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A Comparison of Recent Methods for solving a model 1D Convection Diffusion Equation

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***Abstract*—**In this paper we study some numerical methods to solve a model one-dimensional convection–diffusion equation. The semi-discretisation of the space variable results into a system of ordinary differential equations and the solution of the latter involves the evaluation of a matrix exponent. Since the calculation of this term is computationally expensive, we study some methods based on Krylov subspace and on Restrictive Taylor series approximation respectively. We also consider the Chebyshev Pseudospectral collocation method to do the spatial discretisation and we present the numerical solution obtained by these methods.

***Keywords*—**Chebyshev Pseudospectral collocation method, convection-diffusion equation, restrictive Taylor approximation.

I. Introduction

THE numerical solution of convection-diffusion transport problems arises in many important applications in science and engineering. These problems occur in many applications such as in the transport of air and ground water pollutants, oil reservoir flow, in the modeling of semiconductors, among others. In this paper, we consider the one dimensional convection-diffusion equation, given as

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - \gamma\frac{\partial^2 u}{\partial x^2} = 0,\ x \in (0,1),\ t > 0, \tag{1}$$

subject to the initial condition

$u(x,0) = g(x),\ 0 < x < 1$

and the boundary conditions given by

$u(0,t) = g_0(t),\quad t \ge 0$

$u(1,t) = g_1(t),\quad t \ge 0.$

Much research work has been done on computing a finite difference approximation solution for (1) as shown in [3,7]. In this paper, we focus on a semi-discretisation of (1) so as to obtain a system of ordinary differential equations. The discrete solution requires the computation of a matrix exponent with a vector. Our study is thus based on a comparison of three recent methods for solving the one dimensional convection diffusion equation. We first consider the discretisation of (1) in the next section.

A. Discretisation of the 1-D convection-diffusion equation

We start by considering the grid point $x_i = ih$, where $i = 0,\ldots,n$ a set of regular grid points of the interval [0,1] with $x_0 = 0$ and $x_n = 1$ and $nh = 1$. We use the Taylor series expansion to obtain expressions for the first and second partial derivative of u with respect to x respectively as:

$$u_x(x_i,t) = (u(x_{i+1},t) - u(x_{i-1},t))/(2h) + O(h^2) \tag{2}$$

and

$$u_{xx}(x_i,t) = (u(x_{i+1},t) - 2u(x_i,t) + u(x_{i-1},t))/(h^2) + O(h^2) \tag{3}$$

at a fixed time t. Replacing equations (2) and (3) into (1) gives

$$\frac{du}{dt} + c\left(\frac{u_{i+1,j} - u_{i-1,j}}{2h}\right) = \gamma\left(\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}\right)$$

$$\Rightarrow h^2\frac{du}{dt} = \left(\gamma - \frac{ch}{2}\right)u_{i+1,j} + \left(\gamma + \frac{ch}{2}\right)u_{i-1,j} + (-2\lambda)u_{i,j}$$

Thus we obtain

$$h^2\frac{du}{dt} = ru_{i-1,j} + pu_{i,j} + qu_{i+1,j} \tag{4}$$

where $p = \left(\gamma + \frac{ch}{2}\right),\quad q = (-2\lambda),\quad r = \left(\gamma - \frac{ch}{2}\right).$

The difference method (4) can be written as

$$\frac{dV(t)}{dt} = AV(t) + b, \tag{5}$$

where $V(t) = [u_1(t), u_2(t), \ldots u_n(t)]$, A is the tridiagonal matrix of order $n-1$ given by

$$A = \begin{pmatrix} p & r & & & & \\ q & p & r & & & \\ & . & . & . & & \\ & & . & . & . & \\ & & & . & . & . \\ & & & q & p & r \\ & & & & q & p \end{pmatrix}_{(N-1)\times(N-1)} \tag{6}$$

and

$$b(t) = \left[\left(\frac{ch}{2} + \gamma\right)u_1 \quad 0 \quad . \quad . \quad . \quad 0 \quad \left(\gamma - \frac{ch}{2}\right)u_{N-1}\right]^T.$$

II. Discrete Solution of the ODE System

In this section we show how the expressions obtained after discretising the model convection-diffusion equation can be expressed as a system of ordinary differential equations. We find that the solution of such systems involves terms such as e^{kA} and we investigate ways to obtain the explicit computation of the exponential matrix. Thus the term $e^{kA}y$ is approximated based by the Krylov subspace method proposed in [6].

