AN APPROXIMATION METHOD FOR CONTAMINANT TRANSPORT EQUATION

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ABSTRACT

There are few techniques available to numerically solve contaminant transport equation. In this paper we show that the Sinc-Galerkin method is a very effective tool in numerically solving contaminant transport equation. The numerical results demonstrate the reliability and efficiency of using the Sinc-Galerkin method to solve such problems.

Keywords: Sinc-Galerkin method, contaminant transport equation, numerical solutions.

1. INTRODUCTION

Groundwater flow, contaminant transport, and seawater movement in coastal aquifers are simulated using the USGS three-dimensional heat and transport model (HST3D). The model in its original form solves the groundwater, a single solute species, and heat transport equations. The heat transport equation was converted via parameter transformation to simulate a conservative solute species, namely salt. This use of the model has been verified by comparisons with existing results for documented cases.

The model is utilized to simulate an underground oil fuel leak at an old power station in Ayn Zara; a suburb east of Tripoli on the Mediterranean coastline. The suspected oil leak at Ayn Zara started approximately in 1973 and continued up to 1995, where at that time the leaking underground storage tank was removed.

The model was calibrated for steady state condition in 1957 and for transient conditions in 1972 and 1994 for both flow and salinity concentration. The model was further used to simulate the entire process under actual conditions and using pump-treat and inject remedial action plan up to the year 2001. Simulation results revealed the extent of the seawater encroachment and the oil plume spread up to the year 1995 and the predictions up to year 2010 for both action and no action scenarios.

In this paper, we employ the Sinc-Galerkin method to solve the contaminant transport equation:

$$A\frac{\partial u}{\partial t} = B\frac{\partial^2 u}{\partial x^2} - C\frac{\partial u}{\partial x} + f(x,t), \qquad 0 < x < 1, t > 0 \tag{1.1}$$

subject to boundary conditions

$$u(0,t) = 0, \qquad u(1,t) = 0, \tag{1.2}$$

and the initial conditions

$$u(x,0) = \eta(x), \; 0 < x < 1, \tag{1.3}$$

where the unknown *u(x,t)* is the concentration of the contaminant dissolved in the fluid; the coefficients, *A, B* and *C* are the porosity of the medium, the delusion coefficient, and the Darcy velocity of the fluid, respectively; the right hand side *f(x,t)* is the contaminant source term; and the initial condition *u(x, 0)* is the concentration of the contaminant at time *t = 0*. For more details about the formulation of this equation, see Douglas [3, 10].

In recent years, a lot of attention has been devoted to the study of Sinc-Galerkin method to investigate various scientific models. The efficiency of the method has been formally proved by many researchers [1, 2, 4, 5, 6, 7, 12, 13, 14].

The paper is organized as follows. In Section 2, as a background, the fundamental properties of the sinc functions. The Sinc-Galerkin solution for equation (1.1) is described in detail in section 3. In Section 4, we apply our method to specific problems, compare the results, and close with conclusions.

2. SINC INTERPOLATION

The goal of this section is to recall notation and definitions of the Sinc function, state some known results, and derive useful formulas that are important for this paper. First denote the set of all integers, the set of all real numbers, and the set of all complex numbers by Z, R, and C, respectively.

- $\sin c(z) = \sin(\pi z)/\pi z, \qquad z \in Z$

  Note that $|\sin c(x)| \le 1$ *for any* $x \in R$.
- $S(k,h)(z) = \sin c[(z - kh)/h], z \in Z, h > 0$
- $C(f,h) = \sum_{k=-\infty}^{\infty} f(hk)S(k,h)(x), h > 0$

Here, $C(f,h)$ is called the Whittaker cardinal expansion of $f(x)$ whenever this series converges.

