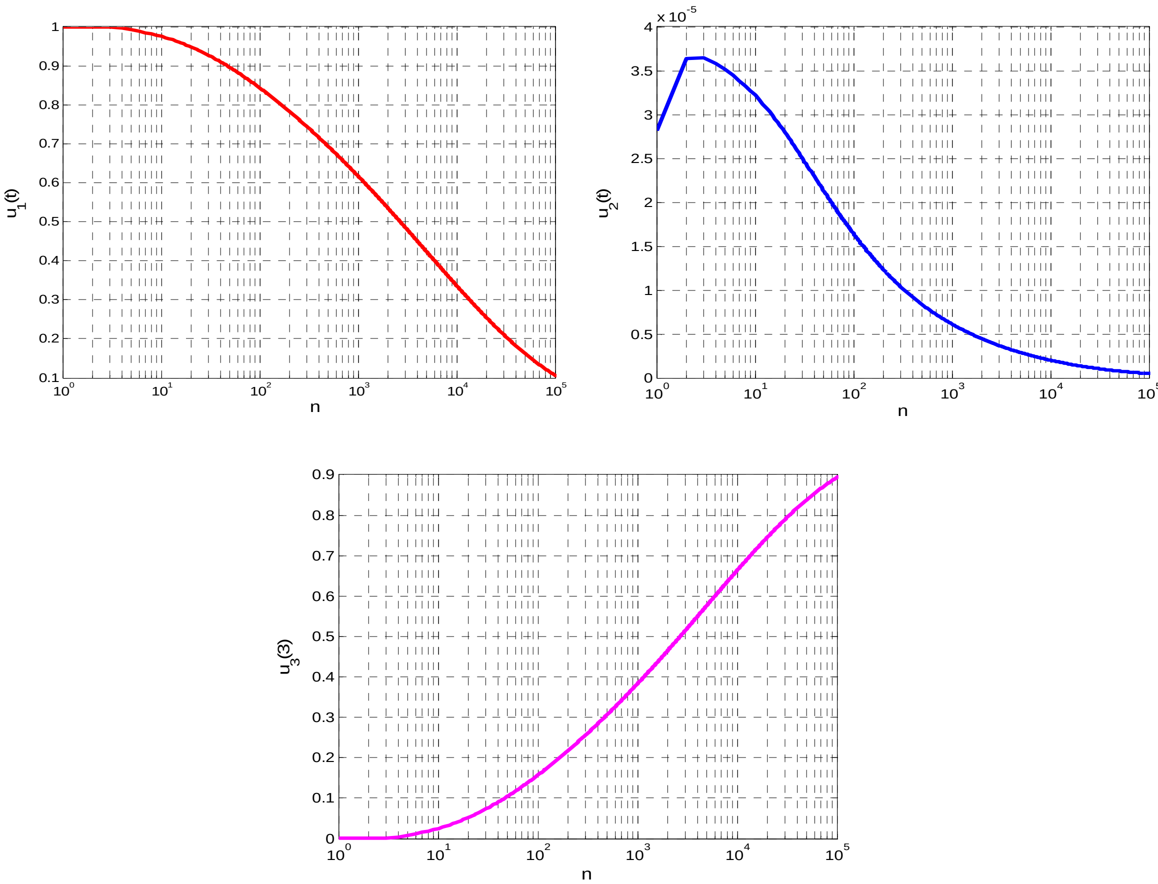

Figure 11. Solution of the Rober problem in Example 6. (n designates the number of instants).

This problem, known as ROBER problem, is very popular in numerical studies and it is often used as a benchmark problem to test the efficiency of stiff numerical integrators. The numerical values of the rate constants used in the test problem are $k_1 = 0{,}04, k_2 = 3\times 10^7, k_3 = 10^4$ and the initial conditions $\{u_{10} \quad u_{20} \quad u_{30}\}^T = \{1 \quad 0 \quad 0\}^T$. The large difference among the reaction rate constants is the reason for stiffness. It was observed that many integration codes, though for small intervals ($0 \le t \le 40$) perform well, they fail if t becomes very large. In this case, u_2 may accidentally becomes negative, and then tends to $-\infty$, causing overflow [6]. The solution in the interval $0 \le t \le 10^4$ is shown in Fig 11. It has been obtained using the Matlab code run on a Fujitsu Celsius H-series computer with $\Delta t = 0.001$ in the interval $0 \le t \le 3$ and $\Delta t = 0.1$ in the interval $3 < t \le 10^4$.

6 CONCLUSIONS

An integral equation method has been developed for the numerical solution of first order linear and nonlinear parabolic differential equations. The developed numerical scheme is applied to the solution of the semi-discrete equations arising in diffusion problems after spatial discretization using modern computational methods. The stability does not demand symmetric and positive definite coefficient matrices $\mathbf{C}, \mathbf{K}$ as the widely used methods, but can solve equations with non symmetric matrices provided that the matrix $\mathbf{C}^{-1}\mathbf{K}$ has positive eigenvalues. This is an important advantage, since the scheme can solve semi-discrete diffusion equations resulting from methods that do not produce symmetric matrices, e.g. the boundary element method. It applies also to equations with time dependent coefficient matrices, i.e. variable. The method is simple to implement. It is self starting, unconditionally stable. As it conserves energy, it performs well when long time durations are considered. It can be used as a practical method for integration of stiff diffusion equations in cases where widely used time integration procedures fail. Several examples are presented, which illustrate the method and demonstrate its efficiency.

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