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Solution of parabolic equations using an eigenvalue method for time advancement

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The use of numerical time advancement techniques typically involve development of matrix systems that are solved in timestepped form. In this paper, an eigenvalue approach is used to exactly solve the fundamental matrix system. In this way, numerical error occurs only in the spatial derivative terms, and not the temporal term.

Key words: time-advancement, eigenvalues, numerical methods, matrix formulations.

1 INTRODUCTION

Numerical solution of partial differential equations (PDE) of the parabolic type is traditionally accomplished by finite difference, finite element, collocation, or other techniques that resolve the problem setting into a set of linear equations (e.g. Ref. 1). Such parabolic equations arise in problems in the fields of heat flow, groundwater flow, and containment transport, among others. In order to advance the usual nodal point vector solution in time, a time-stepping technique is typically employed such as Crank–Nicholson, explicit, or implicit methods, which use matrix solutions computed at small time increments in order to achieve time advancement.

In this paper, we recall the use of eigenvalue solutions that directly and exactly solve the matrix system with respect to the time derivative term. Although complex in application, once formulated into software, the eigenvalue method for solving the time derivative term affords clear advantages over the usual time-stepping techniques. These advantages include:

(1) exact solution of the time derivative component of the matrix system;
(2) ability to solve for the nodal point vector value at arbitrary time t, without solving for nodal values at intermediate time-steps; and
(3) elimination of considerable quantities of repetitive calculations required by the usual time-stepping procedures.

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2 DEVELOPMENT OF THE NUMERICAL MODEL

Although the discussions pertain to parabolic equations in general, we will focus our attention on generalized flow modeling. For the one-dimensional case, unsteady flow (groundwater, heat, and other phenomena) in a homogeneous medium may be described by:

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}, \quad 0 \le x \le L \tag{1}$$

where x and t are spatial and temporal coordinates, respectively; and T is the state variable. In addition to eqn (1), boundary and initial conditions are needed to have a well posed problem.

The general numerical approach is to discretize the spatial domain into smaller domains using N nodal points, which have associated nodal values T_k^i, $k = 1, 2, \ldots, N$ at time-step i, where each time-step is of duration Δt. For evenly spaced nodal points, a matrix solution of eqn (1) may be written in generalized matrix

form as:

$$\mathbf{ST} + \mathbf{\Psi}\dot{\mathbf{T}} = \mathbf{L} \tag{2}$$

where $\mathbf{S}$ is an $N \times N$ symmetric stiffness matrix; $\mathbf{\Psi}$ is an $N \times N$ symmetric capacitance matrix; $\mathbf{T}$ is an $N \times 1$ column vector of nodal values; $\dot{\mathbf{T}}$ is an $N \times 1$ column vector of nodal value time derivatives of the form $\partial T_k/\partial t$; and L is an $N \times 1$ column load vector.

Many numerical techniques may be written in a unifying matrix form analogous to eqn (2) by specifying the capacitance matrix as depending on a parameter η, that is, $\mathbf{\Psi} = \mathbf{\Psi}(\eta)$. For one-dimensional problems we have:

$$\mathbf{\Psi}(\eta) = \frac{\mathbf{L}}{\eta+2}\begin{bmatrix} \eta & 1 & 0 & & & \cdots & & 0 \\ 1 & \eta & 1 & 0 & & \cdots & & 0 \\ 0 & 1 & \eta & 1 & & \cdots & & 0 \\ \vdots & & \ddots & \vdots & & & \vdots & \\ 0 & \cdots & & & 0 & 1 & \eta & 1 \\ 0 & \cdots & & & 0 & 0 & 1 & \eta \end{bmatrix} \tag{3}$$

For $\eta = 2, 3, \infty$, we obtain the Galerkin finite element, nodal domain integration, and finite difference modal equations, respectively.