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Now consider the ordinary differential equation (5). Rewriting the equation gives

$$\frac{dV(t)}{dt} - A[V(t)] = b\,.$$

$$\therefore e^{-tA}V(t) = \int e^{-tA}(b)dt = -A^{-1}be^{-tA} + c.$$

$$\therefore V(t) = -A^{-1}b + ce^{-tA}$$

Using initial condition we obtain

$$V(t) = -A^{-1}b + e^{tA}\left(V(0) + A^{-1}b\right)$$

$$V(0) = -A^{-1}b + e^{0}c \qquad \therefore c = V(0) + A^{-1}b$$

$$\therefore V(t) = -A^{-1}b + e^{tA}\left(V(0) + A^{-1}b\right) \qquad (7)$$

Now, $V(t+k) = -A^{-1}b + e^{(t+k)A}\left(V(0) + A^{-1}b\right)$

$$= -A^{-1}b + e^{kA}\left[e^{tA}\left(V(0) + A^{-1}b\right)\right]$$

$$= -A^{-1}b + e^{kA}\left(V(t) + A^{-1}b\right)$$

Hence to compute solution at time $t+k$, we need to compute $e^{kA}y$ where $y = V(t) + A^{-1}b$, that is

$$V(t+k) = -A^{-1}b + e^{kA}\left(V(t) + A^{-1}b\right) = -A^{-1}b + e^{kA}y \qquad (8)$$

A. The Krylov Subspace Method

Let us consider the tridiagonal matrix *A* instead of *kA*. The method proposed is based on the Krylov subspace which is of the form

$$e^{A}y \approx p_{m-1}(A)y$$

where p_{m-1} is the polynomial of degree of $m-1$. In this paper, the approximation to $e^{A}y$ is taken from the Krylov subspace

$$\kappa_m = span\left\{y, Ay, \ldots, A^{m-1}y\right\}$$

We then have to generate an orthonormal basis $V_m = [v_1, v_2, \ldots, v_m]$, so that the vectors in the Krylov subspace can be manipulated. Taking initial vector: $v_1 = \frac{y}{\|y\|_2}$ we obtain V_m by the Arnoldi's algorithm which is next given by:

Algorithm: (*Arnoldi-modified Gram-Schmidt*).

Compute $v_1 = y / \|y\|_2$.

For $j = 1,2,\ldots, m$ Do:

Compute $w_j := Av_j$

For $i = 1,\ldots j$ Do:

$h_{ij} := (w_i, v_i)$

$w_j := w_j - h_{i,j}v_i$

EndDo

$h_{j+1} := \|w_j\|_2$. If $h_{j+1,j} = 0$, then Stop

$v_{j+1} := w_j / h_{j+1,j}$

EndDo

From this algorithm, a matrix H_m (Hessenberg matrix) and an orthonormal basis V_m can be obtained. We also find the following relations to hold:

$$V_m^{\,T} A V_m = H_m$$

$$AV_m = V_m H_m + h_{m+1,m} V_{m+1} e_m^{\,T}$$

where e_m is the m^{th} unit vector belonging to real space of order *m*. Hence H_m represents the projection of the linear transformation A to the space κ_m, with respect to the basis V_m.

The required approximation can be written to $x = e^{Ay}$ as $x_m = p_{m-1}(A)y$ or equivalently, $x_m = V_m w$ where w is an *m*-vector.

$w = \beta e^{H_m} e_1$ with $\beta = \|y\|_2$ is suggested, leading to the following formula: $e^{Ay} \approx \beta V_m e^{H_m} e_1$ where e_1 is the first unit vector belonging to the real space of order *m*.

B. Restrictive Taylor's approximation for solving convection-diffusion equation (RTA)

In this section we introduce an explicit method for solving (1) which exhibits several advantageous features compared other known methods. The accuracy is not affected when the exact solution is sufficiently large. Moreover, the choice of time step length *k* is relatively large compared with what can be used for the classical schemes, this allows us to have the solution at high level of time. We use the restrictive Taylor (RT) approximation [4, 5] to approximate the exponential matrix given as e^{kA}. The RTs approximation of the function *f(x)* at the point a can be written in the form:

$$RT_{n,f(x)}(x,a) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \ldots + \frac{\varepsilon f^{(n)}(a)}{n!}(x-a)^n, \qquad (9)$$

where the parameter ε is to be determined such that

$$RT_{n,f(x)}(x_0) = f(x_0)\,. \qquad (10)$$

This means that the considered approximation is exact at two points $x = a$ and $x = x_0$.

$$f(x) = RT_{n,f(x)}(x_0) + \Re_{n+1}(x), \qquad (11)$$

where $\Re_{n+1}(x)$ is the remainder term of Restrictive Taylor's series and it given by

$$\Re_{n+1}(x) = \frac{\varepsilon(x-a)^{n+1}}{(n+1)!} f^{(n+1)}(\xi)$$
$$-\frac{n(\varepsilon-1)(x-a)^{n+1}}{(x-\xi)(n+1)!} f^{(n)}(\xi), \qquad (12)$$

where $\xi \in [a,x]$ and ε is the restrictive parameter.