- $C_N(f,h) = \sum_{k=-N}^{\infty} f(hk)S(k,h).$

The properties of Whittaker cardinal expansions have been studied and are thoroughly surveyed in [14]. These properties are derived in the infinite strip D_d of the complex plane where for d > 0

$$D_d = \left\{ \varsigma = \xi + i\eta : |\eta| < d \le \frac{\pi}{2} \right\}. \tag{2.1}$$

Approximations can be constructed for infinite, semi-finite, and finite intervals. To construct approximations on the interval (0, 1) and (0,1) respectively, which are used in this paper, consider the conformal maps.

$$\phi(z) = \ln\left(\frac{z}{1-z} \right), \tag{2.2}$$

and

$$\gamma(w) = \ln(w). \tag{2.3}$$

The map ϕ carries the eye-shaped region

$$D_E = \left\{ z = x + iy : \left| \arg\left(\frac{z}{1-z} \right) \right| < d \le \frac{\pi}{2} \right\}, \tag{2.4}$$

onto the infinite strip D_d. Similarly, the map γ carries the infinite wedge

$$D_w = \left\{ w = t + is : |\arg(w)| < d \le \frac{\pi}{2} \right\}, \tag{2.5}$$

onto the strip D_d.

The "mesh sizes" hx and ht represent the mesh sizes in D_d for the uniform grids {khx}, and {kht}, k = 0,±1,±2, ... The sinc grid points zk 2 (0, 1) in D_E will be denoted by x_k because they are real. Similarly, the grid points wk 2 (0,1) in D_w will be denoted by tk. Both are inverse images of the equi-spaced grids, that is

$$x_k = \phi^{-1}(kh_x) = \frac{e^{kh_x}}{1+e^{kh_w}}, \tag{2.6}$$

and

$$t_k = \gamma^{-1}(kh_t) = e^{kh_w}, \tag{2.7}$$

To simplify the notation throughout the remainder of this section, the pairs ϕ, D_E and Y, D_w are referred to generically as χ, and D. It is understood that the subsequent definition and theorems hold in either setting. Furthermore, the inverse of χ is denoted by ψ.

The sinc-Galerkin method requires the derivatives of composite sinc functions be evaluated at the nodes. We need the following lemma.

Lemma 2.1. [12]: Let χ be a conformal one-to one map of the arbitrary simply connected domain D onto Dd. Then

$$\delta_{jk}^{(0)} = [S(j,h)\circ\chi(\tau)]_{\tau=\tau_k} = \begin{cases}1, & j=k,\\ 0, & j\neq k,\end{cases} \tag{2.8}$$

$$\delta_{jk}^{(1)} = h\left[\frac{d}{d\chi}[S(j,h)\circ\chi(\tau)]\right]_{\tau=\tau_k} = \begin{cases}0, & j=k,\\ \frac{(-1)^{k-j}}{k-j}, & j\neq k,\end{cases} \tag{2.9}$$

$$\delta_{jk}^{(2)} = h^2\left[\frac{d^2}{d\chi^2}[S(j,h)\circ\chi(\tau)]\right]_{\tau=\tau_k} = \begin{cases}\frac{-\pi^2}{3}, & j=k,\\ \frac{-2(-1)^{k-j}}{(k-j)^2}, & j\neq k,\end{cases} \tag{2.10}$$

In equations (2.8) - (2.10) h is step size and T_k is a sinc grid point as in (2.6) or (2.7).

3. THE SINC-GALERKIN METHOD

The Sinc-Galerkin method described in this paper, at one level, simply consists of the assembly of the discrete Sinc-Galerkin in the spatial domain with a Sinc-Galerkin discretization in the temporal domain. The approximate solution to (1.1)–(1.3) is defined by

$$u_{m_x,m_t}(x,t) = \sum_{j=-M_t}^{N_t}\sum_{i=-M_x}^{N_x} u_{ij}S_{ij}(x,t), \tag{3.1}$$

where $m_x = M_x + N_x + 1$, $m_t = M_t + N_t + 1$. The basis functions $\{Sij(x, t)\}$ for $-M_x \le i \le N_x$, $-M_t \le j \le N_t$ are given as the product of basis functions. In this paper we take