In order to solve the time derivative term in eqn (2), the column vector $\dot{\mathbf{T}}$ is replaced by the approximation $\dot{\mathbf{T}} \approx (T^{i+1} - T^i)/\Delta t$ and a well known technique such as the Crank–Nicholson method is employed. Thus, we obtain:

$$\mathbf{S}\frac{T^i + T^{i+1}}{2} + \mathbf{\Psi}(\eta)\frac{T^{i+1} - T^i}{\Delta t} = \mathbf{L} \tag{4}$$

where $T^i = T(i\Delta t)$, and $T^{i+1} = T((i+1)\Delta t)$. By rearranging terms, eqn (4) becomes:

$$\left(\mathbf{\Psi}(\eta) + \frac{\Delta t}{2}\mathbf{S}\right)T^{i+1} = \left(\mathbf{\Psi}(\eta) - \frac{\Delta t}{2}\mathbf{S}\right)T^i + \mathbf{L} \tag{5}$$

In eqn (5) initial conditions at time $t = 0$ are supplied by the known vector $\mathbf{g}$ and boundary conditions are imposed which define the load vector $\mathbf{L}$. The solution vector of nodal values at subsequent time-steps are computed by repetitive solution of eqn (5). Thus, the solution vector at time t is obtained by solving eqn (5) a total of $t/\Delta t$ times.

Returning to eqn (2), $\mathbf{ST} + \mathbf{\Psi}(\eta)\dot{\mathbf{T}} = \mathbf{L}$. If we solve for $\dot{\mathbf{T}}$, we obtain:

$$\dot{\mathbf{T}} = \mathbf{A}(\eta)\mathbf{T} + \mathbf{b}(\eta) \tag{6}$$

where $\mathbf{A}(\eta) = -\mathbf{\Psi}^{-1}(\eta)\mathbf{S}$ is a real symmetric $N \times N$ matrix and $\mathbf{b}(\eta) = \mathbf{\Psi}^{-1}(\eta)\mathbf{L}$ is an $N \times 1$ column vector. Since $\mathbf{A}(\eta)$ is symmetric it has real eigenvalues and a complete set or N orthogonal eigenvectors (henceforth we shall omit explicit reference to η). Observe, $\mathbf{A}$ and $\mathbf{b}$ do not depend on t. Consequently, eqn (6) can be directly solved using eigenvalue techniques so that the solution vector at time t can be obtained in one step.

3 DEVELOPMENT OF THE EIGENVALUE METHOD

If we combine eqn (6) with the initial condition $\mathbf{T}(0) = \mathbf{g}$ we obtain a vector initial value problem (IVP) of the form:

$$\begin{cases} \dot{\mathbf{T}} = \mathbf{AT} + \mathbf{b} \\ \mathbf{T}(0) = \mathbf{g} \end{cases}$$

where $\mathbf{A}$ is a real $N \times N$ banded symmetric constant matrix and $\mathbf{b}$ and $\mathbf{g}$ are real $N \times 1$ constant vectors. This system is quite numerically expedient since $\mathbf{A}$ is symmetric and therefore has real eigenvalues and N orthogonal eigenvectors. It is therefore possible to obtain a closed form solution.

First consider the associated homogeneous system $\dot{\mathbf{T}} = \mathbf{AT}$. Rearranging, we obtain $\dot{\mathbf{T}} - \mathbf{AT} = 0$. Given a solution of the form $\mathbf{T} = e^{\lambda t}\mathbf{u}$, then $\dot{\mathbf{T}} = \lambda e^{\lambda t}\mathbf{u}$; this, upon substitution, yields:

$$\lambda e^{\lambda t}\mathbf{u} - \mathbf{A}e^{\lambda t}\mathbf{u} = 0$$

or:

$$e^{\lambda t}(\lambda\mathbf{u} - \mathbf{Au}) = 0$$

Since $e^{\lambda t} \neq 0$, we may divide both sides of the above equation by $e^{\lambda t}$ to obtain $\lambda\mathbf{u} - \mathbf{Au} = 0$ so that λ must be an eigenvalue and $\mathbf{u}$ must be an eigenvector of $\mathbf{A}$.

Now let $\mathbf{\Phi}(t)$ be the fundamental matrix whose columns are each independent solutions to the homogeneous system. Then, any solution has the form:

$$\mathbf{T} = \mathbf{\Phi c}$$

where $\mathbf{c}$ is a real $N \times 1$ constant vector to be determined.

Since $\mathbf{A}$ is constant and real-symmetric, the fundamental matrix $\mathbf{\Phi}(t)$ will have a particularly convenient form. First, define $\mathbf{P}$ to be the matrix whose columns are the eigenvectors of $\mathbf{A}$ and let $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$, where the λ_i are eigenvalues of $\mathbf{A}$ taken in the same order that the corresponding eigenvectors occur in $\mathbf{P}$. Since $\mathbf{A}$ is symmetric, $\mathbf{P}$ will be orthogonal, i.e. $\mathbf{P}^{-1} = \mathbf{P}^{\mathrm{T}}$ and the following similarity relations hold:

$$\mathbf{A} = \mathbf{P\Lambda P}^{\mathrm{T}}$$

and:

$$\mathbf{\Lambda} = \mathbf{P}^{\mathrm{T}}\mathbf{AP}$$

That is, $\mathbf{A}$ is orthogonally diagonalizable.