The exponential matrix e^{kA} can be formally defined by the convergent power series

$$e^{kA} = I + kA + \frac{k^2}{2!}A^2 + ... = \sum_{n=0}^{\infty} \frac{k^n}{n!}A^n, A^0 = I.$$

In the case of RTs approximation of single function the term ε, (9) can be reduced to the square restrictive matrix Γ in the case of RTs approximation for matrix function, where $\Gamma = \varepsilon I$ and I is the identity matrix.

For example, $RT_{1,\exp(xA)}(k) = I + k\Gamma A$.

III. CHEBYSHEV PSEUDOSPECTRAL METHOD (CPS)

In this section, we focus on solving (1) based on Chebyshev pseudospectral collocation (CPS) [1]. Spatial discretization is done by using the Chebyshev pseudospectral collocation (CPS). Bazan [1] has highlighted one major drawback of [6] lies in the fact that the vector b does not take into account the time dependence. The solution to (1) with respect to the given initial condition is therefore given as:

$$V(t) = e^{At}V(0) + \frac{1}{h^2}\begin{bmatrix} q\int_0^t \exp(A(t-\tau))g_0(\tau)e_1 d\tau \\ + r\int_0^t \exp(A(t-\tau))g_1(\tau)e_{m-1} d\tau \end{bmatrix} \qquad (13)$$

where e_i represents the i^{th} canonical vector in $\Re^{m-1}$ [1]. If $b(t)$ is independent to t which is the case when the boundary conditions in (1) are constants, the unique solution to (1) reduces to

$$V(t) = -A^{-1}b + \exp(tA)\left(V(0) + A^{-1}b\right).$$

Consider the lemma given in [1]

LEMMA 1: Let A have a spectral decomposition $A = PAP^{-1}$. Then a necessary condition for $u(x,t) = \exp(\alpha x + \beta t)$ to solve problem (1) is $g_o(t) = \exp(\beta t)$, $g_1(t) = \exp(\alpha + \beta t)$ and $\gamma\alpha^2 - c\alpha - \beta = 0$. Moreover, the approximate difference finite-based solution becomes in this case

$$V(t) = P\begin{bmatrix} \exp(tA)w_0 \\ + \frac{1}{h^2}\left((\beta I - A)^{-1}\exp(\beta It) - \exp(At)\right)w_1 \end{bmatrix} \qquad (14)$$

where $w_0 = P^{-1}V(0)$ and $w_1 = P^{-1}(qe_1 + \exp(\alpha)ce_{m-1})$.

We can readily conclude that problem (1) is of the form $\exp(\alpha x + \beta t)$. As for (14), it results from using $A = PAP^{-1}$ in (13) and the specified boundary conditions.

We focus on defining a semi-discrete method obtained by discretising (1) with respect to the spatial variable using the pseudospectral Chebyshev method. In the following the first-order $(n+1)\times(n+1)$ Chebyshev differentiation matrix associated with the collocation points

$0 = x_0 < x_1 < ... < x_n = 1,$

with $x_j = \frac{1}{2}[1 - \cos(j\pi/n)]$, $j = 0,1,...,n$ will be denoted by D. Also, if $d_i(resp., l_i)^T$ denotes the i^{th} column (resp., row) vector of matrix D, we write

$$D = [d_1, ..., d_{n+1}] = \begin{bmatrix} l_1^T \\ . \\ . \\ . \\ l_{n+1}^T \end{bmatrix}.$$

Let D_1, D_2, and D_3 be matrices defined by $D_1 = [d_2,...,d_n]$, $D_2 = [l_2,...,l_n]^T$, $D_3 = E^T DE$,

with $E = [e_2,..., e_n]$, where e_i is the i^{th} column of the identity matrix of order $n+1$.

We introduce the semi-discrete version of (1) obtained by discrete differencing using matrix D. Then $\mu = [\mu_0, \mu_1, ..., \mu_n]^T$ denotes a vector of data at positions x_j, $j = 0,1,...,n$, the first order differentiation matrix D gives highly accurate approximations to $\mu'(x_j), \mu''(x_j),...,$ simply by taking $\mu'(x_j) = (D\mu)_j$, $\mu''(x_j) = (D^2\mu)_j$, and so on. Thus the formulae for the entries of D can be computed by the Chebyshev differentiation matrix matlab code given in [1].