$$S_{ij}(x,t) = S_i(x)S_j(t),$$
$$= [S(i,h_x)\circ\phi(x)][S(i,h_t)\circ\gamma(t)],$$

where the conformal map in the spatial domain is given by

$$\phi(x) = \ln\left(\frac{x}{1-x}\right)$$

and the conformal map in the temporal domain is given by

$$\gamma(t) = \ln(t)$$

The unknown coefficients $\{u_{ij}\}$ in equation (3.1) are determined by orthogonalizing the residual with respect to the functions $\{S_{kl}(x,\ t)\},\ -M_x \le k \le N_x,\ -M_t \le l \le N_t$. This yields the discrete Galerkin system

$$\left\langle Lu_{m_x m_t} - f, S_{kl}\right\rangle = 0, \quad -M_x \le k \le N_x, -M_t \le l \le N_t \tag{3.2}$$

The inner product is defined by

$$\left\langle f, g\right\rangle = \int_0^\infty \int_0^1 f(x,t)g(x,t)W(x,t)dx\,dt,$$

where

$$W(x,t) = w(x)v(t) = \frac{\gamma'(t)}{\phi'(x)^2},$$

Here, a product weight function is chosen depending on the boundary conditions, the domain, and the differential equation. In this paper we choose $\omega(\chi) = \dfrac{1}{\phi'(x)^2}$ as the weight in the spatial domain, and $\upsilon(t) = \gamma'(t)$ as the weight in the temporal domain. A complete discussion on the choices of the weight functions can be found in [4, 5, 6].

The most direct development of the discrete system for (1.1) is obtained by substituting (3.1) into (3.2). This approach, however, obscures the analysis that is necessary for applying sinc quadrature formulas to (3.2). An alternative approach is to analyze instead

$$\left\langle Au_t, S_k S_l\right\rangle = \left\langle Bu_{xx}, S_k S_l\right\rangle - \left\langle Cu_x, S_k S_l\right\rangle + \left\langle f(x,t), S_k S_l\right\rangle, \tag{3.3}$$

We need the following lemma.

Lemma 3.1. : The following relations hold

$$\langle Au_t, S_k S_l \rangle \approx A h_t h_x \frac{w(x_k)}{\phi'(x_k)} \sum_{j=-M_t}^{N_t} \sum_{i=0}^{1} \frac{u(x_k, t_j)}{\gamma'(t_j)} \left[\frac{1}{h_t^i} \delta_{lj}^{(i)} \varepsilon_i \right], \tag{3.4}$$

$$\langle Bu_{xx}, S_k S_l \rangle \approx B h_x h_t \frac{v(t_k)}{\gamma'(t_l)} \sum_{i=-M_x}^{N_x} \sum_{j=0}^{2} \frac{u(x_i, t_l)}{\phi'(x_i)} \left[\frac{1}{h_x^j} \delta_{ki}^{(j)} \mathrm{P}_j \right], \tag{3.5}$$

$$\langle Cu_x, S_k S_l \rangle \approx C h_x h_t \frac{v(t_l)}{\gamma'(t_l)} \sum_{i=-M_x}^{N_x} \sum_{j=0}^{1} \frac{u(x_i, t_l)}{\phi'(x_i)} \left[\frac{1}{h_x^j} \delta_{ki}^{(j)} \mu_j \right], \tag{3.6}$$

and

$$\langle f, S_k S_l \rangle \approx h_k h_x \frac{w(x_k) f(x_k, t_l) v(t_l)}{\phi'(x_k) \gamma(t_l)}. \tag{3.7}$$

for some functions ε_i, P_j and μ_i, to be determined.