If we let $\mathbf{Y} = \mathbf{P}^{\mathrm{T}}\mathbf{T}$ and substitute into the homogeneous equation we obtain the decoupled system $\dot{\mathbf{Y}} = \mathbf{\Lambda Y}$. This represents N equations of the form $\mathrm{d}y_i/\mathrm{d}t = \lambda_i y_i$, each having solution $y_i = e^{\lambda_i t}$. Thus, the fundamental matrix for the decoupled system is:

$$\mathbf{D}(t) = \mathrm{diag}\,(e^{\lambda_1 t}, \ldots e^{\lambda_N t})$$

From this we may conclude that the fundamental matrix for the homogeneous system is:

$$\mathbf{\Phi}(t) = \mathbf{PD}(t)$$

Therefore, any solution to the homogeneous system must be of the form $\mathbf{T} = \mathbf{PDc}$, where $\mathbf{c}$ is a vector of constants to be determined.

Now we shall return to the non-homogeneous problem. In order to obtain the solution to the non-homogeneous problem we shall employ the technique of variation of parameters: assume a solution of the form $\mathbf{T}(t) = \mathbf{\Phi u}(t)$. Substituting into IVP and applying the rule for differentiating a matrix product, we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathbf{\Phi u}] = \frac{\mathrm{d}\mathbf{\Phi}}{\mathrm{d}t}\mathbf{u} + \mathbf{\Phi}\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{A\Phi u} + \mathbf{b}$$

However, $\mathrm{d}\mathbf{\Phi}/\mathrm{d}t = \mathbf{A\Phi}$, so we have:

$$\mathbf{A\Phi u} + \mathbf{\Phi}\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{A\Phi u} + \mathbf{b}$$

Clearly $\mathbf{D}$ is non-singular and so $\mathbf{D}^{-1} = \mathrm{diag}\,(\mathrm{e}^{-\lambda_1 t}, \ldots, \mathrm{e}^{-\lambda_N t})$. Since $\mathbf{\Phi} = \mathbf{PD}$, $\mathbf{\Phi}$ is non-singular and $\mathbf{\Phi}^{-1} = \mathbf{D}^{-1}\mathbf{P}^{-1} = \mathbf{D}^{-1}\mathbf{P}^{\mathrm{T}}$. Therefore, $\mathrm{d}\mathbf{u}/\mathrm{d}t = \mathbf{\Phi}^{-1}\mathbf{b} = \mathbf{D}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}$. Integration yields:

$$\mathbf{u} = \int \mathbf{D}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}\,\mathrm{d}t + \mathbf{c}$$

Back-substitution now yields:

$$\begin{aligned}\mathbf{T} &= \mathbf{PDc} + \mathbf{PD}\int \mathbf{D}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}\,\mathrm{d}t \\ &= \mathbf{PDc} + \mathbf{PD}\int \mathbf{D}(-t)\mathbf{P}^{\mathrm{T}}\mathbf{b}\,\mathrm{d}t\end{aligned}$$

The only quantity inside the integral that depends on t is $\mathbf{D}(-t)$. Therefore, upon integrating we obtain:

$$\mathbf{T} = \mathbf{PDc} - \mathbf{PD\Lambda}^{-1}\mathbf{D}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}$$

where $\mathbf{\Lambda}^{-1} = \mathrm{diag}\,(1/\lambda_1, \ldots, 1/\lambda_N)$. Since $\mathbf{\Lambda}^{-1}$ and $\mathbf{D}^{-1}$ are diagonal matrices we can interchange the order of multiplication to obtain:

$$\begin{aligned}\mathbf{T} &= \mathbf{PDc} - \mathbf{PDD}^{-1}\mathbf{\Lambda}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b} \\ &= \mathbf{PDc} - \mathbf{P\Lambda}^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b} \\ &= \mathbf{PDc} - \mathbf{A}^{-1}\mathbf{b}\end{aligned}$$

since $\mathbf{P\Lambda}^{-1}\mathbf{P}^{\mathrm{T}} = \mathbf{A}^{-1}$.