A semi discrete Chebyshev approximation to (1) is provided by the system of $n-1$ ordinary differential equations:

$$\frac{dV}{dt} = AV + b(t)$$

$V(0) = [f(x_1),...,f(x_{n-1})]^T$, $\qquad V(t) = [\mu_1(t),..., \mu_{n-1}(t)]^T$,

$A = \gamma D_2 D_1 - cD_3$,

and $b(t) = g_o(t)(\gamma D_2 - cE^T)d_1 + g_1(t)(\gamma D_2 - cE^T)d_{n+1}$.

If $A = PAP^{-1}$ holds, the solution to the above initial value problem (2.1) is

$$V(t) = P\left[\exp(tA)\begin{pmatrix} w_0 + \int_0^t \exp(-A\tau)g_0(\tau)d\tau w_1 \\ + \int_0^t \exp(-A\tau)g_0(\tau)d\tau w_2 \end{pmatrix}\right]$$

where

$w_0 = P^{-1}V(0)$, $w_1 = P^{-1}(\gamma D_2 - cE^T)d_1$ and

$w_2 = P^{-1}(\gamma D_2 - cE^T)d_{n+1}$.

Finally the solution to the problem (1) follows as:
$V(t) = P\left(e^{tA} w_0\right) + (BI - A)^{-1}\left(e^{Bt} - e^{At}\right)w$, where
$w = P^{-1}\left(\left(\gamma D_2 - cE^T\right)\left(d_1 + e^{\alpha} d_{n+1}\right)\right)$.

IV. Numerical Experiments

In this section, we use the methods described earlier to solve three problems which are given as follows:

Problem 1

$$\frac{\partial u}{\partial t} + 0.1\frac{\partial u}{\partial x} = 0.02\frac{\partial^2 u}{\partial x^2}, \quad 0 \le x \le 1, t \ge 0$$

where the initial boundary conditions are defined such that the exact solution is $u(x,t) = e^{1.1771243444\ 46770\, x - 0.09t}$.

Problem 2

$$\frac{\partial u}{\partial t} + 0.1\frac{\partial u}{\partial x} = 0.01\frac{\partial^2 u}{\partial x^2}, 0 \le x \le 1, t \ge 0,$$

where the initial boundary conditions are defined such that the exact solution is $u(x,t) = e^{9x - 0.09t}$.

Problem 3

$$\frac{\partial u}{\partial t} + 3.5\frac{\partial u}{\partial x} = 0.022\frac{\partial^2 u}{\partial x^2}, 0 \le x \le 1, t \ge 0,$$

where the initial boundary conditions are defined such that the exact solution is $u(x,t) = e^{0.0285479799\ 1928\, x - 0.09t}$.

For our numerical experiments, we let $h = 0.025$, $k = 0.001$ and $m = 5$ for the Krylov subspace projection. We observe that the CPS's accuracy for problem 1 is better than that of SM. RTA gives the least accurate solution when compared to SM and CPS. Thus we can conclude that for problem 1, the parameters defined on CPS gives very accurate approximation.

We note that the SM's accuracy for problem 1 is more accurate than CPS. RTA gives the least accurate solution when compared to SM and CPS. Thus we find that for problem 2, the parameters defined on SM gives very accurate approximation.

We note that the RTA's accuracy for problem 2.3 is more accurate than CPS and SM. SM gives the least accuracy compared to RTA and CPS at $x = 0.5$ and at $x = 0.1$, SM and CPS gives a mean absolute value relatively the same. Thus we see that for problem 3, the parameters defined on RTA gives good accuracy.

V. Conclusion

In this paper, we have studied three methods for solving the one-dimensional convection-diffusion equation. The first method, SM, consists of finding the solution of the system of ordinary differential equations which arises from discretisation of the convection-diffusion with respect to the spatial variable. The resulting exponential matrix term was approximated by a polynomial obtained by using a Krylov subspace method. We next studied the Restrictive Taylor approximation (RTA) method. This time the exponential matrix was approximated by an expression derived from the Taylor series approximation. Finally, we studied the Chebyshev Pseudospectral Collocation method which is used from the spatial discretisation.