Replacing each term of (3.3) with the approximation defined in (3.4)-(3.7) and replacing $u(x_k, t_l)$ by u_{kl} and dividing by $h_x h_t$ we obtain the following theorem, Theorem 3.1. If the assumed approximate solution of the problem (1.1)-(1.3) is (3.1), then the discrete Sinc-Galerkin system for the determination of the unknown coefficients $\{u_{kj}, -Mx < k < N_x, -M_t < j < N_t\}$ is given by

$$A \frac{w(x_k)}{\phi'(x_k)} \sum_{j=-M_t}^{N_t} \sum_{i=0}^{1} \frac{u_{kj}}{\gamma'(t_j)} \left[\frac{1}{h_t^i} \delta_{lj}^{(i)} \varepsilon_i \right] = B \frac{v(t_l)}{\gamma'(t_l)} \sum_{i=-M_x}^{N_x} \sum_{j=0}^{2} \frac{u_{il}}{\phi'(x_i)} \left[\frac{1}{h_x^j} \delta_{ki}^{(i)} P_j \right]$$
$$- C h_x h_t \frac{v(t_l)}{\gamma'(t_l)} \sum_{i=-M_x}^{N_x} \sum_{j=0}^{1} \frac{u(x_i, t_l)}{\phi'(x_i)} \left[\frac{1}{h_x^j} \delta_{ki}^{(j)} \mu_j \right] + \frac{w(x_k) f(x_k, t_l) v(t_l)}{\phi'(x_k) \gamma(t_l)} \tag{3.8}$$

Recall the notation of Toeplitz matrices [9]. Let $I_{m_x}^{(P)}, P = 0,1,2$ be the $m_x \times m_x$ matrices $I^{(P)}$, with jk-th entry $\delta_{jk}^{(P)}$ as given by equations (2.8)–(2.10). Further, $D(g_x)$ is an $m_x \times m_x$ diagonal matrix whose diagonal entries are:
$[g(x - M_x), (x - M_x + 1), \ldots, g(x_0), \ldots, g(x_{N_x})]^T$. The matrices $I_{m_x}^{(P)}, P = 0,1,2$ and $D(g_t)$ are similarly defined though of size $m_t \times m_t$. Introducing this notation in Eq. (3.8) leads to the matrix form

$$AD(w)UD(v) \left[\sum_{j=0}^{1} \frac{1}{h_t^j} I_{mt}^{(j)} D\left(\frac{\varepsilon_j}{\gamma'} \right) \right]^t$$
$$= B \left[\sum_{i=0}^{2} \frac{1}{h_x^i} I_{m_x}^{(i)} D\left(\frac{p_i}{(\phi')^2 w} \right) \right] D(\phi') D(w) U D\left(\frac{v}{\gamma'} \right)$$
$$- C \left[\sum_{i=0}^{1} \frac{1}{h_x^i} I_{mx}^{(i)} D\left(\frac{\mu_i}{(\phi')^2 w} \right) \right] D(\phi') D(w) U D\left(\frac{v}{\gamma'} \right) + D\left(\frac{w}{\phi'} \right) F D\left(\frac{v}{\gamma'} \right) \tag{3.9}$$

Note that $[\ \ ]^t$, denotes the transpose of the matrix $[\ \ ]$. Premultiplying by $D(\phi')$ and postmultiplying by $D(\gamma')$ yields the equivalent system

$$SX + XT = G, \tag{3.10}$$

where

$$S = AH - Ck + I,$$

$$H = D(\phi')\left[\sum_{i=0}^{2} \frac{1}{h_x^i} I_{m_z}^{(i)} D\left(\frac{\rho i}{(\phi')^2 w}\right)\right] D(\phi'),$$

$$k = D(\phi')\left[\sum_{i=0}^{1} \frac{1}{h_x^i} I_{m_z}^{(i)} D\left(\frac{\mu i}{(\phi')^2 w}\right)\right] D(\phi'),$$

$$T = \left[\sum_{i=0}^{1} \frac{1}{h_t^i} I_{m_t}^{(i)} D\left(\frac{\xi j}{\gamma' \upsilon}\right)\right]^t D(\gamma'),$$

$$G = D(w) F D(\upsilon),$$

and

$$X = D(w) U\, D(\upsilon), \tag{3.11}$$

The four matrices S,T,X and G have dimension $m_x \times m_x$, $m_t \times m_t$, $m_x \times m_t$ and $m_x \times m_t$, respectively. Lastly, the $m_x \times m_t$ matrices U and F have kl-th entries given by u_{kl} and $f(x_k, t_l) = f\left(\frac{e^{kh}}{l + e^{kh}}, e^{lh}\right)$, respectively.