Now we force the solution to satisfy the initial condition $\mathbf{T}(0) = \mathbf{g}$ and solve for $\mathbf{c}$ to obtain:

$$\mathbf{c} = \mathbf{P}^{\mathrm{T}}(\mathbf{g} + \mathbf{A}^{-1}\mathbf{b})$$

where we have used the fact $\mathbf{D}(0) = \mathbf{I}$. Substitution now yields the closed form solution:

$$\mathbf{T} = \mathbf{PD}(t)\mathbf{P}^{\mathrm{T}}(\mathbf{g} + \mathbf{A}^{-1}\mathbf{b}) - \mathbf{A}^{-1}\mathbf{b}$$

4 APPLICATION AND COMPARISON TO OTHER NUMERICAL METHODS

For comparison, the eigenvalue method was applied to two simple test problems:

$$\text{(application 1)} \quad \begin{cases} \dfrac{\partial T}{\partial t} = \dfrac{\partial^2 T}{\partial x^2} \\ T(x,0) = 1, \quad 0 < x < 1 \\ T(0,t) = 0 = T(1,t), \quad t > 0 \end{cases}$$

and:

$$\text{(application 2)} \quad \begin{cases} \dfrac{\partial T}{\partial t} = \dfrac{\partial^2 T}{\partial x^2} \\ T(x,0) = 2, \quad 0 < x < 1 \\ T(0,t) = 1 = T(1,t), \quad t > 0 \end{cases}$$

Observe that applications 1 and 2 differ only in their initial/boundary conditions.

To begin, we subdivide the interval $[0,1]$ with $N+2$ evenly spaced node points $x_k \equiv k/N+1$, $k = 0, 1, 2, \ldots, N+1$. If we define $T_k(t) \equiv T(x_k, t)$, then $\mathrm{d}T_k/\mathrm{d}t = \partial T(x_k,t)/\partial t$ for $k = 1, 2, 3, \ldots, N$.

Using finite differences for the spatial derivative we obtain:

$$\frac{\partial^2 T(x_k,t)}{\partial x^2} \approx \frac{T_{k-1} - 2T_k + T_{k+1}}{(\Delta x)^2}$$

Therefore, substitution into the above definition yields the system of N ordinary differential equations:

$$\frac{\mathrm{d}T_k}{\mathrm{d}t} = \frac{T_{k-1} - 2T_k + T_{k+1}}{(\Delta x)^2}$$

Specifically, for $k = 1$ we have:

$$\frac{\mathrm{d}T_1}{\mathrm{d}t} = \frac{-2T_1 + T_2}{(\Delta x)^2} + \frac{T_0}{(\Delta x)^2}$$

and for $k = N$:

$$\frac{\mathrm{d}T_N}{\mathrm{d}t} = \frac{T_{N-1} - 2T_N}{(\Delta x)^2} + \frac{T_{N+1}}{(\Delta x)^2}$$

In matrix form we may write these equations as:

$$\begin{cases} \dot{\mathbf{T}} = \mathbf{AT} + \mathbf{b} \\ \mathbf{T}(0) = \mathbf{g} \end{cases}$$

where:

$$\mathbf{A} = \frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 & & & \cdots & & & 0 \\ \vdots & & & & \vdots & & & & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & & & & \vdots & & & & \vdots \\ 0 & & & \cdots & & & 0 & 1 & -2 \end{bmatrix}$$

and $\mathbf{T} = \begin{bmatrix} T_1 \\ \vdots \\ T_N \end{bmatrix}$

For application 1, $\mathbf{b} = 0$ and $\mathbf{g}$ has components all

Table 1. Comparison of results of applying three numerical methods to application 1 for three interior nodes for node at $x = 0{\cdot}50$

Time	Exact solution	Eigenvalue method	Finite element method	Nodal domain integration	Rel. % error: eigenvalue method	Rel. % error: finite element method	Rel. % error nodal domain integration
0·01	0·999	0·979	0·887	0·901	2	11	9
0·02	0·975	0·931	0·786	0·833	4	19	15
0·03	0·918	0·871	0·697	0·763	5	24	17
0·04	0·846	0·806	0·618	0·700	5	27	17
0·05	0·772	0·742	0·548	0·641	4	29	17
0·06	0·702	0·680	0·486	0·588	3	28	16
0·07	0·637	0·622	0·431	0·538	2	32	16
0·08	0·578	0·568	0·382	0·493	2	34	15
0·09	0·524	0·518	0·339	0·452	1	35	14
0·10	0·474	0·472	0·301	0·414	0·5	36	13
0·11	0·430	0·430	0·267	0·380	0·2	38	12
0·12	0·390	0·392	0·237	0·348	0·6	39	11
0·13	0·353	0·357	0·210	0·319	1	40	10
0·14	0·320	0·325	0·186	0·292	2	42	9
0·15	0·290	0·296	0·165	0·268	2	43	8
0·16	0·262	0·269	0·146	0·246	3	44	6
0·17	0·238	0·245	0·130	0·225	3	46	5
0·18	0·215	0·223	0·115	0·206	4	47	4
0·19	0·195	0·203	0·102	0·189	4	48	3
0·20	0·177	0·185	0·091	0·173	5	49	2