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TABLE I
COMPARISON OF SM, RTA AND CPS'S ABSOLUTE ERRORS AT $x = 0.1$ AND $x = 0.5$ FOR PROBLEM 1

Time *t*	**Absolute errors at *x* = 0.1**			**Absolute errors at *x* = 0.5**		
	SM	**RTA**	**CPS**	**SM**	**RTA**	**CPS**
1	1.2894e-005	6.7584e-004	4.4148e-008	3.9094e-004	2.8050e-003	2.2772e-007
2	3.7845e-007	2.5208e-005	4.7615e-008	6.8890e-005	7.2700e-004	2.9006e-007
3	3.8452e-008	2.3145e-006	4.9108e-008	9.5392e-006	1.4102e-004	3.0894e-007
4	5.0364e-008	2.1025e-006	5.0577e-008	8.4640e-007	3.0323e-005	3.1966e-007
5	5.2083e-008	2.1653e-006	5.2087e-008	2.1159e-007	1.5436e-005	3.2939e-007
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
36	1.2928e-007	5.3916e-006	1.2970e-007	1.4737e-006	6.7588e-005	8.1984e-007
37	1.0981e-007	6.1610e-006	1.3357e-007	2.1112e-005	3.2069e-004	8.4107e-007
38	9.3904e-007	6.4395e-005	1.3738e-007	1.7394e-004	1.8412e-003	8.4085e-007
39	3.6908e-005	1.9355e-003	1.3550e-007	1.1193e-003	8.0338e-003	7.0949e-007
Error	1.3858e-006	7.2434e-005	8.5287e-008	4.6208e-005	3.7577e-004	5.3312e-007

TABLE II
COMPARISON OF SM, RTA AND CPS'S ABSOLUTE ERRORS AT $x = 0.1$ AND $x = 0.5$ FOR PROBLEM 2

Time *t*	**Absolute errors at *x* = 0.1**			**Absolute errors at *x* = 0.5**		
	SM	**RTA**	**CPS**	**SM**	**RTA**	**CPS**
1	8.3458e-006	2.3530e-002	1.5409e-005	1.5434e-004	1.3006e-001	8.8238e-005
2	1.9577e-005	4.1244e-004	1.9703e-005	9.8454e-005	1.2307e-002	1.2347e-004
3	2.4680e-005	2.2087e-004	2.4681e-005	1.5398e-004	2.0218e-003	1.5599e-004
4	3.0909e-005	2.7560e-004	3.0909e-005	1.9533e-004	1.7688e-003	1.9546e-004
5	3.8708e-005	3.4514e-004	3.8708e-005	2.4478e-004	2.1841e-003	2.4479e-004
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
36	4.1400e-002	3.6914e-001	4.1400e-002	2.6141e-001	2.4103e+000	2.6180e-001
37	5.1840e-002	4.6535e-001	5.1846e-002	3.1986e-001	5.3248e+000	3.2752e-001
38	6.4287e-002	1.7393e+000	6.4900e-002	2.8227e-001	5.8540e+001	4.0490e-001
39	3.4727e-002	1.4814e+002	7.9240e-002	1.0857e+000	8.1866e+002	4.4308e-001
Error	9.1349e-003	3.9025e+000	1.0292e-002	7.6577e-002	2.2932e+001	1.1412e-001

TABLE III
COMPARISON OF SM, RTA AND CPS'S ABSOLUTE ERRORS AT $x = 0.1$ AND $x = 0.5$ FOR PROBLEM 3

Time *t*	**Absolute errors at *x* = 0.1**			**Absolute errors at *x* = 0.5**		
	SM	**RTA**	**CPS**	**SM**	**RTA**	**CPS**
1	8.3458e-006	3.8701e-005	2.5637e-005	1.5434e-004	1.1186e-004	7.1696e-005
2	1.9577e-005	3.1223e-005	2.9621e-005	9.8454e-005	1.6231e-004	1.2897e-004
3	2.4680e-005	3.0136e-005	3.0055e-005	1.5398e-004	1.8483e-004	1.6397e-004
4	3.0909e-005	3.0111e-005	3.0109e-005	1.9533e-004	1.9074e-004	1.8086e-004
5	3.8708e-005	3.0133e-005	3.0131e-005	2.4478e-004	1.9122e-004	1.8757e-004
.	.	.		.	.	.
.	.	.		.	.	.
.	.	.		.	.	.
36	4.1400e-002	3.0808e-005	2.6089e-003	2.6141e-001	1.9482e-004	5.8361e-003
37	5.1840e-002	3.0828e-005	1.6659e-002	3.1986e-001	1.9516e-004	7.9375e-003
38	6.4287e-002	3.0982e-005	9.6472e-003	2.8227e-001	1.9196e-004	2.0856e-002
39	3.4727e-002	2.7928e-005	2.7770e-002	1.0857e+000	2.2184e-004	1.2473e-002
Error	9.1349e-003	3.0639e-005	1.6969e-003	7.6577e-002	1.9040e-004	1.5399e-003