To obtain the approximate solution equation (3.1), we need to solve the system for U which requires solving (3.10) for X.

We have excluded the presentation for solving equation (3.10). In order to save space, refer instead to the excellent references [4, 7].

4. NUMERICAL EXAMPLES

We give two examples, in one of them the nonhomogeneous term, f(x, t), has singularities. For purposes of comparison, contrast and performance, examples with known solutions were chosen.

For these examples, d is taken to be $\pi/2$. The step sizes h_x and ht and the summation limits M_x, N_x, M_t and N_t are selected so that the error in each coordinate direction is asymptotically balanced. Once M_x is chosen, the step sizes and remaining summation limits can be determined as follows

$$h_x = h_t = \sqrt{\frac{\pi d}{\sigma M_x}}, \quad N_x = \left[\left|\frac{\sigma M_x}{\beta}\right|\right],$$

and

$$M_t = M_x,$$

and N_t is also arbitrary. In most cases reported $M_t > N_t$ which yields a much smaller discrete system than the choice $M_t = N_t$ that may give results in larger matrices with no corresponding increase in accuracy.

We report Absolute Error which is defined as

Absolute Error = |^{u}exact solution - ^{U}Sinc-Galerkin|

Table 4.1. Maximum Absolute Error for Example 1

M_x	N_t	Maximum Absolute Error
2	2	0.0098
5	5	0.4559 E-03
20	6	0.1116 E-04
35	10	0.7779 E-05
50	15	0.1602 E-07

Example 4.1. Consider the problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x} + f(x,t), \qquad 0 < x < 1, t > 0,$$

If

$$f(x,t) = 3\sin t - 2x\sin t + x(1-x)\cos t,$$

subject to the boundary conditions

$$u(0,t) = 0, \qquad u(1,t) = 0,$$

and the initial condition

$$u(x,0) = 0, \qquad 0 \le x \le 1,$$

then the exact solution is

$$u(x,t) = x(1-x)\sin t$$

The Maximum Absolute Errors obtained are shown in Table 4.1 for Sinc-Galerkin together with the exact solution.

Example 4.2. Consider the problem

$$\frac{\partial u}{\partial t} = 2\frac{\partial^2 u}{\partial x^2} - 0.3\frac{\partial u}{\partial x} + f(x,t), \qquad 0 < x < 1,\ t > 0,$$

subject to the boundary conditions

$$u(0,t) = 0, \qquad u(1,t) = 0,$$

and the initial condition

$$u(x,0) = 0, \qquad 0 \le x \le 1,$$

If

$$f(x,t) = (1-t)e^{-t}x^2(1-x) + \left[12.6x - 0.9x^2 - 4\right]t\,e^{-t}$$

then the exact solution is

$$u(x,t) = x^2(1-x)t\,e^{-t}.$$

The Maximum Absolute Errors obtained are shown in Table 4.2 for Sinc-Galerkin together with the exact solution.

The computations associated with the two examples discussed above were performed by using MATLAB.

Table 4.2. Maximum Absolute Error for Example 2

M_x	N_t	**Maximum Absolute Error**
10	3	0.3615 E-03
20	8	0.3615 E-04
30	10	0.3615 E-05
40	15	0.3615 E-06
60	20	0.3615 E-07
80	25	0.3615 E-08
100	35	0.3615 E-09

5. CONCLUSIONS

As it has been shown in the paper, the proposed Sinc-Galerkin method converts the problem of solving partial differential equation (PDE) to solving a linear system of first order differential equations (ODE) , for unknown Wavelet series coefficients, which can be solved by some automatic ODE solver. Hence, the method can be easily implemented on digital computer.

The numerical results on two models partial differential equations show that the present method is competitive with the exact solutions.

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