equal to 1. For application 2, $\mathbf{b} = [(1/(\Delta x)^2)0 \cdots 0(1/(\Delta x)^2)]^T$ and $\mathbf{g}$ has components all equal to 2.

The analytic solution to application 1 is given by:

$$T_1(x,t) = \frac{4}{\pi}\sum_{k=0}^{\infty}\frac{e^{-(2k+1)^2\pi t}\sin((2k+1)\pi x)}{2k+1}$$

and to application 2 by:

$$T_2(x,t) = 1 + \frac{4}{\pi}\sum_{k=0}^{\infty}\frac{e^{-(2k+1)^2\pi t}\sin((2k+1)\pi x)}{2k+1}$$

Tables 1 and 2 compare the results of applying the eigenvalue method to the two applications with the results of applying various prevalent finite difference and finite element techniques. The results show that the eigenvalue method compares quite favorably to the other presented techniques and demonstrates that it possesses excellent stability and convergence characteristics. These performance characteristics combined with the previously mentioned advantages show that the eigenvalue method is certainly worthy of further investigation.

The eigenvalue method was implemented in MATLAB(c) which utilizes well established numerical linear algebra techniques and thus provides a valid means for investigating the feasibility of the eigenvalue method.

4.1 Limitations of the eigenvalue technique

Because the matrix system of eqn (3) is non-singular, it provides the necessary eigenvalues and eigenvectors for solving the exponential function parameters. Consequently, there are no limitations on the eigenvalue technique other than accuracy issues which are related to nodal point density and placement (which are issues that are not remedied by the eigenvalue technique).

Table 2. Results of applying the eigenvalue method and other methods to application 1 using three equally spaced interior nodes

Time	$\eta = 2$		$\eta = 3$		$\eta = 11$		$\eta = \infty$		Fourth-order subdomain approximation		Adjusted nodal domain integration		Eigenvalue method		Analytic solution	
	0·25[a]	0·50[a]	0·25	0·50	0·25	0·50	0·25	0·50	0·25	0·50	0·25	0·50	0·25	0·50	0·25	0·50
0·01	0·802	1·041	0·823	0·989	0·851	0·989	0·861	0·981	0·864	1·003	0·864	1·013	0·862	0·979	0·923	0·999
0·02	0·701	0·970	0·716	0·941	0·743	0·941	0·755	0·933	0·760	0·961	0·761	0·967	0·756	0·931	0·789	0·975
0·03	0·627	0·881	0·637	0·876	0·660	0·876	0·671	0·873	0·676	0·898	0·678	0·902	0·672	0·871	0·690	0·918
0·04	0·564	0·796	0·572	0·807	0·592	0·807	0·602	0·807	0·606	0·828	0·608	0·830	0·603	0·806	0·615	0·846
0·05	0·508	0·718	0·515	0·739	0·533	0·739	0·543	0·743	0·546	0·759	0·548	0·759	0·544	0·742	0·553	0·772
0·10	0·302	0·427	0·310	0·461	0·327	0·461	0·335	0·472	0·331	0·469	0·331	0·468	0·335	0·471	0·336	0·474
0·15	0·179	0·254	0·187	0·285	0·202	0·285	0·209	0·295	0·202	0·287	0·201	0·285	0·209	0·296	0·205	0·290
0·20	0·107	0·151	0·113	0·176	0·125	0·176	0·131	0·185	0·123	0·175	0·123	0·174	0·131	0·185	0·125	0·177
0·25	0·063	0·090	0·068	0·109	0·077	0·109	0·082	0·116	0·075	0·107	0·075	0·106	0·082	0·116	0·076	0·108
0·30	0·038	0·053	0·041	0·067	0·048	0·067	0·051	0·072	0·046	0·065	0·046	0·064	0·051	0·073	0·047	0·066

[a] Value of X.

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